ANNUAL REPORT 1993

Institut Max von Laue
Paul Langevin
Grenoble - France

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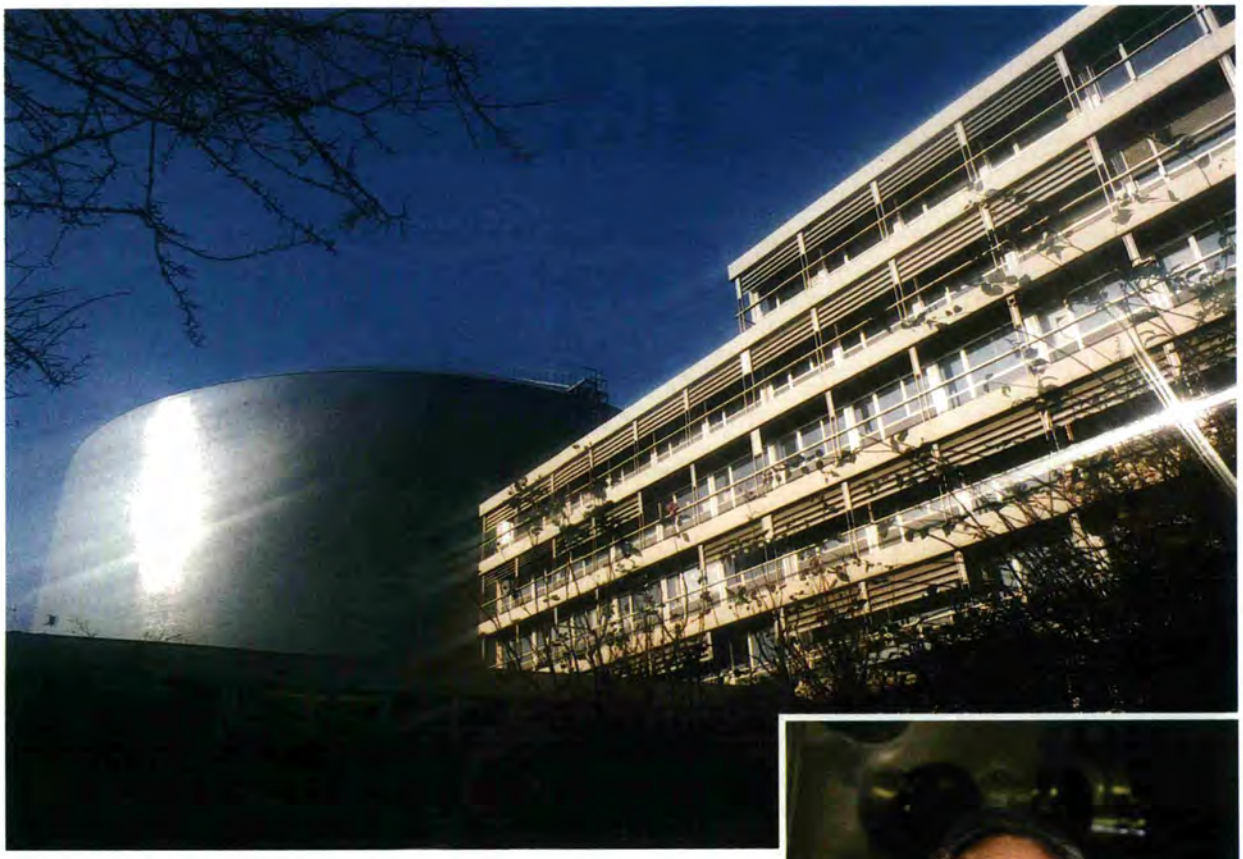


The repainted reactor building.

Jean Charvolin, Director .
On the day of the arrival of the new D_2O reflector tank (seen in the background).

Front cover

The new D_2O reflector tank being lowered into the empty reactor swimming pool on 2 March 1994.

– CONTENTS –

– ORGANISATION OF THE ILL P. 5

– VISITS AND EVENTS P. 8

– DIRECTOR'S REPORT P. 14

– ILL-ESRF-EMBL–COOPERATION P. 20

– COLLEGES : P. 21

COLL. 2 - THEORY P. 22

COLL. 3 - NUCLEAR AND FUNDAMENTAL PHYSICS P. 28

COLL. 4 - STRUCTURAL AND MAGNETIC EXCITATIONS P. 38

COLL. 5 - CRYSTAL AND MAGNETIC STRUCTURES P. 46

COLL. 6 - LIQUIDS, DISORDERED MATERIALS AND METAL PHYSICS P. 63

COLL. 8 - BIOLOGICAL STRUCTURES AND DYNAMICS P. 82

COLL.9a - MOLECULAR SPECTROSCOPY, SURFACES AND MESOPHASES P. 86

COLL.9b - LARGE MOLECULES P. 96

– DIRECTORATE SERVICES : P.101

– SCIENCE DIVISION (DS): P.103

SCIENTIFIC SUPPORT P.104

NUCLEAR AND FUNDAMENTAL PHYSICS (NFP) GROUP P.106

DIFFRACTION (DIFF) GROUP P.110

LARGE SCALE STRUCTURES (LSS) GROUP P.115

THREE-AXIS SPECTROMETER (TAS) GROUP P.118

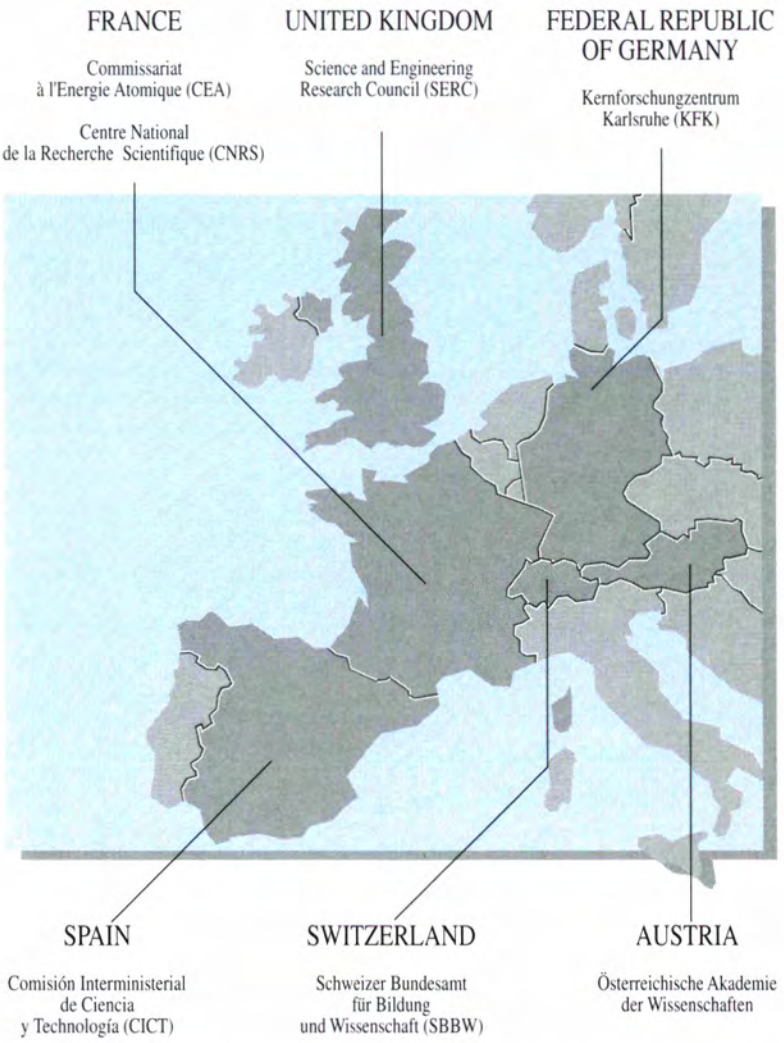
TIME-OF-FLIGHT AND HIGH RESOLUTION (TOF/HR) GROUP P.120

SMALL PROJECTS IN DS P.123

– CONTENTS –

– PROJECTS AND TECHNIQUES DIVISION (DPT) :	P. 127
INSTRUMENTATION BRANCH	P. 130
DEVELOPMENT BRANCH	P. 135
– INSTRUMENTS – PROJECTS – TECHNIQUES	P. 140
– REACTOR DIVISION :	P. 145
DISMANTLING	P. 145
RECONSTRUCTION	P. 148
STUDIES AND METROLOGY	P. 152
BUDGET AND TIMETABLE	P. 152
– ADMINISTRATION DIVISION :	P. 153
FINANCE AND MANAGEMENT INFORMATION SYSTEMS	P. 154
PURCHASING	P. 156
PERSONNEL AND HUMAN RESOURCES	P. 157
BUILDING AND SITE MAINTENANCE	P. 159
– COMMUNICATIONS :	P. 161
SEMINARS	P. 161
WORKSHOPS	P. 166
THESES	P. 167
CONFERENCE CONTRIBUTIONS	P. 168
PUBLICATIONS – ILL-REPORTS	P. 174
AUTHOR INDEX	P. 194
PAPERS ACCEPTED FOR PUBLICATION	P. 202

Associates of the ILL



Countries with scientific membership

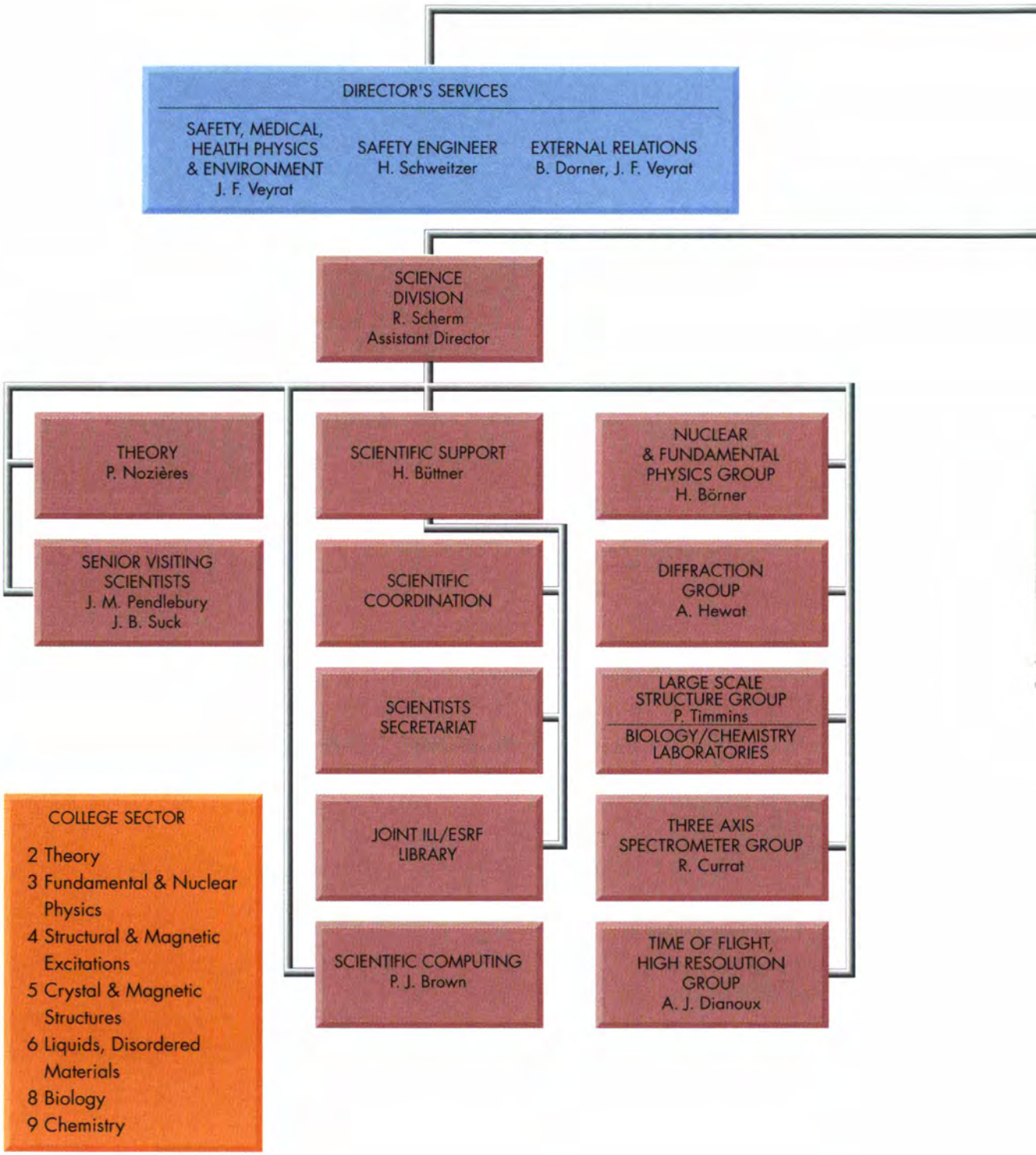
Steering Committee
(at its last meeting)

❍ Hennies (KFK)	❍ Aymar (CEA)	❍ Richards (Univ. Durham)
❍ Schmidt-Küntzel (BMFT)	❍ Bouchard (CEA)	❍ Taylor (RAL)
❍ Schunck (BMFT)	❍ Comès (CNRS)	❍ Ward (SERC)
❍ Steiner (HMI, Berlin)	❍ Sevin (CNRS)	❍ Wilkins (SERC)

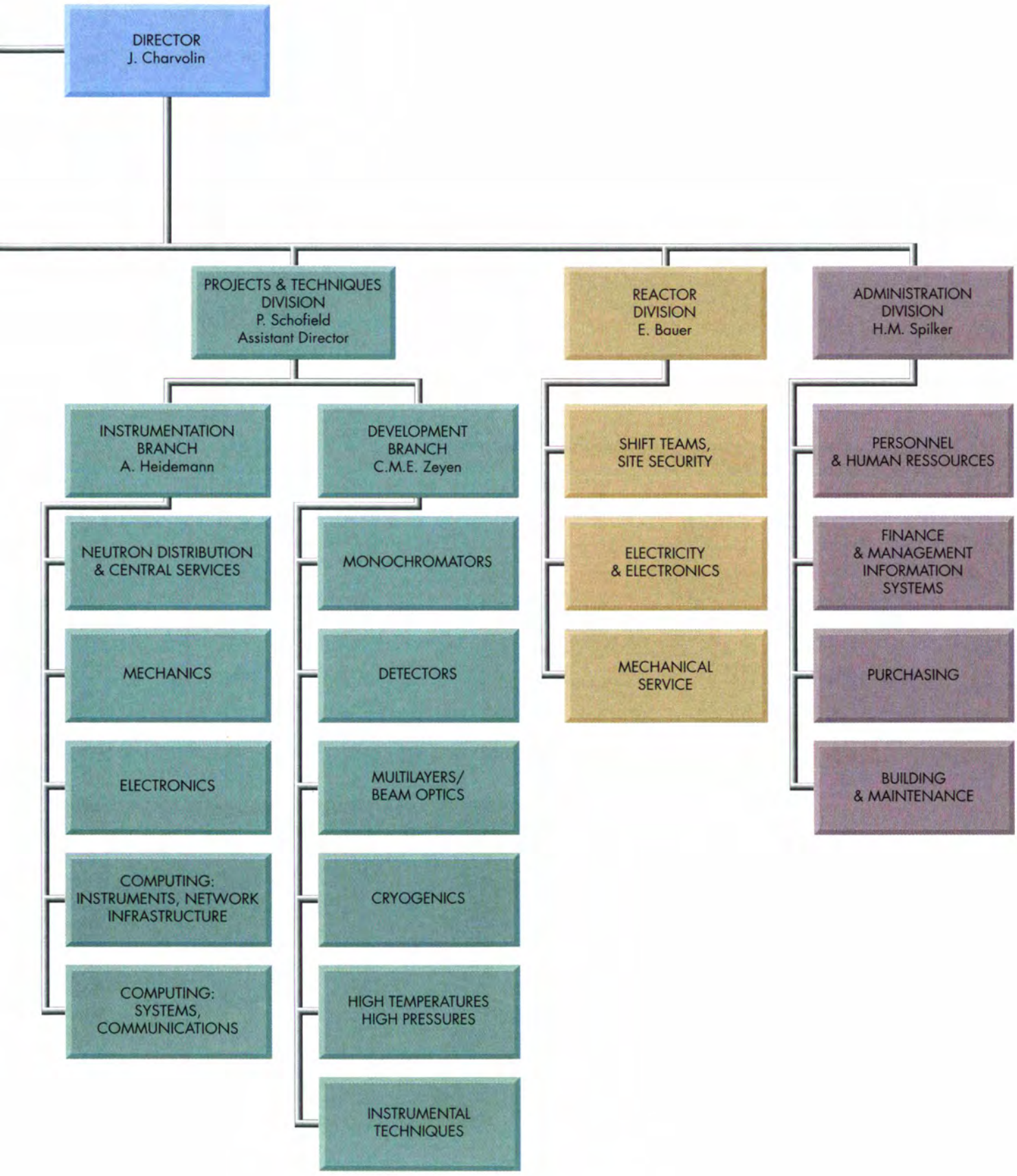
Scientific Council

Plenary Session	Subcommittees
30 participants	66 members

Status: November 1993


DIRECTOR'S SERVICES
SAFETY, MEDICAL, HEALTH PHYSICS & ENVIRONMENT
J. F. Veyrat
SAFETY ENGINEER
H. Schweitzer
EXTERNAL RELATIONS
B. Dorner, J. F. Veyrat
SCIENCE DIVISION
R. Scherm
Assistant Director
THEORY
P. Nozières
SENIOR VISITING SCIENTISTS
J. M. Pendlebury
J. B. Suck
SCIENTIFIC SUPPORT
H. Büttner
SCIENTIFIC COORDINATION
SCIENTISTS SECRETARIAT
JOINT ILL/ESRF LIBRARY
SCIENTIFIC COMPUTING
P. J. Brown
NUCLEAR & FUNDAMENTAL PHYSICS GROUP
H. Börner
DIFFRACTION GROUP
A. Hewat
LARGE SCALE STRUCTURE GROUP
P. Timmins
BIOLOGY/CHEMISTRY LABORATORIES
THREE AXIS SPECTROMETER GROUP
R. Currat
TIME OF FLIGHT, HIGH RESOLUTION GROUP
A. J. Dianoux
COLLEGE SECTOR
2 Theory
3 Fundamental & Nuclear Physics
4 Structural & Magnetic Excitations
5 Crystal & Magnetic Structures
6 Liquids, Disordered Materials
8 Biology
9 Chemistry

NEW ORGANIGRAM



"Walter Mampe Memorial Colloquium" organized by M. Pendlebury on 29 January.

"Walter Mampe Memorial Colloquium"
From left to right : Late W. Paul, J. Kalus and J.-B. Suck.

"Walter Mampe Memorial Colloquium",
M. Pendlebury, N. Ramsey,
and Kathi Mampe, Walter's wife.

Joint ILL-ESRF Colloquium by George Charpak, Nobel Prize winner, held on 31 March.

G. Charpak in discussion with Y. Petroff.

Visit of G. Charpak. J. Charvolin on the left, P. Geltenbort on the right and P. Schofield in the foreground.

Visit of Gerhard Stoltenberg on 15 September. In the entrance hall of the ILL from left to right : Guy Aubert, ENS Lyon, representing the High Field Magnet Laboratory, Stephen Cusack, Director of the EMBL outstation, Jean Charvolin, Director of ILL, Gerhard Stoltenberg, Coordinator for German-French Collaboration, Yves Petroff, Director General of ESRF, Reinhard Scherm, Assistant Director of ILL, and Peter Schofield, Assistant Director of ILL.

Visit of the empty and cleaned swimming pool. From left to right : E. Bauer, Head of the Reactor Division, G. Stoltenberg, V. Knoerich, Ministerial Dirigent at the BMFT/Germany, J. Charvolin, M. Maldacker, Assistant of G. Stoltenberg, H. von Hengstenberg, Generalkonsul in Lyon, H.-M. Spilker, Head of Administration Division ILL.

Gerhard Stoltenberg dresses up for the visit of the reactor, Volker Knoerich in the background.

Visit of G. Stoltenberg. J. Gadbin, Préfet de l'Isère, E. Fischer, Interpreter, J. Charvolin, A. Nemoz, Président de l'Université Joseph Fourier, H. von Hengstenberg.

O. Schärpf presents the instrument D7 to G. Stoltenberg. J. Charvolin, V. Knoerich, B. Dorner, and A. Heidemann listen.

G. Stoltenberg is listening to J.P. Watteau, Recteur de l'Académie de Grenoble. H.-M. Spilker and J. Charvolin on the right.

Participants at the Workshop "Dynamics of Disordered Materials II" organized by A.J. Dianoux (ILL), W. Petry (München), D. Richter (Jülich) on 22-24 March at the ILL.

Workshop "Dynamics of Disordered Materials II" From left to right : Mrs. M. and Mr. U. Dahlborg, A. Wright, P. Pusey, A.-J. Dianoux, J.-B. Suck.

Participants at the Workshop on "Neutrons and X-rays in the Study of Magnetism", organized at the ILL by P.J. Brown (ILL), G.H. Lander (EITU Karlsruhe), J.L. Martinez (Madrid), W.G. Stirling (Keele), C. Vettier (ESRF), 21-23 January 1993.

Workshop on "Bragg Optics" organized at the PTB in Braunschweig, 10-11 May 1993. From left to right : P. Mikula, R. Scherm, J. Kulda, B. Dorner.

The organizers of the Workshop on "Bragg Optics", A. Magerl (ILL) and V. Wagner (PTB).

Participants at the Workshop on "Progress in Gaseous Microstrip Proportional Chambers" organized by P. Geltenbort at the ILL, 21-23 June 1993.

Workshop on "Quasicrystals" organized by C. Janot at the ILL, 2-4 June 1993.

Si 1992 avait été l'année marquée par l'expression de la volonté des Associés de l'ILL de maintenir l'ILL dans son statut de laboratoire multinational, 1993 a été celle pendant laquelle cette volonté a été matérialisée par la signature à Paris, le 25 mars, de l'Avenant prolongeant la Convention Intergouvernementale entre la France, l'Allemagne et la Grande Bretagne, pour au moins dix ans à partir du 1er janvier 1994. Ceci a permis d'entreprendre les négociations avec les Membres Scientifiques actuels et potentiels en vue de l'établissement de contrats valables à partir de ce 1er janvier 1994. Nous préparons actuellement les signatures des nouveaux contrats avec l'Autriche, l'Espagne et la Suisse. C'est évidemment avec une très grande satisfaction que l'ILL voit se reconstituer le cadre juridique liant entre eux les pays, donc les communautés, participant à son exploitation et à sa vie scientifique. C'est aussi un élément de motivation puissant pour la poursuite des actions en vue du redémarrage, qui concernent la remise en état du réacteur, la réinstallation des instruments et la mise en place de la nouvelle structure de l'Institut.

Depuis le démontage de l'ancien bidon réflecteur à la fin novembre 1992 l'accent a été mis sur la préparation du remontage. La piscine a été totalement nettoyée, la résistance mécanique de son revêtement contrôlée et sa géométrie vérifiée. L'état de propreté atteint est remarquable, puisque les équipes peuvent y travailler sans protection particulière, et les contrôles et vérifications nous montrent une piscine dans un état très proche de celui d'origine. Aucune intervention supplémentaire sur la piscine n'a été nécessaire. Elle est maintenant prête à recevoir le nouveau bidon dont la fabrication avance comme prévu et qui devrait arriver début février 1994. Pour terminer avec les aspects techniques je mentionnerai que l'avance de la découpe de l'ancien bidon nous a permis d'examiner directement la grille avec les fissures qui sont à l'origine de la remise en état et de confirmer le mécanisme proposé par l'ILL pour l'apparition de ces dernières. L'ensemble de ces travaux a été conduit du mieux possible grâce au dynamisme et à la compétence des équipes de l'ILL, ainsi qu'à l'esprit de bonne collaboration manifesté par tous les participants à ce projet. La procédure administrative nécessaire pour l'obtention du décret d'autorisation de redémarrage se déroule tout à fait normalement, l'ILL a fait parvenir les dossiers nécessaires aux autorités compétentes aux dates prévues, ils ont été examinés par ces autorités qui mettent en place les dernières actions de la procédure. Le déroulement de l'ensemble des actions, aussi bien techniques qu'administratives, ainsi que l'évolution des dépenses, sont analysés très régulièrement par le sous-comité "Remise en état" qui a conclu, lors de sa dernière visite à l'ILL le 18/10/1993, que les coûts et délais sont actuellement respectés et qu'aucune indication n'apparaît qui conduirait à penser que la date prévue de redémarrage ne puisse être respectée.

Ayant maintenant la quasi certitude que le réacteur redémarrera mi-1994 il importait de lancer le programme de réinstallation des instruments pour que ceux-ci soient disponibles au même moment. Nous commençons par les travaux dans les halls des guides et nous poursuivrons par le remontage des instruments du niveau C, qui avaient été entièrement démontés pour libérer l'accès au réacteur, dès que les doigts de gant seront réinstallés. Pour cela l'Institut doit reconstituer au mieux le potentiel humain nécessaire en rappelant ses scientifiques et techniciens travaillant dans d'autres centres et laboratoires. Nous n'éviterons cependant pas une situation difficile car l'Institut mène maintenant deux importants projets techniques de front, réacteur et instruments, et certaines compétences, que nous ne pouvons pas doubler en raison des limitations d'effectifs, sont nécessaires sur ces deux projets.

Une dernière action nécessaire au fonctionnement futur de l'Institut a été la mise en place de la nouvelle structure en quatre Divisions. Cette action est l'aboutissement d'une longue période de discussions et de réflexions initiées par l'analyse de l'organisation et du fonctionnement de l'Institut effectuée par un Groupe d'études à la demande du Comité de Direction le 27/11/90. Le projet définitif de réorganisation avait été accepté par le Comité de Direction réuni le 02/06/93 à Abingdon et nous avons tenu à le mettre en place le plus tôt possible afin que la délicate période du redémarrage ne soit pas perturbée par un tel bouleversement et que l'Institut soit prêt à fonctionner dans ce nouveau cadre dès le redémarrage de l'installation prévu pour la mi-1994. Le changement de structure a donc eu lieu le 01/07/93, très vite après la dernière

réunion du Comité de Direction. Si l'Institut travaille depuis cette date dans sa nouvelle structure, l'effectif correspondant à cette dernière n'est pas encore atteint ainsi que la distribution finale du personnel dans les nouvelles unités. L'effectif est en effet en pleine évolution suite aux premiers départs dans le cadre de la Convention FNE, aux retours des scientifiques et techniciens qui avaient rejoint d'autres centres ou laboratoires pendant l'arrêt et, enfin, aux recrutements nécessaires, en particulier dans le secteur scientifique. Ce n'est que dans le courant 1995 que nous atteindrons l'effectif de l'ordre de 400 envisagé dans la nouvelle structure. Réorganiser un institut dans le cadre d'un effectif limité implique aussi des mutations internes qui ne peuvent pas être toutes réalisées dès maintenant en raison des priorités actuelles qui ne sont pas celles d'un institut en fonctionnement normal. Les départs et mutations qui accompagnent une telle réorganisation dans une entreprise bouleversent profondément, et parfois péniblement, le réseau de relations qui ont lié ses membres et nous devons souligner que, dans notre cas, cette réorganisation se fait avec la participation constructive du personnel qui sait dominer les doutes et anxiétés que génère une telle situation.

Nous venons d'examiner trois points -réorganisation, remise en état du réacteur, réinstallation des instruments- nécessaires pour permettre à l'ensemble de l'installation de redémarrer à la mi-1994, puis de fonctionner comme souhaité avec 5 cycles et 25 instruments. Nous envisageons 2 cycles en 1994, le premier étant consacré à la mise au point finale des instruments et le second étant ouvert aux utilisateurs. Les propositions d'expériences seront examinées par les sous-comités du Conseil Scientifique en automne 1994 et nous distribuerons le temps de faisceau pour un premier ensemble de 3 cycles, 1 en 1994 et 2 en 1995. Les conditions de ce redémarrage doivent être assurées par un budget comprenant les contributions des Associés, comme prévu dans l'Avenant à la Convention Intergouvernementale et le Protocole d'Accord, signés le 25.3.1993, et par celles des Membres Scientifiques. Ces conditions sont assez contraignantes et, pour l'instant, l'Institut doit consacrer ses efforts au retour à l'activité expérimentale, la reprise de l'activité de développement devant être plus lente. Dans ces nouvelles conditions nous n'offrirons que 25 instruments programmés aux utilisateurs, ce nombre est inférieur à celui d'avant l'arrêt, nous recherchons actuellement une formule qui permette de réintroduire partiellement les instruments déprogrammés dans le programme en négociant les conditions de leur exploitation avec des groupes extérieurs pouvant financer cette opération dans le cadre de "Collaborating Research Group" (CRG). Enfin, un signe très positif est que l'Institut commence à reconstituer l'effectif de son secteur scientifique qui avait beaucoup décru ces dernières années. Huit jeunes scientifiques post-doctoraux seront embauchés dans le début de 1994, les recrutements continueront jusqu'à la fin de 1995 pour atteindre le nombre total de 22 sur ces deux années, les premiers boursiers de thèse seront accueillis dès octobre 1994.

Nous conclurons ce rapport en disant que nous considérons que tout est mis en oeuvre pour que l'Institut reprenne ses activités scientifiques et de service en 1994 et ceci quelle que soit la conjoncture générale. L'Institut tient à réaffirmer ainsi sa vitalité et ses engagements envers les communautés scientifiques qui le soutiennent. Si les budgets 1994 et 1995 nous permettent d'assurer ce retour en exploitation, ils ne permettront pas encore le lancement de nouveaux développements importants. Nous souhaitons une amélioration rapide de la situation budgétaire afin que l'Institut puisse reprendre le plus rapidement possible son rôle de création et de développement en instrumentation neutronique ; et ceci n'était pas le moindre des services que l'Institut rendait à la communauté internationale.

J. Rossat-Mignod, membre du Conseil Scientifique, est décédé brutalement à la fin du mois d'Août. Il fut responsable du "Service de Magnétisme et Diffusion Neutronique" au CENG avant de devenir Directeur du Laboratoire Léon Brillouin à Saclay. Il était bien connu et très apprécié par la communauté internationale neutronique pour sa très haute compétence. A l'ILL, où il comptait de nombreux amis et collaborateurs, sa mort a été ressentie comme la perte d'un de ses membres.

Jean Charvolin

While 1992 was characterized by the expression of the ILL Associates' will to maintain the Institut's status as a multinational laboratory, 1993 was the year in which this was confirmed by the signature in Paris on 25 March of the Protocol extending the Intergovernmental Convention between France, Germany and the United Kingdom for at least ten years from 1 January 1994. This made it possible to open negotiations with the present and potential scientific member countries with a view to concluding contracts valid from that date. We are currently preparing for the signature of new contracts with Austria, Spain and Switzerland. It is clearly with great satisfaction that ILL sees the reconstitution of the legal framework associating the countries, and hence the scientific communities, which share its operation and its scientific life. It is also a strong motivation for the continuation of the operations necessary for the restart, covering the refurbishment of the reactor, the reinstallation of the instruments and the implementation of the new structure of the ILL.

Since the removal of the old reactor vessel at the end of November 1992, the emphasis has been on the preparation for the reinstallation. The swimming pool has been completely cleaned, the mechanical strength of its lining checked and its geometry verified. The state of cleanliness achieved is remarkable, as the reactor teams can work there without any particular protective measures, and the inspections and tests reveal a swimming pool in a state very close to its original condition. No additional intervention work has been necessary on the swimming pool. It is now ready to receive the new reactor vessel, whose manufacture is proceeding according to schedule and which should arrive at the beginning of February 1994. Before leaving the technical aspects I will mention that the progress in cutting up the old reactor vessel has enabled us to examine directly the grid with the cracks which led to the refurbishment, and to confirm the hypothesis proposed by ILL as to the appearance of these cracks. All this work has been done under the best possible conditions, thanks to the dynamism and competence of the ILL teams, and to the excellent spirit of cooperation shown by all those concerned with this project. The administrative procedure necessary to obtain the decree to authorize the restart is progressing normally, ILL having forwarded the necessary documents to the appropriate authorities at the dates specified, where they were examined by these authorities, who are implementing the final stages of the procedure. The progress of all the operations, both technical and administrative, and the expenditure situation, have been analysed regularly by the Subcommittee on Refurbishment, which concluded at its last visit to ILL on 18 October 1993 that the costs and time scale have been respected up to the present, and that there is no indication to suggest that the planned date for the restart might not be respected.

As it is now almost certain that the reactor will restart in mid-1994, it was necessary to launch the programme for reinstallation of the instruments, so that these would be available at the same time. We are starting with the work in the guide halls, and shall continue with the installation of the instruments in level C, which were completely dismantled to allow free access to the reactor, as soon as the beam tube thimbles have been replaced. To this end the ILL has to reconstitute as far as possible the manpower required by recalling the scientists and technicians who have been working in other research centres and laboratories. However we shall not avoid a difficult situation, as the ILL is now running in parallel two major technical projects, reactor and instruments, and certain skills, which we cannot duplicate because of the staff limitations, are necessary for both projects.

A final event necessary for the future operation of the ILL was the introduction of the new structure with four Divisions. This is the culmination of a long period of discussions and reflections initiated by the analysis of the ILL's organisation and operation carried out by a working group at the request of the Steering Committee on 27 November 1993. The final reorganisation proposal was accepted by the Steering Committee at its meeting in Abingdon on 2 June 1993, and we wanted to implement it as soon as possible, so as to avoid the sensitive restart period being affected by such a major change, and to ensure that the ILL is ready to operate within the new framework as soon as the reactor starts up, as planned for mid-1994. The change of structure accordingly took place on 1 July 1993, very soon after the meeting of the Steering Committee. Although the ILL has been operating with the new structure since that date,

the corresponding staff complement has not yet been reached, nor has the final distribution of personnel within the new units. The staff situation is still changing, following the first departures under the FNE early retirement plan, the return of scientists and technicians who had worked at other laboratories during the shutdown, and finally the necessary recruitments, particularly in the scientific sector. It is only during 1995 that we shall reach the staff of about 400 envisaged for the new structure. Reorganisation of an institute with a limited staff level also implies internal transfers which cannot all be effected immediately because of the current priorities which are not the same as those of an institute operating normally. The departures and transfers which accompany such a reorganisation have a profound and sometimes disturbing effect on the network of relations linking the members of an organisation, and we should emphasize that in the ILL's case this is taking place with the constructive participation of the staff, who have overcome the doubts and anxieties arising from such a situation.

We have examined three points - reorganisation, reactor refurbishment and reinstallation of the instruments - which are essential to permit the complete installation to start up in mid-1994, and to operate as required with 5 cycles and 25 instruments. We envisage two cycles in 1994, the first being devoted to the final adjustment of the instruments, and the second being open to the users. Experiment proposals will be examined by the Scientific Council subcommittees in autumn 1994, and we shall allocate the beam time for a first group of 3 cycles, one in 1994 and two in 1995. This restart must be covered by a budget comprising the contributions of the Associates, as provided for in the Protocol to the Intergovernmental Convention and the Memorandum of Understanding signed on 25.3.93, and by those of the scientific member countries. These conditions are somewhat restrictive, and for the time being the ILL must devote its efforts to the return to experimental activity, while the development work has to be resumed more slowly. Under these new conditions we shall only offer the users 25 scheduled instruments. This is less than the number before the shutdown, and we are currently looking for a formula to permit the partial rescheduling of the missing instruments by negotiating conditions for their operation with external groups capable of financing this operation in the context of Collaborating Research Groups (CRGs). It is finally a very positive sign that the ILL is starting to reconstitute its scientific sector staff complement, which had considerably diminished in recent years. Eight young post-docs will be recruited in the early part of 1994, and recruitments will continue until the end of 1995 to arrive at a total of 22 over the two years, while the first thesis students will start in October 1994.

We shall conclude this report by saying that in our view everything has been done to ensure that ILL resumes its scientific and service activities in 1994, whatever the general economic situation. ILL is keen to reaffirm its vitality and its commitment to the scientific communities which support it. However the 1994 and 1995 budgets only provide for the return to operation, and do not yet permit the initiation of major new developments. We should like to see a rapid improvement in the budgetary situation, to enable ILL to resume as soon as possible its role of creativity and development in neutron instrumentation; this was not the least of the services which ILL gave to the international community.

J. Rossat-Mignod, a member of the Scientific Council, died suddenly at the end of August. He had been responsible for the 'Service de Magnétisme et Diffusion Neutronique' at the CENG before becoming Director of the Laboratoire Léon Brillouin at Saclay. He was well known and highly appreciated by the international neutron community for his great competence. At ILL, where he had many friends and collaborators, his death was felt as the loss of one of its own members.

Jean Charvolin

War 1992 das Jahr, das durch die Erklärung der ILL-Gesellschafter, das ILL als multinationales Institut weiterführen zu wollen, geprägt wurde, so war 1993 das Jahr, in dem diese Absicht durch die Unterzeichnung eines Zusatzübereinkommens am 25. März in Paris in die Tat umgesetzt wurde. Dadurch wurde das Regierungsabkommen zwischen Frankreich, Deutschland und dem Vereinigten Königreich für eine Dauer von mindestens zehn Jahren ab dem 1. Januar 1994 verlängert. Dies ermöglichte die Aufnahme von Verhandlungen mit den gegenwärtigen und möglichen weiteren wissenschaftlichen Mitgliedern über den Abschluß von Vereinbarungen für die Zeit nach dem 1. Januar 1994. Wir bereiten gegenwärtig die Unterzeichnung der neuen Vereinbarungen mit Österreich, Spanien und der Schweiz vor. Für das ILL ist es selbstverständlich eine große Genugtuung, die Wiederherstellung des juristischen Rahmens zu sehen, der die Länder und damit auch die wissenschaftlichen Gemeinschaften verbindet, die an seiner Nutzung und seinem wissenschaftlichen Leben beteiligt sind. Dies ist auch ein wichtiges Motivationselement bei den Arbeiten zur Vorbereitung des Wiederanfahrens, die die Instandsetzung des Reaktors, den Wiederaufbau der Experimente und die Einführung einer neuen Organisationsstruktur am ILL umfassen.

Seit dem Abbau des alten Reflektortanks Ende November 1992 wurde der Schwerpunkt auf die Vorbeitung des Wiederaufbaus gelegt. Das Reaktor-Schwimmbecken wurde komplett gereinigt, die mechanische Festigkeit seiner Auskleidung kontrolliert und seine Geometrie überprüft. Das Niveau der erreichten Sauberkeit ist bemerkenswert, so daß die Mannschaften sogar ohne besondere Schutzkleidung arbeiten können. Die Kontrollen und Überprüfungen zeigen uns ein Schwimmbecken, dessen Zustand dem Originalzustand sehr nahekommt. Zusätzliche Arbeiten am Becken waren nicht notwendig. Es ist somit für den Einbau des neuen Tanks vorbereitet. Dessen Herstellung geht wie vorgesehen voran. Mit seiner Anlieferung wird Anfang Februar 1994 gerechnet. Zum Abschluß der technischen Aspekte ist noch anzumerken, daß der Fortschritt beim Zerschneiden des alten Reaktortanks eine direkte Untersuchung des Gitters mit den Rissen, die Ursache der Instandsetzung waren, ermöglichte und die Bestätigung der vom ILL zu ihrer Entstehung aufgestellten Hypothese erlaubte. Alle diese Arbeiten wurden dank der dynamischen und kompetenten ILL-Mannschaften sowie des guten Kooperationsgeistes aller Beteiligter an diesem Projekt zur vollsten Zufriedenheit ausgeführt. Das Verwaltungsverfahren zur Erteilung der Genehmigung zum Wiederanfahren des Reaktors verläuft normal. Das ILL hat die erforderlichen Unterlagen zu den vorgesehenen Terminen an die zuständigen Behörden übermittelt, die sie geprüft und nunmehr die abschließenden Verfahrensmaßnahmen eingeleitet haben. Der Verlauf aller dieser technischen und administrativen Maßnahmen sowie die Ausgabenentwicklung werden regelmäßig vom Unterausschuß "Reaktorinstandsetzung" kontrolliert, der anläßlich seiner letzten Sitzung im ILL am 18.10.93 zu dem Schluß kam, daß Kosten und Termine bis jetzt eingehalten wurden und nichts darauf hindeutet, daß der vorgesehene Termin für das Anfahren des Reaktors nicht eingehalten werden könnte.

Nachdem jetzt praktisch davon ausgegangen werden kann, daß der Reaktor Mitte 1994 wieder anfährt, war es wichtig, mit dem Programm für den Wiederaufbau der Instrumente zu beginnen, damit diese ebenfalls zur gleichen Zeit zur Verfügung stehen. Wir haben mit den Arbeiten in den Neutronenleiterhallen begonnen und werden uns im Anschluß an den Einbau der Strahlkanäle dem Wiederaufbau der Instrumente des Niveau C zuwenden, die komplett entfernt worden waren, um Zugang zum Reaktor zu gewähren. Dazu muß das Institut das notwendige Arbeitskräftepotential optimal wiederherstellen, indem es seine in andere Zentren oder Laboratorien abgeordneten Wissenschaftler und Techniker zurückruft. Eine schwierige Lage wird jedoch nicht vermieden werden können, da das Institut gegenwärtig zwei wichtige technische Projekte-Reaktor und Instrumente- gleichzeitig durchführen muß und bestimmte Sachkenntnisse, die aufgrund der begrenzten Stellenzahl nicht verdoppelt werden können, für beide Projekte benötigt werden.

Eine letzte wichtige Voraussetzung für den zukünftigen Betrieb des Instituts war die Einführung der neuen Struktur mit vier Abteilungen. Sie ist der Abschluß einer langen Phase der Diskussion und des Nachdenkens, eingeleitet durch die Analyse der Organisation und des Betriebs des Instituts durch eine Expertengruppe entsprechend dem Auftrag des Lenkungsausschusses vom 27.11.90. Der endgültige Vorschlag zur Reorganisation war vom Lenkungsausschuß auf seiner Sitzung in Abingdon am 2.6.93 genehmigt worden. Wir haben Wert darauf gelegt, die Umstrukturierung so schnell wie möglich in die Tat umzusetzen, damit die schwierige Periode des Wiederanfahrens des Reaktors dadurch nicht belastet wird und auch um sicherzustellen, daß das Institut nach Anfahren des Reaktors Mitte 1994 in diesem neuen Rahmen arbeiten kann. Die neue Struktur wurde am 1. Juli 1993 -kurz nach der Sitzung des Lenkungsausschusses- eingeführt. Wenn auch das Institut seitdem entsprechend seiner neuen Struktur arbeitet, ist weder die entsprechende Stellenzahl noch

die endgültige Verteilung des Personals in den neuen Arbeitseinheiten erreicht. Die Personalsituation befindet sich in der Tat in ständiger Entwicklung als Folge der ersten Abgänge im Rahmen der FNE-Vorruhestandsregelung (FNE = Fonds National pour l'Emploi) und der Rückkehr der Wissenschaftler und Techniker, die während des Reaktorstillstands in anderen Zentren und Laboratorien gearbeitet hatten und schließlich auch wegen der notwendigen Einstellungen, insbesondere im wissenschaftlichen Bereich. Erst im Laufe 1995 werden wir eine Personalstärke von ungefähr 400 Mitarbeitern im Rahmen der neuen Struktur erreichen. Die Umstrukturierung eines Institutes bei einer begrenzten Stellenzahl bringt auch interne Umsetzungen mit sich, die nicht alle sofort durchgeführt werden können im Hinblick auf die derzeitigen Prioritäten, die nicht dieselben sind wie die eines Instituts im Normalbetrieb. Die Abgänge und Umsetzungen, die eine solche Reorganisation in einem Unternehmen begleiten, haben tiefgreifende und manchmal störende Auswirkungen auf das Netz der Beziehungen der Belegschaftsmitglieder untereinander. Wir sollten erwähnen, daß in unserem Fall das Personal auf konstruktive Weise bei der Reorganisation mitwirkt und die Zweifel und Befürchtungen, die eine solche Situation mit sich bringt, zu überwinden wußte.

Wir haben drei Punkte betrachtet -Reorganisation, Instandsetzung des Reaktors, Wiederaufbau der Instrumente- die wesentlich sind, damit das gesamte Institut seinen normalen Betrieb Mitte 1994 wieder aufnimmt und sodann -wie vorgesehen- mit 5 Reaktorzyklen und 25 Instrumenten fortsetzt. 1994 planen wir 2 Reaktorzyklen, wobei der erste Zyklus der Justierung der Instrumente dient und der zweite Zyklus für Benutzer zur Verfügung stehen soll. Die Experimentiervorschläge werden von den Unterausschüssen des Wissenschaftlichen Rates im Herbst 1994 geprüft, und wir werden bei dieser Gelegenheit Strahlzeit für eine erste Gruppe von 3 Reaktorzyklen -1 Zyklus im Jahr 1994 und 2 Zyklen im Jahr 1995- vergeben. Die Bedingungen für dieses Wiederanfahren müssen von einem Haushalt sichergestellt werden, der sich aus Beiträgen der Gesellschafter -entsprechend dem am 25.3.93 unterzeichneten Zusatzübereinkommen zum Regierungsabkommen und dem Vereinbarungsprotokoll- und aus Beiträgen der wissenschaftlichen Mitglieder zusammensetzt. Diese Bedingungen sind ziemlich einschränkend, so daß das ILL derzeit seine Anstrengungen auf die Wiederaufnahme der experimentellen Arbeit konzentrieren muß. Die Wiederaufnahme der Entwicklungsarbeit wird nur langsam möglich sein. Unter diesen neuen Rahmenbedingungen werden wir den Benutzern nur 25 programmierte Instrumente anbieten können, das heißt weniger Instrumente als vor dem Reaktorstopp. Wir suchen gegenwärtig nach einer Lösung, die uns erlaubt, die aus dem Programm genommenen Instrumente teilweise wieder zu nutzen; zu diesem Zweck verhandeln wir mit externen Gruppen, die für die erforderliche Finanzierung im Rahmen von "Collaborating Research Groups" (CRGs) aufkommen würden, über die entsprechenden Betriebsbedingungen. Ein sehr positives Zeichen ist schließlich, daß das ILL anfängt, seine Personalstärke im wissenschaftlichen Bereich zu erhöhen, der in den letzten Jahren stark gekürzt worden war. Acht junge promovierte Wissenschaftler werden Anfang 1994 eingestellt. Die Einstellungen werden bis Ende 1995 fortgesetzt. In diesen zwei Jahren werden insgesamt 22 Wissenschaftler eingestellt werden. Die ersten Doktoranden werden wir im Oktober 1994 begrüßen.

Zum Abschluß dieses Berichtes möchten wir darauf hinweisen, daß aus unserer Sicht alles getan wird, damit das ILL seine wissenschaftliche Arbeit und seine Dienstleistungen im Jahr 1994 wiederaufnimmt, wie auch immer die allgemeine wirtschaftliche Lage aussehen mag. Das ILL möchte damit seine Vitalität beweisen und seinen Verpflichtungen gegenüber den wissenschaftlichen Gemeinschaften nachkommen. Die Haushaltspläne 1994 und 1995 erlauben uns die Wiederaufnahme des Betriebs, sie ermöglichen uns jedoch noch nicht die Inangriffnahme wesentlicher neuer Entwicklungen. Wir hoffen, daß sich die Finanzlage rasch verbessert, damit das Institut so bald wie möglich seine Rolle bei der Konzeption und der Entwicklung im Bereich der Neutroneninstrumentierung wiederfindet. Und dies war nicht der geringste Dienst, den das ILL der internationalen Forschergemeinschaft geleistet hat.

J. Rossat-Mignod, Mitglied des Wissenschaftlichen Rates, starb plötzlich und unerwartet Ende August 1993. Bevor er seinen Posten als Direktor des Laboratoriums Léon Brillouin einnahm, war er Leiter der Abteilung für Magnetismus und Neutronenstreuung im Kernforschungszentrum Grenoble (CENG). Er war ein bekannter und von der internationalen Neutronen-Gemeinschaft wegen seiner ausgezeichneten Fachkenntnisse sehr geschätzter Wissenschaftler. Am ILL, an dem er viele Freunde und Kollegen hatte, wurde sein Tod wie der Verlust eines eigenen Mitarbeiters empfunden.

Jean Charvolin

Relations with ESRF and EMBL

Following the establishment of a common site for EMBL, ESRF and ILL, reported in the last Annual Report, relations with the ESRF have continued to develop at the management level through direct contacts between the Director of ILL and the Director-General of ESRF, and in regular meetings between the two Heads of Administration.

Two major developments on the common site are worth noting. The EMBL has planned an extension to the ILL/EMBL building (ILL20) to provide additional office and laboratory space, with the possibility of eventual access to ILL staff. Construction will start in 1994. Secondly, the ESRF is constructing a guest house to provide sleeping accommodation for visiting scientists. Some rooms will also be available to ILL visiting scientists.

A number of new agreements have been signed with ESRF, including one on the exchange of technical information and documents, and the establishment of a common secretarial service for the theory groups of the two Institutes. These are in addition to existing agreements on joint services, including the joint building, library, medical service, telephone, site security and restaurant.

At the scientific level, many close contacts continue between the staff of the three Institutes on the site, including the development of an image plate detector for diffraction from large-scale structures, led by EMBL (see Chapter "Projects"). A joint ILL-ESRF Workshop on 'X-rays and Neutrons in the Study of Magnetism' was held on 21-23 January 1993, which illustrated the great potential complementarity of the two sources.

The Institutes have cooperated in two 'public relations' exercises locally. In June, ILL and ESRF took adjoining stands at 'La Science en Fête' in Place Victor Hugo in the centre of Grenoble; in November with EMBL they participated in the 'Semaine Européenne de la Culture Scientifique', including a joint press visit to the site.

The ILL and ESRF together continue to press for much-needed improvements in the provision of international schooling for the children of their non-French staff in local schools. They were founder members with local companies of a new 'Association pour le Développement de l'Enseignement International dans la Région Grenobloise' (ADEIRG). Good relations have been established with the local Education Authorities, which have resulted in some improvements in communication with parents. A number of issues have been taken up, including the question of obtaining contractual terms to attract good foreign teachers.

Peter Schofield

– COLLEGES –

The scientific life of the ILL is organised through the Colleges. The Colleges are the forum for scientific contacts and exchanges. The College Secretaries organize seminars and meetings.

The scientists have their hierarchical positions defined in the Science Division. In this respect, they are instrument responsibles and have the duty of dealing with more technical topics. As regards their scientific activities on the other hand, they are left with the utmost freedom, to choose individually their main fields of interest.

The College Secretaries are elected in June each year for a term of one year, which can be renewed for a second year.

College Secretaries in 1993

		Spring	**Autumn**
College 2:	Theory	J. Voit	M. Fabrizio
College 3:	Nuclear and Fundamental Physics	U. Mayerhofer	J. Last
College 4:	Structural and Magnetic Excitations	J. Kulda	J. Kulda
College 5:	Crystal and Magnetic Structures	M. Reehuis (5a) B. Ouladdiaf (5b)	G.J. McIntyre (5a) B. Ouladdiaf (5b)
College 6:	Liquids, Disordered Materials and Metal Physics	J.C. Cook	I. Anderson
College 8:	Biological Structures and Dynamics	R.P. May	L. Vuillard
College 9a:	Molecular Spectroscopy, Surfaces and Mesophases	J.H. Williams	G. Kearley
9b:	Large Molecules	P. Lindner	P. Lindner

The Colleges (except Theory) correspond one-to-one to the Subcommittees of the Scientific Council. The College Secretaries (with help from the Scientific Coordination Office, H. Büttner) prepare the meetings of the Subcommittees. They classify the proposals by subjects and collect advice on their technical feasibility from the College members. In the meetings of the Subcommittees they act as secretary to the Chairperson. One experienced ILL scientist (if possible a Visiting Senior Scientist) per Subcommittee also attends the meetings.

Theory

Members of the College

P. Bares	C. Misbah
S. Brazovskii	P. Nozières
B. Clements	J. Palmeri
M. Fabrizio	P. Quemerais
B. Fourcade	S. Scheidl
F. Gebhard	A. Valance
A. Gogolin	J. Voit
M. Kagan	M. Walker

General

The activity of the Theory College in 1993 has again been considerably affected by budget restrictions as shown by the reduced number of staff in comparison with previous years. The simultaneous growth of the ESRF Theory Group, which shares the Joint (ILL-ESRF) Building with the ILL Theory College, is a positive asset, giving rise to fruitful collaborations among the theorists of both groups.

During the year, the College composition has changed considerably: S. Brazovskii, J. Voit, M. Walker and J. Palmeri left; the first three returned to their own home institutions, whereas J. Palmeri moved to Montpellier where he obtained a CNRS position. Conversely, after October, four new members joined the College: P. Bares (at ILL for two years), F. Gebhard (for six months), A. Gogolin (for one year) and S. Scheidl (also for one year).

Scientific activity in 1993

The research activity of the Theory College concentrated this year on condensed matter physics, covering various areas which are listed below. Special interest has been devoted to "low dimensional" physics, ranging from correlated fermion systems in reduced dimensions, to various aspects of surface physics, to the thermal behaviour of lipid vesicles and polymerized membranes.

Helium and related topics

B. Clements investigated the structure, stability, excitations and thermodynamics of thin films of liquid ^{4}He on weakly attractive substrates. This work has been done in collaboration with E. Krotscheck (USA), H.J. Lauter (ILL), and M. Sarrela (Finland). Experiments have shown that these films can form well-defined atomic layers of *liquid* ^{4}He, lying parallel to the substrate, and persisting rather deep into the film. Depending on the surface coverage, their theory predicts that superfluid ^{4}He films, adsorbed on a graphite substrate, exist in both uniform and non-uniform surface-covering phases. The transition between the two phases is first order, occurs near layer completion, and can persist for at least three liquid layers. For a sufficiently smooth substrate these layering-transitions should be observed in torsional oscillator experiments. A less pronounced layering structure is found for the alkali metal substrates, but in the case of magnesium, at least one layering-transition should be experimentally detectable.

Thin films of ^{4}He adsorbed to a plane substrate also provide a unique opportunity to study the structure of the "nearly" two-dimensional quantum liquids where, as the thickness of the adsorbed film increases, a transition from an "essentially two-dimensional" to an "essentially three-dimensional" system takes place. Using a generalized Feynman theory, including multi-phonon scattering effects, they have determined as a function of surface coverage the dispersion relations, excitation mechanisms, transition densities, and particle currents. A pronounced softening of the long-wavelength, lowest-energy mode is observed near the layering transition. Because of the layered growth, the film's sound velocity exhibits a series of oscillations. In a monolayer, the nature of the excitations undergoes a noticeable change at the coverage where the velocity of sound starts to *decrease*. This is a crossover from "essentially two-dimensional" to "essentially three-dimensional" behaviour. At long wavelengths, below (above) the crossover coverage, the lowest-energy excitations are longitudinal phonons propagating within the monolayer (surface excitations). At higher wave numbers, a layered-phonon level-crosses with a surface excitation to become the lowest-energy mode. For double- and higher-layer films, the excitations are complicated by multiple (layer-phonon with layer-phonon and layer-phonon with surface excitations) level-crossings.

Pursuing a stimulating discussion with a visiting seminar speaker (M. Liu), J. Palmeri began to reexamine the problem of the dynamics of the phase boundary between the A and B phases of superfluid ^{3}He. He has been attempting to settle the question of what is the dominant friction mechanism on the moving phase boundary.

P. Nozières completed a work he started inspired by a set of lectures given some years ago. He has settled a question never clarified in the past: why does a condensate form in a pure state and not within different degenerate states ? He showed that it is the *exchange* energy which makes the big difference, and which is lastly responsible for the *purity* of the condensate.

S. Scheidl has started a collaboration with D. Feinberg (CNRS). They intend to develop an improved phenomenological description for materials where proximity effects of metallic atoms between superconductive layers are important.

Correlated fermion systems

P. Quemerais and P. Bares, in collaboration with D. Nunez-Regueiro (ESRF) and A. Bianconi (Italy), are investigating the possible existence of polaronic charge density waves induced by the interplay of strong correlation and electron-phonon interaction. This work has been

stimulated by recent experiments on $La_{2-x}Sr_xNiO_{4+y}$ compounds, which suggest that such a combined effect might indeed be relevant in these materials. As a first step, they have considered a one dimensional model of polarons in presence of strong on-site repulsion. Their aim is to get as much exact information as possible in 1D, before passing to the higher dimensions relevant for the experiments. Although the investigation is still in progress, the preliminary results seem quite promising, especially from the viewpoint of a better understanding of the role of electron-phonon interaction in nickelate compounds and high T_c-materials.

F. Gebhard and P. Bares are both experts on low dimensional models solvable by Bethe Ansatz methods. Bares has been investigating the possibility of applying these methods for solving a particular one-dimensional model of light and heavy particles with local interaction.

Together they are trying to construct the eigenstates of the exactly solvable $1/r$-Hubbard model, which might lead to a generalization of the Bethe ansatz technique. Such a model exhibits a metal-to-insulator transition at half filling for a finite strength of the on site repulsion, in contrast to the more popular Hubbard model where this critical value is zero. The hope is to understand the origin and the relevant features of the correlation driven metal-insulator transition, in order to construct more realistic Hamiltonians which might show similar behaviour.

Gebhard is also interested in studying the link between single-site and lattice problems for interacting electrons. Lattice Hamiltonians with a large number of nearest neighbours, or with a random dispersion relation, can be mapped onto single site models which may thus also be used to study the Mott-Hubbard metal-to-insulator transition.

S. Brazovskii's research was devoted to several subjects in the theory of quasi one-dimensional (1D) superstructures and of 1D models of interacting electrons.

He has, together with S. Matveenko (CEI) and P. Nozières, addressed the problem of spin-charge separation in 1D, by analysing current carrying states in a system of interacting electrons, exploiting both the exact results known for the Hubbard model and the bosonization technique. He found that both spin and charge excitations carry currents proportional to their respective momenta. In spite of being in agreement with a single particle picture of a noninteracting 1D Fermi gas, this result contrasts the spin-charge separation concept as it is usually derived from the bozonization or from strong coupling arguments. For weak interaction, this paradox is resolved by taking into account the Fermi velocity dispersion and by reexamining the current operator structure. For strong interactions he found an effect of holon drag by a spinon.

He has also investigated intrinsic defects in Density Wave (DW) crystals. For an isolated point (the 2π-soliton) and for a line (the dislocation) defect, he showed that the Coulomb interaction dominates in determining distributions of the phase φ, of the potential ϕ and of the accompanying electronic structure. The last shows itself e.g. in the collapse of the DW state over a number of chains around the dislocation. In spin DW conventional dislocations lose their priority in favour of a special topological object: a half-integer dislocation combined with a semi-vortex of the staggered magnetization vector.

By reconsidering on microscopic grounds the effects of the electric field on the phase dynamics and relaxation of CDW/SDW, he suggested a transparent form of the dynamic and dissipative equations for the DW phase and for the electric field. His approach is based on a helpful relation between a "generalized condensate density" and a complex dielectric susceptibility of intrinsic carriers. Separately for CDW and SDW, he got the spectra and the attenuation for the TO and LO modes, the low frequency relaxation and the intrinsic nonlinear conductivity.

M. Fabrizio has worked on the behaviour of weakly coupled one-dimensional chains of interacting fermions. His aim was to understand how stable the peculiar one-dimensional behaviour is in relation to the switching of weak transverse correlations induced by direct hopping between the chains. He showed that the one-dimensional behaviour (so called Luttinger-liquid behaviour) is quite unstable as one couples chains together, since any weak interchain hopping generates very strong correlations between the chains, and he was able to determine which correlations are favoured.

Together with A. Gogolin and S. Scheidl, they have started a study of the transport properties of quantum wires in presence of diluted scattering centres. Since it seems experimentally crucial, their model includes an unscreened Coulomb repulsion between the electrons. Therefore 1) they investigated how Coulomb repulsion changes the response of a one-dimensional band to an impurity potential; 2) they will consider how the presence of more one-dimensional bands (as it is usually the case in experiments) modifies this scenario.

A Gogolin's research has been concerned with the theory of quantum wires. In collaboration with N. Prokof'ev (USA), he studied the persistent current phenomenon both for interacting and non-interacting electrons. In the latter case, in presence of a disordered potential, they were able to derive a universal formula expressing the persistent current in terms of the transmission coefficient at the Fermi energy. In presence of electron-electron interaction, they showed how an unusual size dependence of the current amplitude arises from the interplay of disorder and interaction.

P. Nozières continued his work on the behaviour of heavy particles coupled to a light Fermi sea. This problem is of fundamental importance for the physics of heavy fermions and of many correlated systems. In particular, he showed under what conditions the edge singularity produced by a *single* and *fixed* scattering centre, persists if this source

of scattering is left free to recoil. For a *non-localized* particle, he proved rigorously that the singularity survives only in one, but not in higher, dimensions; a result which raises serious doubts on many of the theories proposed for high T_c superconductivity. Besides, he has been investigating other related models, like the resonant level model he studied last year together with C. Varma, where essentially effective spin 1/2 channels interact with screening channels, giving rise to a whole series of interesting phenomena.

Much of J. Voit's research interest was devoted to spectral properties of Luttinger liquids, pursuing a study initiated in 1992. His investigation aimed at showing where and which of the peculiar properties of Luttinger liquids show up, how they can be measured and how they interfere/separate in any given experiment. Such properties have been clearly observed in a wide series of photoemission experiments on Bechgaard salts, which have been analysed by Voit in comparison with the existing theory of Luttinger liquids. The outcome of this analysis is that, in order to account for the experimental data, one is obliged to assume for these materials a model hamiltonian, which includes a long range interaction term. He has also shown how other very interesting features of Luttinger liquids (like the so called "spin charge separation") might be observed in experiments where two particle correlations are worked out, as, for example, in inelastic neutron scattering.

Another field of Voit's activity was concerned with electron-libron coupling in polyaniline. In collaboration with D. Baranowski (Germany) he obtained two important results, both connected to failure of Peierls' "theorem": (i) in the strong correlation limit of the half-filled band, they found several phases with regular lattice spacing. This implies that beyond a critical interaction strength the dimerized Peierls state becomes unstable towards e.g. an ideal paramagnet. (ii) In the weak correlation limit at quarter-filled band, phases with long periods are lower in energy than the period-four Peierls state. They will have important consequences for the interpretation of experiments.

Continuing a collaboration with Anna Painelli and Gian Paolo Borghi (Italy) on a new exact numerical diagonalization method for interacting electrons coupled non-adiabatically to phonons, they developed a new algorithm, which takes advantage of the adiabatic basis of the problem, in order to reduce the critical memory requirements. They found some interesting new results, e.g. that, contrary to earlier wisdom, there are cases of antisqueezing, i.e. where quantum fluctuations reduce the position uncertainty of the phonons increasing the momentum uncertainty.

M. Walker began a collaboration with Keith McEwen (UK) to try to understand the nature of an apparently quadrupolar ordered phase of UPd_3. He also completed work on the identification of the ordered phase of heavy-fermion metal URu_2Si_2 which exists below 17.5K. In addition, he continued work with graduate students on theoretical models for the phase diagram of betaine calcium chloride dihydrate, and for the low-temperature hexagonal phase of C_{70}.

Surface physics

P. Nozières devoted much of his 1993 activity to this subject, since he gave a set of lectures at the Collège de France on "*Crystal surfaces: structure, fluctuations, growth and stability*". Among the various aspects of this problem tackled in his lectures, some have led to new developments. In particular, he carried on research concerning: (i) the mobility of a vicinal surface in connection with the recent experiments on capillarity oscillations; (ii) Grinfeld instability of a faceted or vicinal surface.

C. Misbah investigated some problems connected to vicinal surfaces. He analysed the steady-state cellular structure that may arise during step flow growth (growth from a super-saturated vapour, or by molecular beam epitaxi).

In connection with the problem of the competition between noise and determinism in step flow growth, he extended the Burton-Cabrera-Frank theory to include fluctuations. He derived the non-linear stochastic equation controlling the behaviour of a single step, and thus he could determine the range of parameters where fluctuations compete with deterministic dynamics.

He also studied the behaviour of linear fluctuations of a train of steps. He derived the shape of the excitation spectrum of an asynchronized train of steps. Asynchronized fluctuations lead to qualitatively new effects. In particular the time needed to form a bump on a step scales as l (l = interstep distance), while it scales like l^{-1} for a synchronized train.

M. Fabrizio, in collaboration with E. Tosatti and G. Santoro (Italy), has studied a solid on solid model for fcc (110) surfaces which can describe, depending on the value of the parameters, rough, disordered and reconstructed (2×1) and (1×1) surfaces. They studied this model by mapping it onto a quantum spin-1/2 chain of Heisenberg type. Such a model was then analysed both by numerical diagonalization, as well as by analytical techniques. This allowed them to obtain a complete characterization of the phase diagram of the model.

Liquid crystals, lamellar eutectics, polymerized membranes and lipid vesicles

C. Misbah studied extensively the problem of growth of lamellar eutectics and liquid crystals. He discovered a new broken parity-state, where, in contrast to the state where both lamellae are tilted in the same direction, each lamella has a tendency to choose an opposite tilt angle to that of its neighbours. He suggested new experiments to observe this state.

In connection with liquid crystals, he tackled the problem of the coupling between the nematic-isotropic growing front and the elasticity of the nematic phase, and he analysed it in a special geometry. He showed that weak growth speed corresponds to weak coupling between those two effects, and the contrary for high speed. A part of this work was done with his student A. Valance, who obtained his Doctoral degree on November 29th 1993 with a thesis entitled: "Contribution à la théorie dynamique de croissance des cristaux liquides et des eutectiques lamellaires".

B. Fourcade has mainly worked on the behaviour of lipid vesicles. Phospholipid vesicles of high topological genus have been observed in laboratory experiments. These systems exhibit strong thermal fluctuations, and they differ from the usual thermal undulations of the membranes. They can be described as positional fluctuations of necks connecting to concentric membranes. Together with the group of Bensimon in Paris, he has introduced a model based on an electrostatic analogy. Such a model has been tested numerically and analytically and it shows that the holes or necks can move almost freely on these membranes. He is also investigating two component membranes (with a D.E.A-student, T. Charitat), as well as budding problems (with another D.E.A.-student, G. Rudine).

During 1993, J. Palmeri began investigating an uncontrolled, but perhaps effective saddle point expansion method for going beyond the non-perturbative variational treatment that he developed with E. Guitter to study crumpling transitions for self-avoiding polymerized membranes. Moreover, he attempted to develop a non-perturbative method that avoids the replica trick for studying problems with quenched disorder. He applied such a method, which makes use of the so-called "principle of minimum sensitivity", to the problem of directed polymers and manifolds in random media.

Other condensed-matter topics

M. Fabrizio, together with P. Carra (ESRF), investigated (theoretically), the possibility of using X-ray resonant inelastic scattering (XRIS) as a probe of charge and magnetic correlations in transition metals and rare earths. Their analysis of the scattering cross-section relies on the application of sum rules, recently derived for X-ray absorption and dichroism; it shows that XRIS might provide a powerful new tool for obtaining new information on magnetic and anisotropic materials.

P. Quémerais studied the growth of intermetallic compounds with strong chemical order. He proposed a simple one-dimensional model of growth, based on an electronic process, which is quite helpful for understanding the selection and the propagation of a periodic or quasiperiodic chemical order during the growth process. This mechanism has been proposed as one of the important physical features for the comprehension of quasi-crystal growth.

Secretary: Michele Fabrizio

Elementary excitations in liquid ^{4}He films

B. E. Clements and H. J. Lauter

The structure, excitations, and growth of liquid ^{4}He films, adsorbed on a graphite substrate, are of considerable experimental and theoretical interest. It is an intriguing goal to uncover the underlying mechanisms that drive an apparently simple system to display a complicated growth scenario [1,2], a multitude of thermodynamic phases [3], transient superfluid behaviour [4], and so forth. To understand these phenomena one should first have a good understanding of the film's elementary excitations.

Neutron scattering experiments carried out by Lauter, Godfrin, Frank and Leiderer [5], done on low temperature films and for a broad range of surface coverages, reveal spectra that are rich with structure. In Fig. 1, the experimental dynamic structure function, $S(q, w)$ is shown for a ^{4}He film adsorbed on a graphite substrate. It is well known that adsorbed helium films grow initially by the formation of well-defined *liquid* layers. Fig. 1 corresponds to a triple-layer liquid film.

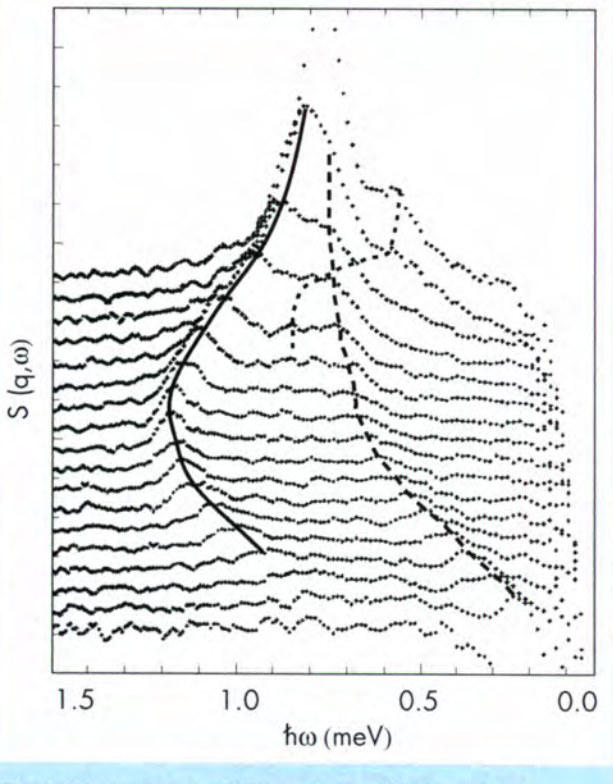


Fig. 1: The experimental S(q,w) for a triple-layer film (crosses). The surface coverage is 0.239 Å^{-2}. The lowest and highest curves correspond to $q \approx 0.25$ Å^{-1} and $q \approx 2.0$ Å^{-1} respectively. Also shown are the phonon-maxon-roton mode (solid curve), the surface mode (long-dashes) and a layer-phonon mode (dots) that level-crosses with the surface mode.

The experiment was performed at the time-of-flight spectrometer IN6. The scattering sample consisted of ^{4}He adsorbed on graphite (Papex), which was kept at a temperature of 0.65 K. The basal planes of the graphite are in the scattering plane. Each experimental curve (the crosses) corresponds to a different wave vector q. The wave vectors range between 0.25 Å^{-1} and 2.0 Å^{-1} and occur at approximately equal intervals. The largest wave vector corresponds to the position of the roton minimum in bulk helium. The $S(q, w)$ have been vertically displaced for each q to provide a clear representation of the excitations.

In the figure, additional curves have been drawn to indicate the positions of the various excitations. It is clear from the figure that, already for three layers, there is a rather strong signal coming from a mode that will evolve into the bulk phonon-maxon-roton spectrum. In Fig. 1 this mode is the highest-energy dispersion curve. The low-energy surface excitation (ripplon) is equally clear from this figure. This mode is absent when the scattering is performed on a full cell. This provides proof that this mode is indeed related to the liquid-gas interface. There are two more important observations. First, between the phonon-roton excitation and the surface mode there is a plateau in the strength of $S(q, w)$. The plateau is most obvious for the larger wave vectors. It appears that there is too much scattering to be explained by the phonon-roton mode (whose experimentally determined maximum line width is obvious from the figure), the surface mode, and the multiphonon contributions. The latter, which are highly temperature dependent, can probably be ruled out as a possible cause for the large plateau by looking at energies above the phonon-roton mode. There it is seen that multiphonon excitations produce very little scattering at this temperature. Second, there is a low-energy, high wave vector mode with substantial strength located below the roton minimum.

An explanation for the plateau and the extra mode is provided by theoretical calculations. In close collaboration with Eckhard Krotscheck of Texas A&M University, and Mikko Saarela of the University of Oulu, a generalized Feynman theory of excitations has been developed and applied to these systems [6]. In Fig. 2, our theoretical $S(q, w)$ is shown for a triple layer ^{4}He film on a graphite substrate. The intensity of the mode is measured by the shade of the greyscale. To keep the figure as clear as possible, we have chosen to omit multiphonon effects here. From Fig. 2, it is clear that the theory predicts several modes. At short wave vectors the surface mode is the lowest-energy mode present. The theory shows that, for wave vectors below 1.5 Å^{-1}, this mode propagates on the surface of the film and has a strong component of the particle's motion that is out of the plane of the film. At high energies (15 - 20 K) a strongly coverage dependent mode has formed that will eventually become the bulk phonon-maxon-roton dispersion curve. Several intermediate energy modes are also apparent. The theory shows that these modes are "layer-phonons", i.e., longitudinal phonons that propagate *within* a given liquid layer. Layer-phonons begin having significant strength at wave vectors around 1.0 Å^{-1}.

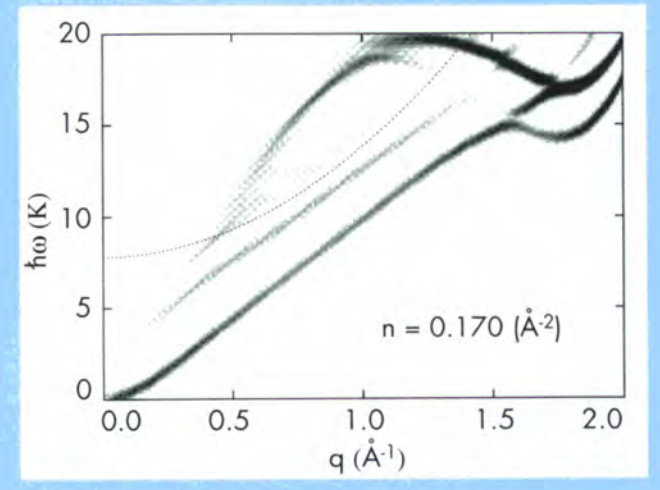


Fig. 2: Map of the theoretical dynamic structure function S(q,w) in Feynman approximation for a triple-layer film with a surface coverage of 0.17 Å^{-2}. The dotted parabolic line is the boundary which separates discrete from continuum states, in the Feynman theory. The darkness of the greyscale indicates the scattering intensity.

We have proposed that these layer-phonon modes are responsible for the effects mentioned above. The possibility of seeing at least one of these layer-phonon modes in the experimental data is evident from Fig. 1. A rather clear mode has been indicated by the dotted curve in that figure. Similar to the theoretical lowest energy layer phonon, the experimental mode has a dispersion curve that runs quite close to the surface mode - for intermediate wave numbers ($q \approx 1.2$ Å^{-1}) it gives the experimental surface mode a bimodal appearance. Interestingly, this mode appears to level-cross with the surface mode at $q \approx 1.5$ Å^{-1}, and for q near the roton minimum, where it has emerged out of the continuum, the full strength of the mode is shown. It is also very convincing that the sharp kink seen in the lowest-energy mode, in Fig. 1 is very similar to the sharp kink observed in the theoretical values where level-crossings occur ($q \approx 1.5$ Å^{-1}). In both the experimental and theoretical $S(q, w)$ the surface mode is no longer the lowest-energy mode for wave vectors above the level-crossing. For the experimental case, this is evident by studying the line width of the surface excitation through the level-crossing

region; below and above the level-crossing there is a clearly defined "shoulder" in $S(q, w)$ which is the surface mode. In the theoretical analysis, we arrive at this conclusion by studying the particle current below and above the level-crossing. At wave vectors below (above) the level-crossing the *lowest-energy* excitation is a surface mode (layer-phonon). It is also clear from Fig. 2 that there is the possibility of multiple (layer-phonon with layer-phonon) and (layer-phonon with surface excitation) level-crossings. Finally, in the full-cell bulk limit, both experiment and theory show that the layer-phonon mode has non-negligible strength and retains an energy lower than the *bulk* roton! The theory shows that the layer-phonon propagates in the first layer of the liquid-solid interface.

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Nuclear and Fundamental Physics

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H.G. Börner
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G. Fioni
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A. Jungclaus
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Summary

As the only experiment at the ILL which took data during the reactor shutdown the magnetic electron spectrometer from BILL continued to be used for a precision measurement of the ^{177}Lu β–spectrum. BILL had been moved to the old PF1 site the year before. Another, different, heavy neutrino rearch experiment was performed in a collaboration with the University of Heidelberg.

Before coming to the ILL J. Last had been involved in the design of an electron pair spectrometer APEX (Argonne Positron Experiment) to measure positron lines in "very-heavy-ion" collisions below the coulomb barrier. APEX was completed this year and started to take data. J. Last's contribution to the experiment was the development of a position sensitive NaI(Tl) array for the APEX trigger detector [1].

At the UCN facility PF2 work on the neutron Electric Dipole Moment (EDM) experiment has continued. V. Nesvizhevsky from Gachina spent several months at the ILL to study the systematic errors in neutron bottle life time experiments with the special emphasis on the MAMBO II set-up.

The PN1 upgrade was completed during 1993 with successful testing of the ion optics of the new electro-magnet system with an α source. Current activities include feasibility studies on the PIAFE project in which it is proposed to place a thermal fission source at an in-pile position using the H9 beam tube.

The spectrometer GAMS 2/3, after upgrading, has been reinstalled at the C-level of the reactor. The prototype interferometer GAMS 5T (Munich-ILL-collaboration) has been assembled and is currently being tested. The new GAMS 5 spectrometer, which will replace GAMS 1 has been designed. Its assembly will start in 1994.

During 1993 A. Williams and U. Mayerhofer were detached to the ESRF with the latter rejoining College 3 at the beginning of December. G. Fioni temporarily left the ILL in July to work at the ISN on the PIAFE project. He will return to the ILL at the end of January 1994. The restructuring of the ILL also brought three new members to College 3: W. Drexel and P. Geltenbort who will be responsible for PF2 and P. Ageron who is interested in experiments with slow neutrons.

In memory of W. Mampe College 3 held a one day colloquium on 29th January, 1993. His family, friends and physicists met at this occasion to listen to talks which covered the broad range of Walter's scientific interests (See also the article by M. Pendlebury at the end of the College 3 chapter).

Scientific Highlights in 1993

At the Cold Polarized Neutron Beam Facility PF1

Scientific activity at PF1 in 1993 was almost entirely devoted to two heavy neutrino searches. One of them continued to use the BILL magnetic spectrometer while the other one was done with a scaled down version of the successful PERKEO neutron decay spectrometer.

The ILL collaboration with the Technical University Munich continued to search for a heavy neutrino contribution to nuclear β-decay. First restricting limits for the mass region up to 30 keV were established. Subsequently a new and improved detector system has been developed and installed at the BILL magnet by S. Schönert from the TUM. It should now be possible to extend the sensitivity for heavy neutrino admixtures for up to masses of several 100 keV.

In collaboration with the University of Heidelberg the PERKINO (sic!) magnet was set up to measure the β-spectrum of ^{35}S with silicon detectors using a virtually loss-free method originally developed for free neutron decay. Our aim was to study the systematic effects which electron backscattering could have on the spectral shape in the region around the energy end point. The principle of the experimental setup is shown in Fig.1. Various coincidence conditions and energy cuts can be imposed on the data. It is thus possible to extract the spectrum of electrons which are backscattered from a silicon detector surface. These spectra perfectly agree with results from complicated Monte-Carlo calculations using the EGS4 program library (see Fig.2). As a result of the experiment we were able to set stringent limits on the amplitude of heavy neutrino admixtures in the

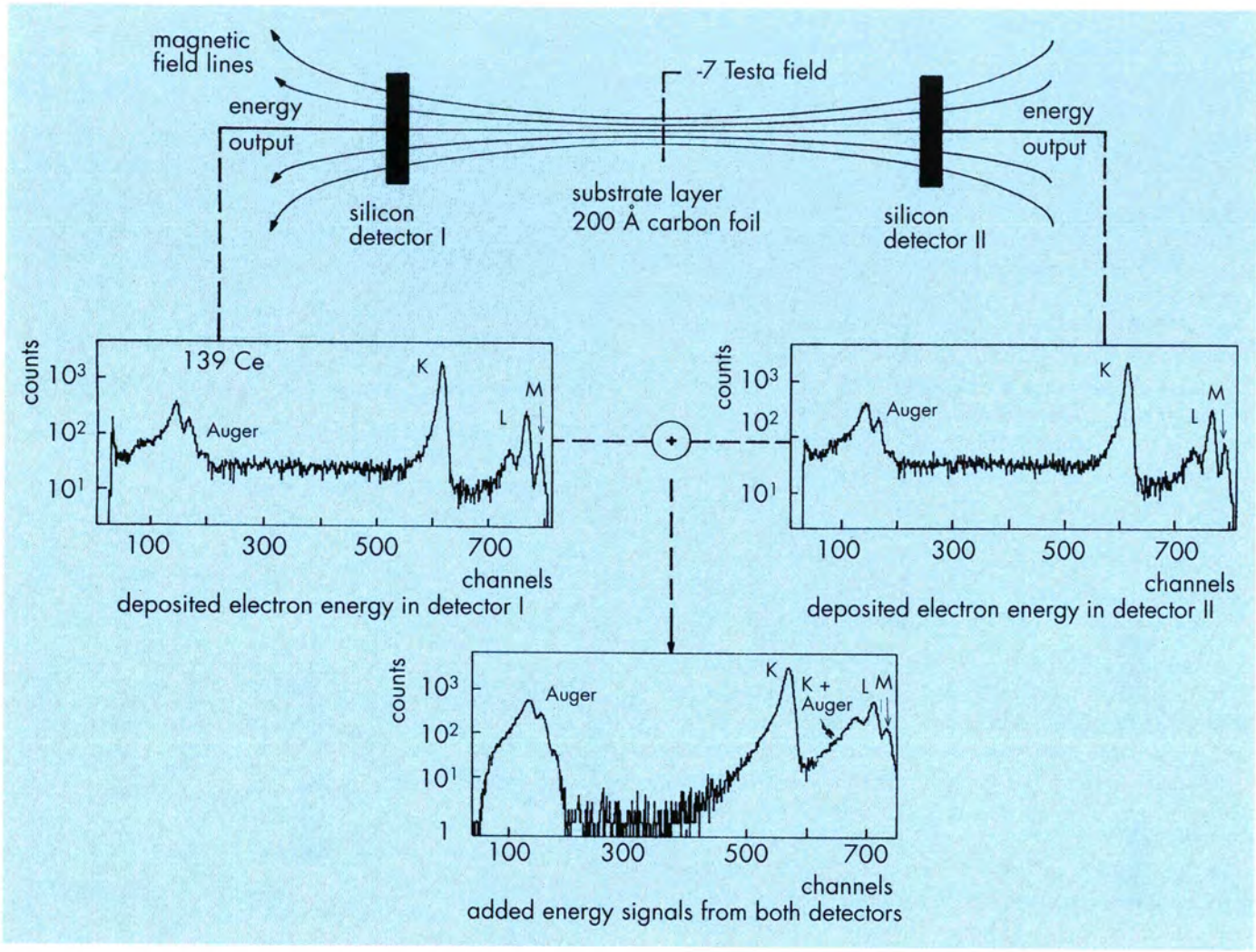


Fig. 1: The principle of loss-free β-spectroscopy: electrons emitted by the conversion electron source are trapped between two silicon detectors by the magnetic field and can, even after multiple backscattering, lose energy only to the detectors. When the single spectra (middle) are summed electronically the backscatter tail disappears (bottom).

same system which so far had produced the most significant heavy neutrino signals (Fig.3). We found that the energy spectrum of electrons scattered from solid matter could create a heavy neutrino kink when superposed to the original β-spectrum (Fig.4). The results were published in [2].

At the Ultra-Cold Neutron Facility PF2

Work on the current neutron EDM project using UCN at ILL by the Sussex-RAL-ILL-Washington-PNPI collaboration has continued. The mercury magnetometer under development has just recently reached the stage where it has the required signal-to-noise ratio. The next step is to study its response to high electric fields.

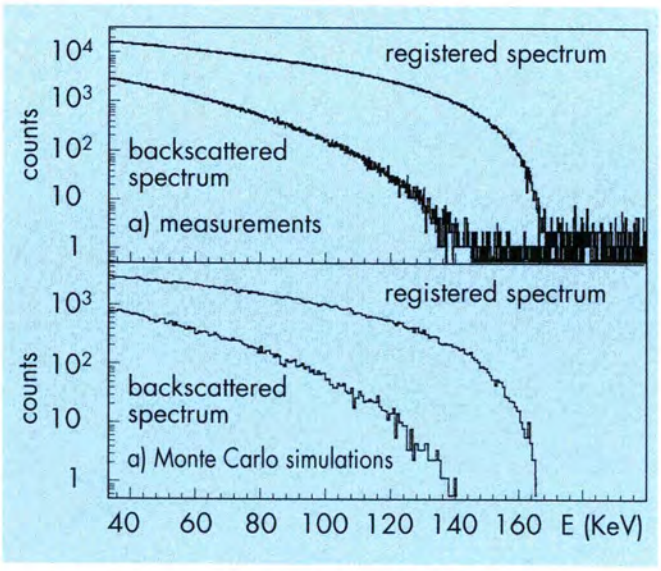


Fig. 2: a) Measurements of the initial and the backscattered electron spectrum; b) Monte Carlo simulation of the initial and the backscattered electron spectrum.

For the Mambo II project an intensive study has been carried out by ILL thesis student F. Schorr and visiting scientist V. Nesvizhevsky to predict all the contributions to the measurement errors which will arise when it is used in future to measure the neutron lifetime.

This year saw the publication of the neutron lifetime measurement $\tau_n = 882.6 \pm 2.7$ s derived from the Kurchatov Institute - ILL experiment carried out at the ILL in 1990 [3]. The experiment is shown in Fig. 5. It is the only neutron lifetime experiment using UCN storage which has used the detection of up scattered UCN at thermal energies as well as the direct detection of UCN. The storage vessel had walls of stainless steel coated with Fomblin oil. A removable liner allowed the wall surface area exposed to the neutrons to be changed by a factor of about 2.5 where this factor applied also approximately on a local basis over all parts of the trap. Besides changes of surface area, measurements were made at room temperature and at –55 °C where the Fomblin was frozen. The detected neutron up scattering rate compared with the number of UCN stored, was used as a measure of the wall losses.

A number of talks on UCN were presented at the Colloquium in Memory of Walter Mampe in January. One of the most interesting problems discussed was that of the much greater than expected wall losses for UCN in material traps where steps have been taken to control surface hydrogen [4,5]. Data for beryllium presented in the former paper are shown in Fig. 6. Standard theory relates the losses on the trap walls to the total loss cross-sections and number densities of the wall atoms. These cross-sections can also be measured in other experiments using the transmission of very cold neutrons. Curves 1a, 3a and 4c show similar increases with temperature which are consistent with what can be expected for the inelastic up scattering of beryllium and its increase with temperature. At the lowest temperatures

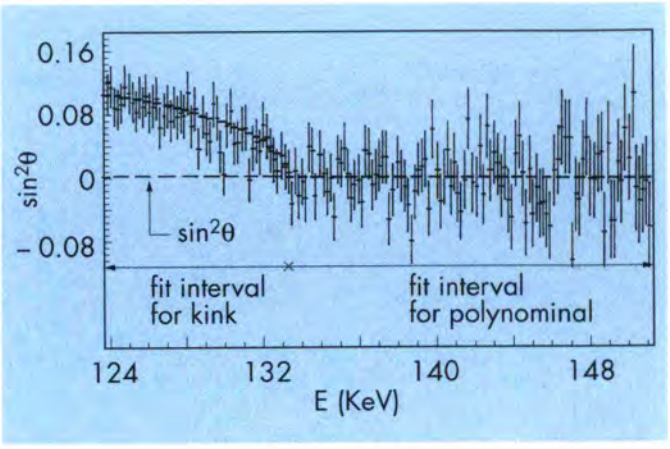


Fig. 4: Appearance of a kink in the single detector spectrum due to electrons backscattered onto the detector, and theoretical fit of heavy neutrino kink to the data [1].

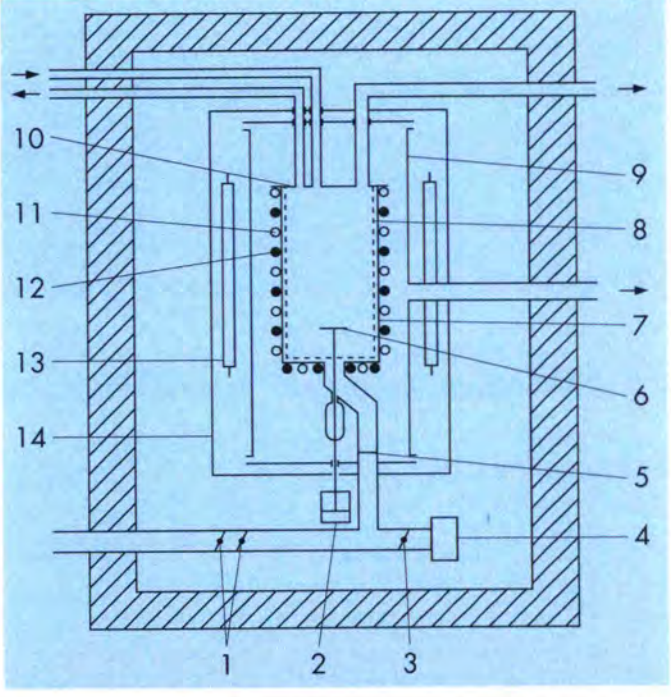


Fig. 5: Experimental layout. (1) Entrance gates of the guide for the ultracold neutrons; (2) mechanism which controls the plate-shaped inlet/outlet gate 6 of the storage vessel; (3) gate of the detector of ultracold neutrons; (4) the detector of the ultracold neutrons; (5) thin (0.1 mm) aluminum diaphragm which separates the high-vacuum chamber of the storage vessel from the neutron guides; (6) plate-shaped gate; (7) storage vessel; (8) auxilliary surface; (9) outer vacuum jacket of apparatus; (10) scatterer which removes "supercritical" ultracold neutrons from the spectrum; (11) coiled tube for cooling the storage vessel; (12) heater for the storage vessel; (13) detectors of thermal neutrons which result from inealstic scattering of ultracold neutrons by the surface of the storage vessel; (14) cadmium shielding.

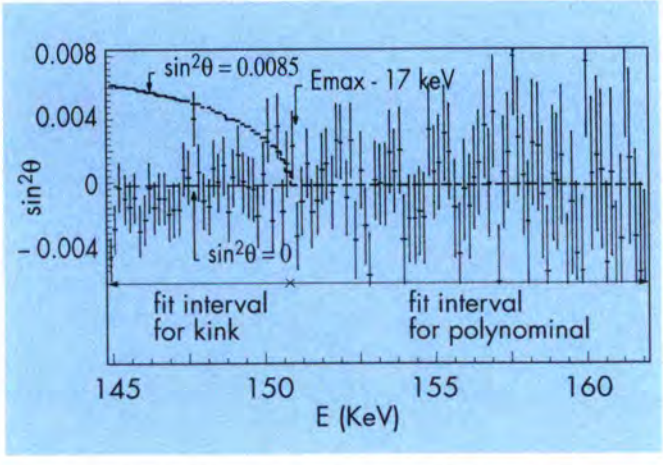


Fig. 3: Residuals of best fit of orthogonalized polynomials to ^{35}S ß–spectrum.

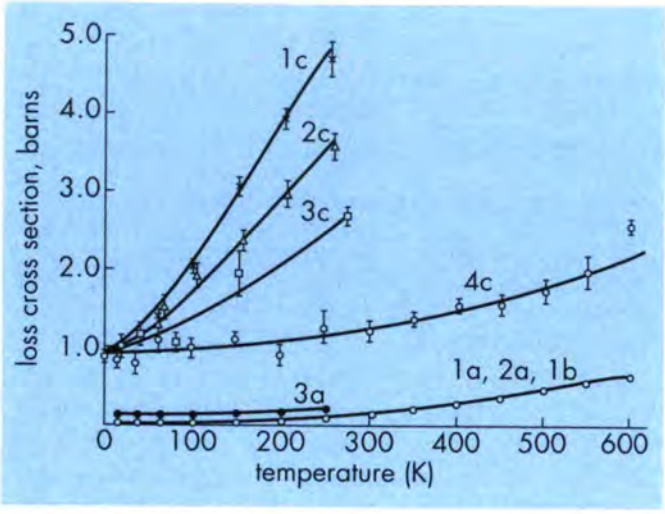


Fig. 6: (1a) Fused Be; (2a) quasi-single-crystal Be; (3a) pressed sintered beryllium; (1b) theoretical temperature dependence of the beryllium loss cross section ($\sigma_a+\sigma_{in}$) calculated in the Debye model; (1c) "spherical" deposited Be trap, not degassed; (2c) deposited cylindrical trap, degassed (5 h at 250°C); (3c) all-Be trap, degassed (8 h at 300°C); (4c) "spherical" deposited trap, degassed (28 h at 350°C, with purification of the evaporated He And D_2).

shown, the dominant contribution to the loss cross-section should be capture in beryllium. The value observed for curve 1a is consistent with the accepted value of 9 mb for the capture cross-section. (The somewhat higher cross-section seen in transmission through the sintered beryllium sample of curve 3a is expected in view of the inhomogeneity scattering). At low temperatures, curve 4c from trapping experiments shows a value which is approximately 100 times greater than the capture cross-section. The absence of up scattered neutrons suggests that the associated loss process in case 4c involves capture, at least at low temperatures. These enhanced losses amount to a probability of loss of $1 \cdot 10^{-5}$ per wall collision.

M. Pendlebury visited Japan to see some projects on ultra cold neutrons there. In particular the results of experiments on UCN production in liquid helium by down scattering of 9 Å neutrons were discussed [6]. The Yoshiki fridge has been run on a cold guide at JAERI. Up to now, UCN have to pass out through the radiation shielding windows to room temperature regions before they can be detected. As in the case of the fridge which has been run at ILL, the passage through the windows seems to produce larger than expected losses. Measurements at ILL by physicists from TU Munich, RAL and HMI on up scattered neutrons derived from UCN stored in the helium have indicated that the number of UCN produced in the helium is close to the number expected from theory. Now, Japanese physicists are developing a scintillation detector for UCN which will work at 4 K with the aim of detecting the UCN directly in the liquid helium. They are also starting to build an instrument to measure the neutron EDM which will be connected to the fridge source and also operate at low temperature. A UCN fridge source operating on a cold guide like H53 at ILL should be able to accumulate UCN to a density of about 2000 cm^{-3}.

At the PN1 facility LOHENGRIN

Production rates of exotic isotopes along the astrophysical r-process path

Investigations based on data from the Lohengrin spectrometer for far asymmetric fission of ^{236}U (Fig. 7) have shown that a simple correlation can be established between the yield and the reaction Q-value of the process. This correlation is exemplified in Fig. 8 and shows a linear correspondence if yields are displayed on a logarithmic axis:

$$\ln(yield) = aQ + b$$

The regression analysis gives a=0.544 and b=–95.861. Here only ground state masses are taken into account, the neutron binding energy from the thermal neutron capture reaction is omitted. The correlation coefficient for the data points between mass 70 and mass 87 is about 0.97, which allows the calculation of yields to a factor of 3 if estimates for Q-values for exotic nuclei can be taken from tables. The striking feature is that the above relation holds over

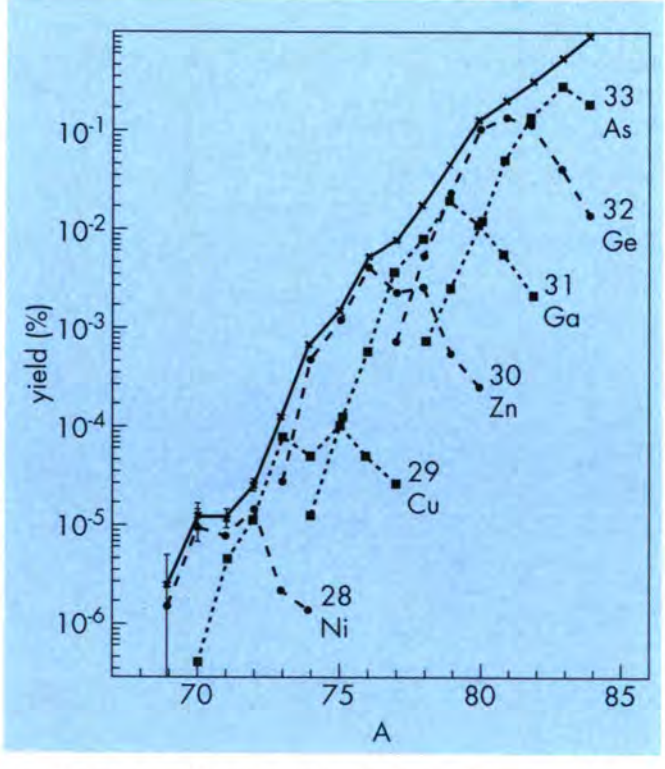


Fig. 7: Isotopic yield and mass distribution for far asymmetric fission of $^{235}U(n,f)$ (From J.L. Sida et al., Nucl. Phys. A502 (1989) 233c).

almost 5 orders of magnitude in the yield, and that mostly the estimate of exotic isotope production can be calculated from an interpolation rather than an extrapolation in the given mass region.

From the above formula production rates of fragments for the standard PIAFE projects source (6.3 kW thermal power, $2.2 \cdot 10^{14}$ fissions$\cdot s^{-1}$) (see chapter "Projects") have been calculated and compared to the expected production rate for the planned Isospin Laboratory Project, based on spallation induced by a 1 GeV, 100 μA proton beam in a 1 Mol UC-target (40 kW thermal power).

In Figs. 9 and 10 this comparison is shown for zinc and germanium. To correct for losses in the extraction and separation stages the production rates have been scaled down to 4.5 %. The following features may be recognized from the comparison: for very neutron rich species above mass 70 and yields from fission are orders of magnitudes higher than for spallation, and thus fission should be the preferred reaction if a radioactive beam facility is to be built. The very reason for the higher yield in fission is, that it proceeds cold, especially for far asymmetric fission. Thus, neutron evaporation is strongly suppressed, a feature which is exemplified by the pronounced fine structure in the yield curves. In contrast, for spallation it is known that this reaction is very efficient for producing neutrons by evaporation and fragmentation, a fact which shifts the mass distribution curves to the neutron deficient side and washes out any fine structure. The second advantage for fission is its rather narrow mass distribution and the correspondingly high yields for very neutron rich species between mass 70 and 160. This strongly enhances the figure of merit which puts the value of the usable intensity in the relation to the overall waste created in any reaction. This ratio reaches about 5 % for the most abundant species in nuclear fission.

H. Faust spent 3 months at the Studsvik Laboratory to establish the principles for a standard PIAFE source which could be implemented in the H 9 beam tube. During his detachment to the ISN/Grenoble, G. Fioni was working on calculations of the beam optics for the PIAFE setup proposed at the ILL site.

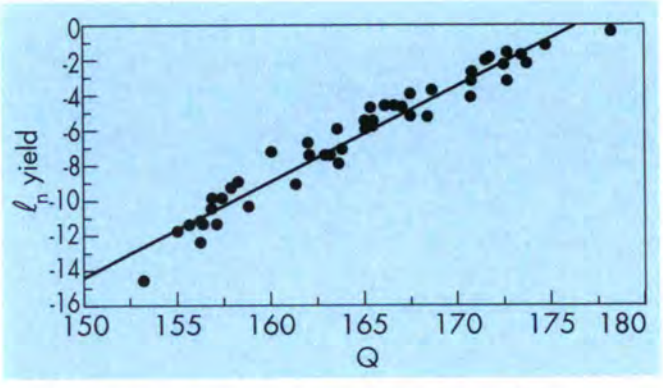
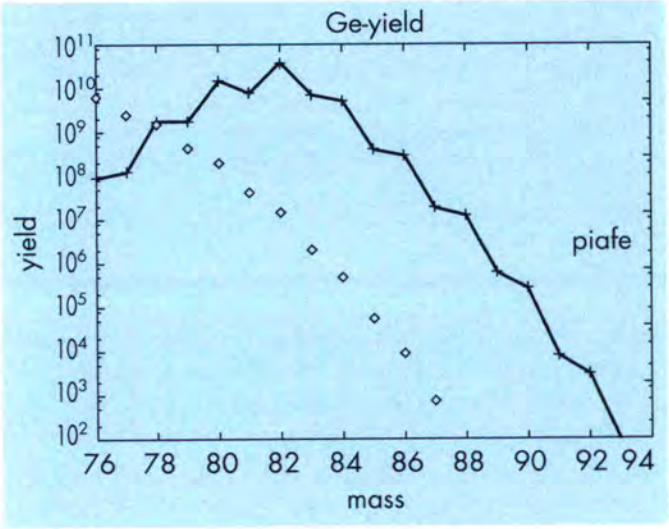


Fig. 8: Correlation between the logarithm of the yield for far asymmetric fission to the reaction Q-value. The straight line is a fit to the data.

At the PN3 facility GAMS

Levels above 2 MeV and the onset of chaos

In 1981, a detailed level scheme for ^{168}Er, based on GAMS measurements was published [7]. The "completeness" features of this reaction led to a level scheme that was complete for negative parity states up to about 2200 keV and for positive parity states to about 2000 keV. It was thought prudent to halt the development of the ^{168}Er level scheme at about these energies due to the difficulties inherent in extending it into the next energy



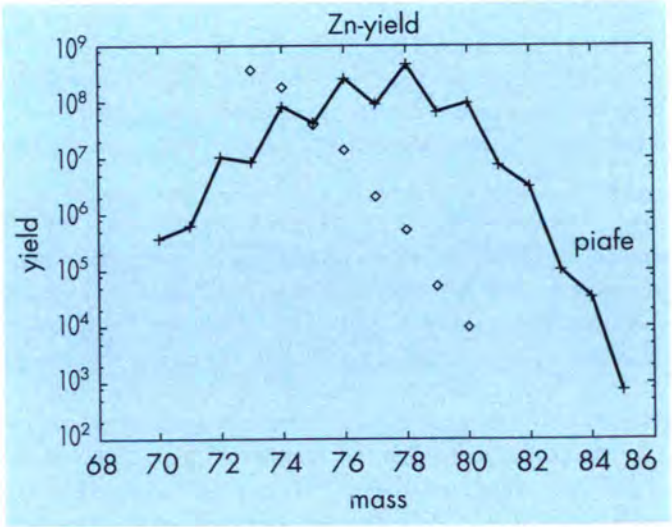


Fig. 9-10: Rates for exotic zinc and germanium isotopes for a standard PIAFE source compared to the IsoSpin Laboratory (ISL) project. In both cases the production rates have been scaled down to 4.5 % to account for the expected losses in the extraction and mass separation process.

region and to the desire to preserve the completeness property. These results formed the basis for a number of successful tests of the IBA model and the completeness of the scheme has made this nucleus a touchstone testing ground for subsequent experimental and theoretical work. Recently, the original 1981 data have been further analyzed and new data were added in order to propose a considerable extension of the level scheme along with rotational band assignments up to energies (well above the pairing gap) as high as nearly 2800 keV [8]. These data were used to argue that there is a distinction in intensity for final states of low and higher K (K=0,1 vs. K=2-5) and therefore to conclude that K remains a good quantum number in the neutron resonance energy regionwith an excitation energy E_x ~ 7-8 MeV [9]. This conclusion, which is contrary to the usual perception that this energy regime is chaotic at low spin and that the neutron capture levels are complex compound nuclear states, has aroused considerable interest.

In order to further elucidate this situation we have carried out extremely high statistics γ - γ coincidence data for ^{168}Er following thermal neutron capture on ^{167}Er. These measurements were carried out at the BNL-reactor. Our results alter considerably the experimental and theoretical work on ^{168}Er cited above and affect the conclusions concerning the quality of the K quantum number in the neutron resonance region: The claims that K remains good and that this energy region is non-chaotic are shown to be based in part on band assignments that need to be seriously re-examined.

Interpretation of GRID profiles

First principles Molecular Dynamics (MD) simulation were further developed to describe GRID profiles (Rossendorf-ILL, Helsinki-ILL collaboration). The study of Gamma Ray Induced Doppler broadening allows to obtain insight into the slowing down process of atoms in solids as well as information about short lived nuclear lifetimes. The new calculations (an example is shown in Fig. 11) show that directional correlations in single crystals can provide information about the site in which specific atoms are located in the lattice. With these theoretical treatments we expect to develop the basis for new GRID-measurements to be carried out after the reactor restart.

Secretary: Jürgen Last

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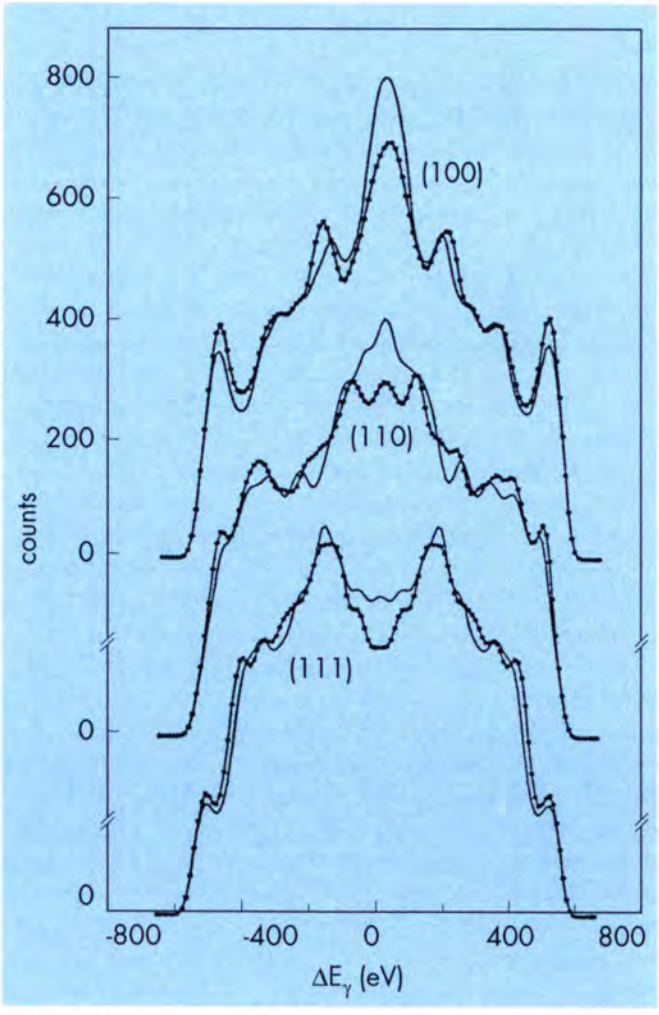

Fig. 11: Examples for Doppler-broadened lineshapes due to the slowing down of recoils in monocrystalline silicon. The Doppler-broadened lineshapes are predicted by MD simulations for the secondary γ-decay with E_γ = 2.43 MeV following the nuclear reaction $^{28}Si(n,\gamma)^{29}Si$. The structure in the lineshape reflects the dependence of the slowing down process of the recoiling nuclei on the recoil direction in the crystal. With changing alignments between the spectrometer axis and the crystal orientations (denoted in the figure) the lineshape changes substantially. The universal potential (marked lines) and the Moliere potential (thin lines) result in different lineshapes which should be experimentally resolveable. The calculations were done by K.H. Heinig, Rossendorf.

One Day Colloquium in Memory of Walter Mampe

On the 29th of January, 1993 physicists and friends came together from all parts of the world to join in remembering Walter Mampe and discussing the field of study which had inspired his research. They did this in the presence of his immediate family and bore witness to the immense regard they had for Walter in both personal and scientific domains. In all, some 115 persons attended.

Walter being a most energetic and outgoing individual, had contributed significantly to very many collaborations, too many to present them all in a one day meeting. The program was therefore concentrated on those topics which the organizers felt had been closest to his personal interests and which had stimulated his original contributions.

Peter Armbruster, who was recently a director of ILL and one of the organizers of the colloquium, opened the colloquium and introduced the first speaker, Norman Ramsey who had worked regularly with Walter over the last 18 years. Professor Ramsey gave his lively and moving personal recollections of Walter as a colleague and particularly as a friend, both at work and at leisure. He went on to describe Walter's scientific career highlighting many of the projects with which he had been concerned. Walter's work began with measurements in nuclear physics made with the beta spectrometer in Munich where his thesis supervisor was Till von Egidy. Till gave the second talk in which he traced a path, from the time when Walter was his student, to some of the most recent developments in nuclear physics concerned with the question of when nuclear states are chaotic and when they are not chaotic and by what criteria this can be judged. The ideas have been developed using the data that have been accumulated by the wide ranging efforts of nuclear physicists over the last few decades. The BILL electron spectrometer at ILL was an outstanding machine making a notable contribution. Walter worked for three years on the development of BILL and after he had completed it in 1974, he became the first person responsible for its regular operation for visiting users. A year later, when BILL was well established, he handed over to Klaus Schreckenbach. Klaus described some of his experiences then. The spectrometer weighed 7 tons and stood 3 m high with parts which extended deep into the reactor. It was a big responsibility. He could not help but remember the remark within some pages of operating instructions where Walter had written laconically. 'If you hear by any chance a loud bang from the 150 A, 200 V power supply, that is, unit 10, and you see a flame coming out of it, you are sure that you have made a mistake'. In spite of such dire warnings, the whole instrument worked extremely well with incomparable energy resolution for many years. Klaus recounted how, in addition to its productivity for nuclear physics, it had been the ideal machine for many experiments in fundamental physics, the field to which Walter had then moved.

Walter's first project in this new area was a precision measurement of the neutron magnetic moment. It involved working closely with, among others, Harvard thesis student Geoffrey Greene. At the successful conclusion of the project which reached a precision of 2 parts in 10^7, both were stimulated to pursue this kind of work. Geoff was present to describe that first project and more recent fundamental constants experiments with neutrons which still involve the ILL. As an outcome Walter became committed to stay at the ILL to become a Staff Scientist in fundamental physics.

Immediately he began to supervise his first thesis student Roland Gähler and to be involved with a series of beautiful experiments in neutron optics described in talks by Gähler and Anton Zeilinger. Also at that time (1977) the first ultra cold neutron source came into operation introducing a field which immediately became Walter Mampe's principal research interest and the theme of an ongoing collaboration with the author, others, and in particular, Paul Ageron who talked about all the UCN developments at the ILL. The first collaborations concerned the neutron electric dipole moment, described by Ramsey and taken up again by Bob Golub who spoke about UCN production in superfluid helium and new ways in which liquid helium might be used to measure the electric dipole moment with even higher precision in the future.

Another of the very early UCN projects was the magnetic storage ring for neutrons described in the talk by Professor Wolfgang Paul. In its later version of 1987 the magnetic storage ring was set up at the new ILL UCN source on level D which incorporated the use of the ILL cold source with the turbine of Albert Steyerl. By this time the storage ring had been developed to the point of giving one of the best neutron lifetime measurements. When its large superconducting magnet was in operation, data was taken under personal supervision both day and night and Walter Mampe's input was considerable. Besides his work with UCN, Walter also had responsibilities for experiments with cold neutrons such as those on the neutron decay angular correlation coefficients which were described by Tom Bowles from Los Alamos National Laboratory where Walter had been a visiting scientist. The results of those experiments are combined with the neutron lifetime value to give the basic parameters of the weak interaction of the nucleon at low energies.

In addition to greatly smoothing the way for these many collaborations, Walter had his own projects which started at the first UCN source where he studied the storage of neutrons in traps with very clean surfaces so as to understand better the loss processes. Later these projects lead naturally to a program of experiments to measure the neutron lifetime by storage in material traps. Out of this grew a very fruitful friendship with Chris Bates who had discovered the high efficiency of Fomblin liquid walls in remarkable experiments at the small reactor in Risley near Manchester. Driven with much skill and determination by Walter, this program of experiments resulted by 1989 in

what was, at the time, the most precise neutron lifetime measurement of 887.6 ± 3.0 s. Two years later, Russian colleagues, for whom Walter had a special regard, were able to make lifetime measurements with similar precision in Russia and these were in good agreement with those of ILL. Their program and their reminiscences of times spent with Walter were presented vividly in the talks by Anatoly Serebrov, Lev Bondarenko and Vasiliy Morozov. The measurements at Gatchina described by Tolia had employed a very cold trap with beryllium or solid oxygen surfaces. Lifetime experiments with material traps have to be designed so that the extraneous wall losses can be corrected for with high precision. The original aim of the Gatchina experiments had been to avoid the problem by reducing these wall losses to below one tenth of one percent of the beta decay rate. To their surprise, they could not bring about such a large reduction. They achieved losses of 3 %, compared with 15 % in the Fomblin traps, nevertheless, given the flexible nature of the Gatchina apparatus, a good lifetime measurement has resulted. Why the losses remain about one hundred times greater than anticipated remains puzzle, in spite of considerable subsequent thought and experimentation. Vasiliy Morozov described separate experiments at the Kurchatov Institut aimed at further elucidating loss mechanisms on clean surfaces. These have also revealed unexplained enhancements. In the early years, large losses were found to be linked to the ubiquitous presence of hydrogen. By now it is thought that this is understood and under control through vacuum baking and cooling procedures. Perhaps there is some other feature causing surprises!

There is much to learn yet in the physics of particles as was emphasized by Dirk Dubbers in his talk which reviewed ten fundamental questions that neutron experiments can continue to help to resolve. Thus the colloquium looked forwards as well as backwards, and in his concluding remarks Ken Smith expressed the feeling of gratitude of all those present for what Walter Mampe had contributed in so many different ways to promote the ongoing collective endeavour.

Mike Pendlebury

Scientific opportunities with the fundamental physics cold and ultra-cold neutron sources

Jürgen Last and Mike Pendlebury

Already home of high intensity slow neutron beams before 1991, the ILL will, after the reactor restart, offer to the fundamental physics community two unique facilities with the highest cold and ultra-cold neutron fluxes currently available. Both facilities, PF1 and PF2, are scheduled to begin their regular operation after an initial test and commissioning phase towards the end of 1994. In the following we will discuss the lay-out and scientific perspectives of the cold neutron beam facility PF1 and the ultra-cold neutron source PF2 (TGV).

PF1: The new and enhanced cold neutron beam facility

When in 1990 SN7, then still located at the far end of the old neutron guide hall, was again given the status of a scheduled instrument, it was only to operate a few more reactor cycles under its newly regained name PN7. Until the reactor shutdown, after nearly 20 years of operation, this facility featured one of the most intense cold neutron beams in the world with an equivalent capture flux of $\phi=3\cdot10^9$ n·cm^{-2}·s^{-1} and, after the installation of one of O. Schärpf's super-mirror polarizers with polarization strengths regularly between P=0.96-0.98 at $\phi_{pol}=5\cdot10^8$ n·cm^{-2}·s^{-1}, it had the highest figure of merit $P^2\cdot\phi_{pol}$. Experiments at PN7 also benefited from the relatively low background rates due to the 110 m long, slightly curved neutron guide.

In fundamental physics the use of cold neutrons is often preferable to thermal neutrons. At intensities comparable to those of thermal neutron beams, cold neutrons are typically 4 times slower and thus remain longer in the measurement volume. For n-decay experiments this immediately results in a 4 times higher count rate. In the energy range of cold neutrons the capture cross-sections follow strictly the 1/v dependence. Thus slower neutrons have enhanced capture probability and avoid complicated resonance corrections in experiments that require high precision beam calibration. Also a slower neutron beam can be polarized to more nearly 100% and the polarization vector more easily turned into any direction by a simple magnetic guide field.

All these advantages were reflected in the high demand for beam time at PN7 which was usually three to five times more than the available reactor time. There is a wide spectrum of scientific activities with a significant proportion of experiments on free neutron decay, where we count 4 lifetime and 3 correlation coefficient measurements. Another large group of experiments

measures parity violating features in neutron nucleus interactions. The latter included processes like nuclear fission and n-γ reactions after polarized neutron capture.

Over the years the PN7 beam quality became degraded due to the introduction of several interruptions in the H14-2 guide and deterioration of the natural nickel coated guide itself. To partly remedy this situation, it was proposed in 1992 and subsequently decided to rebuild PN7, which meanwhile had become PF1 for Physique Fondamentale, at the end position of the H53b guide inside the newer guide hall ILL22. The same location at the ^{58}Ni coated cold neutron guide which had been formerly been used by the n $\bar{n}$ collaboration.

The primary H53b guide ends inside the "EVA" casemate. There it has a usable cross-section of 6 by 12 cm^2, a fourfold increase over H14-2. It follows a 4 m long ^{58}Ni coated guide segment with the same cross-section which will guide the neutrons into the PF1 casemate and to the polarization set-up. Measurements of the n $\bar{n}$ collaboration established a capture flux of $1 \cdot 10^{10}$ n·cm^{-2}·s^{-1} and we hope that this number can be preserved. Thus one can expect at best a total flux increase of about one order of magnitude. Experimental set-ups which cannot take advantage of the significantly enlarged beam cross-section will only benefit from the 3 times higher capture flux.

PF1 will offer considerably more space to the user. The experimental area, now securely protected by a wall of concrete blocks is 4 m wide and 8 m long. This will simplify TOF measurements. Adjacent to the experimental zone, an area 4 by 4 m^2 is available for experiment preparation and testing so that an experiment can be set up while there is still another experiment taking data. This way we hope to reduce the loss of valuable beam time in the set-up phase.

In these years occupied by the ILL reactor refurbishment, the fundamental physics community has tried to perform experiments which were originally scheduled for PN7 at NIST, Gatchina or elsewhere. Others have used the time to design and build completely new experiments. There are plans for at least 4 different new measurements of angular correlations in neutron decay. These experiments alone will keep PF1 busy for two or maybe three years. There are also proposals for new experiments on parity violation in nuclear systems, that can now be carried out at higher count rates and with better statistics. Also crucial for the understanding of the structure of the fundamental interactions are time-reversal invariance (TRI) measurements, and there are already two new proposals in this class for PF1. Whether the neutron life-time will ever be measured again in a beam experiment at PF1 is an open question. It seems as if ultra-cold neutron techniques are more suitable for such measurements.

Last but not least we expect a number of technological developments to be made at PF1. A neutron focussing device which should give a factor 5 flux increase on a 1 cm^2 "hot spot" is already under development. Also, the significant "contamination" of the H53b beam with very cold neutrons of wavelengths greater than 9 Å could be extracted with a suitable beam bender. Such neutrons can be used to feed a future supra-thermal source for ultra-cold neutrons or in neutron interference experiments.

PF2: Ultra-cold neutron source TGV and experimental facility

The ultra-cold neutron (UCN) source assembly on level D comprising a vertical guide from the cold source feeding the Steyerl turbine (TGV) was commissioned in the autumn of 1985 and was in regular use early in 1986. The major input of finance and technical effort was provided by the TU Munich while much close collaboration and technical work was also required from the ILL Reactor Division.

Until this year the source had the status of a special instrument for which the TU Munich was responsible. Recognizing the increasing demand for and interest in UCN, the ILL has decided to make this a scheduled facility and has assigned the instrument name PF2. Accordingly a leasing agreement has been made with the TU.

At the commissioning in 1985 the number density of unpolarized UCN with speeds less than 6 m/s at the position of the experiments, which is about 4 m from the turbine, was found to be 50 cm^{-3}. This was a hundredfold improvement compared with the earlier ILL SN5 thermal source for UCN, a change which completely transformed the experimental possibilities. It remains at present the world's strongest source of UCN. Another excellent feature of the source has been its nearly constant UCN output level over the five years of running since it was installed. In fact no serious trouble was encountered until a small leak in the vertical guide appeared just before the shutdown in 1991. The TGV guide also provides a beam of 100 Å neutrons with a wavelength resolution of 20 %, which are being used for the development of a long wavelength interferometer. The next strongest UCN source is that of the WWR-M reactor at PNPI, Gatchina near St. Petersburg. After the renewal the PNPI source reaches about 1/3 of the intensity of the ILL source but its output tends to decrease in time so that the average has been 1/5.

Anticipating the arrival of the new UCN source the neutron lifetime experiment organized by W. Mampe, employing Fomblin liquid coated walls, was rebuilt taking account of the experience gained from a preliminary trial on SN5. The measurements were completed by the end of 1988 yielding a lifetime result of 887.6±3.0 s, which at that time, was a threefold improvement in precision compared with any other published result. By then, the systematic error was three times the statistical error; further progress would require a more elaborate apparatus. A related lifetime measurement then took its place combining ideas from ILL and the Kurchatov Institute. This was completed in 1990 with the result 882.6±2.7 s. The world average of neutron lifetime results published since 1987 is 886.2±1.6 s.

The neutron electric dipole moment measurement which had reached a statistically limited error of $3 \cdot 10^{-25}$ e·cm running on SN5 between 1982 and 1985 was modified slightly and transferred to the new UCN source 1986 where it ran until 1989, reaching a statistical error of $2 \cdot 10^{-26}$ e·cm. It too had become limited by systematic errors which were, by then, double the errors from counting statistics. Nevertheless, close to one order of magnitude improvement and another world minimum error had been obtained. For the time being at least the high intensity UCN source had won, causing two large experiments to withdraw to adopt a more advanced design. In both cases new instruments have been built and new measurements are planned at PF2 for the time when the neutrons return.

The high UCN intensity has also made it possible to develop a versatile monochromator for UCN. Gravity was used to select and control the energies and the device has been used to make the most precise measurement to date of stored UCN loss rates versus UCN energy. It has also confirmed a slight warming of the neutrons after long intervals of storage which had already been suspected from storage data from the liquid walled trap. This may be explained by environmental vibrations which must be shielded against for the next lifetime experiment.

The feasibility of using UCN at PF2 to measure the electron asymmetry in polarized neutron decay A is also under study. As part of this exercise there are plans to test whether a simple superconducting magnet field configuration can be used to generate essentially 100.0 % polarization in UCN and if so, to what extent this high degree of polarization can be maintained during storage in a material trap. The signal counting rate for an asymmetry experiment will be less than in cold beam experiments such as PERKEO II, but there may be advantages in respect of background and polarization measurement. The subject of anomalous losses of UCN discussed on an earlier page must be pursued with more detailed experiments at higher flux. Applications to use PF2 have already been received.

Most of these experiments only need to be supplied with UCN for intervals of a few seconds with gaps of as much as thousand seconds in between. It is ideal for running experiments in parallel using a switching system. An associated problem is working space. The principal investment planned for adapting PF2 better to its future role is for extending the beam switching system and for extending the floor area available to experiments.

Structural and Magnetic Excitations

Members of the College

Internal members

T. Baumbach	H.J. Lauter
S. Bramwell	A. Magerl
T. Chattopadhyay	A.P. Murani
R. Currat	H. Mutka
Ch. Doll	S. Pouget
B. Dorner	O. Schaerpf
B. Farago	B. Schmid
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J. Bossy (CNRS)	L.P. Regnault (CENG)
G. Dolino (UJF)	H. Schober (CENG)
C. Filippini (CNRS)	M. Vallade (UJF)
B. Fåk (CENG)	Ch.Vettier (ESRF)

Introduction

The scientific activities of College 4 went on through another year of the ILL reactor shutdown without a significant reduction of their scope. Despite the absence of neutrons, college members pursued their research projects, combining theoretical work and data evaluation at ILL with neutron experiments at other reactor centers. Laboratoire Leon Brillouin at Saclay and the Japan Atomic Energy Research Institute (JAERI) at Tokai, Japan, played a prominent role in providing beams of sufficient flux for the time consuming inelastic scattering experiments. In the case of JAERI, a generous Foreign Scientist Invitation Program permitted four college members to bridge the large distance from Europe to Japan and to carry out several weeks' experiments each. The preliminary results of three of them are mentioned in what follows.

Scientific Trends and Highlights in 1993

Phonon eigenvectors in silicon

A number of existing phenomenological models of lattice dynamics of silicon has been recently complemented by the potentially more exact results of *ab initio* calculations [1]. Although most of the different approaches reproduce the observed dispersion relations with comparable accuracy, significant differences exist between the predicted eigenvectors, drawing attention to their direct experimental observation.

In a series of experiments performed during 1992 and 1993 on the TAS1 spectrometer at the JRR-3 reactor of JAERI (Japan Atomic Energy Research Institute, Tokai, Japan) the problem of determining phonon eigenvectors from the observed intensities of coherent inelastic scattering was revisited [2] in preparation for future activities of this type on the TAS instruments at ILL. Only scan geometries fulfilling the conditions for good resolution have been employed so that the observed peaks could be resolved from the spurious ones. The inelastic structure factors were then extracted from the complete set of integrated intensities, observed at different **Q** and ω values, via a single scale factor analogously to the current practice in crystallography.

Fig. 1a displays observed dispersion relations for the Σ_1 acoustic and optic branches along [110]. As a consequence of an accidental degeneracy their polarization is elliptical, passing from purely longitudinal [110] at the Brillouin zone origin to purely transverse [001] at the zone boundary for the acoustic branch and vice versa for the optic branch. From the structure factors, Fig. 1b, measured in different Brillouin zones, the angle ϕ governing the proportion of the two polarization components of the acoustic branch was determined, Fig. 1c, together with the rotation sense - being positive for the acoustic branch. For the optic one the polarization angle is $\pi/2$-ϕ and the rotation sense negative. Once the polarization components are resolved, it is straightforward - using the quantum-mechanical branch crossing formalism - to extract the frequencies of the unperturbed LA and TO1 branches, displayed by dotted lines in Fig. 1a, as well as the off-diagonal interaction term Δ, Fig. 1d, responsible for the coupling. In this way the 2x2 dynamical matrix providing complete description of the dynamics of the two branches is fully reconstructed from the experimental data. Full lines in Fig. 1a-d represent results of the *ab initio* quantum mechanical calculations of the lattice dynamics of silicon which find in the present results - comprising also frequencies and eigenvectors in the other high symmetry directions - an excellent experimental confirmation.

Measurement of phonon dispersion curves in Cr_2O_3

The study of Cr_2O_3 [3], having rhombohedral symmetry, was undertaken to follow up the investigation of the ionicity and the polarisability of the oxygen ion, which was started by measuring phonon dispersion curves up to the highest frequencies of about 40 THz in quartz (SiO_2) and in sapphire (Al_2O_3). The crystal of Cr_2O_3 with a volume of about 4 cm^2 was examined on the PRISMA time-of-flight spectrometer at ISIS (with a limited success) and in March 1993 on the triple axis spectrometer TAS-1 at the JRR-3 reactor at JAERI.

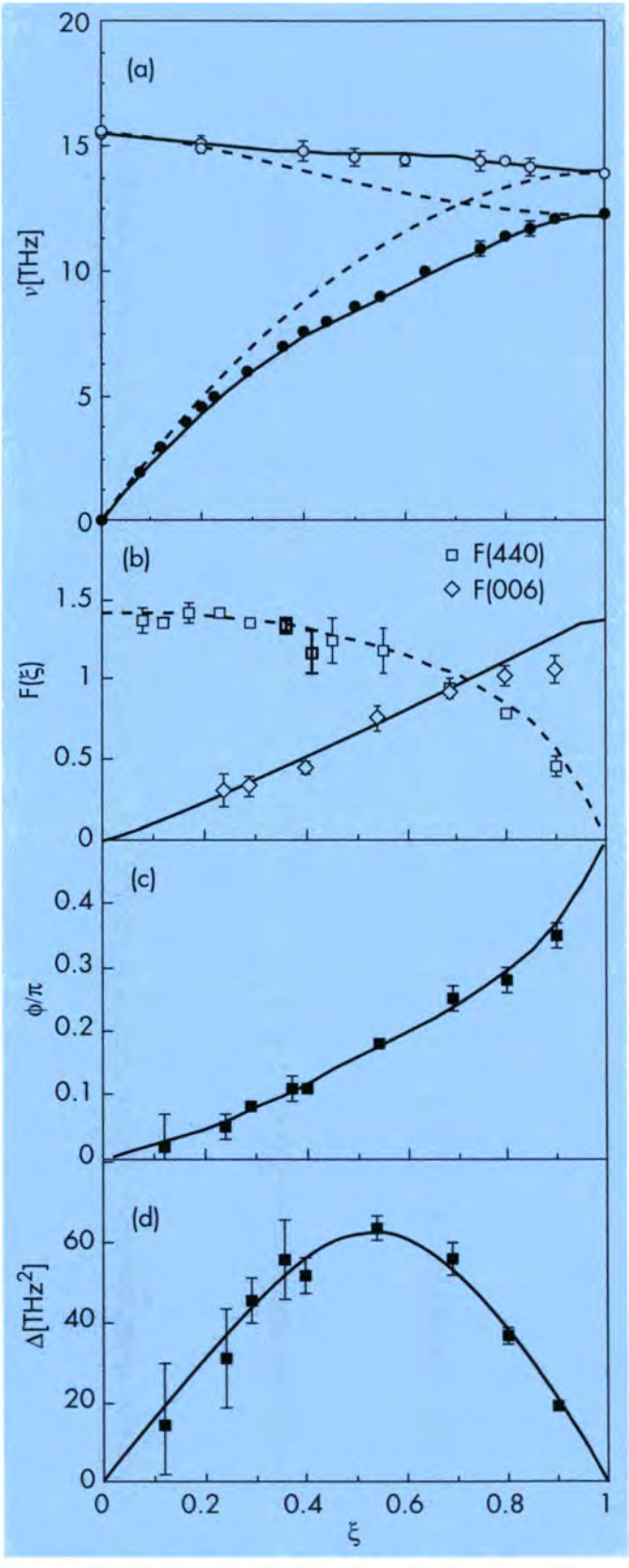

Fig. 1: Phonon dispersion relations for the Σ_1 branches along [110] in silicon (a); inelastic structure factors for the acoustic phonons observed in the 440 and 006 Brillouin zones (b), polarization angle in the (110) plane (c) and the corresponding interaction term of the dynamical matrix (d). The solid curves are based on results of the ab initio calculations.

The investigations were concentrated on the [ξξξ] direction. The three lowest modes out of each of the five "even longitudinal" ones and the five "odd longitudinal" ones were measured and identified, as well as the two lowest double degenerate "transverse" modes. Three more of the "transverse" modes were measured and could be identified by calculations of their frequencies and intensities from a lattice dynamical model. The shell model calculations with 9 parameters reproduce the data satisfactorily well. Studies of other symmetry directions, requiring an extended energy transfer range, are waiting for the IN1 spectrometer after the restart of the ILL reactor.

Incommensurate and ferroelectric phase transitions in $Sn_2P_2Se_6$

The dynamical behaviour of the semiconducting compounds $Sn_2P_2S_6$ and $Sn_2P_2Se_6$ has been recently investigated by optical spectroscopy. While the first compound exhibits a direct paraelectric to ferroelectric second-order phase transition at 340 K, in the isomorphous Se-based compound, the same type of structural change takes place in two steps: a second-order transition from paraelectric to a long-wavelength dipolar-modulated phase at T_i=220 K, followed by a first-order ''lock-in'' transition to the homogeneous ferroelectric state, at T_c=193 K. These two compounds, as well as their solid solutions $Sn_2P_2(Se_xS_{1-x})_6$, are used in non-linear ultrasonic devices because of their strong piezoelectric properties.

From a more fundamental point of view, the x-T phase diagram of the mixed compounds exhibits a rather rare kind of high-order critical point, the so-called Lifshitz point (x_L=0.28; T_L=295 K). For $x<x_L$, a direct paraelectric-to-ferroelectric second order phase transition is observed, while for $x>x_L$, as in $Sn_2P_2Se_6$, the intermediate modulated phase is stable over a finite temperature interval $\Delta T(x) = T_i(x)-T_c(x)$. As $x \rightarrow x_L^+$, both the stability range $\Delta T(x)$ of the modulated phase and the modulation wave vector for $T_c(x) < T < T_i(x)$ vanish continuously. The critical behaviour associated with Lifshitz points has been studied so far in nematic ferroelectric liquid crystals and in helimagnets such as MnP.

The first inelastic neutron scattering data [4] were obtained with a 1 cm^3 single crystal of $Sn_2P_2Se_6$. The experiment was carried out on the TAS1 thermal-beam 3-axis spectrometer at the JRR-3 reactor at JAERI. Preliminary elastic measurements to determine the position of the satellite reflections in the modulated state ($T_c<T<T_i$) confirmed previous X-ray data. The polarization of the modulated ionic displacements is found to be directed along the **a**-axis of the pseudo-orthorhombic cell (a = 9.652 Å, b = 7.679 Å, c = 6.810 Å; α = 90°, β = 91.4°, γ = 90°), i.e. transverse to the modulation wave vector $\mathbf{q_s} \approx 0.085\mathbf{c}^*$ and $0.1\mathbf{c}^*$ at 193 K and 214 K, respectively.

Hence, in the paraelectric phase, one expects to observe the mixing of a soft transverse polar optic mode (TO-mode), propagating along **c*** and polarized along **a**, with an acoustic (TA) branch of same polarization. Fig. 2 shows the inelastic response at (4,0,-ζ), for ζ = 0.2, 0.3 and 0.4. The upper frequency peak (near 3.5 meV for ζ = 0.3) corresponds to the TA mode, while the low frequency tail (from 2 to 3 meV for ζ = 0.3) was tentatively identified with the TO mode response. This tail gradually disappears on cooling, as seen in Fig. 3, until, below T_c = 193 K, a normal (i.e. symmetrical) TA response is recovered. This behaviour suggests that the tail arises mostly from a TA-TO interference effect, as opposed to a true one-phonon response. It is hoped that further measurements of the coupled-mode response as a function of temperature, in selected Brillouin zones, will enable one to extract the independent TA and TO mode-parameters.

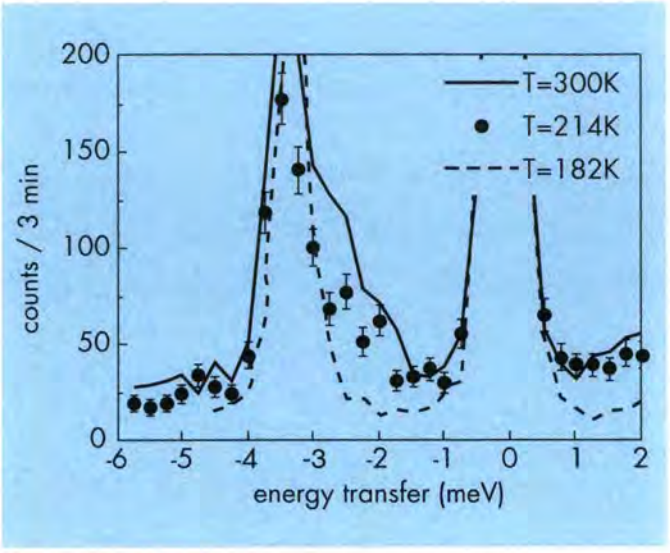

*Fig. 3: Temperature dependence of mixed TA-TO response in $Sn_2P_2Se_6$ at **Q** = [4, 0, - 0.3].*

Magnetic excitations in $CsFeCl_3$ in a magnetic field perpendicular to the c-axis

In $CsFeCl_3$ the Fe^{2+}-ion with effective spin one has locally a singlet ground state (m = 0). The ferromagnetic interactions along the c-direction and the antiferromagnetic interactions perpendicular to it are too weak as compared to the anisotropy to introduce long-range order in the absence of an external field. The excitation spectrum was investigated at LLB by inelastic neutron scattering in an external magnetic field up to 6 T, applied perpendicularly to the c-axis [5]. It was found that, with increasing magnetic field, the whole dispersion sheet is shifted towards higher frequencies and a splitting appears. A local Hamiltonian which neglects exchange interactions between all neighbours can give a qualitative explanation of the intensity of the magnetic excitations in dependence of the magnetic field. A more sophisticated theory, RPA-diagonalisation of the Heisenberg Hamiltonian used to describe the magnetic behaviour of $CsFeCl_3$, yields - apart from a mismatch for the modes at high energy transfers - a satisfactory description of the magnetic excitations of $CsFeCl_3$ in dependence on the magnetic field as displayed in Fig. 4.

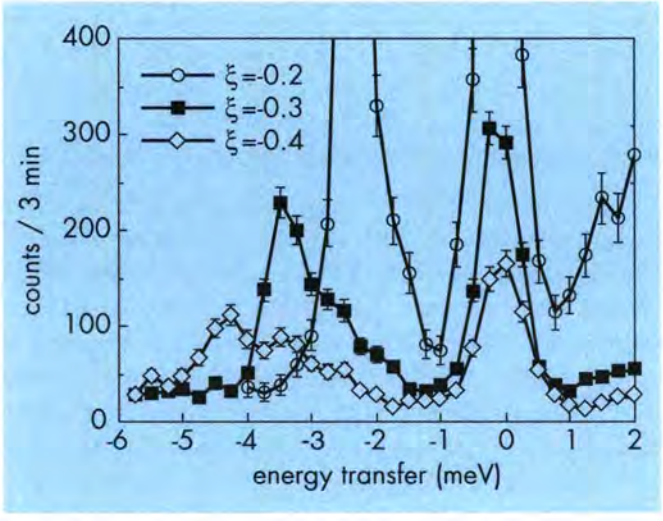

*Fig. 2: Mixed TA-TO line shape at 300 K in $Sn_2P_2Se_6$ at **Q** = [4, 0, - ξ].*

1D Heisenberg antiferromagnets with half-integer spin - universal properties?

Inelastic neutron scattering at ILL in the 1D phase on the spin S=3/2 Heisenberg chain $AgCrP_2S_6$ indicated a spin-wave velocity $C \approx 4.6J$, well in excess of the classical value $2JS = 3J$. This result emphasizes the strong quantum character of the S=3/2 Heisenberg chain and the similarity with the S =1/2 system that has a gapless excitation spectrum with a spin-wave velocity $C = \pi J/2$, i.e. π/2 times the corresponding classical value. Universal properties are expected for the half-integer systems, but it is not immediately evident that the relevant quantum effects are measurable for spins larger than 1/2. The universal behaviour could be checked via the relation between zero temperature susceptibilities and spin-wave velocities, it is expected that $\chi(T=0) = 1/(2\pi C)$ valid for spin S=1/2 holds also for other half-integer spins. At present, for S = 3/2, this relation can be examined only by extrapolation as depicted in the Fig. 5 that displays the existing calculated susceptibilities together with the experimental points [6]. While the zero temperature susceptibility cannot be measured (the weak 3D interaction induces order) and has not been calculated, the extrapolation of the temperature dependence agrees with the value obtained using the measured spin-wave velocity. This result is compatible with the theoretical predictions that suggest universal critical properties for half-integer spins.

Finite size effects in two-dimensional magnets

Whilst most crystals studied at ILL contain about 10^{24} atoms, the statistical mechanics which is used to calculate their behaviour is only exactly correct for a hypothetical system containing an infinite number of particles. Usually one needs not worry about the fact that real systems are finite, since $N = 10^{24}$ is a very large number, and finite-size corrections to the statistical mechanics of the infinite system are generally negligible. Theoretical work at ILL and the E.N.S. in Lyon [7], has stressed that for two-dimensional systems this is generally not true, and one must always take finite-size effects into account. The essential reason for this is that in two dimensions properties depend upon log(N) rather than N. Coupled to the obvious fact that macroscopic two dimensional systems only contain some $(10^{24})^{2/3} = 10^{16}$ particles, one can see that log(N) cannot necessarily be treated as an almost-infinite number.

A spectacular example of the breakdown of the applicability of the "thermodynamic limit" (i.e. the approximation $N = \infty$) is seen in the behaviour of magnets which approximate the two dimensional XY model; in other words layered magnets or ultra thin films with easy-plane anisotropy. In the case of layered magnets, it can be shown that weak interlayer coupling determines an effective finite size, which is smaller than the actual sample size.

Recent work [7] has re-examined inelastic neutron scattering data for the layered easy-plane ferromagnet Rb_2CrCl_4 measured on IN12 in the 1980's [8]. This material is expected to show a Kosterlitz-Thouless phase transition, where the unpairing of defects in the ferromagnetic spin structure causes a collapse, with increasing temperature, of the effective spin wave stiffness K_{eff}. In the infinite system the collapse is sudden and is known as the "universal jump". A theory which takes into account finite size effects predicts that the universal jump is severely rounded. The theory can be rigorously tested because it predicts that K_{eff} can be derived equivalently from neutron diffraction measurements of the spontaneous magnetization (itself a finite-size effect), and from the weak-field bulk magnetization, as well as more directly from inelastic neutron scattering measurements of the spin wave frequencies.

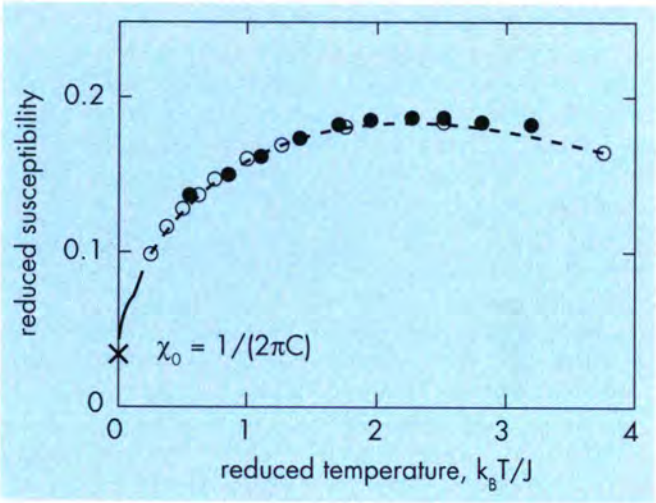

Fig. 5: The susceptibility of the quasi-1D antiferromagnet $AgCrP_2S_6$ in reduced units $\chi J/(g\mu_B)^2$. The open circles represent the quantum Monte-Carlo simulation for S=3/2 by Sandvik&Kurkijärvi (Phys. Rev. B, 1991), while full circles reproduce the measured temperature dependence scaled by the exchange constant J/k_B= 100 K, and the zero temperature value (X) is calculated using the measured spin-wave velocity C = 4.6J.

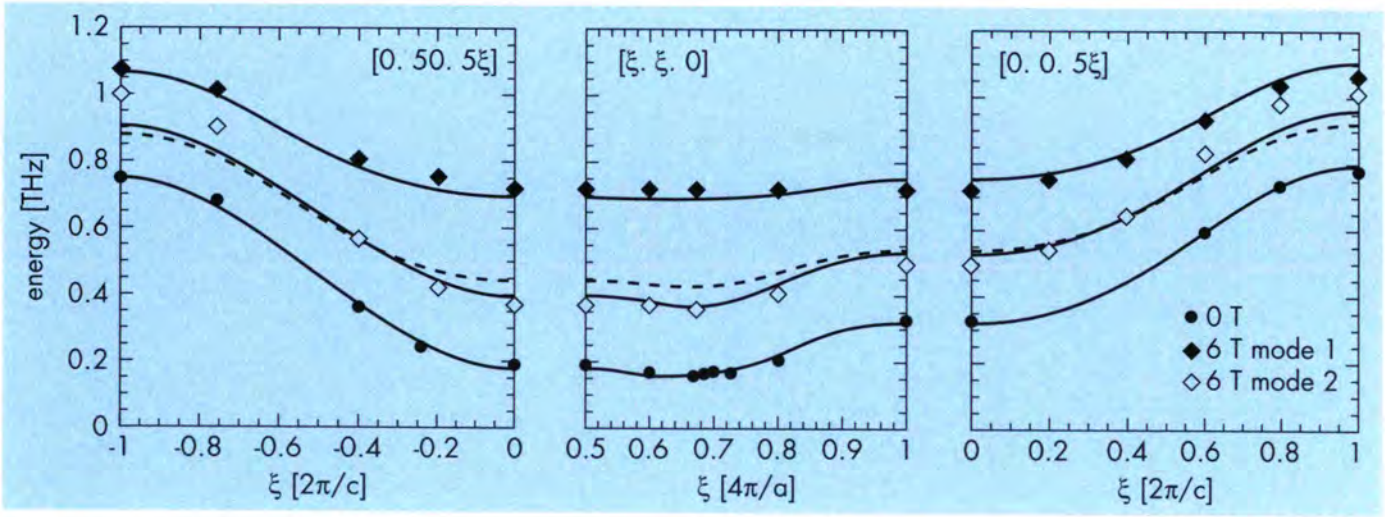

Fig. 4: Magnetic excitations in $CsFeCl_3$ at 1.6 K for three different symmetry directions: the doubly degenerate mode at zero field (•) and the modes separated at a field of 6 Tesla perpendicular to the c-axis (symbols u and ◊). The full lines are calculated from a Heisenberg Hamiltonian in RPA theory. The dashed line indicates the middle between the zero field frequencies and the upper mode at 6 Tesla.

Fig. 6 compares K_{eff} for Rb_2CrCl_4 determined by these three techniques. The temperature scale is normalized by a temperature T_{KT} which is the transition temperature of the hypothetical infinite system. The figure also plots the slope of the curve calculated by renormalization group theory at a temperature T*, just above T_{KT} which is a special temperature for the finite system. Given the diversity of techniques involved, the agreement between the theoretical prediction and the three experimental curves is impressive, clearly demonstrating the occurrence of a defect-unpairing transition in Rb_2CrCl_4.

Influence of dilution on the static critical behaviour of 3D-Heisenberg reentrant compounds

Under a random dilution of their magnetic atoms, some frustrated magnetic systems develop a peculiar behaviour known as reentrance: when decreasing the temperature from the paramagnetic state, they first undergo, at T_C, a transition towards an ordered magnetic phase; then, at a lower temperature, strong irreversibilities appear, characterizing the onset of a spin glass like phase.

An experimental study of the influence of dilution on the static critical behaviour has been performed at LLB in the insulating frustrated system $CdCr_{2(1-x)}In_{2x}S_4$, based on the 3D-Heisenberg ferromagnet $CdCr_2S_4$ [9]. Unusually high values of the critical exponents γ and ν (2 and 1, respectively) have been determined for the x=0.05 reentrant compound by means of SANS measurements above T_C. Such behaviour is illustrated by Fig. 7 which presents the observed correlation lengths. In the absence of frustration, such results are theoretically expected in the limiting case close to the geometrical percolation threshold. Surprisingly, diffraction experiments done in the ferromagnetic phase led to the 3D-Heisenberg value for the critical exponent β.

One of the effects of frustration thus appears to be an enhancement of the disorder introduced by dilution, leading to the limiting values γ=2 and ν=1 for a weak 5% dilution. Although it has not been observed, the existence of an asymptotic pure behaviour for small positive reduced temperatures is strongly suggested by the combined results obtained above and below T_C. A highly interesting point is the very probable absence of crossover in the ferromagnetic phase, which means two different behaviours on each side of the transition. This is attributed to the presence of a long range order, inducing a non zero local mean magnetic field. The expected influence of such a field is to reduce the effects of disorder, which appears to prevent the system from developing a dilution induced static critical regime.

Secretary: Jiri Kulda

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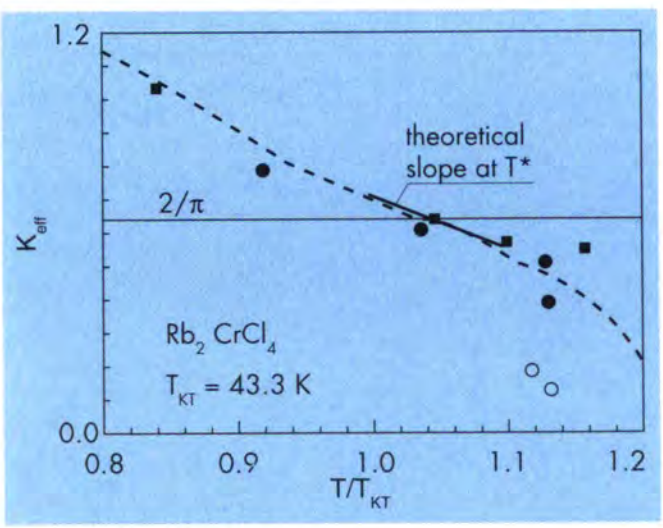

Fig. 6: Spin wave stiffness parameter K_{eff} measured by inelastic neutron scattering (circles), compared to that derived from spontaneous magnetization (dashed line), bulk magnetization (squares), and the theoretical prediction.

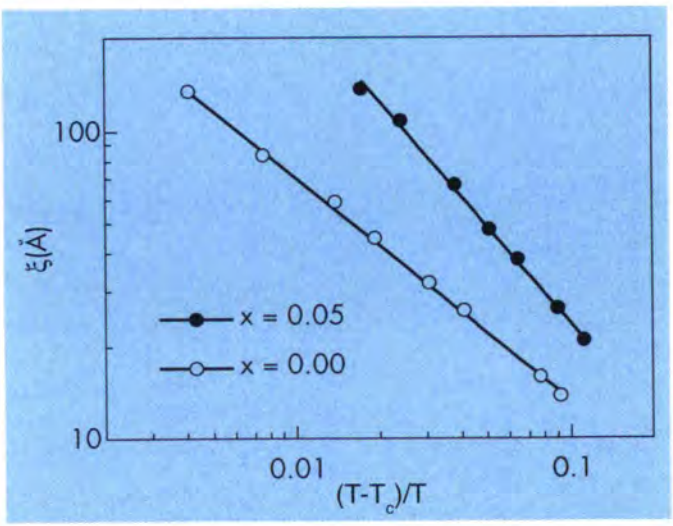

Fig. 7: Influence of dilution in $CdCr_{2(1-x)}In_{2x}S_4$ on the critical behaviour of the correlation length, above T_C. The critical exponent ν, obtained from the slope of the straight lines, is increased by disorder from 0.70 in the pure case to 1.0 for x = 0.05.

The $\gamma \Rightarrow \alpha$ phase transition in Ce

Amir P. Murani

The $\gamma \Rightarrow \alpha$ phase transition in cerium metal has been the subject of a large number of investigations. The fcc γ-Ce stable at room temperature shows normal Curie-Weiss magnetic susceptibility. On application of pressure ($\gtrsim$ 6 kbar) or on cooling (below 110 K), its volume contracts abruptly by ~14 % maintaining the same fcc structure [1]. The transition to the new phase, called α-Ce, is accompanied by a marked drop in the magnetic susceptibility which now shows enhanced Pauli paramagnetism [2,3] characteristic of non-magnetic systems which do not posses well defined local moments.

The first theories of the $\gamma \Rightarrow \alpha$ transition associated it with transfer of the localized (magnetic) 4f electron to the conduction bands. Certain experiments [4], however, showed that the valence did not alter significantly at the transition, and triggered new ideas based on the Mott transition model (localized 4f electron in γ-Ce $\Rightarrow$ delocalized 4f band in α-Ce) [5]. Other theories, based on the Kondo-lattice [6] and Anderson impurity models [7] have put forward the idea of the Kondo volume collapse due to increased hybridization of the localised f-electron with the conduction electrons in the α phase.

We have performed a neutron inelastic scattering investigation of the temperature induced $\gamma \Rightarrow \alpha$ phase transition in Ce, which we believe could aid our choice of the most appropriate model to describe the phase transition. The measurements on the HET time-of-flight spectrometer at ISIS were, in fact, performed on Ce alloyed with 7 at. % Sc which stabilizes the fcc phase against (dhcp) β-Ce formation. Gschneidner et al. [1] have reported that addition of about 7 at. % Sc suppresses formation of β-Ce almost completely (< 1 %) and (unlike Th or other additives) addition of up to 10 at. % Sc has negligible effect on the volume change $\Delta V/V$ at the transition compared with that for pure Ce [1].

The $\gamma \Rightarrow \alpha$ transition is of first order and shows significant hysteresis. On cooling the transition occurs at ~ 110 K while the reverse transition is observed at ~ 170 K on warming [1,2]. We have made use of the hysteresis to carry out measurements on the two phases *at the same temperature,* (viz. 125 K), first performing measurements in the γ-phase at 125 K then cooling the sample to 20 K (α-phase) and finally warming up again to 125 K (α-phase) where measurements were repeated under identical conditions. A one to one subtraction between the two data sets eliminates all possible non-magnetic contributions due to phonons, multiphonons as well as traces of hydrogen. The difference in the phonon spectra between the two phases is small compared with the resolution. The resultant difference signal measured with neutrons of incident energy 2100 meV (the highest energy currently practicable on the HET) using two different energy resolutions is shown in Fig. 1 where the positive intensity structure is predominantly the γ-phase response while the extended "negative intensity" tail is mainly the α-phase signal. In the diagram the continuous curve represents the higher statistical accuracy (poorer resolution) data corrected for the Ce^{3+} form-factor variation.

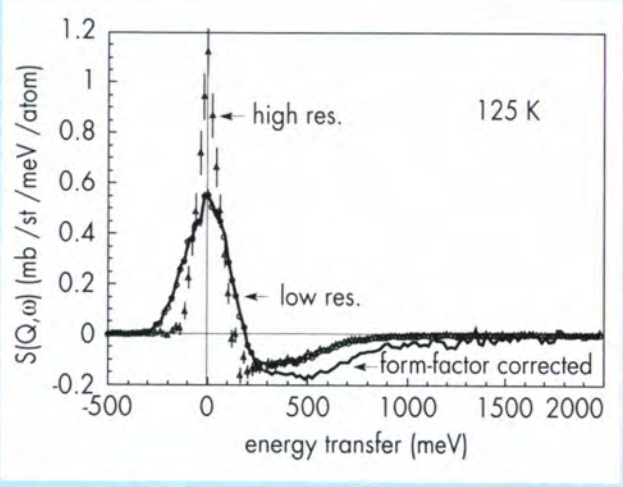

Fig. 1: Spectral intensity difference between γ and α-Ce at 125 K measured using neutrons of incident energy 2100 meV with two different energy resolutions. The continuous curve shows the low resolution (higher statistical accuracy) data corrected for variation of intensity with ω (hence Q) for fixed scattering angle $\langle 2\theta \rangle$, assuming the Ce^{3+} form factor dependence.

If we assume the modified sum rule $\int S(Q,\omega)d\omega \propto \mu_Q^2 = \mu_0^2 F^2(Q) \langle n_f \rangle$ to be valid, where $\langle n_f \rangle$ is the 4f occupancy, then numerical integration of the form-factor corrected data (shown in Fig. 1) up to 1500 meV yields the change in the 4f occupancy at the transition $\Delta \langle n_f \rangle$ of 0.2 ± 0.1. Furthermore, if we assume $\langle n_f \rangle = 1$ for γ-Ce, we obtain $\langle n_f \rangle = 0.8 \pm 0.1$ for α–Ce, consistent with positron annihilation [4] and Compton scattering [8] data which indicate close to fully trivalent state (occupancy ~1) even in the α-phase. The latter measurements, however, did not distinguish between localized and band-like 4f states while, as discussed below, the present neutron data suggest that ~ 0.8 electrons remain *localized* in α-Ce.

Low temperature (20 K) magnetic scattering in α-Ce (obtained taking La as the non-magnetic reference) using neutrons of incident energy 600 meV is presented

in Fig. 2 in the form $\chi''(\omega)/\omega$, where the continuous and the dashed curves show the best fits to the Lorentzian and the Kuramoto-Müller Hartmann (KMH) spectral functions [9] yielding $\omega_o \sim 170$ and 156 meV, respectively. The other parameter of the KMH fit α ($= \pi\langle n_f\rangle/N$), found to be 0.43 ± 0.03, yields the occupancy $\langle n_f\rangle = 0.83$ (assuming the degeneracy N=6), in good accord with the result obtained from the integrated spectral intensity.

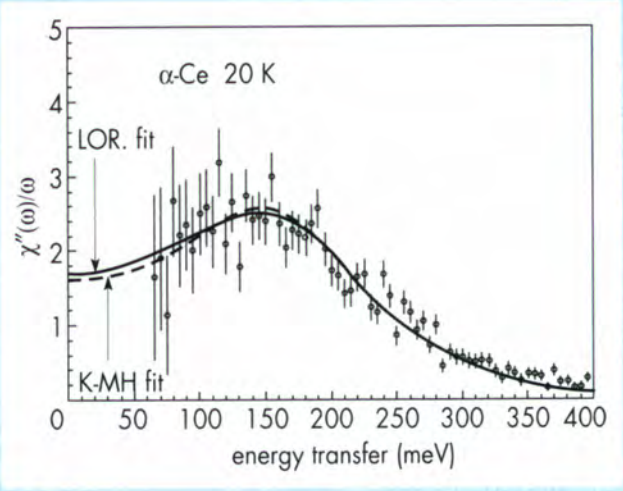

Fig. 2: Low temperature (20 K) dynamic susceptibility response of α-Ce represented as $\chi''(\omega)/\omega$. The continuous curve represents the Lorentzian spectral fit and the dashed curve shows the fit to the Kuramoto-Müller Hartmann function [9]. Ce^{3+} form-factor variation has been included in the fits.

It is interesting that the Kondo temperature T_o (T_K) for α-Ce obtained from our neutron data is fairly close to that predicted from the linear specific heat coefficient γ via the Fermi liquid relation [10] $\gamma = \pi^2 k_B^2 \langle n_f\rangle/3\omega_o$, where $\omega_o = T_o$ (T_K). With $\omega_o = 170 \pm 10$ meV and $\langle n_f\rangle = 0.8 \pm 0.1$ we obtain $\gamma = 10.5 \pm 1.5$ mJ mole^{-1} K^{-2}, in reasonable accord with 12.8 mJ mole^{-1} K^{-2}, obtained from specific heat measurements [3], allowing for some (s, p, d) conduction electron contribution. A similar evaluation for the susceptibility from the relation $\chi(o) = \mu^2\langle n_f\rangle/3\omega_o$, yields $\chi(o) = (3.1 \pm 0.4) \times 10^{-4}$ emu mole^{-1}. This is slightly smaller than the bulk value of 5.32×10^{-4} emu mole^{-1} at 50 K but the discrepancy, we believe, can be understood.

The γ minus α difference signals measured with 450 and 2100 meV neutrons have been analyzed assuming a narrow *quasi-elastic* response for γ-Ce, or broadened crystal field states, Γ_7 and Γ_8, giving rise to a quasi-elastic and an inelastic component. For the α phase we have assumed a broad inelastic Lorentzian spectral response (c.f. Fig. 2). We have also included form-factor variation of intensity with energy transfer ω (and hence Q) with the fitted functions. For γ-Ce the single component quasi-elastic fit yields a width of 7.5 ± 0.5 meV while the two component crystal field fit yields a quasi-elastic width of 5.5 ± 0.5 meV (at 125 K). In Fig. 3 the thick continuous curve (and the short dashed curve) represents the overall best fit to the 450 meV data. The residue in the region of ~ 260 meV represents the spin-orbit excitation. This is shown in the inset together with the curve (dashed) which parametrizes the spin-orbit excitation (width 40 ± 5 meV, position 260 ± 10 meV) taking into account the S-O excitation in α-Ce (see below) and the appropriate form factor for the $^2F_{5/2} \Rightarrow {}^2F_{7/2}$ transition [11].

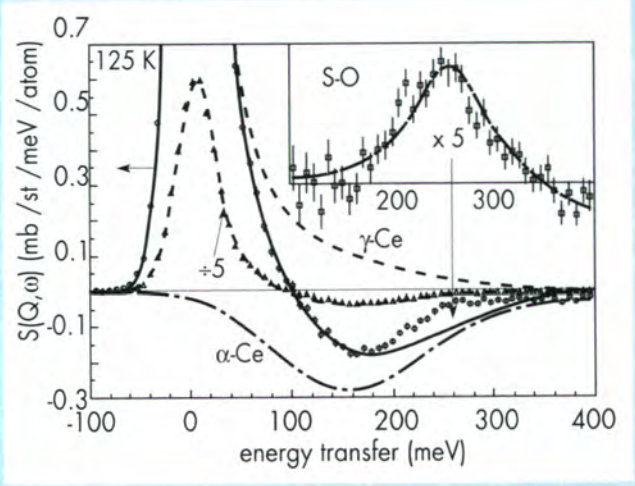

Fig. 3: Two component least-squares fit to the γ–α difference signal (E_i = 450 meV). The continuous and short dashed curves represent the Ce^{3+} form- factor corrected overall fit. The residue is plotted on an expanded vertical scale in the inset where the long dashed curve parametricizes the S-O excitation, taking into account the $^2F_{5/2} \Rightarrow {}^2F_{7/2}$ structure factor [11] as well as the S-O excitation in α–Ce.

The data for $E_i = 2100$ meV presented above in Fig. 1 are reproduced in Fig. 4 together with the resulting fits. The continuous curve represents the overall fit obtained for *the same parameters as for the 450 meV data.* Only the vertical scale is adjusted by 12 % between the two data sets which can be accounted for by possible systematic errors in the vanadium calibration and uncertainty in the scattering angle ($\pm 0.5^\circ$ at 4.5°). The dashed and dash-dotted curves represent the ground ($^2F_{5/2}$) state components for the γ- and α-phases. The residual intensity is shown on an expanded vertical scale in the inset together with the curve obtained for the same

parameters (components are shown dashed) as used to fit the S-O region in the lower energy data, Fig. 3. We believe the peak at ~ 450 meV represents the S-O excitation in the α-phase, although its relatively high energy as well as broad width (~ 100 meV) may appear rather unusual. It is emphasized that the S-O excitation evidenced in α-Ce is *not an artifact* of the fit or the fitted spectral forms, although its exact position, shape and width may depend on the spectral functions (Lorentzian or KMH) chosen to represent the ground state response. In fact, the S-O excitation is *clearly observable* in the *as measured* difference signal in Fig. 1, particularly in the form factor corrected data (continuous curve). Its relatively small intensity compared with the main response is in good quantitative accord with theory, taking into account the respective form factors [11].

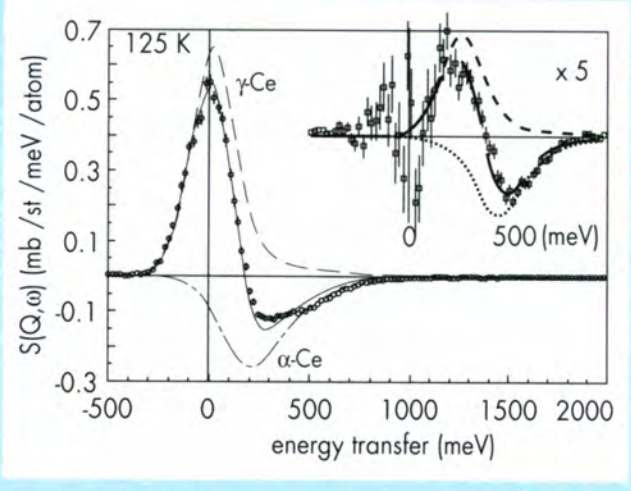

Fig. 4: Model fit to the γ – α difference intensity for E_i = 2100 meV (for the same parameters as the 450 meV data, see text). The two components of the fit are shown by the dashed (γ-Ce) and the dash-dotted (α-Ce) curves. The residue is shown on an expanded vertical scale in the inset, together with a fit assuming S-O excitations in both phases, shown by the dashed curves.

In conclusion, we have identified a single ion spectral response in α-Ce, well described by the KMH spectral function (T_K ~ 1800 K) or an inelastic Lorentzian (T_K ~ 2000 K). Numerical integration of the difference signal between γ and α-Ce measured with high energy neutrons at the same temperature and over the same Q-range thus suggests that the 4f electron remains ***localized*** in α-Ce to the extent of around 8 parts in 10. Further evidence for localized 4f states in α-Ce is provided by the observation of broad yet well defined higher-lying spin-orbit excitation at finite Q's. These results together with the observed magnitudes of the characteristic (Kondo) energies of α-Ce (T_K ~ 2000 K) and γ-Ce (T_K ~ 100 K) provide strong support to the "Kondo volume collapse" theories of the $\gamma \Rightarrow \alpha$ transition [12].

Acknowledgements

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Crystal and Magnetic Structures

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Introduction

Life in College 5, already disrupted by the reactor refurbishment, was further perturbed by the reorganization of the ILL in 1993. Several of our members now occupy more managerial positions: Jane Brown is now Head of the Scientific Computing Group, Alan Hewat is Manager of the Diffraction Group, and Claude Zeyen is Head of the Instrument Development Branch. Most members of the Diffraction Group also spent several weeks shifting to ILL4. This move puts most members of College 5 in much closer proximity than before which should be beneficial to scientific activity in the long term.

In spite of these changes, scientific activity within the College has continued apace both at home and abroad. Three College members continued detachments to other neutron scattering facilities in 1993; Manfred Reehuis to the Hahn-Meitner Institut to help to bring on-line the four-circle diffractometer and to introduce the Berliners to the D15 position-sensitive detector on loan during the shutdown, Juan Rodriguez-Carvajal to Laboratoire Léon Brillouin, in part to be responsible for the D1A powder diffractometer also on loan, and Thomas Vogt to Brookhaven National Laboratory to help construct a new powder diffractometer and develop novel monochromators of sandwiched germanium. Closer to home Jean Pannetier spent the major part of the year doing industrial research in the Groupe Investigations Structurale at the Centre de Recherche de Voreppe of the Pechiney company.

In similar vein several College members took the opportunity of the shutdown to make shorter extended visits to other facilities: Steve Bramwell to TRIUMF in Vancouver where he was involved in μSR experiments and in theoretical studies of frustrated magnets; Jane Brown to Coimbra, Portugal, as Visiting Gulbenkian Professor in the Physics Department and then on to Brookhaven National Laboratory to work with Gen Shirane on magnetic inelastic scattering from ferromagnetic compounds showing quadrupolar interactions; Garry McIntyre to Lucas Heights in Australia to assist in the experimental program on the four-circle diffractometers and to demonstrate the benefits of position-sensitive detectors; Claude Zeyen to the ISSP to advise in the construction of the three-axis spin-echo spectrometer PONTA and to JAERI to use the three-axis spectrometer TAS-1 and the precise neutron optics machine PNO. Most College members have also done experiments at various neutron and x-ray centres in Europe and further afield, and have always been warmly welcomed. These visits often reveal elegant solutions to experimental problems about which we, with the luxury of 'high flux', have not worried. Being the reversal of the usual scientific tourism they also establish new and different contacts and foster goodwill for the future experimental program at the ILL.

The past year has also seen the departure of most of the remaining thesis students: José De Carvalho Paixão, Klaus Hinrichs, Olivier Isnard, Gerd Lautenschläger, Helen Murphy and Zoran Mursic. Mark Nutley will finish at the end of 1993, leaving only Claire Wilson who is due to depart just as the next batch of students arrives in the autumn of 1994. Many of these students have been forced by the reactor shutdown to perform all of their experimental work elsewhere, and to spend the rest of the time at the ILL in relative isolation compared to their peers at the home universities. Rather than demoralize, as might be expected, this premature introduction to 'suitcase' science has but strengthened their ability to work independently and to adapt quickly to new experimental situations. Not that this is a scenario that we would recommend for future students!

In addition to the contributions both to the organization and to the content of the Workshop on Magnetism and the IAEA Materials-Research Workshop described in detail below, several College members assisted in planning the scientific programs of microsymposia of the 16th IUCr

congress in Beijing and associated satellite meetings held in August and September of 1993. As in previous years several members of the College helped organize or lectured at the annual HERCULES (Higher European Research Course for Users of Large Experimental Systems) course for young scientists held in the spring-time. A fine three-volume set of lecture notes, edited by J. Baruchel, J.L. Hodeau, M.S. Lehmann, J.R. Regnard and C. Schlenker, has recently been published by Les Editions de Physique and Springer-Verlag.

With a little help from other members of the College, Alain Filhol has produced an English version of "Video ILL Interactive", Macintosh software which presents the scientific activities of the ILL in the form of interactive animation and simulation of various typical experiments. The original French version was produced for the technology exposition held annually in Grenoble, where it has always been very well received by scientists and laymen alike, and the new English version was similarly very much appreciated by participants in the IAEA Workshop. This type of publicity has immediate visual impact, and with further support should be made more widely available.

Amidst much globetrotting in search of beam-time and conference interaction, scientific activity at the ILL has often concentrated on analysis of the remaining difficult problems of experiments done the years before the shutdown. What the scientific highlights of 1993 lack in numbers they more than compensate in depth and diversity!

Scientific Highlights in 1993

Crystallography

The paraelectric and ferroelectric phases of betaine phosphite

During the last decade orientational glasses have attracted considerable attention. These compounds exhibit a transition from a crystalline high-temperature phase to a glassy low-temperature state, which is characterized by a collective freezing of reorienting moments in an orientationally disordered phase. The best-known examples are alkali halide - alkali cyanide mixtures, such as $(KBr)_{1-x}(KCN)_x$, and solid solutions of PbH_2PO_4 and $(NH_4)H_2PO_4$.

Recently new systems of this type have been discovered, namely, mixed crystals of ferroelectric betaine phosphate, $(CH_3)_3NCH_2COO.H_3PO_4$ (BP), and ferroelectric betaine arsenate, $(CH_3)_3NCH_2COO.H_3AsO_4$ (BA), and mixed crystals of BP, and antiferroelectric betaine phosphite, $(CH_3)_3NCH_2COO.H_3PO_3$ (BPI), both of which, according to dielectric and specific-heat measurements, exhibit a frustrated polar state over a wide concentration range. These compounds adopt hydrogen-bonded structures, where the hydrogen bonds order along linear chains while the weak interactions across the chains determine whether the ordered state is ferroelectric or antiferroelectric. Only limited structural information is available, even for the pure compounds.

At the instigation of physicists at the University of Darmstadt, a program of investigation of the structural properties of these glasses was begun just before the reactor shutdown, beginning with determination of the structure of pure BPI in its different phases. From dielectric measurements it is known to undergo a transition to a ferroelectric state at 216 K, and possibly another transition at 177 K. In the first experiment the structure of BPI was therefore investigated at 295 K, 190 K and 10 K by single-crystal diffraction on D10 [1,2].

The structure determined in this experiment for the paraelectric phase is shown in Fig. 1. This phase of BPI belongs to space group $P2_1/c$ with two half-occupied sites related by inversion centres for both H(13) and H(15) (Fig. 2). Ordering of one or both of these protons by removal of the inversion centre will give a ferroelectric structure with the same unit cell as at room temperature but with the lower symmetry of $P2_1$. In going from $P2_1/c$ to $P2_1$ the reflection condition, h0l, l = 2n, is removed but the additional reflections may be very weak if the 50 remaining atoms in the new asymmetric unit are still very nearly centrosymmetrically related. This was indeed the case, but

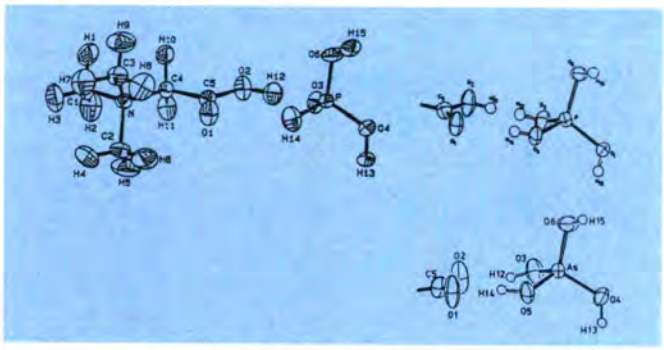

Fig. 1: The asymmetric unit of betaine phosphite at 295 K in the paraelectric phase. Inset: the regions near H(12) and H(14) in betaine phosphate and betaine arsenate.

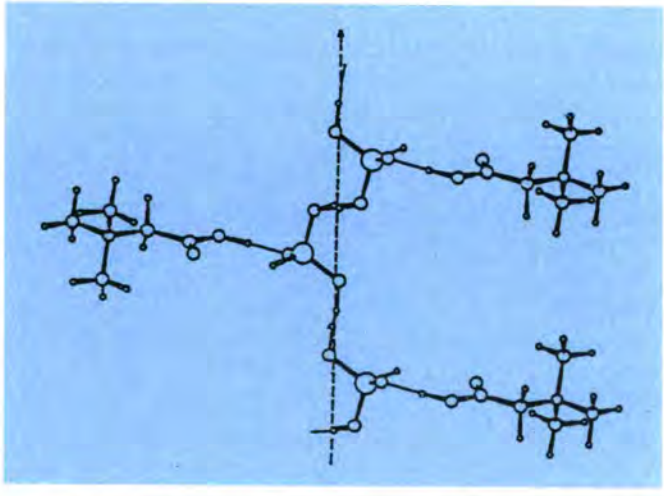

Fig. 2: Schematic drawing of the chaining of the betaine and hydrogen phosphite molecules units along the monoclinic b-axis (dashed) of the paraelectric phase of betaine phosphite.

the h0l, $l \neq 2n$, reflections were clearly visible at both 190K and 10K. The structure refinements showed ordering of both H(13) and H(15) at both temperatures, in the chemically more plausible arrangement of two (crystallographically independent) H_2PO_3 groups rather than one HPO_3 group and one H_3PO_3 group.

Ordering of the hydrogens alone did not however entirely explain the diffraction intensities in the ferroelectric phase; as expected from the observed ferroelectricity the rest of the structure also becomes 'significantly' noncentrosymmetric, with the atoms of the phosphite group showing the largest degree of noncentrosymmetry at both the lower temperatures. Furthermore the bridging hydrogen atoms appear to be fully ordered at 190 K, yet the marked average increase in intensity of the h 0 l, $l \neq 2n$, reflections in going from 190 K to 10 K strongly suggests that the ordering (in the sense of a phase transition) is only partial at 190 K. If true this strongly contrasts with the otherwise seemingly similar KH_2PO_4 family where the hydrogen ordering and the distortion of the heavy-atom lattice go hand-in-hand.

Thus far no evidence has been found for a structural transition in BPI between 190 K and 10 K, although the most recent investigation at Laboratoire Léon Brillouin of the temperature dependence of the additional reflections of the ferroelectric phase has suggested the formation of an intermediate phase around 210 K. Perhaps this is where gradual ordering of the bridging hydrogens occurs?

At all temperatures it was clear that in BPI there is just a single H(12) site near O(2), in contrast to BP where two half-occupied sites between O(2) and O(3) are preferred. The total transfer of H(12) to the betaine zwitterion, as opposed to the partial transfer in BP and the total retention in the H_3AsO_4 group in BA (inset to Fig. 1), is consistent with the increase in acidity in going from H_3AsO_4 to H_3PO_4 to H_3PO_3.

A lot of work lies ahead before we can hope to understand fully the pure end members let alone the frustrated phases of the mixed crystals. The large asymmetric units, particularly in the lower temperature phases, demand extensive and precise diffraction data and careful analysis to extract physical characteristics of the different phases and phase transitions. This is particularly so in the frustrated mixed phases where additional occupational and positional disorder occurs in the salt groups [viz. O(5)/H(14) in BP-BPI, and P/As in BP-BA, see the inset to Fig. 1]. Deuteration would alleviate the experimental problem of absorption, but can also change the nature of the phase transition. Indeed, deuterated BA has an antiferroelectric, rather than ferroelectric, low-temperature phase and mixed crystals of hydrogenous BA and deuterated BA also form a frustrated polar phase; but that is a story for a later annual report!

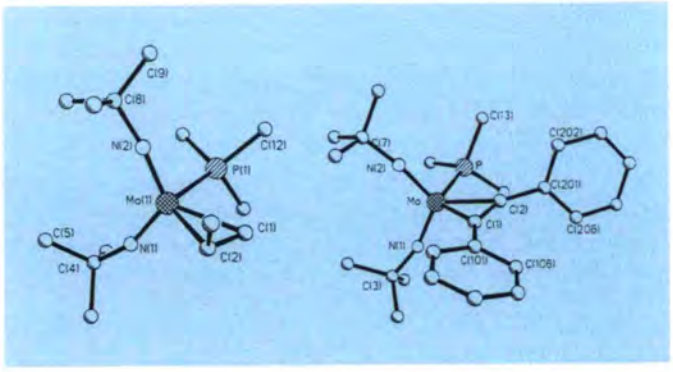

Fig. 4: The molecular structures of two Mo bis(imido) complexes a) [Mo(NBut)$_2$(CH$_2$=CHMe)(PMe$_3$)], b) [Mo(PMe$_3$(NBut)$_2$(PhC≡CPh)].

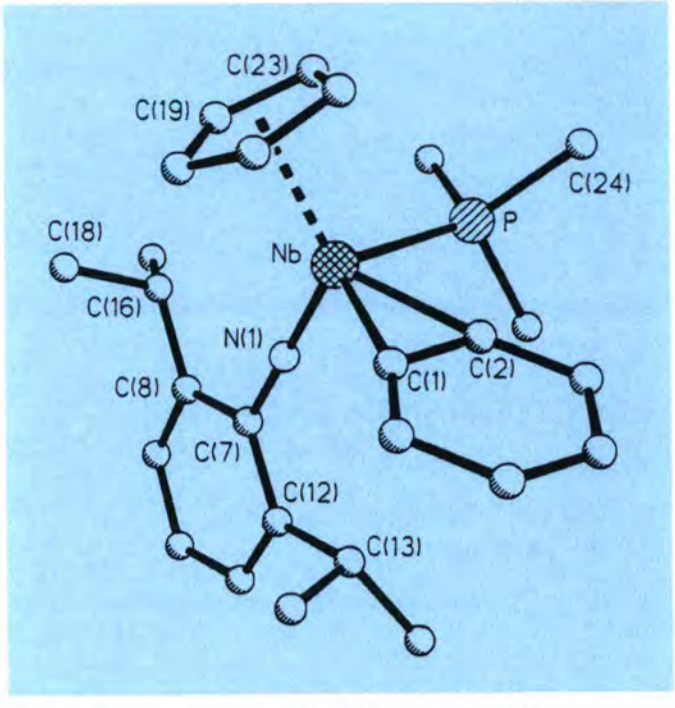

Fig. 5: Molecular structure of the Nb benzyne complex [Nb(η^2-C$_6$H$_4$)Cp(N-2,6-Pr$^i_2$C$_6$H$_4$)PMe$_3$].

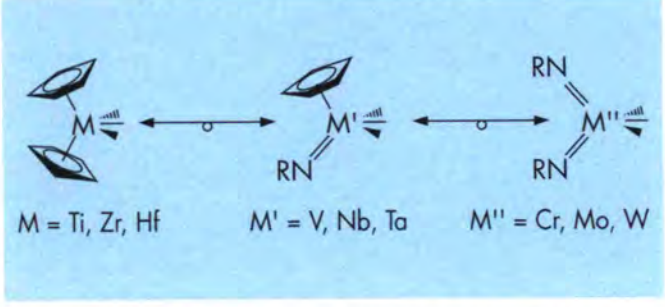

Fig. 3: Isolobal species of group 4, group 5 and group 6 metals. RN is an imido group.

Half-sandwich niobium imido and molybdenum bis(imido) complexes: metallocene analogues

Bent group 4 metallocene derivatives (Cp_2MCl_2, where M=Ti or Zr, and Cp = cyclopentadienyl) are of current interest as precursors to Ziegler-Natta polymerization catalysts. Fenske-Hall molecular-orbital calculations carried out on group 5 half-sandwich imido and group 6 bis(imido) fragments show that they may be considered to be isolobal (Fig. 3) and electronically isovalent with the group 4 metallocenes. The frontier orbitals available for the coordination of further ligands have been calculated to lie in a plane perpendicular to that defined by the metal, the imido nitrogen and the centroid of the cyclopentadienyl ligand for group 5 complexes, and to the plane of the two imido nitrogens and the metal for group 6 compounds. The structures of three of these compounds - two Mo bis(imido) complexes (Fig. 4,) [3], and a rare example of a Nb benzyne complex (Fig. 5) [4] - have been determined by single-crystal X-ray diffraction. These structures were found to be consistent with the predicted geometry around the metal. The structures of a number of other Mo bis(imido) and Nb half-sandwich imido complexes have also been determined. (Collaboration with Durham University).

Neutron diffraction study of the Bauschinger effect in a high carbon steel

The Bauschinger effect was noted as early as 1886 by J. Bauschinger as "by loading in tension or compression above the elastic limit, the elastic limit for compression or tension respectively is lowered significantly, the more so, the greater is the initial loading above the limit". Despite extensive research in the intervening years however, this effect, which is common to all inhomogeneous materials remains poorly understood. This is largely because the roles of mismatched stresses between the phases and of dislocation-based work hardening, as the load is reversed, have not been conclusively identified. To date the only attempt to distinguish between these two effects has been the X-ray work of Wilson and Bate [5]. In this respect, Bragg diffraction is a very useful tool enabling one to measure the strains in individual phases *via* peak shifts, while the dislocation density is related to the peak width. A study of the Bauschinger effect has now been made by neutron diffraction.

As in the early work on the Bauschinger effect, this study was undertaken on a 1.1 % carbon steel heat-treated to give ~17 % of spheroidal cementite particles. The neutron experiments were carried out at the reactor of NPI Rez near Prag on a dedicated three-axis spectrometer equipped with elastically bent silicon monochromator and analyser crystals. Thanks to a combination of real and reciprocal space focusing, it permits profile analysis at resolution conditions approaching those offered by X-ray equipment [6]. Neutrons have, however, the distinct advantage over X-rays that they penetrate centimetres rather than microns of material and thus unequivocally provide information about the bulk state of internal stress.

Specimens were prestrained to 1.5, 4.5 and 8 % compressive strain, prior to reverse (tensile) straining. The development of internal stress was monitored by intermittent unloading and diffraction peak measurement (the strain being calculated from the shift of the centre of a Gaussian peak). The results are shown in Fig. 6 plotted against cumulative strain ($\Sigma|\varepsilon|$). It can clearly be seen that internal matrix strains build up in similar sense (but of opposite sign) under forward straining in both tension and compression. The load is transferred from the matrix to the elastically deforming particles, but plastic relaxation, local to the particles, limits the rate of increase of load transfer and after a few percent plastic strain the rate of increase of matrix strain falls considerably.

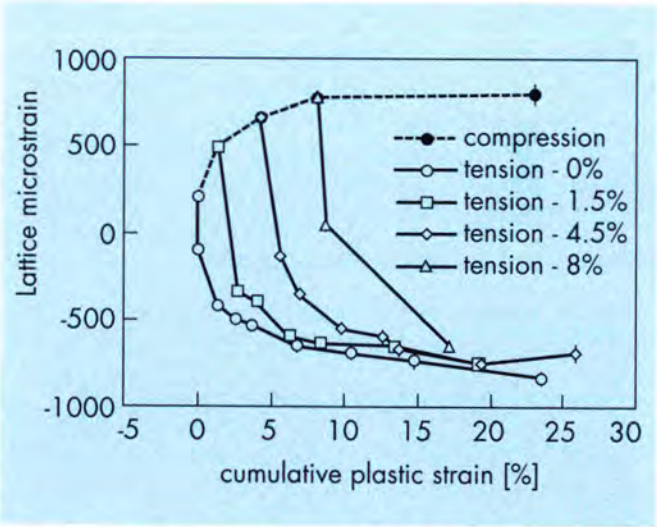

Fig. 6: The development of matrix strain as a function of cumulative plastic straining for different compressive prestrains. The monotonic loading curves are shown in bold lines.

While the load transfer increases the yield stress in the forward direction, it decreases it upon reverse straining, giving rise to the Bauschinger effect. This is because, upon unloading, the load transfer leaves residual stresses in the matrix, acting in a sense opposite to the forward deformation. Hence upon load reversal the residual stresses facilitate a rapid reversal of the internal matrix strain, which is fully achieved when the plastic strain approximately equals the prestrain. The variation in diffraction peak width (FWHM) with forward and reverse straining is

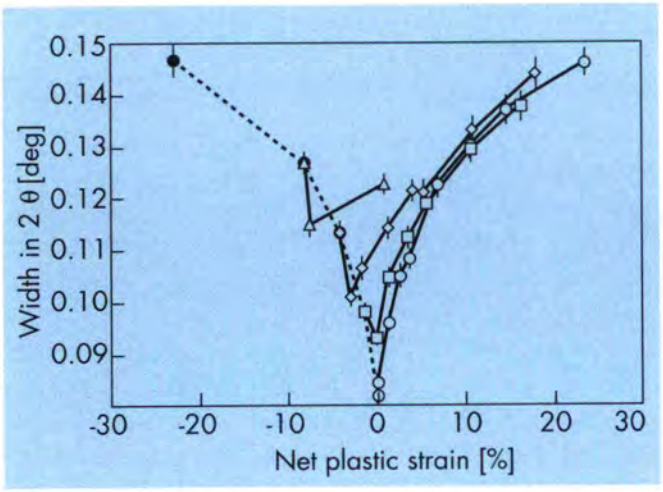

Fig. 7: The variation in diffraction peak width as a function of net (tensile) strain for different compressive prestrains. The monotonic loading curves are shown in bold lines. Symbols as in Fig. 6.

displayed in Fig. 7. Again, there appears to be little difference between evolutions due to forward loading in tension and compression. Immediately upon load reversal the width decreases abruptly - reflecting relaxation of residual matrix strains, also responsible for peak position shifts. After a transient period the width becomes related to the net strain rather than to the cumulative strain, reflecting the evolution of the dislocation substructure under new conditions.

Crystallography and Magnetism

Magnetic ordering and excitations in electron-doped superconducting materials

The magnetic properties of high temperature-superconductors and related materials have been investigated in great detail following the suggestion that these might play an important role in the superconducting mechanism. The Cu ions in these materials carry an unpaired spin and therefore it is possible that the magnetic fluctuations are responsible for the Cooper pairing. Indeed, fluctuating two-dimensional antiferromagnetic spin correlations in CuO_2 planes have been reported to exist up to very high temperatures in these compounds and persist even in the samples which are doped to become superconductors and in which no magnetic transition occurs. The magnetic properties of the hole-doped superconductors $La_{2-x}Sr_xCuO_4$ and $RBa_2Cu_3O_x$ (R = rare-earth element) have been investigated quite extensively. Superconductivity has also been discovered in the class of materials $R_{2-x}M_xCuO_4$ (R = Pr, Nd, Sm and Eu; M = Ce, Th) for which electrons, rather than holes, are the charge carriers. Systematic investigation of the magnetic properties of the electron-doped superconductors could further elucidate the possible relationship between magnetism and superconductivity.

The magnetic ordering of the parent undoped materials R_2CuO_4 has been investigated for a number of rare-earth ions. The Cu magnetic moments in R_2CuO_4 order at temperatures in the range 250 - 285 K. The rare-earth moments, when they are non-zero, order at much lower temperatures (1-6 K). Systematic neutron-scattering investigations on R_2CuO_4 (R = Pr, Nd, Eu and Gd) were performed initially at the ILL. After the unfortunate shut down of the ILL reactor several ILL scientists continued these investigations at other neutron scattering centres.

Gd_2CuO_4 behaves differently to the rest of the R_2CuO_4 family Although Gd_2CuO_4 is as easily doped with Ce or Th as the other members of the family, it does not, as they do, become superconducting. Several explanations have been suggested for the absence of superconductivity in this compound, but they are not convincing. Gd_2CuO_4 also shows weak ferromagnetism below the copper ordering temperature. The magnetic ordering of Gd_2CuO_4 was studied at low temperatures by neutron diffraction at ILL [7] and it was found that below T = 6.4 K the gadolinium moments order antiferromagnetically with the wave vector **k** = (0,0,0). Ferromagnetic Gd layers parallel to the a-b plane

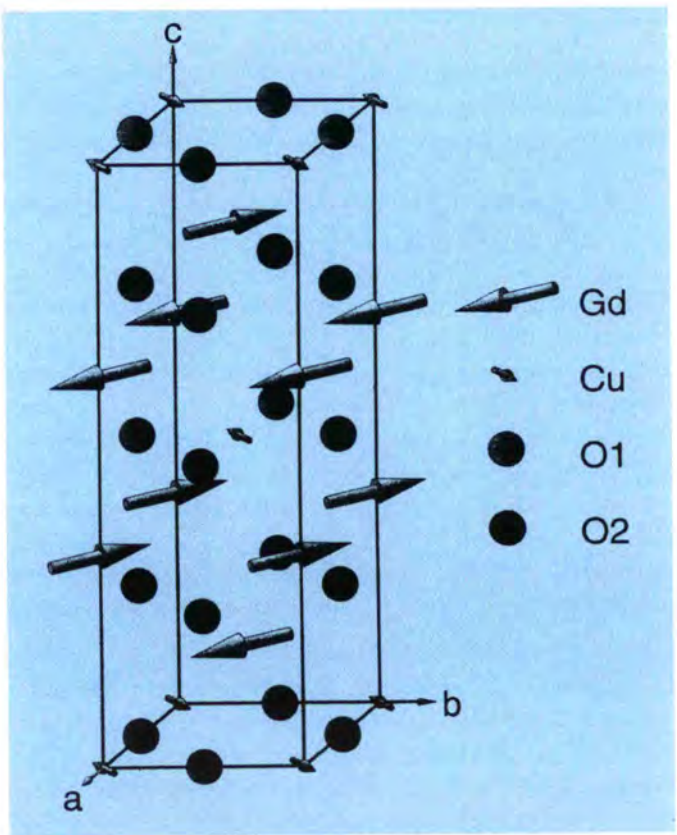

Fig. 8: Magnetic structure of Gd_2CuO_4 below $T_N(Gd)$= 6.4 K. Note that the spin directions of the Cu and Gd sublattices are at right angles. The structure model assumes a single-k ordering of the Cu sublattice. A double-k non-collinear spin arrangement is also possible.

are antiferromagnetically stacked along [001]. The magnetic ordering of the copper sublattice has also been investigated by neutron diffraction at PSI [8]. The Cu^{2+} ions in Gd_2CuO_4 order at T_N = 285 K to a La_2NiO_4-type antiferromagnetic structure with the propagation vector **k** = (1/2,1/2,0). Fig. 8 shows the magnetic structure of Gd_2CuO_4 below 6.4 K. The intensity of the 1/2 1/2 1 magnetic reflection increases continuously with decreasing temperature to 45 K. Below this temperature it starts to decrease and shows a minimum at about 20 K (Fig. 9). There is a further sharp anomaly at about 7 K at which the intensity of the reflection becomes practically zero. A search for magnetic reflections at Q = (1/2,1/2,0), (1/2,1/2,2) and (1/2,1/2,3) and other incommensurate positions at 7 K did not reveal any magnetic intensity [9]. This result indicates that at this temperature three-dimensional ordering of the copper sublattice disappears. The disappearance of three-dimensional magnetic ordering of the Cu sublattice just above the ordering temperature of the Gd sublattice is intimately connected with the weak ferromagnetism observed in Gd_2CuO_4 [10]. Since weak ferromagnetism is forbidden both for non-zero propagation vectors and in the tetragonal space group I4/mmm of Gd_2CuO_4, some structural distortion which changes the periodicity and lowers the symmetry must be present. A model in which the oxygen atoms are displaced perpendicular to the ideal Cu-O-Cu bond direction in accordance with the X-ray measurements was proposed [10]. Of the two possible displacement patterns the more likely is the one for which there is a real antisymmetric exchange interaction of the Dzyaloshinski-Moriya type between the nearest neighbours within the CuO_2 planes. It has been assumed that these displacements are perfectly correlated in each CuO_2 plane, but there exists no correlation of displacements from plane to plane. This model provides a possible explanation for the nature of the transformations of the magnetic structure which occur at temperatures below 50 K.

The magnetic ordering of the Cu ions in a single crystal of Eu_2CuO_4 has been determined at NIST [11]. Magnetic reflections corresponding to the wave vector **k** = (1/2,1/2,0) develop below the Néel temperature T_N = 265(5) K, showing a long-range antiferromagnetic ordering of the Cu moments in Eu_2CuO_4. The low-temperature saturated moment was determined to be 0.4(0.1) μ_B, with the spin directions restricted to the a-b plane. Magnetic field-dependent studies show no hysteretic behaviour at intermediate temperatures, which strongly suggests that the antiferromagnetic spin structure is of the non-collinear double-k type previously observed in Sm_2CuO_4 as well as Nd_2CuO_4 at intermediate temperatures.

The dispersion of the singlet-doublet magnetic excitons of the Pr^{3+} ions in the singlet-ground-state system Pr_2CuO_4 was measured by inelastic neutron scattering at NIST [12]. The excitons exhibit significant dispersion both within the basal plane as well as along the c-axis direction, directly demonstrating the Pr-Pr exchange interactions. These exchange interactions must be mediated through the CuO_2 layers involved in the formation of the superconducting state.

The magnetic ordering of Nd_2CuO_4 at milliKelvin temperatures has also been investigated by neutron diffraction at HMI [13]. At about T = 400 mK the 1/2 1/2 0 reflection which is forbidden for the magnetic structure determined at higher temperatures starts increasing in intensity and shows no indication of being saturated down to 33 mK, the lowest temperature attained during the experiment. Other allowed reflections like 1/2 1/2 1, 1/2 1/2 2, 1/2 1/2 3, etc. also show anomalous increases in intensity below 400 mK. These results strongly suggest induced nuclear magnetic ordering in Nd_2CuO_4 below 400 mK.

The Surface Superconducting Region in Lead

Above the critical applied field, H_c, for a bulk superconducting state of a type-I superconductor superconductivity persists within a narrow surface layer of the material, a phenomenon known as surface superconductivity and predicted within Ginzburg-Landau theory. The magnetic flux profiles within the surface superconducting region of lead films has been measured by polarized-neutron reflectometry on CRISP at ISIS and the validity of the Ginzburg-Landau equations examined [14].

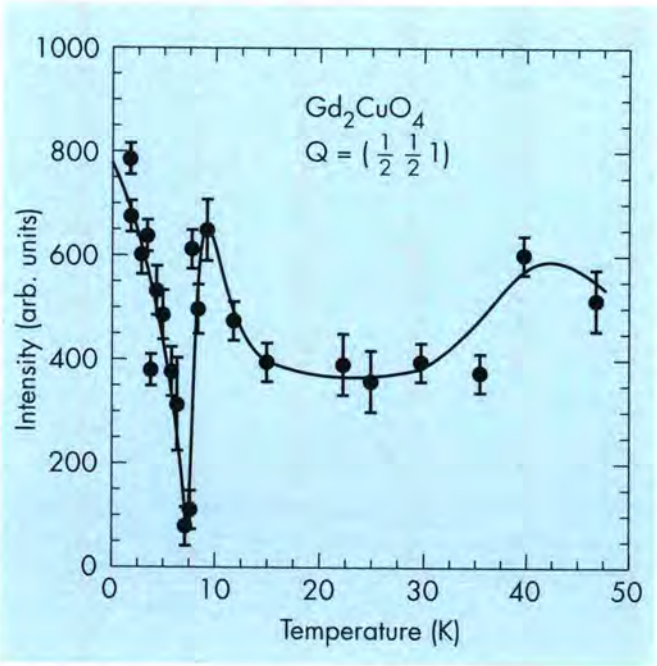

Fig. 9: Temperature variation of the integrated intensity of the 1/2 1/2 1 magnetic reflection in the temperature range from 1.5 to 45 K showing a broad minimum at about 20 K and a further sharp minimum at about 7 K. The first anomaly is associated with the weak ferromagnetism, whereas the second anomaly is interpreted to be due to the disappearance of the three-dimensional ordering of the Cu magnetic moments. Two-dimensional magnetic ordering in the CuO_2 plane must still exist due to the strong Cu-O-Cu superexchange interaction.

In these studies, the transition from the bulk superconducting state to the surface superconducting state and the subsequent entire destruction of superconductivity within the material as a function of the applied field has been directly observed (fig 10). Analysis of the measured flipping ratio profiles has shown that in both the bulk superconducting region and the surface superconducting region, at applied fields away from the upper critical field, H_{c3}, Ginzburg-Landau theory is valid and provides an accurate model of the magnetic induction profiles within the material. At higher applied fields, close to H_{c3}, the field dependence of the magnetic induction profiles may be modelled by assuming that the characteristic Ginzburg-Landau parameter κ, increases rapidly with an increasing applied field.

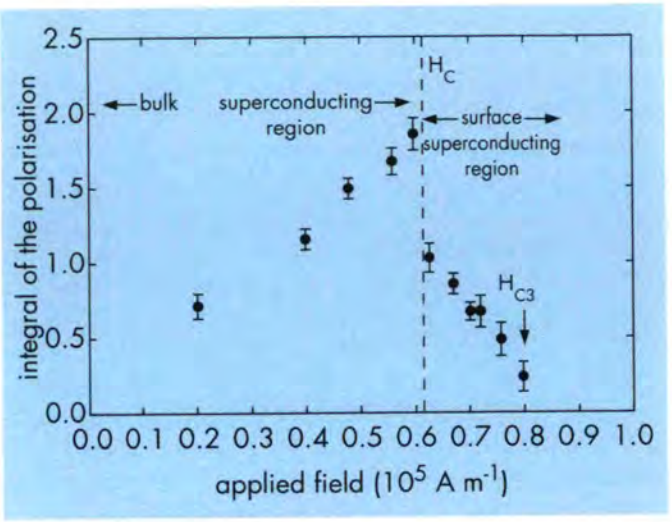

Fig. 10: The integral of the polarization over momentum transfer plotted against the applied field, for a lead film at 1.5K. H_c is the critical field for the bulk superconducting state and H_{c3} is the critical field for the surface superconducting state.

Phase Transition in Pd_2TiIn

Recent measurements of the bulk susceptibility and resistivity of Pd_2TiIn indicated a phase transition at 110 K. A broad peak in the susceptibility occurs around 110 K suggesting an ordered magnetic ground state. Above 110 K the susceptibility follows a Curie-Weiss law. This result was surprising since none of the constituent elements is itself magnetic. In order to try to establish the nature of the ground state, a powder neutron-diffraction experiment was performed using DN5 at Siloé.

Between 300 K and 92 K the neutron diffraction patterns are consistent with a single phase $L2_1$ structure with a space group $Fm\bar{3}m$ (O_h^5). Below 92 K the patterns are characteristic of a crystallographic distortion from a cubic fcc structure to a body-centred tetragonal one with space group I4/mmm (D_h^{17}). The cell parameters of the cubic and tetragonal structures are related by $a_t = a_c / \sqrt{2}$ and $c_t = a_c$. The thermal variation of the lattice parameters and the unit cell volume determined from the neutron diffraction experiment are shown in figures (11) and (12) respectively. At 92 K there is a huge discontinuity in the lattice parameters, consistent with a first order transition. The a parameter is seen to increase abruptly, $\Delta a/a = 0.35$ %, while the c parameter decreases, $\Delta c/c = 0.68$ %. In contrast the volume shows no anomaly at 92 K.

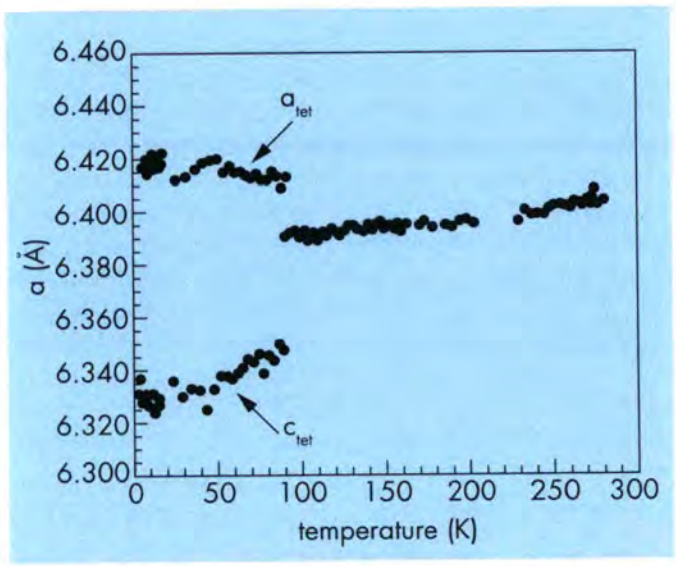

Fig. 11: The thermal variation of the lattice parameters of Pd_2TiIn.

Nor, in contrast to the static susceptibility data, did the neutron diffraction pattern show any evidence of long-range antiferromagnetic order, i.e. there were no additional magnetic peaks. Due to the extinction conditions associated with the body centered structure (h+k+l = 2n) the 001, 100, 111 and 102 reflections are systematically absent. The absence of these peaks leads to the following conclusions: either there is no long-range antiferromagnetic order with a significant moment, or there is only a ferromagnetic or ferrimagnetic coupling of magnetic moments on two crystallographically different sites, i.e. between Pd and Ti atoms. This would give a small contribution to the intensity of the nuclear Bragg reflections which would not easily be detected in a powder experiment.

The results are consistent with an instability of the local moment which would give rise to the structural phase transition [15]. More detailed analysis of the magnetic measurements suggest that the ground state is probably ferrimagnetically ordered, which would produce only a small magnetic contribution to the intense nuclear Bragg peaks. In order to solve this problem, polarized neutron diffraction measurements on a single crystal are required.

The magnetic structure of UCo_2P_2

While UFe_2P_2 and UNi_2P_2 crystallize with the body centered tetragonal $ThCr_2Si_2$ structure (I4/mmm), UCo_2P_2 has a structure, which can be derived from that of $ThCr_2Si_2$

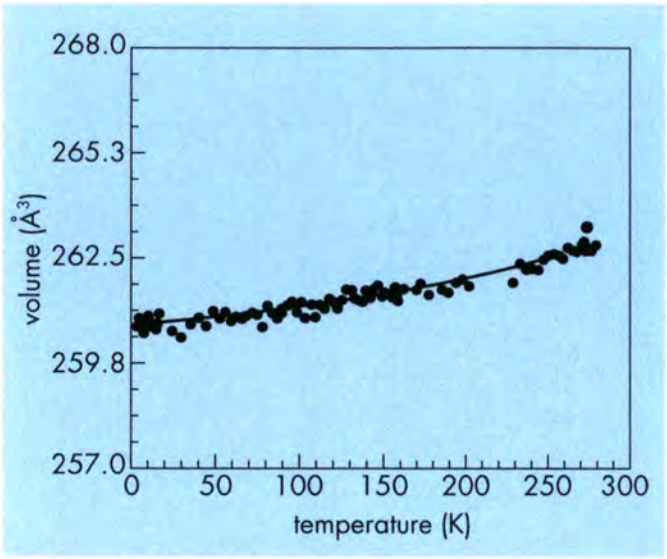

Fig. 12: The variation of unit cell volume as a function of temperature of Pd_2TiIn.

by an interchange of half of the Cr and Si positions. The resulting $CaBe_2Ge_2$-type structure has the space group P4/nmm (fig. 13). In UCo_2P_2 the Co(1) and the P(1) atoms are at 2a and 2b respectively, and the U, Co(2) and P(2) atoms are at positions 2c each with different z values.

Both the uranium and the cobalt atoms of UCo_2P_2 carry magnetic moments. Their order was investigated for polycrystalline samples with a SQUID magnetometer and by neutron diffraction on D20 just before the shutdown [16]. The magnetic cell (Fig. 13) is doubled along the c axis [$\mathbf{k}$ = (0, 0, 1/2)]. The magnetic moments of the uranium atoms are aligned antiferromagnetically and parallel to the c axis with μ_{exp} = 1.58(5) μ_B and a stacking sequence + + - -, + + - -. Of the two cobalt sites only one shows order with the magnetic moments μ_{exp} = 1.14(7) μ_B again aligned parallel to c and therefore parallel to the adjacent uranium moments. In going to higher temperatures the order of the uranium moments disappears at 170 K, while the cobalt moments still show considerable (antiferromagnetic) order. The field dependent susceptibility measurements in the SQUID magnetometer indicate that the magnetic order of the cobalt moments can be changed to be ferromagnetic by applying a magnetic field.

The magnetic H-T phase diagram of $MnWO_4$

Previous results, which were obtained by neutron diffraction experiments on powders and single crystals, revealed that $MnWO_4$ undergoes several magnetic phase transitions below 13.5 K in zero magnetic field [17]. The magnetic phases are labelled AF3 (12.3 K ≤ T ≤ 13.5 K), AF2 (8.0 K ≤ T ≤ 12.3 K) and AF1 (1.2 K ≤ T < 8.0 K).

The symmetry of the underlying magnetic structures in phases AF3 and AF2 is identical. It is incommensurate with the crystallographic lattice and can be described by a propagation vector $\mathbf{k}$ = (-0.214, 1/2, 0.457). In AF3 the magnetic moments are semi-ordered. The component parallel to the a-c plane is sinusoidally modulated in amplitude, whereas the component perpendicular to the a-c plane, i.e. parallel to the [0 1 0] direction, is disordered. The phase transition from AF3 to AF2 on cooling involves an additional ordering of the component of the magnetic moments in the [0 1 0] direction, leading to an elliptical spiral structure in AF2. The basal plane of the elliptical spiral is spanned by the b-axis and the direction of the magnetic moments in AF3, the so-called easy direction. In phase AF1 the magnetic structure is commensurate with the crystallographic structure, being described by a propagation vector $\mathbf{k}$ = (± 1/4, 1/2, 1/2), i.e. with a magnetic unit cell 4a, 2b, 2c. The magnetic moments are collinear and parallel to the easy direction in the a-c plane, forming an angle of 37° to the a axis, like the ordered part of the magnetic moments in AF3.

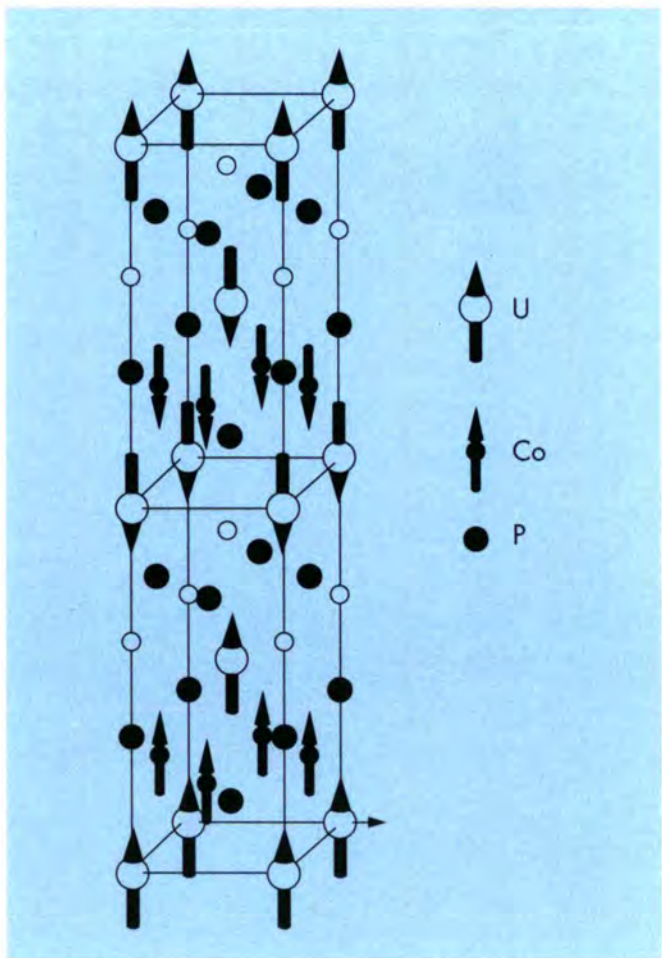

Fig. 13: Crystal and magnetic structure of UCo_2P_2. The moments of the Co(2) atoms which lie between two antiferrromagnetically coupled uranium layers, are disordered.

Susceptibility and magnetization measurements revealed that there is at least one further first-order phase transition, when a magnetic field is applied parallel to the easy axis. The transition field is H = 2.1 T. The field induced magnetic phase was characterized in more detail by a neutron diffraction experiment, which was performed on the normal-beam diffractometer DN3 at the Siloé reactor of the CEN Grenoble. The field and temperature ranges investigated were 0 - 5 T and 1.5 - 16 K respectively. The magnetic field was applied parallel to the easy axis.

It was found that the field-induced magnetic phase is identical with phase AF2. By monitoring systematically the count rate in the maximum of reflections corresponding to the magnetic superstructures of the three magnetic phases as a function of temperature and magnetic field, all phase boundaries in the given field and temperature range were determined. The phase diagram obtained from this experiment is shown in Fig. 14. It appears that phase AF2 occupies the largest part of the magnetic H -T phase diagram, including a field-dependent ferromagnetic component, which is 0.26 μ_B at H = 3.8 T and T = 1.5 K.

Special care had to be taken in order to detect the transition from AF3 to AF2, because the satellite positions of both magnetic phases are exactly identical. At the transition from the paramagnetic state to AF3 on cooling we looked at a magnetic satellite which is strong when the ordered magnetic moments are restricted to the a-c plane, i.e., in phase AF3. As the main difference between the phases AF2 and AF3 is the existence of an ordered component of the magnetic moments parallel to the b axis in phase AF2, at the transition AF3 - AF2 a magnetic satellite was selected, which gains considerable intensity only in phase AF2, i.e. one which is very sensitive to the presence of this component. This is visualized in Fig. 15, where the behaviour at zero field of two such reflections is shown on cooling from the paramagnetic state.

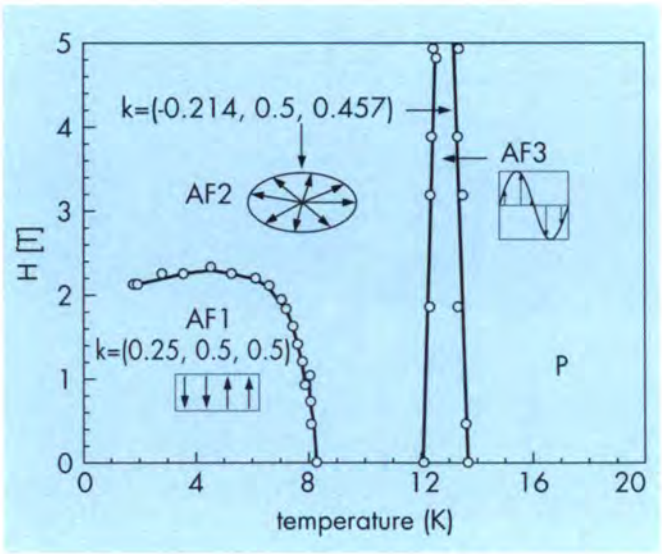

Fig. 14: Magnetic H-T phase diagram of $MnWO_4$, when the applied external magnetic field is along the easy direction.

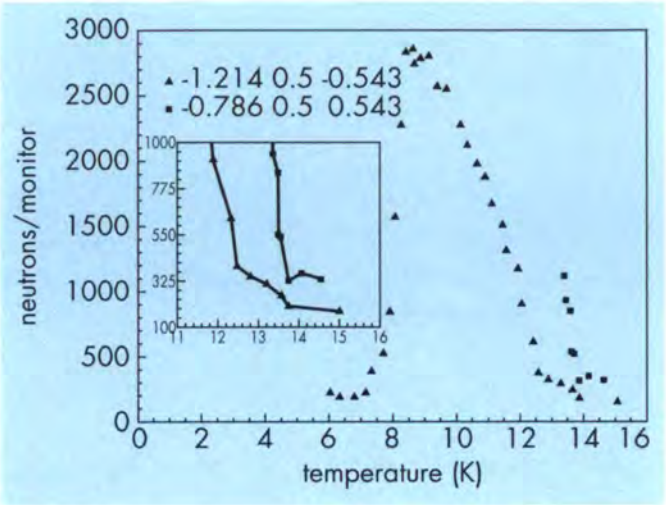

Fig. 15: Temperature dependence of the count rate in the maximum of the reflections (- 1.214, 1/2, - 0.543) and (- 0.786, 1/2, 0.543) of $MnWO_4$. The intensity of reflection (- 1.214, 1/2, - 0.543) is small between 13.8 K and about 12 K; it is significantly increased at about 12 K, i.e. at the phase transition AF2-AF3, whereas the reflection (- 0.786, 1/2, 0.543) gains intensity already at about 13.8 K, i.e. at the transition to phase AF3 on cooling from the paramagnetic state.

The observed transitions result from a competition between isotropic exchange interactions and the weak anisotropy (L = 0 for Mn^{2+}) of the crystal field. Considering the entropy contribution, which was determined by a specific heat measurement, as well as the dipole-dipole interaction, the differences in exchange and anisotropy energy at the phase transition AF1 - AF2 (E(AF1) - E(AF2)) can be determined by the use of mean-field equations. We find ΔE_{ex}= 2.89 J/mol and ΔE_{ani} = - 4.75 J/mol.

Secretaries: Garry J. McIntyre (5a)
Bachir Ouladdiaf (5b)

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The Use of Neutrons and X-rays in the Study of Magnetism

I.L.L., 21-23 January 1993

It is now more than 40 years since Cliff Shull and Ernie Wollan carried out the first neutron experiments on magnetism, studying polycrystalline MnO. In the intervening years, neutron scattering has revolutionised our microscopic understanding of magnetism. The pre-eminent position of neutron scattering as a microscopic probe of magnetism is now being challenged by an increasing number of x-ray techniques, employing synchrotron radiation. Although the interaction of electromagnetic radiation with magnetic electrons is much weaker than the neutron magnetic moment-electron spin interaction, this is compensated to a considerable extent by the enormous photon flux and high brightness of recent (and future) synchrotron sources. X-ray magnetic scattering has made many significant contributions to our knowledge of magnetism over the last few years. The high wavevector resolution, well-defined polarisation and wavelength tunability provided by synchrotron radiation have led to an improved understanding of the magnetic structure of rare-earth metals (the "spin-slip" model), to the discovery of resonant-exchange enhancement at absorption edges, and to a vast body of spin-dependent absorption phenomena studied using both linear and circular polarisation techniques. But neutron scattering has not stood still, with advances in both techniques and applications.

What is interesting is that there is not a confrontational spirit between the proponents of neutrons and x-rays in magnetism. Rather a spirit of educated compromise is emerging as it is realised that the two techniques used together can add significantly to our comprehension. This complementarity is attested to by the Workshop held at I.L.L. in January 1993, organized by W.G. Stirling (Keele), G.H. Lander (Karlsruhe), C. Vettier (ESRF), J.L. Martinez (ILL/Madrid) and P.J. Brown (ILL). Over 100 scientists participated in a series of 23 invited talks. In addition 62 posters were presented and a wide-ranging panel discussion took place. The meeting united members of the neutron and x-ray communities who discussed topics as varied as magnetic x-ray dichroism and flux-line lattices in high-temperature superconductors. The invited talks have been published as a special edition of Physica B [1]; these proceedings are a most valuable indication of current advances in the study of magnetism. The organisers are grateful to the I.L.L. and the E.S.R.F. for financial support and to Diana Dijoux and Serge Claisse for their enthusiastic help with the organisation.

We dedicate this workshop to the memory of our friend and colleague Jean Rossat-Mignod, whose untimely death in August 1993 brought short a most productive scientific career. We shall all miss his scientific drive and originality, but, more importantly, his friendship and humour.

Bill G. Stirling and Gerry Lander

Reference [1] Physica B 192, 1 & 2 (1993)

IAEA Materials-Research Workshop

College 5 members were responsible for organizing an Interregional Training Course on Nuclear Methods in Materials Research under the aegis of the International Atomic Energy Agency,Vienna. Eighteen students from wider Europe and the developing countries spent two weeks at the ILL in May in both lectures and practical exercises. The four IAEA-invited lecturers, from Portugal, France, Britain and Australia, taught the systematics of powder diffraction and small-angle scattering for the study of materials, while ten local lecturers, mainly from ILL and ESRF, highlighted and broadened the course with first-hand accounts of X-ray and neutron topography, kinetic measurements by diffractometry, polymers, high temperature superconductors, phase transitions by powder diffractometry, neutron spectroscopy, multilayer and monochromator production and testing, etc. Exercises and program exchanges on personal computers, and visits to local reactors and the ESRF were much appreciated by the course participants.

Sax A. Mason

Empirical and calculated thermal-diffuse-scattering corrections for single-crystal diffraction data

Garry J. McIntyre

Introduction

For monochromatic X-rays or neutrons the elastic Bragg reflections are observed superimposed on incoherent scattering and inelastic phonon scattering. The incoherent scattering is essentially removed by the background subtraction, but the inelastic phonon scattering, also called thermal diffuse scattering (TDS), peaks at the same positions as the Bragg reflections, and generally can be removed only by calculation based on the elastic constants.

Unfortunately, for many compounds the elastic constants are not known, and corrections to the observed data for TDS are not made, the principal consequence being a reduction in the apparent thermal displacement parameters. Given the differences amongst scan geometries used by different experimenters on different diffractometers, it is little wonder that there is often poor agreement amongst thermal displacement parameters from different experiments on the same compound! Here we shall see that with minor modification of the experimental technique, particularly in measurements with a 2-D position-sensitive detector (PSD), a purely empirical correction can be made.

A little background to TDS

For X-rays the ratio of the one-phonon TDS intensity to the integrated Bragg intensity is [1],

$$\alpha_1 = I_1/I_B = (k_B T/v_c) \iiint J_1(\mathbf{q}) d^3q \qquad (1)$$

where the integration is over the reciprocal space volume swept out in the scan, and

$$J_1(\mathbf{q}) = (1/q^2) \Sigma_j [\mathbf{h}.\mathbf{e}_j(\mathbf{q})]^2/[\rho V_j(\mathbf{q})] \qquad (2)$$

is the one-phonon scattering at $\mathbf{q}$ from the reciprocal-lattice point $\mathbf{h}$, where k_B is Boltzmann's constant, T is the temperature, ρ is the crystal density, v_c is the unit cell volume, $V_j(\mathbf{q})$ is the velocity of the acoustic lattice wave with vector $\mathbf{q}$, and the $e_j(\mathbf{q})$ (j =1,2,3) are unit vectors in the direction of polarisation of the lattice wave.

$J_1(\mathbf{q})$ can be calculated from the elastic constants c_{ijmn} [2],

$$J_1(\mathbf{q}) = (h^2/q^2) \Sigma_{i,j} h_i h_j (A^{-1})_{ij} \qquad (3)$$

where $A_{ij} = \Sigma_{m,n} c_{ijmn} q_m q_n$ and the h_i and q_i are the direction cosines of $\mathbf{h}$ and $\mathbf{q}$ respectively.

If the finite resolution of the diffractometer can be ignored the $1/q^2$ dependence of $J_1(\mathbf{q})$ permits reduction of the 3-D integral over the volume of the scan to a 2-D integral over the surface S of the scan volume, which, as well as allowing the singularity at the origin to be avoided, considerably reduces the calculation time [3]. The expression for α_1 then reduces to

$$\alpha_1 = (k_B T/v_c) \int_S J_1(\mathbf{g}) g dA \cos\xi \qquad (4)$$

where $\mathbf{g}$ is the vector to the surface element dA on the surface S and ξ is the angle between $\mathbf{g}$ and the normal to dA.

For neutrons, the calculation of $J_1(\mathbf{q})$ is a little more complicated since equ. (2) is strictly valid only for the scattering of neutrons that are faster than the velocity of sound in the crystal, from a crystal with elastic isotropy. Calculation of a valid correction for slower-than-sound neutrons or for neutrons scattering from crystals with significant anisotropy is complicated [4]. A reasonable approximation is to accept in the summation of equ. (2) just those lattice waves with velocity less than the neutron velocity [5]. Fortunately most crystallographic structural studies at reactor sources are made at neutron wavelengths for which equ. (2) does apply.

Even less background to PSD's

The recent introduction of 2-D PSD's has brought about a minor revolution in single-crystal diffractometry [6]. One important advantage is that of optimal delineation of peak and background in the 3-D array of counts observed around each reflection (Fig. 1). This is particularly important for weak peaks on a high background. For weak peaks the envelope that minimizes the relative error due to counting statistics lies in fact *within* the instrumental resolution volume [7] - hardly a condition that satisfies the derivation of the TDS correction in equ. (4)!

With minor modification though, equ. (4) can be applied both to weak and to strong peaks, and correction for TDS is easier for 2-D PSD data than for conventional detector data to the extent that a purely empirical correction can be made.

Correction of PSD data for TDS

a) The idealised situation

A very important implication of equ. (4) is that if the finite instrumental resolution can be ignored the amount of TDS included in a pyramid whose apex is at the reciprocal lattice point (relp) is directly proportional to the height of the pyramid, i.e., to the distance from the relp to the integration boundary. Consequently, for integration envelopes of the same shape but different

size, the amount of TDS included in the integration volume is directly proportional to the average radius of the volume, whereas the amount of incoherent (flat) background is proportional to the cube of the radius. Similarly the contribution of two-phonon TDS is proportional to the square of the radius (Fig. 1).

By sampling each reflection in 3-D, as is done in scans with a 2-D PSD, we could correct empirically for TDS, and even deduce the elastic constants. The precision in such an empirical method would be poor for weak reflections, especially if sitting on a high 'flat' background, but, because of the slow global variation of TDS with the scattering vector, the corrections for these reflections can be estimated from those of nearby strong reflections.

Alternatively, if the elastic constants are already well known, the TDS correction to the peak and background integration volumes can be calculated by evaluating equ. (4) for a series of pyramids that fill the integration volume, in the same manner as in existing algorithms for single-detector data.

A convenient division is in terms of the polar coordinates θ and ϕ. Often an ellipsoidal integration envelope is assumed, since it is a good approximation to the instrumental resolution volume. If the integration ellipsoid is described by,

$$e_x^2x^2 + e_y^2y^2 + e_z^2z^2 = 1$$

and θ and ϕ are with respect to the principal axes of the ellipsoid then

$$g = (e_x^2\sin^2\theta\cos^2\phi + e_y^2\sin^2\theta\sin^2\phi + e_z^2\cos^2\theta)^{-1/2} \quad (5)$$

and in equ. (3) $gd\mathrm{A}\cos\xi = g\sin\theta d\theta d\phi$

b) The real situation

Unfortunately, if full advantage of the PSD is taken to minimize the counting statistics of background subtraction by using integration envelopes similar to or smaller than the resolution volume, we are far from the ideal situation. *A correction for finite resolution must be included.*

$\Rightarrow J_1(\mathbf{q})$ in equ. (4), is replaced by $\int R(\mathbf{q}')\, J_1(\mathbf{q} - \mathbf{q}')\, d^3\mathbf{q}'$

If we consider just one pyramid, i.e. just one direction in reciprocal space from the relp, the convolution becomes one of $R(\mathbf{q}')$ with g. For convenience the convolution is broken into two parts:

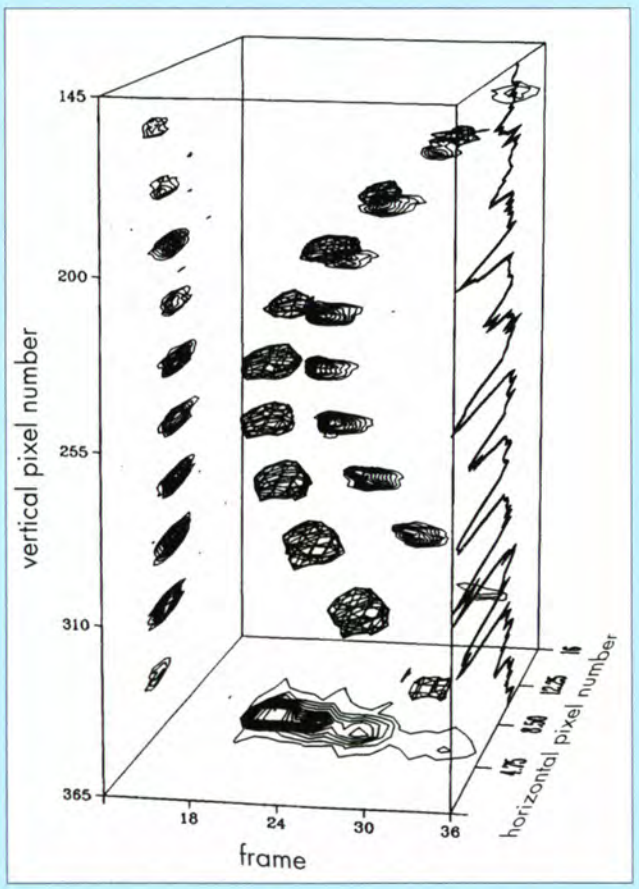

Fig. 1: The 3-D distribution of counts observed around the 2 6 l reciprocal lattice row of monoclinic $NiSO_4.6H_2O$ in a single scan on D19. The iso-intensity contour shown is 10% of the maximum count observed in this scan, and for the strongest reflections corresponds very closely to the size of the reflection integration envelope.

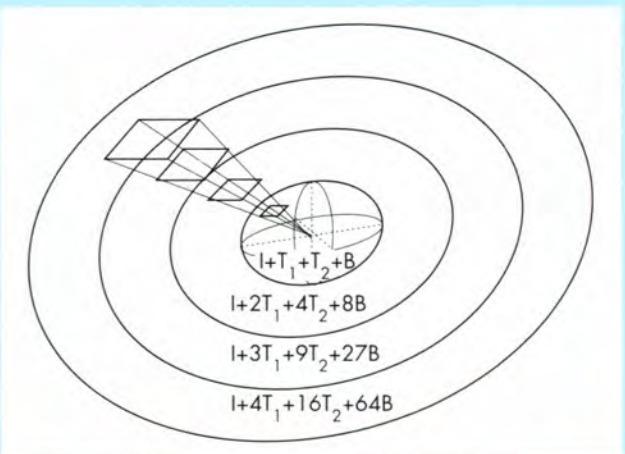

Fig. 2: The relative contributions of Bragg intensity, TDS and background to the total intensity within integration volumes of the same shape but different size in the idealized situation of an infinitely small resolution function. I is the integrated Bragg intensity, T_1 the one-phonon TDS, T_2 the two-phonon TDS, and B other (uniform) background.

a) Fraction of the resolution volume inside the integration volume

We can assume that the integration volume has the same shape as the iso-probability contour of the resolution ellipsoid. If in our example of an ellipsoidal resolution function we choose as integration variables, $x' = e_x^2 x$, $y' = e_y^2 y$, $z' = e_z^2 z$, and shift the ideal g outside the integral, then $R = R(r') = R((x'^2 + y'^2 + z'^2)^{1/2})$ and the integration over R is within a sphere of unit radius. The direction of the pyramid axis is no longer θ,ϕ in these coordinates but since x', y' and z' span identical ranges, the integral itself is independent of θ and ϕ. With the help of Fig. 3, we can deduce that the convolution of the resolution function with the distance to the integration boundary is,

$$g \int R(x'^2+y'^2+z'^2) [\sqrt{(1 - x'^2 - y'^2)} - z'] \, dx'dy'dz' \quad (6a)$$

where the integral is over just those points for which $x'^2 + y'^2 + z'^2 \leq 1$.

b) Fraction of the resolution volume outside the integration volume

The integrand is now the distance through the integration volume, parallel to $(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ weighted by the resolution function. Similarly this can be transformed to integration *outside* a unit sphere, with g of the ideal situation as a prefactor,

$$g \int R(x'^2+y'^2+z'^2) \sqrt{(1 - x'^2 - y'^2)} \, dx'dy'dz' \quad (6b)$$

where the integral is over just those points for which $x'^2 + y'^2 + z'^2 \geq 1$ and $x'^2 + y'^2 \leq 1$.

The total resolution factor is the sum of (6a) and (6b), and can be evaluated numerically for the range of ratios of integration-envelope radius to resolution function FWHH expected in an experiment (Fig. 4). The resolution factor is the same for all 'integration' pyramids of one reflection.

The background is estimated from the counts in an outer shell that is not necessarily contiguous to the peak envelope, but with inner and outer boundaries that would normally be chosen to have the same shape as the peak integration envelope. The contribution of one-phonon TDS to this background 'measurement' is simply proportional to the difference between the inner and outer radii multiplied by (different) resolution factors given by equ. (6a).

The resolution factor for two-phonon TDS is derived in a similar manner, and is,

$$g \int R(x'^2+y'^2+z'^2) [\sqrt{(1 - x'^2 - y'^2)} - z']^2 \, dx'dy'dz' \quad (7a)$$

$$+ g \int R(x'^2+y'^2+z'^2) |z'| \sqrt{(1 - x'^2 - y'^2)} \, dx'dy'dz' \quad (7b)$$

Within the usual assumptions of TDS theory, an *exact* correction for TDS can thus be made, even with finite instrumental resolution. The sampling afforded by the present 2-D PSD's, especially in X-ray diffraction, will ultimately limit the precision of this correction and its use as a method to estimate elastic constants. The very fine sampling offered by newer detectors based on charge-coupled devices might be used to advantage in this regard. With continously variable apertures it would

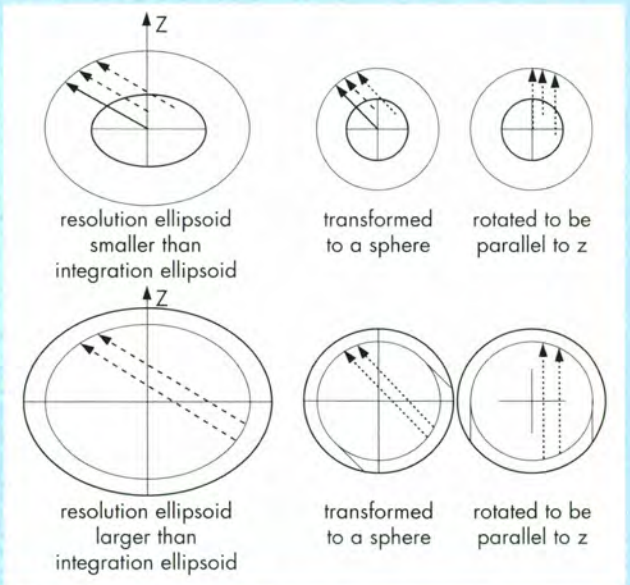

Fig. 3: Reduction of the resolution convolution to integration within a unit sphere. The dashed ellipse or circle is the boundary of the integration envelope; the heavy ellipse or circle is one iso-probability contour of the resolution function, all in reciprocal space. The arrows are the vectors for one pair of polar angles from selected points within the resolution function to the integration envelope.

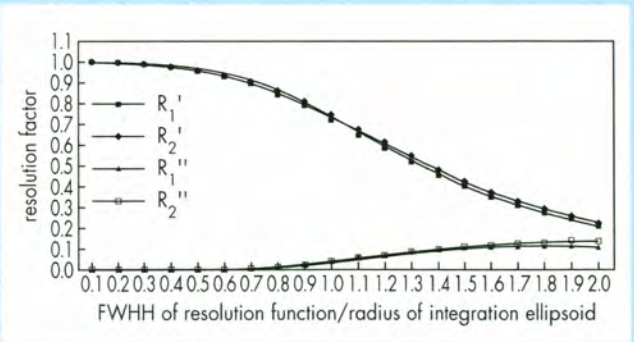

Fig. 4: Resolution factors for one- and two-phonon TDS for a 3-D Gaussian resolution function versus the ratio of the resolution function FWHH to the radius of the integration envelope. The integration envelope is assumed to be an iso-probability contour of the resolution function. The total resolution corrections for one- and two-phonon TDS are $R_1' + R_1''$ and $R_2' + R_2''$ respectively.

even be possible to make an empirical correction with a single detector, but with much poorer precision than with a 2-D PSD.

Conclusions

The differences in the dependence of the contributions to observed Bragg reflections, from one-phonon TDS, from two-phonon TDS, and from background, on the size of the integration volume can be exploited to correct for TDS and to estimate the elastic constants empirically, provided each reflection is sampled in three dimensions, as in scans made with a 2-D PSD. Finite resolution introduces additional geometric factors which can be calculated *exactly* if the integration volumes are iso-probability contours of the 3-D resolution function. These are strong reasons, in addition to that of minimum relative error due to counting statistics, for making 'routine' single-crystal diffraction measurements with a 2-D PSD.

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Spherical Neutron Polarimetry and Magnetic Diffraction*

Francis TASSET

Introduction

In the neutron-scattering cross-section, the basic magnetic scattering amplitudes are vector quantities, the magnetic interaction vectors **Q(k)**. These are projections on the plane perpendicular to the scattering vector k of the magnetic structure factors **M(k)**, those vectors being in fact the various Fourier components of the periodic magnetic density **M(r)**. For complex magnetic structures, in particular non-collinear ones, it has been shown [1, 2] that the measurement of the magnetic intensity alone may not be sensitive enough to determine a unique solution. Neutron Polarimetry, which measures in addition changes in the neutron polarization, can give more direct information on the directions of the magnetic interaction vectors. Therefore neutron polarimetry is an important method for distinguishing amongst "different magnetic orders which may have the same or very similar magnetic cross-sections" [3].

There are actually two forms of neutron polarimetry which we shall now briefly describe:

– Uniaxial Polarization Analysis (UPA), is the analysis of the initial and final polarization component parallel to an applied magnetic field. It was first introduced in 1968 at Oak Ridge by Moon, Riste and Koehler [4]. In magnetism, it has contributed to the study of paramagnetic scattering [5], can detect non collinear components in ferri-magnetic arrangements [6], and help to separate magnon and phonon peaks in case of ambiguity.

– Spherical Neutron Polarimetry (SNP), which better exploits magnetic scattering, requires a measurement whereby all three components in both the incident and the scattered polarization are set and measured independently.

Presently, with our polarimeter CRYOPAD (Cryogenic Polarization Analysis Device) [7], we are able to accomplish such measurements in zero applied field. In section 2 we shall explain why UPA is the only simple technique compatible with an applied magnetic field or a magnetised sample. In section 3 we shall restate the theoretical formula which gives the change of the neutron polarization vector in the microscopic magnetic interaction. This complicated formula is necessary to interpret SNP, and we show that it comprises the spectroscopic subset, introduced with UPA. In Section 4 we present a single generic figure for the possible changes in the neutron polarisation vector induced by magnetic structures containing centre

of symmetry and magnetic/nuclear interference terms. The depolarization effect due to the presence of 180° magnetic domains is incorporated, it illustrates the importance of SNP being able to distinguish a true rotation from a simple depolarization effect.

Spherical Polarimetry

Basic principle

The principle of the measurement is very simple as illustrated in Fig.1. The polarization vector of the incident beam is set in the desired direction, then the corresponding cross section and the direction and strength of the scattered beam polarization vector is determined for a given Bragg reflection.

Zero-field implementation, the CRYOPAD

Although it looks simple, such a complete measurement of the scattered neutron polarisation is not easy. If, as usual, we use a magnetic field to guide the polarization at the sample position, it plays an adverse role. The transverse component of polarization created by our sample (see sections 3 and 4) starts Larmor precession at high speed; due to field inhomogeneities and dispersion in speed, it relaxes and is lost very quickly.

To handle a proper measurement of this component its precession from the sample axis to the analyzing system must be controlled precisely. Spin Echo techniques could be developed in that direction, but with CRYOPAD we attack the problem in a different way: the sample is kept in zero field, low enough to suppress "parasitic precession" and to isolate the true effect of scattering and measure it, as in figure 1.

Using Magnetic Meissner Shields

The polarizer and the analyzer system used on IN20 are based on saturated magnetic crystals and they require high magnetic fields (2000 Oe) which unfortunately give substantial stray fields. Knowing that even the earth field must be eliminated, we have to provide magnetic shields around the sample chamber. Superconducting Meissner magnetic shields are the ideal solution to this problem. With Niobium being transparent to neutrons and to their polarization we have designed an almost closed cylindrical sample chamber. The exit point for the scattered beam being far enough from the entry point, we ought to apply two different guide fields of arbitrary directions in order to transport adiabatically the polarization to and from the sample chamber. But this ideal scheme is not directly applicable due to the boundary condition at the superconducting surface. Because all magnetic fields are necessarily tangent to such surfaces (B_n=0, parallel flux flow condition) it is necessary, in order to analyse an arbitrary, non transverse direction to proceed in two steps and use two successive screen/field combinations [7]. First, we use a calibrated transverse field to make the spins precess until the polarization becomes transverse. Then it enters into a strong nutation guide field which can be oriented in the transverse plane. Using these two magnetic fields, precession and nutation angles are precisely determined by using algorithms based on the detection of zero final polarization values [8]. The final polarization is measured with the classical analyzing system available on IN20 comprising a DC neutron spin flipper, a polarizing Heusler crystal and a neutron detector. A similar, reversed arrangement is provided to control the incident polarization direction. More detailed explanations on CRYOPAD can be found in references [3, 7, 8].

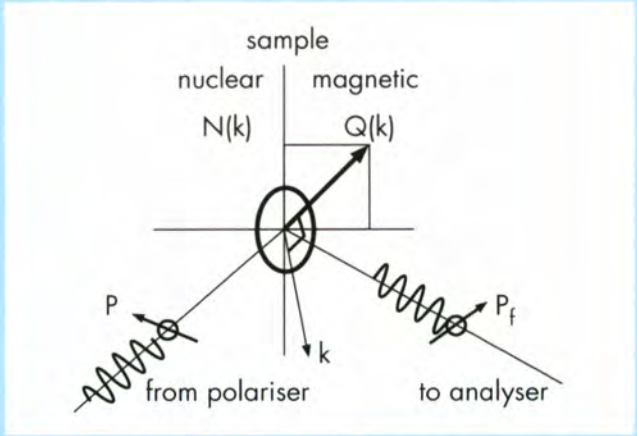

*Fig. 1: **The Polarimetric neutron diffraction experiment:** the polarisation vector of the incident beam **P** is set in the desired direction. Neutrons scattered at momentum transfer $\hbar k/2\pi$ experience the corresponding Fourier component of the nuclear potential $N = N(\mathbf{k})$ and of the effective magnetic interaction vector $\mathbf{Q} = \mathbf{Q}(\mathbf{k})$. The direction and strength of the final polarisation $\mathbf{P}_s$ are kept in zero field until they are measured downstream (see text).*

The microscopic theory for neutron polarimetry

The vectorial formalism

The change in neutron polarization for a mixed magnetic nuclear scattering process has been worked out in its present form by Blume[9]. With **k** being the scattering vector, N= N(**k**) the nuclear structure factor and **M**=**M**(**k**) the magnetic structure factor, we have to introduce the magnetic interaction vector **Q** = **Q**(**k**) which is the projection of **M** on a plane orthogonal to **k**

$$\mathbf{Q}(\mathbf{k}) = \hat{\mathbf{k}} \wedge (\mathbf{M}(\mathbf{k}) \wedge \hat{\mathbf{k}}) \qquad (1)$$

Then we have the following expressions for the scattered neutron intensity I and the scattered polarization vector $\mathbf{P}_s$ where $\mathbf{P}$ is the polarization before scattering:

$$I = NN^* + N\,\mathbf{P}.\mathbf{Q}^* + N^*\mathbf{P}.\mathbf{Q}^* + \mathbf{Q}.\mathbf{Q}^* + i\mathbf{P}.(\mathbf{Q}^*\wedge\mathbf{Q}) \quad (2)$$

$$\mathbf{P}_s I = \mathbf{P}NN^* + \mathbf{Q}N^* + \mathbf{Q}^*N - i\,(\mathbf{P}\wedge\mathbf{Q}N^* - \mathbf{P}\wedge\mathbf{Q}^*N) + \mathbf{Q}\,(\mathbf{P}.\mathbf{Q}^*) + \mathbf{Q}^*\,(\mathbf{P}.\mathbf{Q}) - \mathbf{P}\,(\mathbf{Q}.\mathbf{Q}^*) - i(\mathbf{Q}^*\wedge\mathbf{Q}) \quad (3)$$

N and $\mathbf{Q}$ have to be expressed in the same units using the following scale factor:

$$1\mu_B = 0.2695\ 10^{-12}\ \text{cm} \quad (4)$$

The four scattering cross sections in UPA

When introducing the UPA method, Moon, Riste and Koehler [4] did not use Blume's vectorial theory for neutron polarization rotation. Instead they derived a more spectroscopic set of four partial scattering amplitudes connecting the two initial and final neutron spin states. With our notations the corresponding expressions for the partial cross sections are:

$$\sigma^{++} = |N + \mathbf{Q}^Z|^2 \quad (5)$$

$$\sigma^{--} = |N - \mathbf{Q}^Z|^2 \quad (6)$$

$$\sigma^{+-} = |\mathbf{Q}^X + i\mathbf{Q}^y|^2 \quad (7)$$

$$\sigma^{-+} = |\mathbf{Q}^X - i\mathbf{Q}^y|^2 \quad (8)$$

If we assume that we know the initial polarization vector $\mathbf{P}$ is in the z direction used in their formulae (n^+ and n^- being the number of parallel and antiparallel neutron spins in the incident beam), these spin-flip and non spin-flip cross sections can be substituted into the following appropriate definitions in order to determine the predicted scattered polarization P_s^u.

$$\mathbf{P} = P\hat{z};\ P = \frac{n^+ - n^-}{n^+ + n^-};\ P_s^u = \frac{n_s^+ - n_s^-}{n_s^+ + n_s^-};\ I = \frac{n_s^+ + n_s^-}{n^+ + n^-};\quad (9)$$

where

$$n_s^+ = n^+\sigma^{++} + n^-\sigma^{-+};\qquad n_s^- = n^-\sigma^{--} + n^+\sigma^{+-};\quad (10)$$

Using now the value for $\mathbf{P}_s.I$ from Blume's equation (3) we find that the UPA scattered polarization P_s^u can be expressed simply as:

$$P_s^u \equiv \frac{\mathbf{P}_s.\mathbf{P}}{\mathbf{P}} \quad (11)$$

This means that the UPA final polarization P_s^u is one component of the rotated final polarization $\mathbf{P}_s$, the component which is collinear with the initial $\mathbf{P}$. There is no contradiction between the two theories: Blume's theory predicts the true change (rotation and length) of the polarization vector while Moon, Riste and Koehler partial cross sections can only tell us the ratio of the scattered to initial polarizations in a single, yet arbitrary, z direction. We conclude that these partial cross section can be used safely when applying a magnetic field at the scattering centre as long as the incident polarization has been strictly driven (or has relaxed) to this field direction (i.e. no transverse component should exist at the scattering axis which might be re-injected into the scattered longitudinal polarization). We note also that the analyzer must measure only the longitudinal component in the scattered beam, but this is a built-in property in the ferromagnetic analyzer crystal generally used.

The outcome of vectorial polarimetry

Let us suppose that we have been able to grow a single crystal which is a random alloy of the two existing isomorphous phases α Fe_2O_3 and Cr_2O_3. Like the pristine phases, the unit cell is rhombohedral with four transition metal atoms in two centrosymmetric pairs on the 3-fold axis. These two phases normally have different periodic magnetic arrangements in the unit cell, which is symbolized by α and β in Fig. 2. At low enough temperature, both are collinear arrangements with the spins aligned on the unique axis, but they differ in an essential way: spins in α obey the centre of symmetry, spins in β do not. Therefore magnetic structure factors

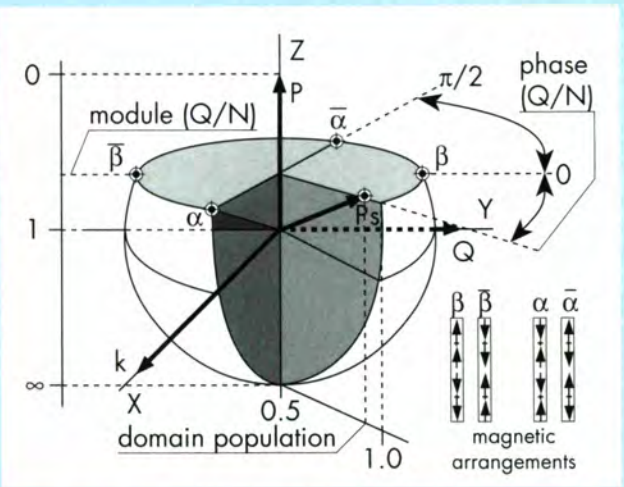

Fig. 2: ***Neutron Polarimetry on centric antiferromagnetic arrangements****: the measurement of the scattered polarisation vector* $\mathbf{P}_f$ *from mixed magnetic nuclear reflections gives information on the ratios* **Q/N**, *including the phase, and on the magnetic domain populations (see text). The four basic arrangements shown in the box produce pure rotations and the corresponding final polarisation tips are indexed on the sphere. Only the incoherent superposition of domains can produce a reduced polarisation* **Ps**.

in α are in phase with nuclear ones, in β they are in quadrature. In addition each structure has two 180° domains which we have shown as $\bar{\alpha}$ and $\bar{\beta}$.

Blume's Formula (3) is difficult to handle in its generality [10] but it is made easier to understand by studying its geometrical concequences in a particular case. Suppose that we have the initial polarization vertical, that we have put the 3-fold magnetic axis in the horizontal plane and that we are looking at a Bragg reflection in the same horizontal plane with CRYOPAD. From the scattered polarization vector $\mathbf{P}_s$, SNP can extract three pieces of information.

1) The length of the magnetic interaction vector in units of the nuclear amplitude is given by the residual z vertical component of polarization.

2) The phase of the magnetic interaction vector relative to the nuclear phase is given by the direction of the horizontal component. If it is in the direction of the scattering vector **k**, it indicates phase quadrature (ex: N is real Q is imaginary); if it is orthogonal to **k** (as **Q** is) then they are in phase.

3) Having a 180° domain simply reverses the direction of **Q**. Therefore the corresponding points α, $\bar{\alpha}$ and β, $\bar{\beta}$ corresponding to pairs of domains have the same z component and Π phases. For single domain scattering we expect no change in the initial polarization (assumed to be 100%), therefore the points lie on the unit sphere of final polarization vectors.

The existence of several domains in the sample will give an "incoherent" superposition of such scattering contributions. The z component of polarization, being the same for each domain, remains constant. On the other hand the horizontal components of the polarization vectors are not collinear, so that their weighted sum is reduced in length and the polarization tip moves toward the z axis. This true depolarization effect which affects only the horizontal components tells us about the proportion of 180° domains.

Using the UPA arrangement, only the z vertical component of polarization could have been collected, information 2) and 3) would be lost. SNP is thus the superior method.

Conclusion

The theory of Spherical Neutron Polarimetry has been given 30 years ago but, because of serious experimental difficulties, it has only been exploited lately in systematic neutron diffraction measurements. Therefore, magnetic neutron scattering was not exploited to its full potential, in particular for the determination of magnetic structures. By building the instrument CRYOPAD we could remedy this situation in the case of non magnetized samples in a strictly zero field. This allowed us to solve several difficult antiferromagnetic structures and to show the potential of the method. The measurement is of a superior nature because it gives the transverse components of the final polarisation which distinguish a true depolarisation from a simple rotation. But the zero field condition is central to the technique used and cannot be overcome easily. Therefore measurements on magnetized samples and those requiring an applied magnetic field will still rely on the classical Uniaxial Polarisation Analysis technique despite its other limitations.

Acknowledgments

The work described in this paper has been accomplished in collaboration with P. J. Brown, J. B. Forsyth and V. Nunez. For technical assistance we are greatly indebted to S. Pujol who built the CRYOPAD and J. Allibon who wrote the acquisition software.

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Liquids, Disordered Materials and Metal Physics

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Although 1993 represents another year without neutrons at ILL the strong support from colleagues at other neutron scattering centres and institutes has enabled college scientists to continue and diversify their respective lines of research as witnessed by the interesting range of results highlighted below. Towards the end of the year the excitement of the approaching reactor start-up began to be felt as preparations continued to prepare the instruments. We look forward to a successful 1994.

Low frequency excitations in glasses

The origin of the Boson peak, which appears in amorphous systems as an inelastic excess intensity (around 0.1-5 meV) over the calculated Debye contribution, is not well understood theoretically. Attempts at elucidating its origin have been made by comparing the Boson peak as measured on polymer glasses with different microstructure which differ by the mobility of their melt. The Boson peak is shown in Fig.1 at temperatures far below T_g for several amorphous polymers and is compared to trans-1,4-polybutadiene, a highly crystalline polymer, which does not show the excess intensity.

The interesting aspect of this comparison is the fact that the Boson peak position shifts towards lower frequencies, when passing from sterically hindered polymers, like poly(isobutylene), towards very flexible polymers, like poly(dimethylsiloxane) or poly(vinylchloride). The peak position is plotted in Fig 2 as a function of the monomeric friction coefficient (deduced from shear viscosity) and shows a clear correlation between a diffusional property above T_g and a vibrational property below T_g. As a reminder we note that neutron spin echo experiments on very different glass formers had clearly shown that the observed microscopic relaxation above T_g follows the same temperature dependence as the friction coefficient, which has been deduced from the macroscopically measured shear viscosity. The Boson peak is attributed to vibrational or librational modes in the disordered system and in consequence it is proposed that the mobility of molecular units above T_g determines how the system is frozen or

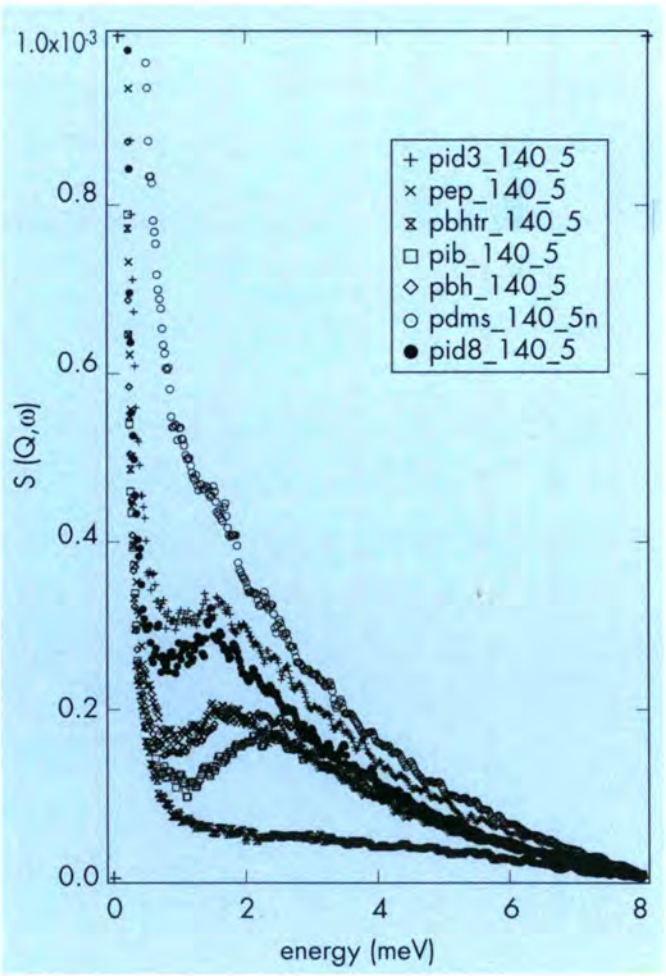

Fig. 1: Boson peak of several polymer glasses with different mobility measured on IN6. The crystalline polymer trans-polybutadiene does not show this excitation.

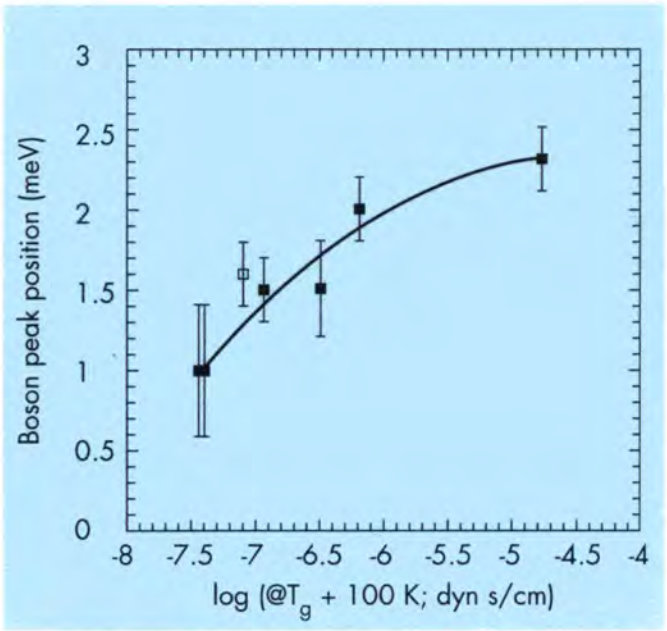

Fig. 2: Energy for the Boson peak maximum as a function of the monomeric friction coefficient at T_g = 100 K. Obviously a higher friction coefficient is related to a higher energy for the peak maximum.

trapped within the metastable states of the complex energy landscape of the glass. Another known experimental result, namely the fact that network glasses exhibit the Boson peak at even higher energies fits nicely into this picture.

Recently it has been proposed that phonon assisted tunnelling should be the origin of the Boson peak. Kanya and co-workers have compared model calculations for tunnelling within an asymmetric two level potential with measurements on poly (isobutylene) (-[CH_2-$C(CH_3)_2$]-). They attributed the observed excess intensity to tunnelling and found an inelastic form factor which reaches a maximum just at the limit of the experimental Q-range. The aim of experiments on polyisobutylene carried out at the thermal triple axis instrument BT4 at NIST [1], was to extend the Q-range above 6 Å^{-1}, where for the proposed parameters a maximum of the inelastic form factor and a further minimum should be observed. Several temperatures and two different sample thicknesses gave the result that the inelastic intensity can well be explained by vibrational properties only. The inelastic intensity, corrected for Bose occupation factor and the Debye Waller factor deduced from the elastic scattering, follows nicely a Q^2-dependence for all temperatures as shown in Fig. 3 and thus contradicts the proposed tunnelling model as origin.

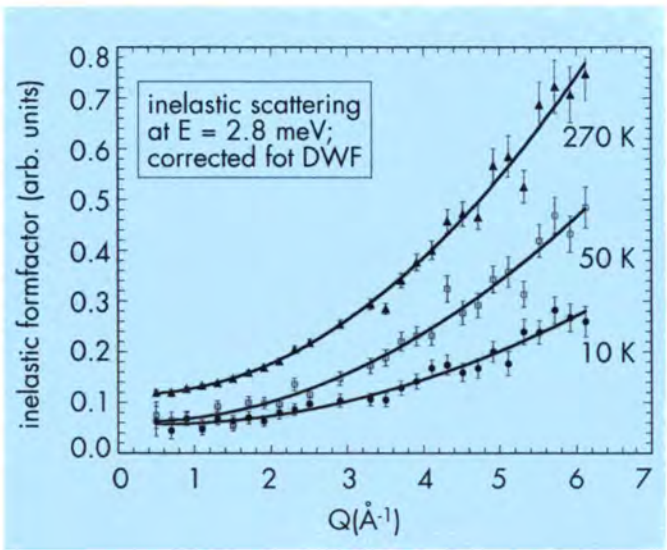

Fig. 3: Inelastic form factor of the Boson peak for polyisobutylene corrected for the Debye-Waller factor as deduced from the elastic scattering. The solid line shows a Q^2-dependent fit to the data as expected for vibrations.

Glass transition dynamics

J. Wuttke and W. Petry continued their investigations into the glass transition dynamics of simple organic liquids in collaboration with F. Fujara and H. Sillescu (Univ. Mainz). As a model case which is intermediate between fragile molecular systems and strong network glass formers,

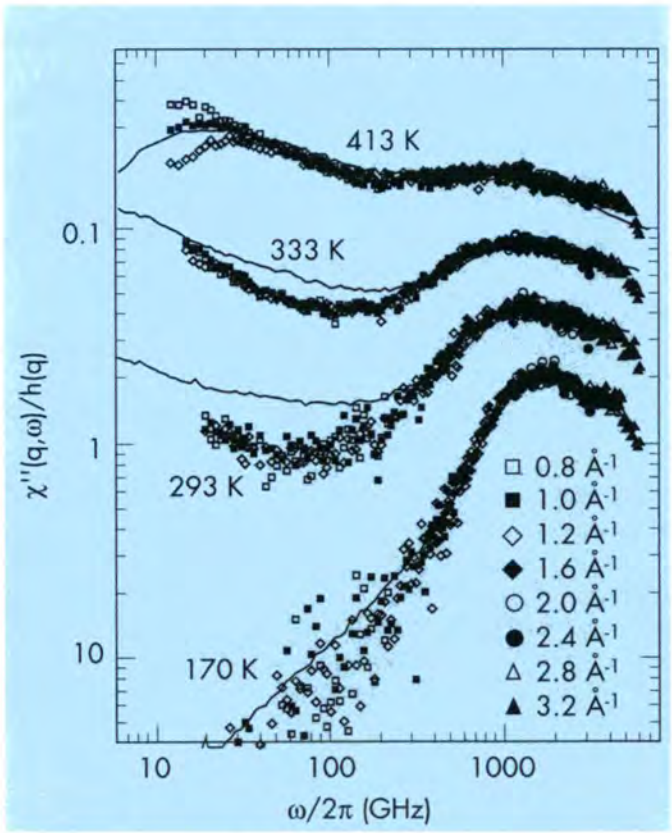

Fig. 4: Susceptibility $\chi_N''(\omega) = \omega S(q\omega)$ of neutron scattering, divided by a factor $h_N(q)$ in order to show the (q,ω)-factorization property of both the Boson peak and the intermediate β-relaxation region. Light scattering (continuous lines) shows essentially the same dynamic regimes, even if there are some obvious quantitative differences.

the associated liquid glycerol was studied by two complementary techniques, incoherent neutron scattering and depolarized light scattering. Neutron scattering experiments on $C_3H_5(OD)_3$ were performed with G. Coddens at the Mibémol time-of-flight spectrometer at Saclay; light scattering in normal glycerol was measured with J. Hernandez, G. Li, and H. Cummins at the City College of New York.

In the susceptibilities $\chi''_{N,L}(q\omega) = \omega S_{N,L}(q\omega)$, two maxima can be attributed to structural relaxation (α-peak) and to excess phonon scattering (boson-peak). Both present characteristics that are known from many other glass forming materials. In addition, there is a smooth, non-trivial contribution filling the gap between both peaks which resembles the anharmonic localized motion (fast β-process) observed previously in fragile liquids and described by mode coupling theory (MCT). In this region (as well as for the harmonic excitations in the Boson peak) the spectral shape of the neutron scattering susceptibility $\chi''_N(\omega) = \chi''_N(q\omega)/\hbar_N(q)$ is independent of q (Fig. 4).

This property makes it possible to compare $\chi''_N(\omega)$ directly to the susceptibility $\chi''_L(\omega) = \chi''_L(q\omega)/\hbar_L$ of light scattering measured at a much smaller q (4.10^{-3} Å^{-1}). Over the full range, both methods probe the same dynamics. Even in the q-dependent α-relaxation regime the curves coincide, indicating that depolarized (2nd order) light scattering couples to particle motion on a molecular length scale. Further experiments are needed to decide whether quantitative differences between both data sets are physical.

In the temperature range 270-413 K, scaling behaviour is found over three decades in frequency around the minima of $\chi(\omega)$ (Fig. 5). The master curve, however, does not follow the predictions of MCT (the asymptotic slope of the high frequency wing should be smaller than 1/2, and it should be smaller than the negative slope of the low frequency limit). The scaling of MCT, if at all, holds in a considerably smaller frequency window where scaling extends down to 243 K. The deviations at low frequencies suggest that the influence of vibrational motion and possibly of bond-breaking processes is much stronger in network glass-formers than in fragile materials.

Collective dynamics in mixtures of liquid Rb and molten RbBr

Mixtures of simple liquid metals and their molten salts are a very interesting class of liquids also from the point of view of their atomic dynamics, as the interplay of optic and acoustic modes in the salt rich mixtures should lead to an extinction of acoustic modes in a well defined region of momentum transfers. In addition they offer the possibility to change the interatomic interaction from a predominantly metallic one on the metal rich side of the phase diagram to dominating ionic interaction at medium and high salt concentrations. Measurements of the partial static structure factors indicate that this transition from nearly free electron behaviour to first influences from charge ordering starts to be observable already at a salt concentration of 20 mole%, i.e. a concentration of only 10 mole% of the non-metallic ions.

The collective atomic dynamics in a mixture of 80% Rb and 20% RbBr was therefore studied at two different temperatures well above the liquidus of the mixture using the cold neutron TOF spectrometer IN6 with an energy of the incident neutrons of 4.7 meV [2]. In contrast to liquid Rb, where collective excitations are observed as maxima and shoulders in the dynamic structure factor S(Q,ω), no such structure is evident in S(Q,ω) of the mixture at both temperatures, in complete agreement with earlier investigations of ionic melts. However, from the maxima of the longitudinal current-current correlation function $J_l(Q,\omega)$

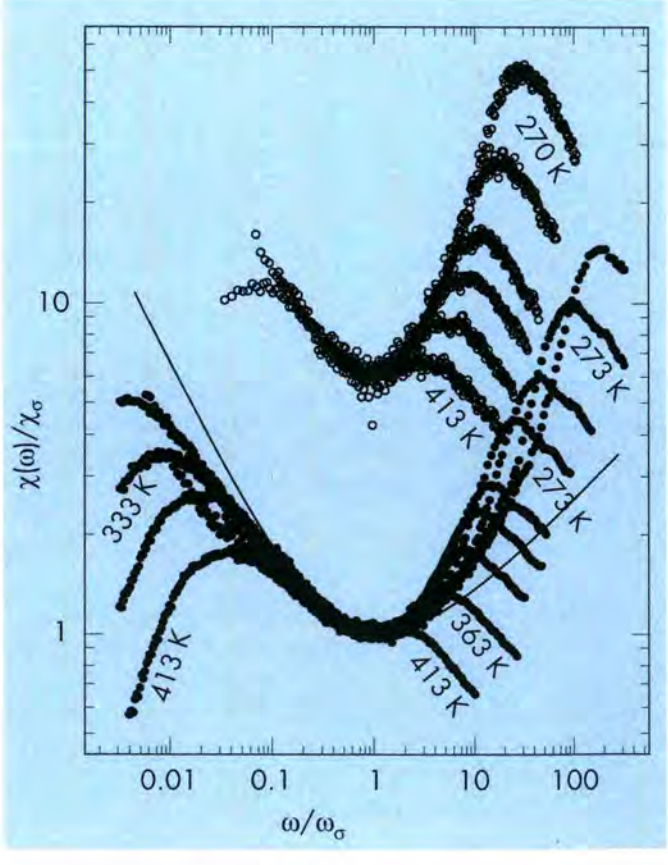

Fig. 5: Rescaled susceptibilities $\chi''(\omega/\omega_{min})/\chi_{min}$; neutron (top) and light (bottom) scattering data are separated vertically for clarity. There is a wide scaling regime for temperatures from 270 to 413 K, extending over three decades. If lower temperatures (243-263 K) are included, the scaling loses accuracy, except in a narrow range of not more than one decade where it can be fitted with the master function of MCT ($\lambda = 0.72$).

dispersions were obtained. In Fig. 6 the dispersion of liquid Rb measured at 776K and obtained in the same manner is compared with the dispersions of the mixture measured at 966K and 1160K.

The collective dynamics of the atoms in a mixture of 80 mole% liquid Rb with 20 mole% molten RbBr as far as reflected in the maxima of the longitudinal current correlation function lead to dispersion $\omega_J(Q)$ with two minima in the region of momentum transfers investigated ($10 \leq Q \leq 30$ nm^{-1}). The position of the first at Q_{min} can be simply related to the principal peak at Q_p in the static structure factor and even partly reflects its extension in Q-space. The second minimum can be related to the second maximum in $S_{MX}(Q)$. It could therefore reflect the influence of a change in the interatomic potential due to a change in the screening mechanism after adding 20 mole% salt to the liquid metal. At the higher Q-values covered here, the free particle dispersion starts dominating the dispersion curve.

Local order in polyatomic and complex systems

Disordered systems of increasing complexity might still present clearly identifiable local atomic arrangements. Although isotopic marking of a reference atom is a very attractive and efficient method to access the local structure in such systems, many other approaches have been successfully tried, giving insight into the local and medium range ordering. Combination of neutron and X-ray scattering, isomorphous, chemical and isotopic substitution, concentration dependence and temperature variation (liquid, undercooled liquid, glass) are used in the following studies which are characteristic examples of recent developments in this field. Of course, this is also an area where further progress is expected from the use of simulation to test various models of local and medium range order.

The total structure factor S(Q) of liquid $LiNbO_3$ has been obtained in a temperature range 1623K > T > 1490 K which includes undercooling [3]. From an analysis of the total pair correlation function G(r) compared with the results of an X-ray scattering experiment as well as with the crystalline structure, it has been possible to extract with precision the nearest neighbour distances $r_{Nb\text{-}O}$, $r_{O\text{-}O}$, $r_{Li\text{-}O}$ and the corresponding coordination numbers. The Nb atoms remain octahedrally coordinated up to one hundred degrees above the melting point. Interconnection of these octahedra by corner-sharing and tightening of their arrangement via Li atoms with a small coordination number ($n_{Li\text{-}O} \sim 3$), is also shown. At this local order level, no clear explanation is found of the large density difference observed between liquid and solid $LiNbO_3$.

A systematic investigation of liquid aluminium-transition metal alloys $Al_{80}M_{20}$, via isomorphous substitution, has allowed us to find some indications of local icosahedral order in the number-number structure factor S_{NN} of quasicrystal forming liquids, which were absent in other liquids such as $Al_{80}Ni_{20}$. These indications are the existence

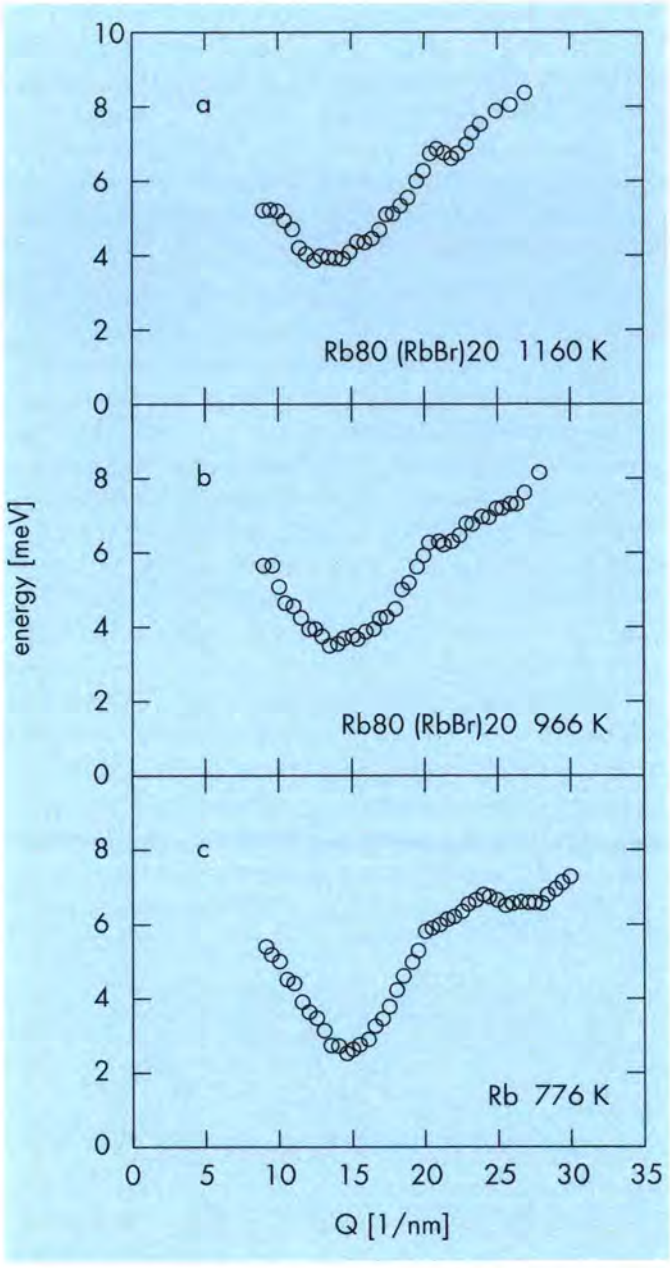

Fig. 6: Dispersion relation $\omega_J(Q)$ as obtained from the maxima in the longitudinal current correlation function $J_l(Q,\omega) = \omega^2 S(Q,\omega)/Q^2$ for $Rb_{80}(RbBr)_{20}$ measured at 1160K (a), 966K (b) and Rb measured at 776K (c). Compared with Rb one clearly sees the influence of the change in the interaction potential (harder and 2nd minimum at 22 nm^{-1}) and of the broader static structure factor on the dispersion curves of the mixtures.

of a sharp first peak, the shape of the second peak, which tends to form a double component peak at positions 1.7 Q_1 and 2 Q_1 (Q_1 being the first peak position) and the height ratio between the two first peaks close to the value of 0.49 given by a Landau description of icosahedral order. The construction of Voronoï polyhedra in quasicrystal forming $Al_{80}M_{20}$ liquids simulated by molecular dynamics has confirmed this point of view, but the percentage of atoms

with complete icosahedral symmetry is limited to a few percent. A study of the quasicrystal forming liquid alloy $Al_{71}Pd_{19}M_{10}$ with M = $Mn_y(FeCr)_{1-y}$ was undertaken using the isomorphous substitution between Mn atoms and the σ-FeCr mixture to confirm these results. The three partials of a pseudo-binary representation of this system (Al and Pd being nearly equivalent) were obtained. The S_{NN} itself was directly measured for the case y = 0.254, and it superimposes very well in reduced Q/Q1 coordinates on the S_{NN} of liquid $Al_{80}Mn_{20}$ in which icosahedral order had been seen by molecular dynamics [4] (Fig. 7).

Numerous studies on vitreous solid electrolytes have shown that it is possible to increase significantly the ionic conductivity of these glasses by addition of a doping agent (e.g. AgX) in a weak ionic conductor (e.g. $AgPO_3$). Several models have been proposed to describe the role of the added halides in the conductivity mechanism, but microscopic investigations were lacking. Since it is impossible to extract the full set of partial structure factors in such quaternary atomic systems, an extensive set of determinations of the total structure factor have instead been undertaken, varying the nature of the halide (Cl, Br, I), the AgX concentration and the Cl isotopic concentration for an AgCl mixture (^{35}Cl, $^{35,5}Cl$, ^{36}Cl, ^{37}Cl). In all cases, the $AgPO_3$ structure is unaffected by the addition of AgX and the system can be considered as biphased. This is so true, that the fraction of $AgPO_3$ structure could be subtracted from the total structure factor, giving access to the remaining AgX pattern. Moreover, the low Q range of the structure ($0.2 < Q < 2$ Å^{-1}) is very sensitive to the nature of the X nucleus, its isotopic enrichment and to the AgX concentration. A detailed study done for five AgI concentrations shows that the prepeak observed between 1 and 0.5 Å^{-1} has a position which decreases linearly versus the increasing volumic fraction in AgI suggesting a structure with nanoaggregates of AgI of increasing size embedded in a $AgPO_3$ matrix [5].

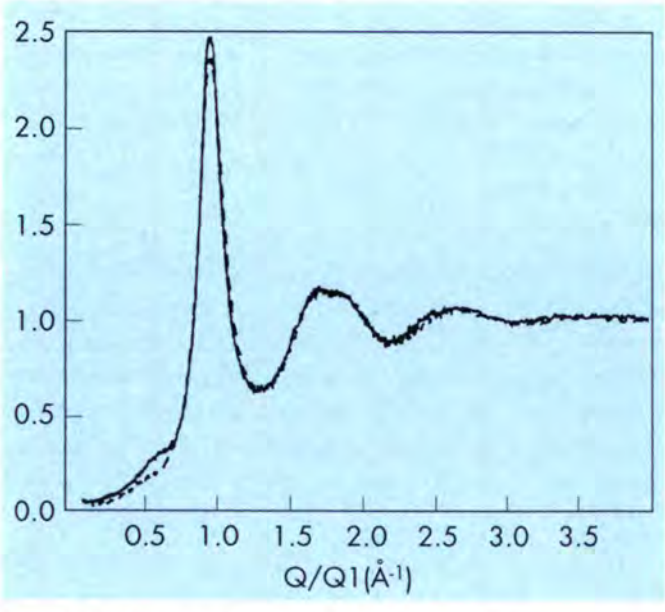

Fig. 7: Total structure factor S(Q) for liquid $Al_{71}Pd_{19}[Mn_{0.254}(FeCr)_{0.746}]_{10}$ (continuous curve) and $S_{NN}(Q)$ function for liquid $Al_{80}Mn_{20}$ (broken curve) as a function of Q/Q_1.

As mode coupling theory of the glass transition which predicts dynamical anomalies close to a critical temperature T_c located above T_g, is expected to work better the more "fragile" the glass former, OTP (orthoterphenyl) was considered to be a proper model system with relatively symmetrical and rigid molecules. This has led to a series of experiments and to the proof of the existence of T_c at about 290 K in this system. However, nothing was known about the structure of OTP, although the structure factor S(Q) is of the utmost importance for the interpretation of the dynamical behaviour as it is assumed that S(Q) varies smoothly in the temperature range where dynamical anomalies are observed. Studying the temperature dependence of the static stucture factor of OTP we find that in contrast to what is known from simple liquids, the main peak of S(Q) is split into two maxima which behave quite differently. Supercooling the system down to T_g, the maximum at Q = 1.4 Å^{-1} is not much affected, while the one at 1.9 Å^{-1} is significantly enhanced. This effect cannot be related to a change of intramolecular configurations (the intramolecular structure playing a role at larger Q values and being apparently unaffected by temperature variation) but is due to the intermolecular structure. However, it varies smoothly, with no discontinuity around T_c. The physical origin of this temperature dependence of S(Q) and its effect on the Q dependence of the dynamics around T_c are being investigated [6].

The investigations into the structure and dynamics of quasicrystals has continued with experiments using X-rays and neutrons (see Blue Box). In particular the anomalous X-ray diffraction close to the Pd K-edge has enabled the determination of the Pd partial structure factor. The results contradict the idea that atomic surfaces in the 6-dimensional images should be sharply faceted polyhedral objects. Recent theoretical results suggest that the atomic surfaces might have fractally shaped borders.

Collective Excitations in ^{4}He

The dynamic structure factor S(Q,ω) in the collective excitation regime of liquid ^{4}He has been measured over a wide range of temperature and wavevector on IN6 [7]. The results summarised in Fig. 8 show the variation of the scattering function with temperature at wavevectors of 0.4Å^{-1}(phonon), 1.2Å^{-1} (maxon) and 1.9Å^{-1} (roton). Note that for clarity the data used to produce these figures have been smoothed so they provide only a qualitative illustration of the temperature variation of the scattering. The temperature dependence in the low Q region appears simple. The scattering consists of a single, sharp peak which broadens with temperature; the multiphonon component

is relatively weak and well separated from the single excitation peak. The rate of broadening of the one-phonon peak appears to change at or near to the lambda transition temperature, T_λ, but a well defined peak remains visible in the normal fluid phase. At the maxon wavevector, the low temperature scattering function is seen to consist of a sharp peak superimposed on a broad multiphonon background, which changes little with temperature. The sharp peak however, is seen to disappear at T_λ, suggesting that it is in some way a "signature" of the superfluid phase, connected with the existence of the Bose condensate. The situation is similar at the roton wavevector. Here the sharp peak is also seen to disappear at T_λ and the scattering in the normal phase is peaked at an energy (of the order of 0.5 meV) lower than that of the sharp peak characteristic of the superfluid (0.74 meV at T=1.3 K). At all wavevectors the high-energy tail of $S(Q,\omega)$ is observed to change very little with temperature. In general the variation of $S(Q,\omega)$ with temperature is very marked in the superfluid phase but almost non-existent in the normal fluid, particularly at high Q. The overall wavevector dependent temperature variation of the excitation spectrum provides support for recent theories in which the linear dispersion part of the spectrum is seen as consisting mainly of a zero sound mode, similar to that observed in Fermi liquids, while the maxon and roton excitations arise from the excitation of a single quasiparticle. The single particle excitations are coupled to the density fluctuations by the presence of a non-zero Bose condensate. They thus establish the connection between the Bose broken symmetry and the sharp one-phonon excitations seen in the superfluid phase.

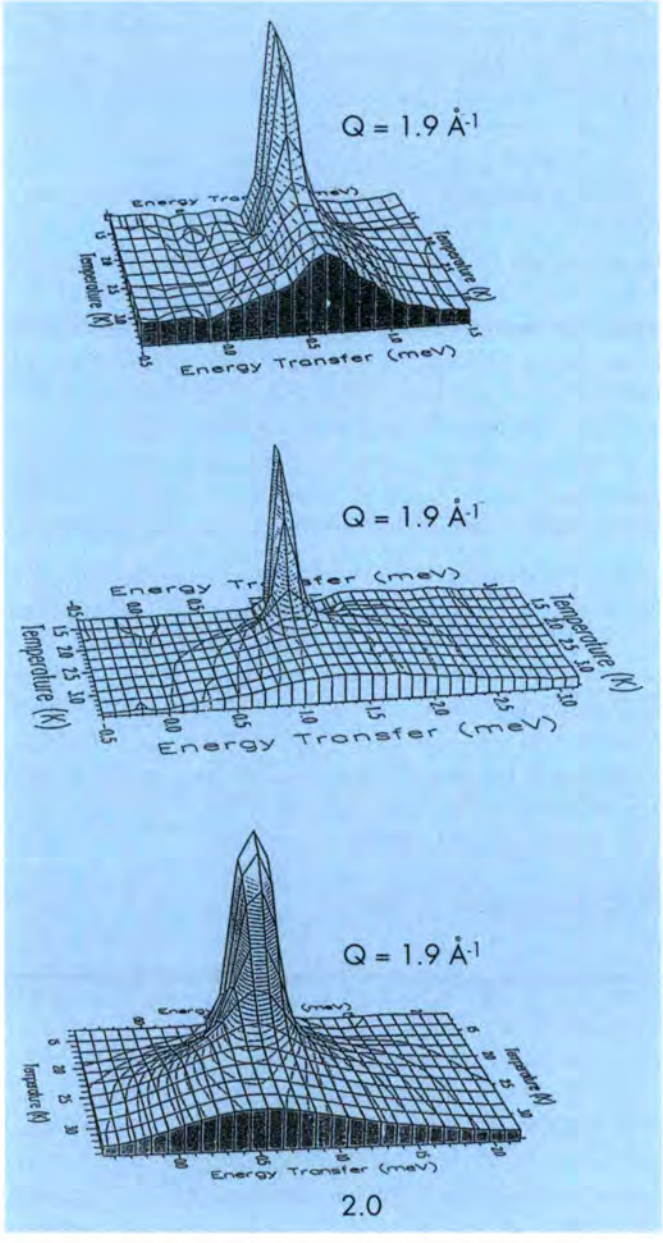

Fig. 8: Figure 1. Three dimensional representation of the temperature dependence of $S(Q,\omega)$ for ^{4}He at Q=0.4 Å^{-1}, 1.2 Å^{-1} and 1.9 Å^{-1}.

The surface dynamics has also been measured from liquid ^{4}He films adsorbed onto graphite (see Blue Box college 2). The data show evidence of layer phonons that propagate within the liquid layer in good agreement with theory.

Investigation of rough interfaces in multilayers by specular and non-specular X-ray reflection

Interface and surface roughness is of crucial importance in thin layer physics and is a decisive factor for their technological applicability. It strongly influences the physical properties of multilayers such as the quantum efficiency of semiconductor superlattices and the magnetic coupling in magnetic multilayers.

X-ray scattering methods are non destructive and allow a statistical description of interfaces. The point properties of the interfaces (r.m.s. roughness) can be investigated by specular X-ray reflection (SXR). Using non-specular X-ray reflection (NSXR) the in-plane correlation (lateral correlation length, fractal dimension of the interface) can be determined.

Both X-ray methods have recently been used successfully to study single surfaces. Yet NSXR has rarely been applied to multilayers, as important features present in the experimental data obtained from multilayers could not be explained theoretically. The previous theoretical description only included the effect of specular surface reflection without taking into account the specular reflection at the interfaces.

Describing the specular interface reflection within the full dynamical theory, a formalism based on a Distorted-Wave-Born-Approximation (DWBA) was developed, which overcomes the problems of previous work [8]. Considering now the specular reflection from the surface

as well as from the interfaces we are able to simulate the coherent and incoherent cross sections of diffuse scattering from multilayers with rough interfaces including:

1) the interaction between specular interface reflection and diffuse scattering (generating Bragg-like peaks in the Non-Specular X-Ray Reflection),

2) the effect of resonant diffuse scattering (RDS) in vertical partial correlated superlattices. (Thus we can distinguish between vertical non-correlated and correlated interface roughness),

3) the contribution of diffuse scattering in transmission geometry, observable above the surface only due to Umweganregung caused by specular interface reflection.

We demonstrate the effect of partially vertical correlated interface roughness for the example of a GaAs/AlAs-superlattice in Fig. 9 showing the calculated reciprocal space mapping of the primary diffuse scattering in the kinematical approximation (Fig. 9a) and in a DWBA, considering the reflection at the surface and the refraction within the layers (Fig. 9b).

In the kinematical approach the diffuse scattered intensity of partial vertical correlated interfaces is concentrated in strips of resonant diffuse scattering (RDS), being parallel to the sample surface and going through the lattice points of the one dimensional reciprocal lattice of the multilayer. Limited by the geometrical horizon of the sample the measured intensity would be restricted between the Ewald spheres ε_1 and ε_2 which mark where the incident or exit angles become zero.

Considering simultaneous specular reflecting from the sample surface and the refraction of X-rays in the layers in the calculation gives rise to:

1) a bending of the RDS sheets due to the X-ray refraction,

2) an enhancement of intensity at the critical angle of total external reflection for the incident or scattered beam, creating the so called Yoneda wings.

The specular interface reflection causes additional sharp resonances in the distribution of diffusely scattered intensity, if the incident or the scattered beam fulfills the Bragg condition of the superlattice (Bragg-like peaks). Their positions in the reciprocal space are marked by crosses in Fig. 9b. The occurrence of the Bragg-like peaks is a pure dynamical effect of multiple scattering and can be understood by the concept of Umweganregung [9]. They are described within an extended DWBA as can be seen in Fig. 10 which shows the experimental and the fitted NSXR rocking scans of a GaAs/AlAs superlattice.

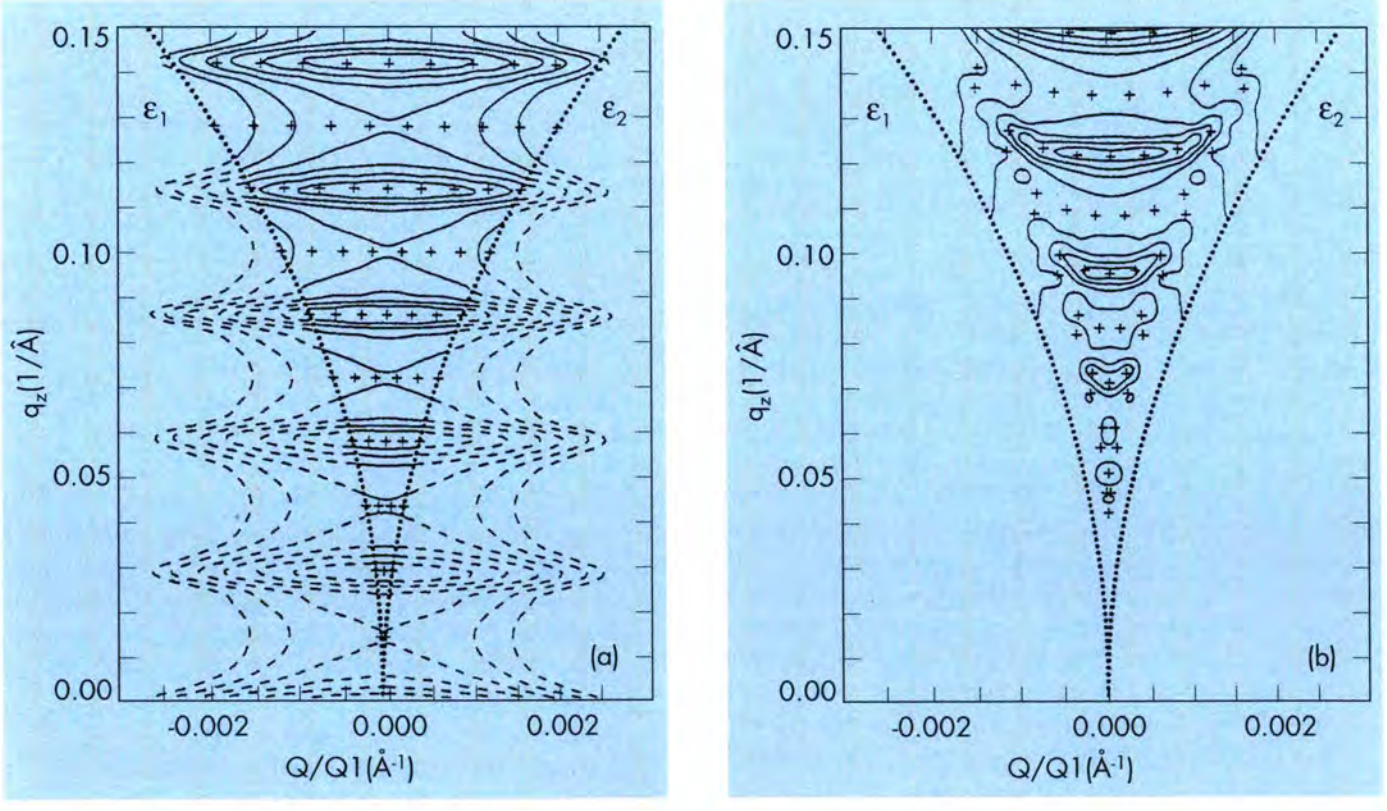

Fig. 9: Non-specular intensity distribution in the reciprocal plane for the case of vertical partial correlated interface roughness;
a) calculation within the first Born approximation without X-ray refraction
b) calculation within a DWBA taking into account the specular X-ray reflection from the surface and refraction in the layers.
The dotted lines represent the Ewald circles $\varepsilon_{1,2}$. The NSXR intensity in the inaccessible regions is denoted by dashed lines. Crosses denote the positions of the Bragg-like peaks, neglected in this approximation but considered in Fig. 10

The broad central hump arises from resonant diffuse scattering (RDS) and gives evidence of the existence of vertical correlation between the rough interfaces. In addition, two Yoneda wings may be seen on each side of the central peak with several Bragg-like peaks between them, well described by the theory.

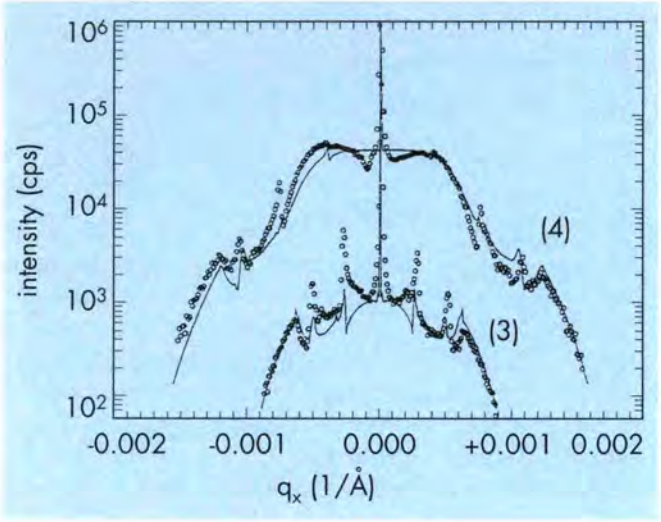

Fig. 10: ω scans (points) measured along the trajectories going through the 3rd (line (3)) and the 4th Bragg peaks (line (4)). Line (4) is shifted upwards by a factor of 10. The lines are the best theoretical fits from our extended DWBA, which describes also the Bragg-like peaks.

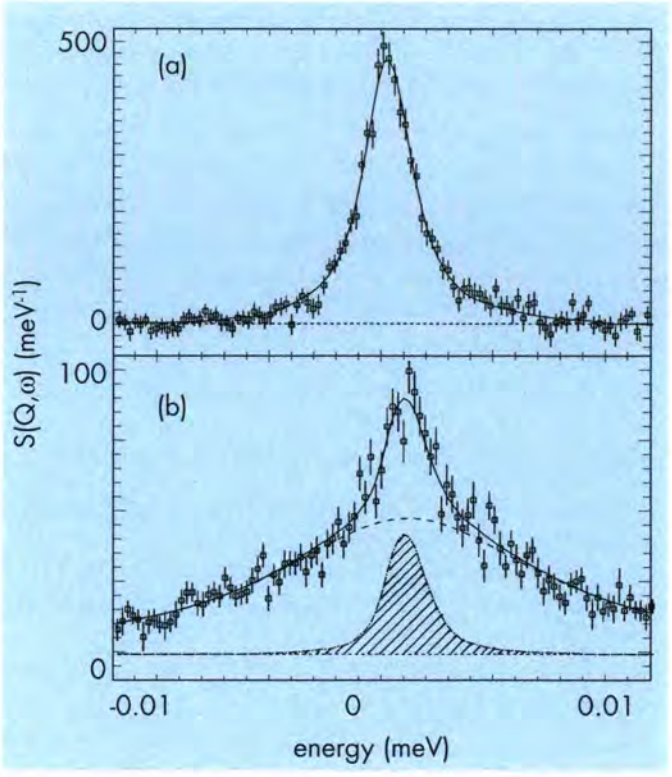

Fig. 11: Quasielastic neutron scattering spectra for a $Ni_{72.5}Sb_{27.5}$ crystal in one specific crystal orientation at Q values of (a) 0.41 Å^{-1} and (b) 1.82 Å^{-1}. T = 800°C.

The theoretical treatment also allows the description of specular and non-specular reflection of neutrons by rough multilayers.

Self-diffusion in intermetallics

The Ni diffusion mechanism in the intermetallic alloys NiSb and Ni_3Sb has been elucidated by QNS measurements on single crystals, performed on IN10. In the B8 phase NiSb the Ni atoms perform jumps between the regular Ni sites (octahedral interstices of the hcp lattice made up by the Sb atoms) and the double tetrahedral interstices (DTI), which are very scarcely populated. The experiments on the DO_3 phase Ni_3Sb [10] necessitated a more sophisticated sample environment, as the alloy studied is stable above 530° C only. Therefore, the single crystals had to be grown in a special in-situ growth furnace, oriented on IN3, and then transported to IN10 without cooling down the furnace. Due to the shutdown of the ILL reactor, these results are preliminary, but the data seem to agree with a very simple jump model: nearest-neighbour jumps of the Ni atoms between the two Ni sublattices. The same mechanism had been found to be operative in the DO_3 phase Fe_3Si by Mössbauer spectroscopy. The Ni diffusivity in Ni_3Sb is very high, leading to very pronounced quasielastic broadening even at moderate temperatures (Fig. 11)and facilitating the separation of the QNS signal into two Lorentzians.

The systems Ni_3Sb and Fe_3Si have also been investigated by neutron diffraction on DMC at the PSI [11] as a function of the alloy concentration and temperature. It has been shown that deviations from stoichiometry are compensated in very different ways in the two alloys of the same structure: whereas in Fe_3Si antistructure atoms of Fe on Si sites are formed, Ni_3Sb compensates the excess of Sb by vacancies on the Ni sublattices.

The phonon dispersion of Fe_3Si alloys (Fig. 12) has been studied on 1-T at LLB [12] in order to decide if the fast Fe diffusion in these alloys is related to soft modes. Although there are low-energetic modes and a very distinct softening of the lattice at high temperatures, there is almost no dependence of the phonon energy on the alloy concentration. Mössbauer studies have indicated that the Fe diffusivity in Fe_3Si is strongly dependent on the alloy concentration, thus the observed fast diffusion cannot be explained by lattice dynamical effects alone.

High temperature lattice dynamics and diffusion in niobium

Recently a close relation was established between particular low energy phonons and high diffusion coefficients in cubic metals. Due to the temperature (T) dependence of phonons in metals the diffusion barriers are

no longer constants, but sensitively depend on T. For instance in bcc-Zr phonons stiffen with increasing T and consequently the migration barrier for vacancy diffusion increases with T. Cr shows the opposite behaviour. Here migration barriers are high at low T and no anomalously low phonons are found, whereas migration barrier and phonons are low at high T. The d-electron density is supposed to be the control parameter. Nb with 3d electrons lies between Zr and Cr and therefore should show an intermediate behaviour.

To prove this the phonon dispersion has been measured at 293K, 773K, 1773K and 2223K (measurements at IN3 ILL, 1T Saclay, DN1 Siloe, HB1 Petten) [13]. Fig. 13 shows a summary of all dispersion measurements which are represented by the results of Born-von-Karman fits. A detailed inspection of this figure shows that (except L0.5(110)) Brillouin zone boundary phonons decrease continuously with T. Two important exceptions

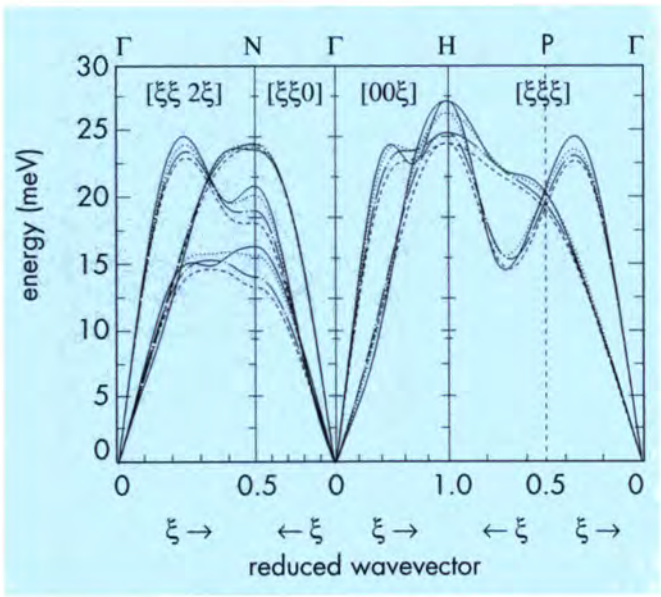

Fig. 13: Born-von-Karman fits of phonon dispersion in Nb at — 293K, - - - 773K, — · — 1773K and – – – 2223K.

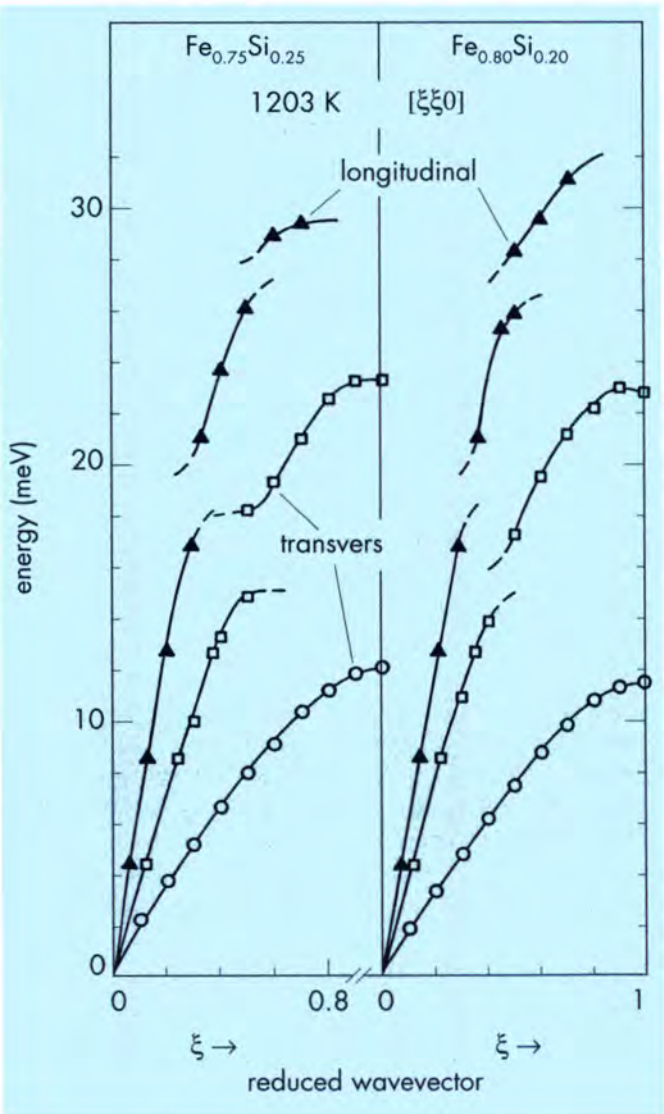

Fig. 12: A detail of the phonon dispersions of $Fe_{75}Si_{25}$ and $Fe_{80}Si_{20}$.

from this normal decrease have to be mentioned: the L2/3(111) phonon increases from 293K to 773K, stays at a plateau up to 1773K and decreases above 1773K. The shear constant C' qualitatively shows the same T dependence.

Due to the dominant role of these low energy phonons in the calculation of the migration barrier

$$H^M = \alpha (G^0)^{-1} a^2, \text{ with } G^0 = \int \frac{Z(\omega)}{M\omega^2} d\omega ,$$

(where G^0 is the static lattice Green's function, α a geometrical factor, a the lattice parameter, $Z(\omega)$ the density of states and M the mass) H^M shows a similar variation with T.

We conclude with the following picture of the diffusion anomalies in the group 4 to 6 metals: from bcc-Zr through Nb to Cr the d-electron density increases, the motion of [111] nearest neighbour rows in these metals is more and more hindered and consequently diffusivities decrease. This effect is particularly pronounced at low T, whereas close to the melting point diffusivities normalise to a common value.

Hydrogen in Metals

The rare-earth dihydrides β-RH_{2+x} form an fcc structure in which, ideally for x=0, the hydrogen occupies all of the tetrahedral (t) sites. In the superstoichiometric region, $0 < x < x_{max}$, the excess hydrogen occupies the octahedral (o) sites. Further addition of hydrogen above x_{max} leads to the precipitation of the hexagonal γ-RH_3 phase. In the dihydride phase the excess hydrogen gives rise to concentration dependent changes in the electronic structure which manifest themselves in metal-semiconductor transitions related to ordering of the octahedral H sublattice.

In particular β–TbH_{2+x} has been shown to possess several x-dependent magnetic ordering phases below ~40 K. At higher temperatures (150-200 K), neutron diffraction studies on TbD_{2+x} ($0 < x < 0.25$) have shown that the octahedral H orders for $x > 0.1$ into a Ni_3Mo structure in which 3 vacant (420) planes are followed by an occupied plane, a structure which is stoichiometric at $TbD_{2.25}$ [14].

The concentration and temperature dependence of the ordering phenomena have been followed using neutron diffraction and inelastic neutron scattering at NIST and PSI. Figure 14 shows the concentration dependence of the local mode due to octahedral site H in TbH_{2+x} measured at NIST using a Be/PG filter spectrometer. It is easy to distiguish the vibrational spectrum arising from H occupying t and o sites in these systems since the former occurs in the region near 120 meV while the latter is observed near 80 meV. At low concentration and low temperature a single relatively sharp vibration feature is observed centred at 80.5 meV due to isolated H in a cubic environment. As the concentration is increased the vibrational spectrum splits giving rise, at x=0.25, to a clearly bimodal structure with a higher energy peak at 83.1 meV having twice the intensity of the lower energy peak centred at 76.7 meV. A similar transition is seen as a function of temperature and can be clearly related to the ordering of octahedral H. In the fully ordered Ni_3Mo structure, each o site H is an intersecting member of identical chains $(\text{-H-Tb-})_n$ in the [100] and [001] directions and a $(\text{-H-Tb-v-Tb-})_n$ chain in the [010] direction where v represents a vacancy in the H sublattice. Thus the doubly degenerate high energy mode corresponds to vibrations in the [100] and [001] directions whereas the low energy singlet is due to vibrations in the [010] direction. The results show the importance of the H-H interactions in these systems which extend to at least second nearest neighbour distances [15].

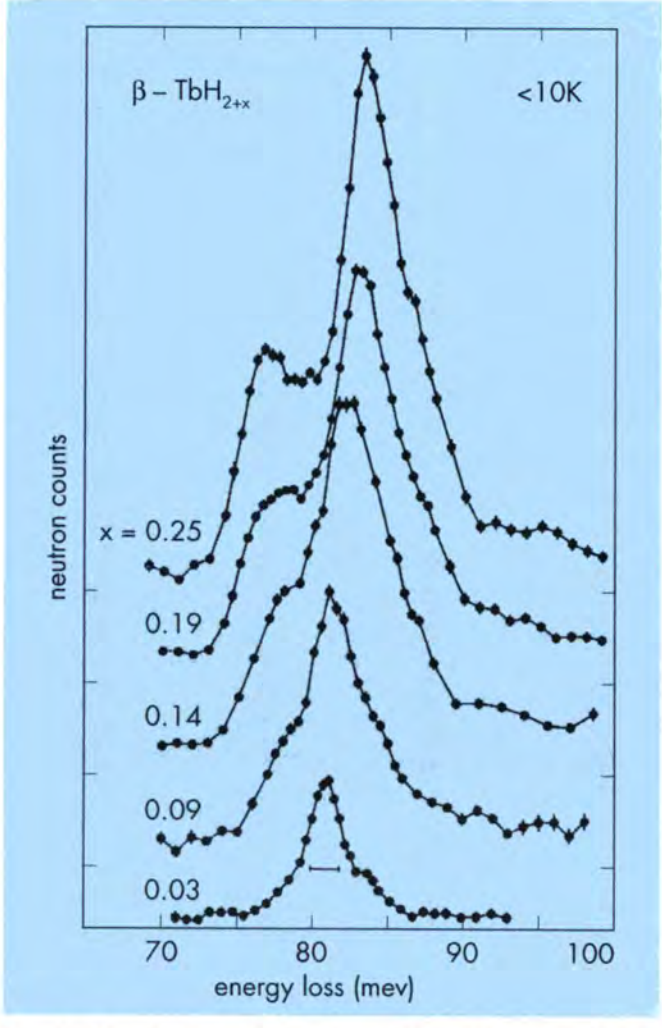

Fig. 14: The vibrational density of states due to H on octahedral sites in β-TbH_{2+x} for different values of x. The continuous lines are guides to the eye.

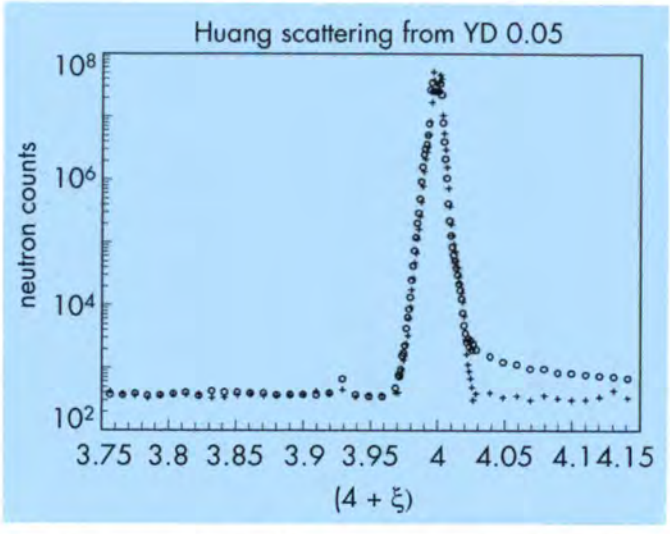

Fig. 15: Comparison of the Huang scattering in the (110) (001) plane of $YD_{0.05}$ (o) and pure Y (+). The scans were taken in the [-ξ,—ξ, 4+ξ] direction about the (004) reflection.

In a complementary study on the hexagonal α-$R(H/D)_x$ systems the neutron Huang scattering due to isolated D atoms has been measured in $YD_{0.05}$ in collaboration with K. Aizawa at JAERI [16]. The results shown in Fig. 15 indicate strongly asymmetric Huang scattering in particular directions which will enable the distortion field surrounding an isolated D atom to be determined and compared with ongoing μSR measurements on these systems.

Secretary: Ian Anderson

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Report on the Workshop "Dynamics of Disordered Materials II" held at the Institut Laue-Langevin, 22-24 March, 1993.

Following the success of the first workshop on "Dynamics of Disordered Materials" held in September 1988, a second meeting took place in Grenoble during March 1993 with the objective of reviewing the considerable progress made. The meeting was jointly organized by the Institut für Festkörperforschung of the Forschungszentrum Jülich and the Institut Laue-Langevin in Grenoble. The proceedings of the workshop will be published at the end of 1993 as a special issue of Physica A and will contain 13 review articles and 44 contributed papers, in both theory and experiments on disordered materials, addressing in particular the dynamics of glasses and the glass transition.

The main thrust of the workshop was directed towards an experimental evaluation of the mode coupling theory of the glass transition (MCT). In particular, scattering methods such as dynamic light scattering and neutron scattering experiments as well as computer simulations were presented in which the undercooled liquid strongly supports mode coupling predictions. Materials as different as polymers, molecular and ionic liquids, colloidal systems and liquid metals were investigated. While this general agreement seems to hold for fragile glasses, strong glasses like network glasses seem to be less well accounted for.

At lower temperatures in the close proximity of the glass transition the situation is less clear. Besides the high frequency "mode coupling" β-relaxation a slow relaxation intrinsically coupled to the α-relaxation is observed microscopically which cannot easily be interpreted by MCT. Another very important issue in this low temperature regime relates to the question of cooperativity close to T_g. Important new developments seem to give indirect evidence for the existence of such a cooperativity length which increases towards T_g. Furthermore, light scattering experiments have established the presence of large scale density fluctuations reaching into the micron regime.

Another important topic concerns the soft phonons in glasses. These were originally observed as a so-called Boson peak in Raman scattering and later on characterized in detail by inelastic neutron scattering. These soft phonons are an intrinsic ingredient of the glassy state and relate to structural instabilities. Considerable progress has been reported in this field, leading towards a unified understanding of these soft vibrations, including the low temperature two-level tunnelling excitations.

Besides this main theme, a series of other aspects of glasses were illuminated stretching from the dynamics of metglasses to biological systems dealing with phenomena such as the effect of confined geometries on water dynamics, the polymerization transition in sulphur or the concentration fluctuations in polymer blends.

The following invited lecturers presented a wide range of review talks covering all aspects of the workshop:

- A.J. Dianoux (Institut Laue-Langevin, Grenoble, France) "Neutron scattering by disordered materials: an introduction"
- M. Fuchs (T.U. München, Garching, Germany) "α-Peak shapes discussed within the mode coupling theory"
- H.R. Schober (IFF, Jülich, Germany) "Soft phonons in glasses"
- J. Colmenero (U. del Pais Vasco, San Sebastian, Spain) "Dynamics of the α-relaxation in glass-forming polymers. Study by neutron scattering and relaxation techniques"
- R. Zorn (IFF, Jülich, Germany) "Neutron scattering experiments on the glass transition of polymers"

• K. Kawasaki (Kyushu University, Fukuoku, Japan) "Relaxation and growth of concentration fluctuations in polymer blends"

• J.-P. Hansen (ENS, Lyon, France) "Kinetic glass transition in liquids and colloidal suspensions: what do we learn from molecular dynamics simulations ?"

• E.W. Fischer (MPI für Polymerforschung, Mainz, Germany) "Light scattering and dielectric studies on glass forming liquids"

• H.Z. Cummins (City College-CUNY, New York, USA) "Light scattering spectroscopy of the liquid-glass transition: Comparison with idealised and extended mode coupling theory predictions"

• F. Fujara (U. Mainz, Germany) "Signatures of the glass transition in van der Waals liquids seen by neutrons and NMR"

• E. Rössler (Freie Universität, Berlin, Germany) "Dynamical phase transition in supercooled simple liquids and polymers - a NMR approach"

• P.N. Pusey (U. of Edinburgh, U.K.) "The dynamics of amorphous states of colloidal systems"

• F. Parak (U. Mainz, Germany) "Protein dynamics"

• M. Descamps (U. Lille I, Villeneuve d'Ascq, France) "Orientational and structural relaxation in a glassy crystal"

Compared to the last workshop a richness of very detailed new quantitative results evolved facilitating a more quantitative comparison with model predictions. However, the complexity and in particular the enormous dynamic range accompanied by the missing translational symmetry still poses a tremendous challenge, which in the future should be met by concentrated efforts using as many experimental methods as possible on the same materials. Nevertheless, we hope that the proceedings of this workshop describing the present day situation will stimulate further work in this very interesting and exciting domain.

The organizers thank the contributors for preparing their manuscripts promptly. We express our gratitude to the Institut Laue-Langevin and the Forschungszentrum Jülich for their financial assistance. We would also like to acknowledge J.P. Hansen and H.Z. Cummins for their critical summary and are grateful to B. Maier and his staff who helped to organize the workshop, and to Mrs. Brigitte Aubert as the workshop secretary.

Grenoble, München, Jülich

Albert-José Dianoux,
Winfried Petry, Dieter Richter

Precise experimental determination of the structure of noble fluids: two- and many-body contributions

Fabrizio Barocchi, Pierre Chieux, Renato Magli

The structure of a fluid (liquid or gas) is considered to be known when the spatial distribution of the atoms in the system, at a precise time t, is known. In principle this can be accomplished only with the knowledge of all the irreducible spatial correlation functions involved in the system. However, theory and experiments, at present, can deal only with the simplest of these functions, i.e. the so called pair correlation function $g(r_{12})$.

Experiments give information on $g(r_{12})$ by means of measurements of the static structure factor S(k) which is related to the spatial Fourier transform of the pair correlation function as follows [1]:

$$S(k) = 1 + n \int [g(r_{12}) - 1] \exp(- i\mathbf{k} \cdot \mathbf{r}_{12}) d\mathbf{r}_{12} \qquad (1)$$

where n is the number density. S(k) can be measured by either X-ray or neutron diffraction, k is the wavevector transfer in the diffraction experiment and $\mathbf{r}_{12}$ is the distance vector between two atoms.

In the field of fluid structural studies the following statements about S(k) have often been accepted. (1) The behaviour of S(k) in dense fluids is dominated by strong microscopic repulsive forces present at short range, and only very small details of S(k) are connected to the peculiar properties of $g(r_{12})$. (2) S(k) cannot be measured in a wide enough k-range and with an accuracy no better than a few parts per hundred. As a consequence S(k) data in fluids are not very useful for detailed studies of $g(r_{12})$.

We will show that by means of a neutron diffractometer such as D4, S(k) can be obtained with a precision of a few parts per thousand [2]. Therefore precise tests of existing modern integral equation theories for $g(r_2)$ and investigations of the nature of microscopic interactions in fluids can be performed [3].

For studying structural properties in simple fluids, it is convenient to define the direct correlation function $c(r_{12})$ which is given by the Orstein-Zernike relation [1]:

$$g(r_{12}) - 1 = c(r_{12}) + n \int d^3 \mathbf{r}' \, c(r') \, [g|\mathbf{r}_{12} - \mathbf{r}'|) - 1] \qquad (2)$$

From equations (1) and (2) it is easy to see that for the Fourier transform c(k) of $c(r_{12})$ the following relation holds:

$$c(k) = [1 - S^{-1}(k)]/n. \qquad (3)$$

When the density of the fluid is sufficiently low, g(r) can be expanded with respect to the density n, this is the so called "virial expansion" and is given by

$$g(r_{12}) = g_o(r_{12}) + n g_1(r_{12}) + O(n^2) \quad (4)$$

where

$$g_o(r_{12}) = \exp[-\beta u_2(1, 2)] \text{ with } \beta = 1/k_B T \quad (5)$$

$$g_1(r_{12}) = g_1^{(2)}(r_{12}) + g_1^{(3)}(r_{12}) \quad (6)$$

$g_1^{(2)}(r_{12})$ indicates the part of $g_1(r_{12})$ that depends only on the two-body potential while $g_1^{(3)}(r_{12})$ depends also on the three-body potential and only the first two terms in equation (4) are retained.

From equations (1), (3) and (4), S(k) and c(k) can also be expanded. In particular we write,

$$c(k) = c_o(k) + n c_1(k) + O(n^2) \quad (7)$$

where

$$c_o(k) = \int [g_o(r_{12}) - 1] \exp(-i\mathbf{k} \cdot \mathbf{r}_{12}) d\mathbf{r}_{12} \quad (8)$$

$$c_1(k) = c_1^{(2)}(k) + c_1^{(3)}(k) \quad (9)$$

As a consequence it is seen that a measurement of the density behaviour of S(k) at low enough density gives access to the pair and three-body terms of c(k). The pair term $c_o(k)$ is directly related to the pair potential $u_2(r)$ and this last function can therefore simply be derived by means of a Fourier inversion of an experimental $c_o(k)$. Moreover, once the pair potential is known a measurement of $c_1(k)$ also gives the possibility of deriving information on the three-body potential $u_3(1,2,3)$.

For the case of dense fluids another approach is necessary. We may use the modified hypernetted chain expression (MHNC) to relate the interaction potentials to g(r), which writes [4],

$$g(r_{12}) = \exp[-\beta u_2(r_{12}) + g(r_{12}) - 1 - c(r_{12}) + C(r_{12}) + E(r_{12})] \quad (10)$$

$C(r_{12})$ is the dressed three-particle vertex:

$$C(r_{12}) = n \int d^3 \mathbf{r}_3 \, g(r_{13}) \, g(r_{23}) \{\exp[-\beta u_3(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_l)] - \quad (11)$$

and $E(r_{12})$ is the so called bridge function.

With some initial estimate of $E(r_{12})$ and a model for both the pair and three-body potentials, the MHNC equation can be solved iteratively and the calculated $g(r_{12})$ compared with the experimental one to check the validity of the model potentials and the precision of the integral equation as well.

Recent measurements of the static structure factor in fluid noble gas have been performed with a very high statistical accuracy, even at low gas density. Rigorous data analysis procedure has made it possible to reach a final precision in S(k) sufficient for the density expansion studies of c(k).

Argon at low density

S(k) was measured in ^{36}Ar at T = 140 K and at four densities, i.e. n = 0.902, 1.399, 1.900, 2.393 at.nm^{-3} (the density of the liquid at the triple point is n = 21.15 at.nm^{-3}). Fig. 1 shows as an example the experimental c(k), for one thermodynamic state obtained on the D4 instrument [2].

Figure 2 shows the experimental density behaviour of c(k) [5]. The linearity predicted by the virial expansion of equation (7) for a low-density gas is very well

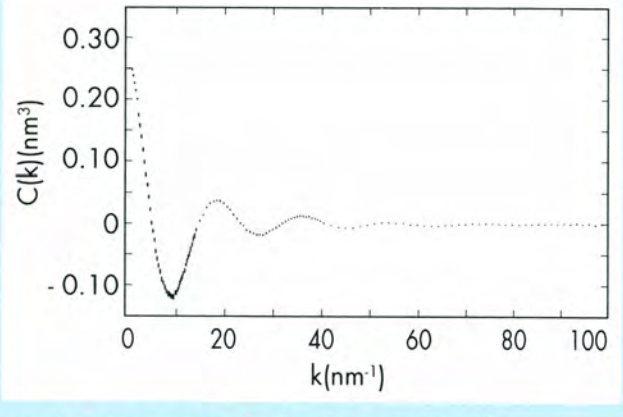

Fig. 1: c(k) at n = 0.9 at/nm^3 and T = 140 K for ^{36}Ar.

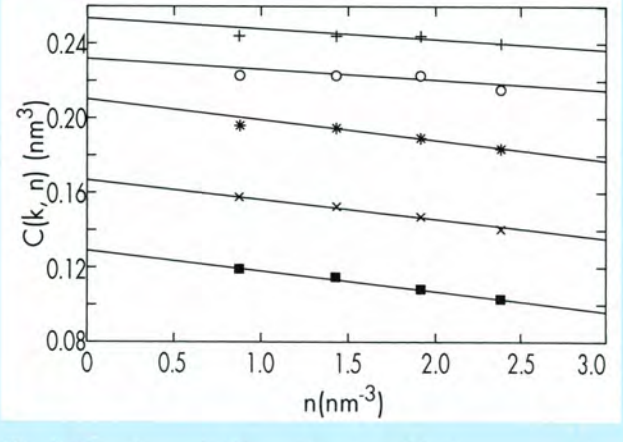

Fig. 2: Experimental c(k) as a function of density at various k-values (symbols, from top to bottom : k = 1.35, 1.82, 2.31, 2.80 and 3.34 nm^{-1}, respectively) and weighted linear fits to the data (continuous lines) for ^{36}Ar. [5].

represented by the experimental results, therefore the pair term $c_0(k)$ and the three-body term $c_1(k)$ can be derived from a linear least squares fit of the experimental density behaviour of c(k) at all the measured k-values.

In Fig. 3, the experimental determination of $c_0(k)$ is compared to a theoretical calculation based on equation (5) using the pair potentials of Aziz [7] or Barker [8] (difference between these potentials cannot be distinguished on the scale of this figure).

In Fig. 4, the virial coefficient $c_1(k)$ is compared to theoretical predictions using only the Barker Fisher Watts (BFW) pair potential [8] or including also the Axilrod-Teller-Muto (ATM) three body potential for Argon [9,10] or its modification [11].

We observe that the agreement between calculation and experiment is very good except at low k values, where the experimental $c_0(k)$ is systematically less than the predicted one, the reverse being the case for $c_1(k)$. These deviations are significantly larger than the estimated errors (error bars given in fig. 4 are correlated to the various instrumental settings).

It is possible to Fourier transform the experimental $c_0(k)$ to determine by means of equation (5) an experimental pair potential $u_2(1,2)$. Extrapolation of the experimental data to k = 0 and truncation at high k affect $c_0(r)$ only at a maximum of 1 % in the region of the peak; quantum corrections to $c_0(r)$ are of the same level [12]. It is worth noticing here that the measurement of the zero density limit of c(k), i.e. $c_0(k)$ gives a unique method of determining the microscopic pair potential in classical systems by means of a direct inversion of the experimental data.

The experimental potential given in Fig. 5 agrees very well at long range with the literature value, however some disagreement is found in the well where

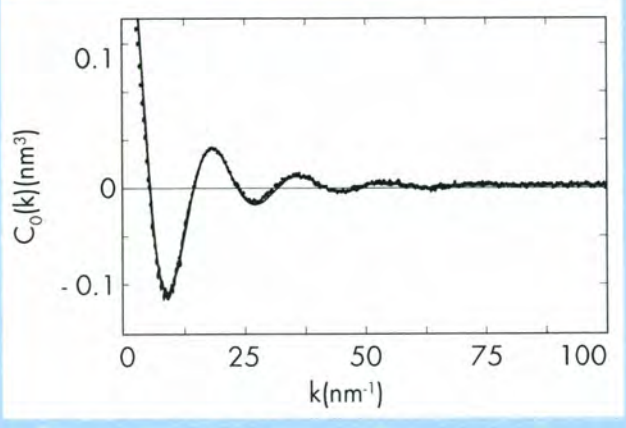

Fig. 3: $c_0(k)$ from extrapolation of c(k) to n = 0 (dots) and calculated from pair potentials taken from the literature (curve) for ^{36}Ar. Typical error bars are shown.

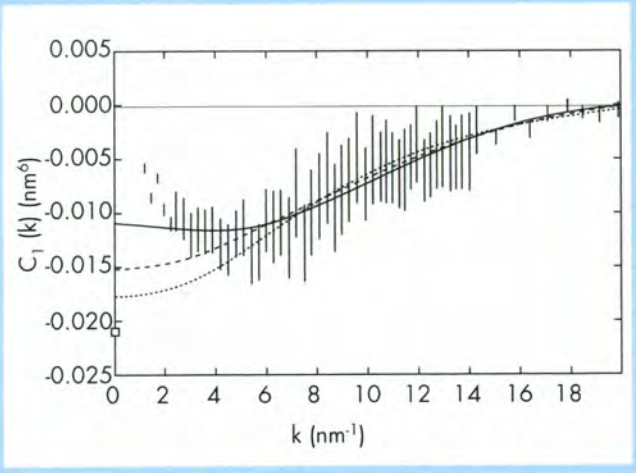

Fig. 4: $c_1(k)$ from linear density-expansion of c(k) (error bars) and as calculated from Barker-Fisher-Watts pair potential alone (continuous line) or including the Axilrod-Teller three-body potential (dotted line) or its modification by Loubeyre (dashed line). The k = 0 value (square) has been calculated by means of the equation of state for Argon [6].

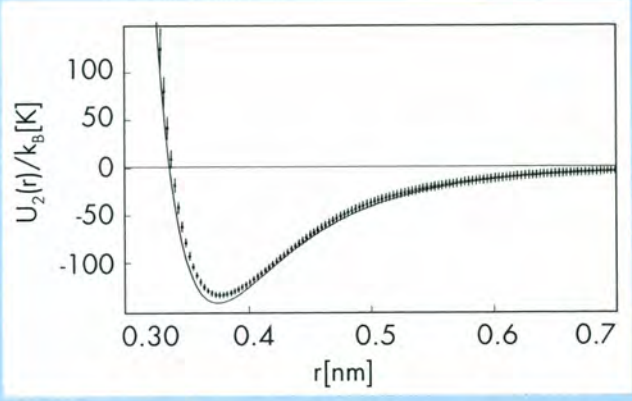

Fig. 5: The pair potential from this work (dots) is compared to the one taken from the literature [7] (curve) for ^{36}Ar.

the experimental well depth is $\varepsilon/kB = 134 \pm 3$ K and the value of r at which the potential equals zero is $\sigma = 0.338 \pm 0.001$ nm while the Barker potential gives $\varepsilon/k_B = 140.2$ K and $\sigma = 0.336$ nm.

Krypton at high density

S(k) ($3.6 < k < 16.2$ nm^{-1}) of dense fluid krypton, has been measured [13] on D4 at seven different thermodynamic states from the triple point to around the critical temperature (T values ranging from 130 K to 200 K, and densities from 11.9 to 17 nm^{-3}). In order to study the relation beween S(k) and the microscopic interaction potential, these experimental data have been compared (see figure 6) to a theoretical calculation performed by

iteratively solving the MHNC integral equation (10). Two models which are considered accurate (Aziz [7] and Barker [14]) have been chosen for the interaction pair potential entering MHNC. The calculation has been extended to take into account the presence of three body interactions using Axilrod-Teller-Muto (ATM). Theoretical and experimental S(k) values are not distinguishable at the scale of the figure [13].

In order to magnify the effects, we consider the deviation $\Delta S(k) = S_{exp}(k) - S_{MHNC}(k)$. We observe that it remains below 0.02 to 0.05 depending on density and that for $k \geq 50$ nm^{-1} it falls within the noise of the experiment. The larger deviations (~ 0.05) obtained at the higher density (T = 130 K) are in great part due to the inadequacy of the MHNC equation. The calculated modifications due to three body effects are weak and apparent only at low k values. Fig. 7 displays $\Delta S(k)$ for an intermediate density and temperature, it also displays the deviation observed for the Lennard-Jones potential which gives particularly poor results in the region of the main maximum of S(k). [5].

When the comparison is performed in the r-space in terms of g(r) it is again necessary to plot $\Delta g(r_{12}) = g_{exp}(r_{12}) - g_{MHNC}(r_{12})$ in order to observe the small deviation remaining between theory and experiment (see Fig. 8), which gives an indication of additional forces of many body character repulsive at short range and attractive at larger distances.

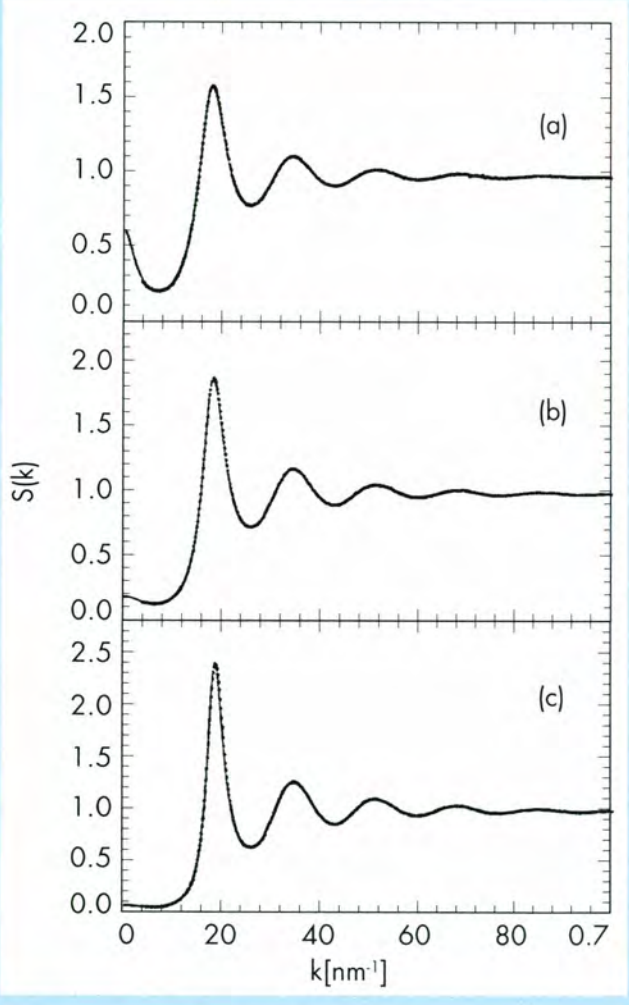

Fig. 6: S(k) over the k < 100 nm^{-1} range of measurement at (a) = 199 K, n = 11.86 nm^{-3}, (b) T = 169 K, n = 14.57 nm^{-3}, (c) T = 130 K, n = 16.83 nm^{-3}. The continuous curve is the result of the triplet MHNC equation with the Aziz pair interaction plus the three-body ATM term. Value at k = 0 is from the compressibility data.

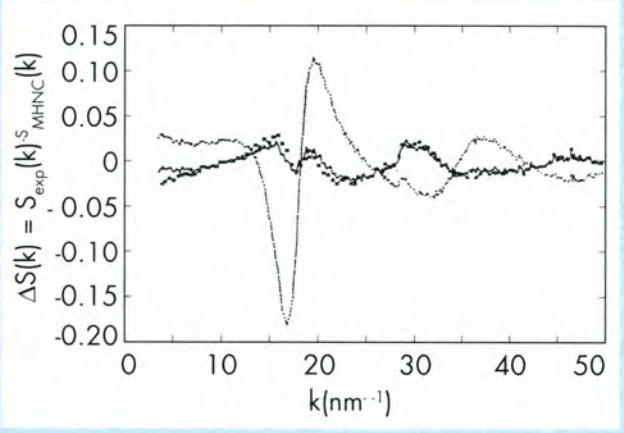

Fig. 7: The difference $\Delta S(k) = S_{exp}(k) - S_{MHNC}(k)$ for the Aziz pair interaction with (continuous curve) and without the ATM three-body term (crosses) and for the Lennard-Jones interaction (dotted curve) for Kr at T = 169 K and n = 14.57 nm^{-3}.

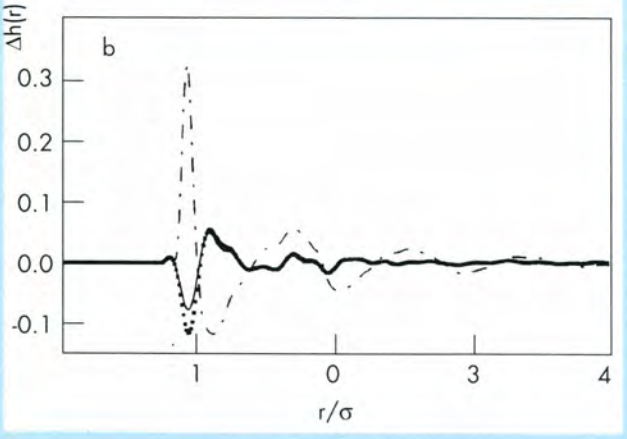

Fig. 8: Difference $\Delta g(r) = g_{exp}(r) - g_{MHNC}(r)$. $g_{MHNC}(r)$ is computed for the Aziz pair interaction including (continuous curve) or not (dotted curve) the ATM three-body interaction and also for the Lennard-Jones interaction (dot-dashed curve).

Finally the measurements of S(k) at closely (1 to 6 % variation) spaced densities [15], give access to the isothermal density derivative $\partial S(k)/\partial n$. This quantity is important because it contains information on 3 body correlations and also because it is very sensitive to the interaction potential. We show, figure 9, the comparison between experimental and theoretical results at k values ≤ 40 nm^{-1} i.e. where the pressure effects are noticeable. Again the accurate potentials of Barker and Aziz are in good agreement with experiment and the three-body contributions important only at very low k-values.

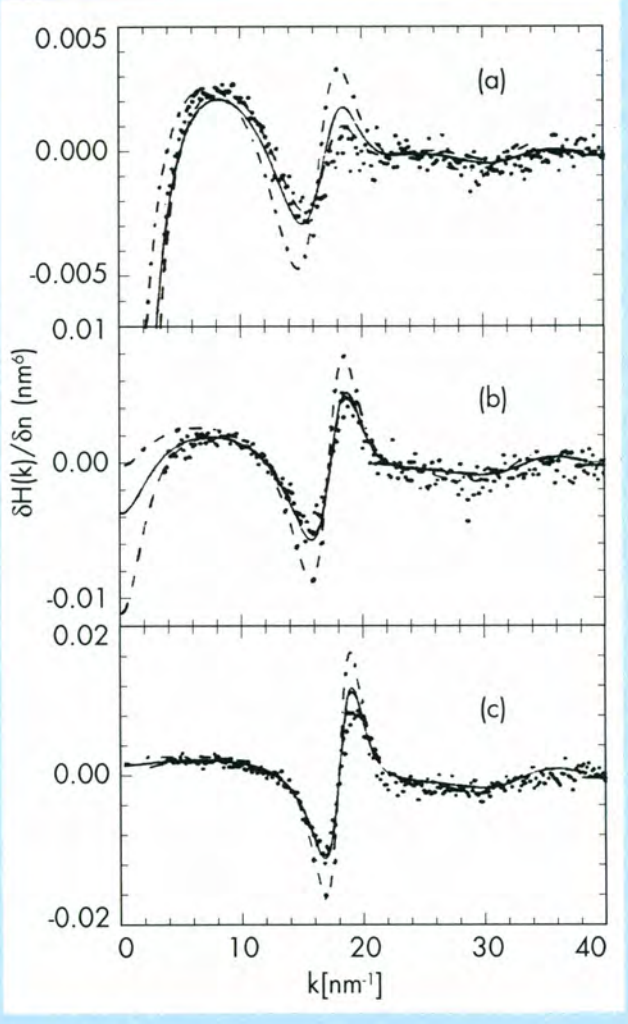

Fig. 9: $\delta S(k)/\delta n$ for the Aziz pair interaction with (continuous curve) and without the ATM three-body term (dashed curve), for the LJ interaction (dot-dashed curve), and from experimental data (•) at (a) T = 199 K, (b) T = 169 K, (c) T = 130 K. Value at k = 0 is from the compressibility data.

We can conclude that a very precise (within a few parts per thousand) determination of S(k), over a large k range can now be performed and the comparison with theory gives the opportunity to investigate in detail our knowledge of the structure of fluids and the connection between the microscopic interaction and the space correlation of the atoms in the system.

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Structure and properties of quasicrystals

Ch. Janot

Atomic order in solids is best defined in terms of the Fourier transform of the mass density. In an ordinary crystal, this transform can be written as a series:

$$\rho(\underset{\sim}{r}) = \frac{1}{V}\sum_{\underset{\sim}{G}} \rho(\underset{\sim}{G}) \exp(i\underset{\sim}{G}\cdot\underset{\sim}{r}) \qquad (1)$$

in which:

$$\underset{\sim}{G} = h\underset{\sim}{a}_1^* + k\underset{\sim}{a}_2^* + l\underset{\sim}{a}_3^* \qquad (2)$$

are vectors of the reciprocal lattice whose basis vectors are the $\underset{\sim}{a}_i^*$ (h, k, l are integers, Miller indices).

The same definition still holds for quasicrystals except that more than three basis vectors $\underset{\sim}{a}_i^*$ are required to span the reciprocal space. For instance, in the case of icosahedral quasicrystals, six basis vectors must be considered, so that:

$$\underset{\sim ico}{G} = \sum_{i=1}^{6} h_i \underset{\sim}{a}_i^* \qquad (3)$$

with the $\underset{\sim}{a}_i^*$ directed from the centre to vortices of an icosahedron.

Comparing Eqs. (2) and (3) demonstrates that quasicrystals will behave as crystals when investigated via diffraction methods, i.e., as periodic structures but periodic structures which would fill a six-dimensional space. This permits the use of regular crystallography rules to approach the structure, except that Bragg peaks must be given 6 Miller indices instead of 3. Formally, the knowledge of $\underset{\sim}{G}$ and $\rho(\underset{\sim}{G})$ in Eq. (1) gives $\rho(\underset{\sim}{r})$, i.e., the physical 3-dimensional structure of the quasicrystal.

During the year 1993, we have clarified several controversial aspects of the structure of a particular quasicrystal that belongs to the AlPdMn system. Single grains of this quasicrystal can be grown to centimetre-size dimensions via a Czrochralski procedure (Figure 1). The quasiperiodic perfection which is achieved is revealed in high-resolution X-ray and γ-ray diffraction measurements which show mosaic spreads less than 0.001° full width at half maximum (less than one third of the intrinsic Darwin width of Si(111)). The anomalous transmission of X-rays due to dynamical diffraction (the Bormann effect) has also been observed [1].

Basically, the structure of the AlPdMn quasicrystal is a hierarchical packing of atomic clusters called pseudo-Mackay icosahedra (PMI). A PMI-cluster is made of three successive "concentric" shells of atoms: an inner shell of 8 atoms distributed randomly on the sites of a small dodecahedron, then an icosahedron of 12 atoms and finally an icosidodecahedron of 30 atoms. The external diameter of a PMI is a little less than 10 Å and the centre distance of two nearest neighbour PMI is about 20 Å. A section of the AlPdMn structure is presented in Fig. 2; rings of atoms are visible; they correspond to the equatorial section of PMI. It can also be inferred from the figure that the PMI combine to form larger (inflated) PMI in such a way that the centres of the PMI are arranged in exactly the same fashions as are

Fig. 1: Optical micrograph of a single grain of the AlPdMn icosahedral quasicrystal obtained via Czochralski growth (scale in cm).

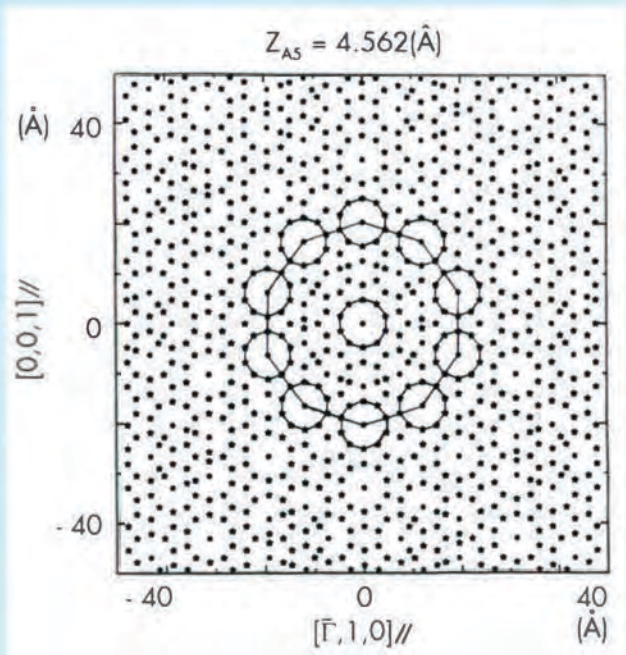

Fig. 2: Example of planar section through the structure of the AlPdMn quasicrystal. Equatorial cuts of PMI are underlined and the τ^3-inflated PMI as well.

the centres of the atoms. The scale factor is τ^3 ($\tau = 2\cos 36°$ the golden mean). An examination of the whole 3-dimensional structure shows that the inflation growth mechanism develops iteratively.

Several experiments have been carried out at the National Synchrotron Light Source Brookhaven. In particular the centric character of the icosahedral AlPdMn phase has been checked by measuring Bijvoet pairs above the Pd-K edge with a single grain [2]. The anomalous X-ray diffraction close to the Pd edge has also been measured with the result that the partial structure factor F_{Pd} of the palladium substructure has been determined [3]. Beyond a definitive confirmation of the existence of a very strong chemical order, these data have brought a contradiction to the idea that atomic surfaces in the 6-dimensional images should be polyhedral objects sharply faceted. The results must be considered in the context of recent theoretical suggestions [4] that the atomic surfaces might have fractally shaped borders.

Understanding of the dynamics of quasicrystals has also made some progress in 1993. Further inelastic neutron scattering data have been collected on triple-axis machines at the LLB and (old) IN10 data have been interpreted along with Mössbauer spectroscopy measurements. The calculation of the dynamical response of quasicrystals remains difficult since the projection of atomic displacements on a plane wave basis does not reduce the number of independent parameters. Proposed models for the vibrational states of quasicrystals are actually based on numerical calculations on large cell periodic approximants [5]. Inelastic neutron scattering measurements [6] have demonstrated the existence of pseudo-dispersion branches and pseudo-Brillouin zones in the acoustic regime. Beyond that, the situation remains confused. No gaps are observed even when branches cross. But "phonon modes" broaden progressively for momentum transfers larger than 0.3-0.4 $Å^{-1}$ (energy $8x10^{-3}$ eV), while the "phonon branches" bend over and finally become dispersionless for momentum transfers above 0.85 $Å^{-1}$ (energy $12x10^{-3}$ eV). The broadening might be due to interactions of the acoustic modes with a "sea" of pseudo-optic localized modes. This idea is supported by the fact that the broadening shows up at momentum transfers corresponding to a length scale of about 10 Å, which is precisely the size of the PMI atomic clusters. The purely elastic neutron scattering has also been measured on a AlFeCu quasicrystal using the high resolution spectrometer IN10 in the fixed energy window mode ($\Delta E = 10^{-6}$ eV). Typical temperature scans of scattered intensities at two momentum transfer values q are shown in Figure 3. A linear Debye-Waller like decay is visible in the whole temperature range with $q \leq 0.41$ $Å^{-1}$ and only below 700°K or so with $q \geq 0.88$ $Å^{-1}$. But this would correspond to a very large DW factor, about 50 to 100 times as large as the aluminium DW. This is interpreted by the existence of phason modes, inducing correlated atomic jumps. In the larger q range and above 800°K, an enhanced drop of intensity is observed. This is confirmed, at higher energy resolution ($2.86x10^{-8}$ eV) by Mössbauer spectroscopy data [7]. This additional drop can be attributed to high energy vibrational states, "localized" over a length scale between 7-15 Å.

Altogether the atomic vibrations in quasicrystals seem to generate fully extended "propagating phonons" of low energy (below 10^{-4} eV or so) and some sort of decoupled eigenmodes of "cavities" corresponding to (about) 10 Å rigid unit modes. This is consistent with the structural analysis and would also explain the very low thermal conductivity of quasicrystals [8].

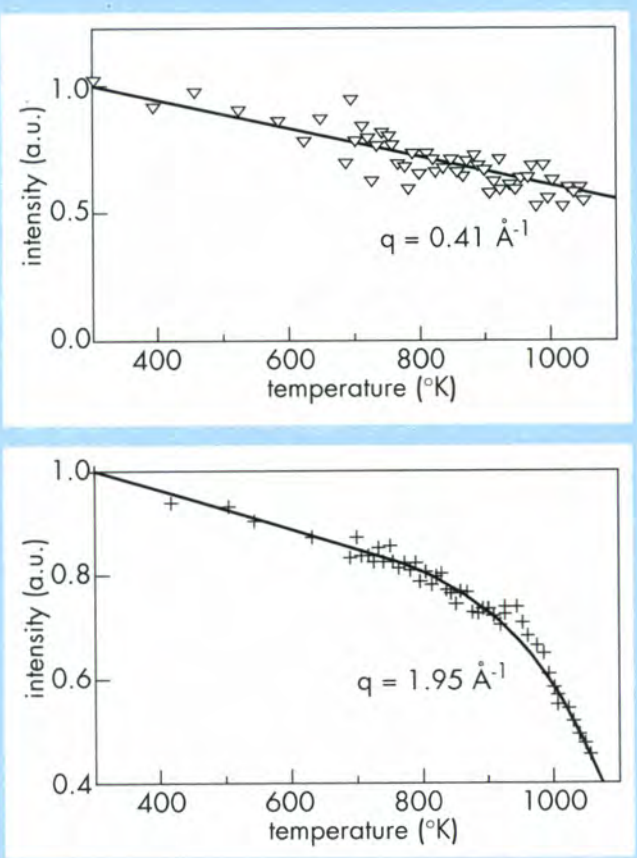

Fig. 3: Typical temperature scans of purely elastic neutron scattering measured for an AlFeCu quasicrystal with a fixed window energy of 10^{-6} eV.

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Biological Structures and Dynamics

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Introduction

As in 1992, following ILL's reactor shutdown, many activities and projects involving the use of neutrons had either to be stopped completely, or could only be pursued partially elsewhere. This has confirmed the fact that most facilities offered by the ILL cannot be replaced. The trends of 1992 have been followed and scientific activity has been maintained through analysis of previous results and by methodological work as well as by extending activities to X-ray diffraction or biochemistry. Collaboration with our colleagues from the Institut de Biologie Structurale (IBS) and with those at the Grenoble outstation of the European Molecular Biology Laboratory (EMBL) has been carried on and still forms a vital element for the scientific life of our college.

Progress in biochemical and molecular biology methods—for example, the cloning and expression of appropriately designed protein mutants and modified nucleic acids, or specific deuterium labelling of large functional complexes—is revolutionizing structural studies including those by neutron scattering and diffraction. A special issue of Biophysical Chemistry devoted to Neutrons in Biology, edited by J. Zaccai, a member of the college, will present a number of original papers on these aspects, describing work at ILL and other neutron reactors around the world. It will be available at about the same time as the start-up of the ILL reactor next summer.

Scientific Trends and Highlights in 1993

Quasi-Laue diffraction instrumentation

Detector development for the Quasi-Laue diffractometer, which was part of the proposed modernization programme, has continued and is described in some detail in the contribution from the Large Structures Group to this Annual Report. In addition further image-plate detector tests have been done.

The most important of these involved the use of a MAR-RESEARCH image-plate scanner converted to detect neutrons. The measurements were done at the V1 instrument of the Hahn-Meitner Institute by a mixed EMBL/ILL team in collaboration with members of the Freie Universität, Berlin. To detect neutrons a plate covered with gadolinium oxide paint was placed in front of the X-ray detector during exposure and removed during read out. A multi-wire detector was also used for comparison [1].

The tests showed that recording of neutron reflections using image plates on the V1 spectrometer is possible, but that protection of the plates against gamma-rays will be required for routine data collection. Another approach for recording of neutrons is by the use of gadolinium doped plates. This was for technical reasons not tried, but earlier measurements at Saclay have shown that this gives a much better peak to background ratio. It is therefore most likely that this approach will be the one followed for the prototype version of the neutron image plate detector presently under construction.

Structure of dodecyl sulphate – protein complexes at subsaturating concentrations of free detergent

The anionic detergent sodium dodecyl sulphate (SDS) effects solubilization of, for instance, membrane, ribosomal and viral proteins. SDS is widely used for size separations of these proteins as well as of water–soluble proteins or protein subunits, by gel electrophoresis and by molecular–sieve

chromatography. Knowledge of the structure of SDS–protein complexes is useful for understanding and for further developing these important biochemical methods. SDS binds to water–soluble proteins approximately in proportion to the polypeptide length. On average, the saturated complexes contain one SDS molecule per two amino–acid residues at moderate ionic strength.

Earlier investigations of SDS–protein complexes by a number of physical techniques resulted in a number of partly incompatible structural models. The first neutron small-angle scattering experiments had revealed the low resolution structure of the complex between SDS and the single polypeptide of a water–soluble enzyme (452 amino acid residues). The saturated complex consists of three globular micelles which are connected by short flexible polypeptide segments.

Shortly before the reactor shut–down new experiments (in collaboration with Uppsala University, Sweden) were performed at subsaturating concentrations of free SDS in equilibrium with the complex. The data show a decrease in stoichiometry from one bound dodecyl sulphate (DS) anion per two amino acid residues near the critical micelle concentration (CMC) to one per four residues at half the CMC. At 0.3 CMC, a two–micelle complex is formed by the recombination of the small amino-terminal micelle with the middle one; and the centre-to-centre distance between the carboxyl–terminal micelle and the middle one decreases from 7.5 nm to 6.2 nm. These structural data allow us to better understand earlier results obtained with high–performance agarose gel chromatography of the same SDS–protein complexes [2].

Functional motions in membrane proteins studied by inelastic neutron scattering

The study of protein motions has gained considerable importance in the search to understand biological function at the molecular level. Because of their wavelengths and energies, thermal and cold neutrons are particularly adapted for such studies. The Purple Membrane of *Halobacterium halobium* contains a single protein, bacteriorhodopsin, which functions as a light-driven proton pump. Inelastic neutron scattering experiments on IN6 and IN13 performed before the reactor went down have appeared in print this year. As described in last year's Annual Report, a detailed study of the dynamics of this membrane in different conditions of temperature and hydration showed strong correlation between the type of dynamics and the ability of the protein to perform different aspects of its function. Thus when the membrane protein is vibrating harmonically, it can be activated by absorbing a photon to release a proton on the outside of the cell (where the proton chemical potential is higher than in the cytoplasm). On the other hand, soft anharmonic motions in the protein are required for it to return to its ground state by binding a proton on the cytoplasmic side. In 1993, the analysis of the neutron results has been taken further by using a recent structural model for the protein and performing molecular dynamics calculations, and collaborations have been initiated for complementary (light absorption) spectroscopic studies. These have led to ideas for new neutron experiments on deuterium labelled samples that are now being planned for when the reactor starts up again [3].

Structure of Porins

Porins are a class of proteins found in the outer membrane of Gram-negative bacteria. They allow the selective passage through the membrane of polar molecules up to a cut-off value in molecular weight that varies somewhat between different porins. The X-ray structures of several different Porins have been solved in the last few years, each one revealing a secondary structure composed mainly of ß-sheet. Crystals of membrane proteins are produced after solubilization of the protein in detergent that is believed to mimic the membrane lipid in its interaction with hydrophobic parts of the protein. The crystallising particle is in fact a mixed protein/detergent micelle. In the X-ray studies to date, however, no detergent structure has been observed, due probably to disorder and low contrast. We reported last year on the organisation of detergent in crystals of Porin from the purple bacterium *Rhodobacter capsulatus* [4]. We have now obtained results from crystals of the protein from *E. Coli* [5]. The results from the two bacterial sources are rather different. In the *Rhodobacter capsulatus* case, the protein molecules and the detergent form two dimensional sheets in the crystals apparently mimicking a bilayer membrane, although there is as yet no direct evidence of a bilayer. There is no interaction between the C8E4 detergent molecules in successive sheets, i.e. there is no 3-dimensional continuity of the detergent phase, and the crystal is formed solely through protein-protein contacts. In the case of the *E. Coli* protein the porin molecules form an extended three-dimensional network with only rather tenuous contacts between detergent micelles. In this case the detergent, N,N dimethyl decyl amine oxide was deuterated in the hydrophobic tail and despite the low resolution (13Å) it appears possible to identify the tail and headgroup regions of the detergent molecules. This will allow us to analyse more closely the form of the interactions between detergent and proteins and to determine whether not only hydrophobic but also polar interactions play a role in the stabilisation of the protein detergent complex.

Low resolution neutron diffraction on 50S ribosomal crystals from *halobacterium marismortui*

Ab initio phasing methods developed for phasing the low resolution neutron diffraction data from 50S ribosomal crystals (from *halobacterium marismortui*), based on direct methods, led to density maps for the 0% D_2O and the 100% D_2O data sets. Both maps were modelled by two density levels. In the 100% D_2O map the high level should represent the proteins and the lower level the RNA; and *vice versa* in the 0% D_2O map. RNA and protein domains showed

reasonable similarities between the two maps. It was then decided, in order to improve the phasing methods, to concentrate the effort on test data instead of experimental ones. Presently, starting from the test data we are trying to improve the phasing method, principally by combining direct methods with supplementary information. These test data should also indicate the confidence level and the limitations of our methodology [6].

High resolution crystallographic studies on a new family of small plant proteins rich in cysteins using X-ray diffraction

The hydrophobic protein from soybean (HPS) for which the structure was solved last year to 1.8 Å resolution shows similarities to non-specific phospholipid transport protein (LTP) from plants. They both belong to a new family of proteins characterized by a motif of 8 Cysteins forming a similar pattern of 4 disulfide bridges. Recent NMR results show similarities in the three-dimensional structures despite a low sequence homology. In order to study the lipid binding function of the LTPs, we cocrystallised the proteins with phospholipids. Two proteins are under study: a wheat LTP and a maize LTP. For both of them, two crystal forms were obtained diffracting to 2.5 Å on a standard rotating anode. Heavy atom derivatives are under study, weak derivatives have been obtained already. A first density map to 6 Å resolution has been calculated. In order to interpret this map we have to improve the heavy atom derivatives [7].

Storage-ring X-ray work

The enforced shut-down of the reactor coinciding with the start-up of the ESRF synchrotron has given the opportunity for the ILL scientists both to learn more about synchrotron radiation and to strengthen the contact with their neighbours. It was therefore only natural for members of the college to participate in some of the first commissioning experiments and measurements in protein crystallography.

The measurements - done in collaboration with and with help from the EMBL staff - were conducted on the Troika beam line, which uses an insertion device (ID9) of the storage ring. Indeed, they were the very first measurements done right after the final installation of the insertion device, an undulator, and they were therefore not only interesting from a protein crystallography viewpoint, but were also used to learn more about these powerful sources.

For the measurements the Troika instrument was equipped with an additional diffractometer, which was a MAR-RESEARCH image-plate detector on loan from the adjacent EMBL outstation. The monochromator was a single Si (220) crystal in reflection, and the imageplate was located on the sample table of the Troika instrument. As this is placed on air-cushions, it was very easy to change wavelength in the range from 0.7 Å to more than 1.5 Å, and both standard protein crystallographic and multiple anomalous dispersion (MAD) studies for structure solution were carried out.

The normal protein crystallographic studies were carried out as an introduction to the MAD measurements. They involved projects from EMBL, ILL and the neighbouring IBS, and gave very satisfactory results. The MAD measurement, which relies on the high energy resolution of the Troika set-up, was done in collaboration with a group from Columbia University, New York. In this case four or five sets of measurements were done around the absorption edge of a heavy atom present in the protein structure, and by combining this information the structure has now been solved. During the measurement two modes were used, namely one where the magnet gap was kept constant and one where - for the first time - it was varied to obtain maximum intensity for the wavelength in question, and both approaches gave useful results [8].

Extracellular matrix protein isoform separation for crystallographic work

The presence of isoforms, also called microheterogeneity, is a consequence of the post translational modifications of the polypeptide backbone. This is generally due to phosphorylation, sulphation, or glycosylation. These modifications are frequent in extracellular proteins such as those from the extracellular matrix.

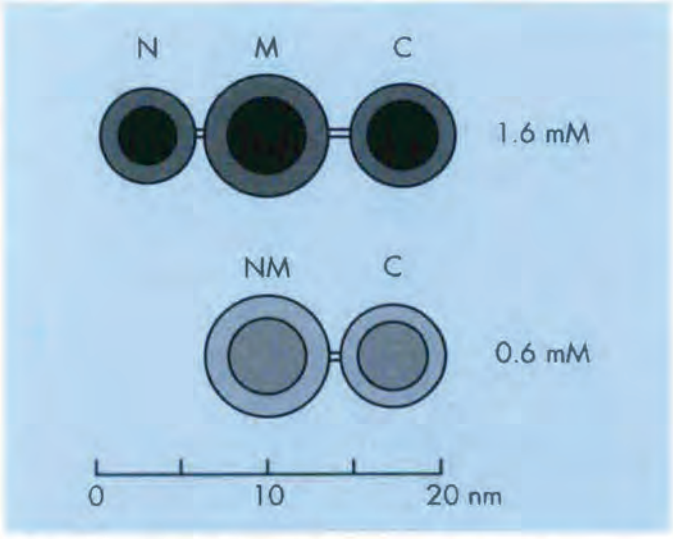

Fig. 1: Schematic scale models of the mutual disposition of the three protein–decorated micelles in buffer containing 1.6 mM SDS (0.9 CMC, top) and of the two protein–decorated micelles in buffer containing 0.6 mM SDS (0.3 CMC, bottom). The independent micelles N (N–terminal), M (middle) and C (C–terminal) of the three–micelle complex are connected, at saturation, by flexible oligopeptide linkers about 5 or 6 amino acid residues long; with decreasing SDS concentration to subsaturating levels, the small micelle N coalesces with micelle M; and micelle C approaches micelle M. The difference in contrast between the dodecyl chain cores and the surrounding protein–sulphate shell is shown by a different shading.

It has been shown that the microheterogeneity has been responsible for some of the problems encountered with the crystallization of proteins. Crystals obtained from isoform mixtures are generally small and diffract poorly.

Isoelectric focussing allows the separation of the isoforms according to their isoelectric points. With mass spectrometry, high resolution isoelectric focussing is currently the most sensitive method of protein analysis. Preparative scale isoelectric focussing under non denaturing conditions has been hampered by the lack of solubility of many proteins at (or near) their isoelectric point. This problem has led to the discovery of new solubilizing agents through a collaboration between the ILL biochemistry laboratory and a CEA -INSERM laboratory in Grenoble. This separation technique will now be applied to improve crystals that have been obtained with osteocalcin as well as with a fragment of fibronectin through a collaboration between the ILL and the IBS [9].

Secretary: Laurent Vuillard

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Molecular Spectroscopy, Surfaces and Mesophases

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Introduction

Despite the reactor shutdown and the departure of many college members, there has been considerable scientific activity. Much of this has resulted from visits to other laboratories, particularly LLB Saclay, and it is hoped that the links formed between ILL scientists and those of other institutes will be mutually beneficial for years to come.

Low-energy excitations, density of states experiments

Amorphous - crystalline ethylbenzene (ILL, NIST)

The dynamics of ethylbenzene was investigated using the three-axis instruments BT4 and BT9 at NIST (Frick, Trevino, Erwin). Previous experiments using an elastic scan on IN13 revealed that the mean squared displacement $\langle u^2 \rangle$ has anomalous behaviour with increasing temperature. A strong increase of $\langle u^2 \rangle$ with respect to lower temperatures is observed between 120 K and 140 K before it drops to a much lower value. Following a further, weaker increase it again decreases.

New experiments on deuterated ethylbenzene at NIST showed that these dynamic anomalies are connected to recrystallization phenomena (Fig. 1). Two different crystalline phases were found above 140 K. Comparing the low-frequency scattering of amorphous and crystalline ethylbenzene (Fig. 2) it can be seen that the intensity at low frequencies for the amorphous sample is strongly enhanced with respect to the crystalline sample. Fig. 2 shows a strong low-frequency hump below 8 meV in the range where the crystalline sample has a much lower and almost frequency-independent intensity. Thus before recrystallizing the low-frequency modes increase drastically in amplitude and show anharmonic behaviour. These are the dynamic precursors of the structural rearrangement from a disordered solid towards the crystal.

Dynamics of pristine and doped polyacetylene (ILL, LLB)

Polyacetylene, $(CH)_x$, is the simplest example of a conjugated polymer. Interest in the physical properties of this molecule has increased since it has been found that it can be chemically doped to 'metallic' levels of conductivity, values as high as 145 000 Scm^{-1} having been reported. In the doping process, carriers are generated by charge transfer, but the spectacular increase in conductivity is due to changes in the electronic structure of the polymer backbone. The mechanisms that lead to metal-like values for the conductivity have been studied theoretically, mainly in lightly-doped systems. In heavily-doped regimes (examined here) a complete delocalization of carriers is assumed.

Until recently vibrational data for polyacetylene were limited to a few Raman and infrared intrachain modes and thus theoretical efforts have concentrated on the dynamics of the isolated chains. However, the modes which dominate the vibrational atomic mean-squared displacements are those at lower frequencies (< 20 meV). Recent inelastic neutron scattering experiments from stretch-oriented *cis*-rich and *trans*-rich polyacetylene have enabled the vibrational density of states, $G(\omega)$ of the system to be determined in the directions parallel and perpendicular to the average chain axes, with good resolution in the low-frequency region. The experimental $G(\omega)$s were found to be highly anisotropic and exhibit considerable differences between the *cis*- and *trans*-conformers.

A detailed interpretation of the observed vibrational spectra based on the neutron data alone is not possible. However, information can be obtained by performing

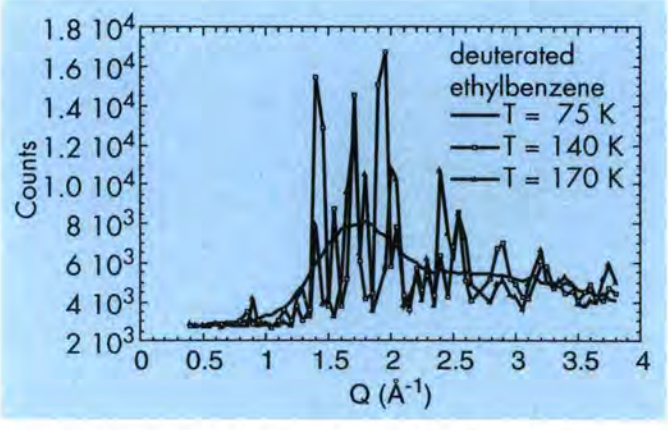

Fig. 1: Static structure factor of deuterated ethylbenzene for a quenched sample (thick line) and patterns at two temperatures (140K and 170K) of the annealed sample.

molecular-dynamics simulations and calculating neutron scattering properties from the resulting atomic trajectories. Recently, simulations of crystals of *cis*-and *trans*-polyacetylene molecules of different chain lengths have been reported [1]. Because the dynamics of interest is vibrational, harmonic analysis can (in principle) be applied to these systems. However, molecular-dynamics simulation, in which the harmonic approximation is not required, is expected to give a better representation of the effective potentials for the large-amplitude, low-frequency vibrations. In this work the density of states was calculated from the molecular-dynamics trajectories by numerical Fourier transformation of the velocity autocorrelation functions.

The low-frequency dynamics (0-20 meV) of sodium-doped *trans*-polyacetylene has recently been investigated using a combination of incoherent neutron scattering spectroscopy and molecular-dynamics simulations. These simulations were performed using a molecular-mechanics potential-function with a model system explicitly including the three-dimensional crystal environment [2]. Time-dependent mean-squared displacements and vibrational densities of states are

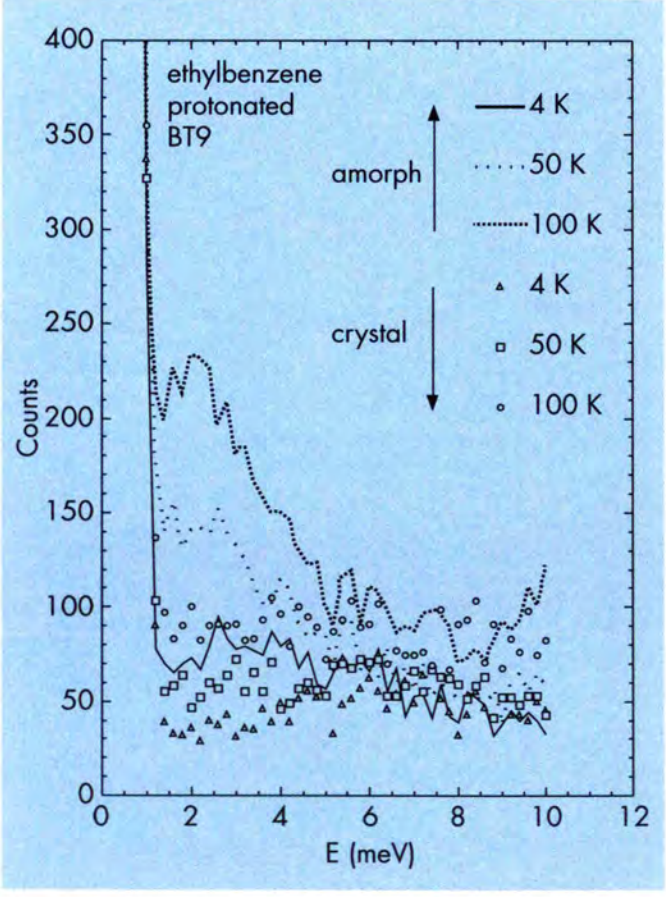

Fig. 2: Low frequency scattering of quenched ethylbenzene (lines) in comparison with crystalline ethylbenzene (symbols) as measured on the thermal triple axis spectrometer BT9, NIST.

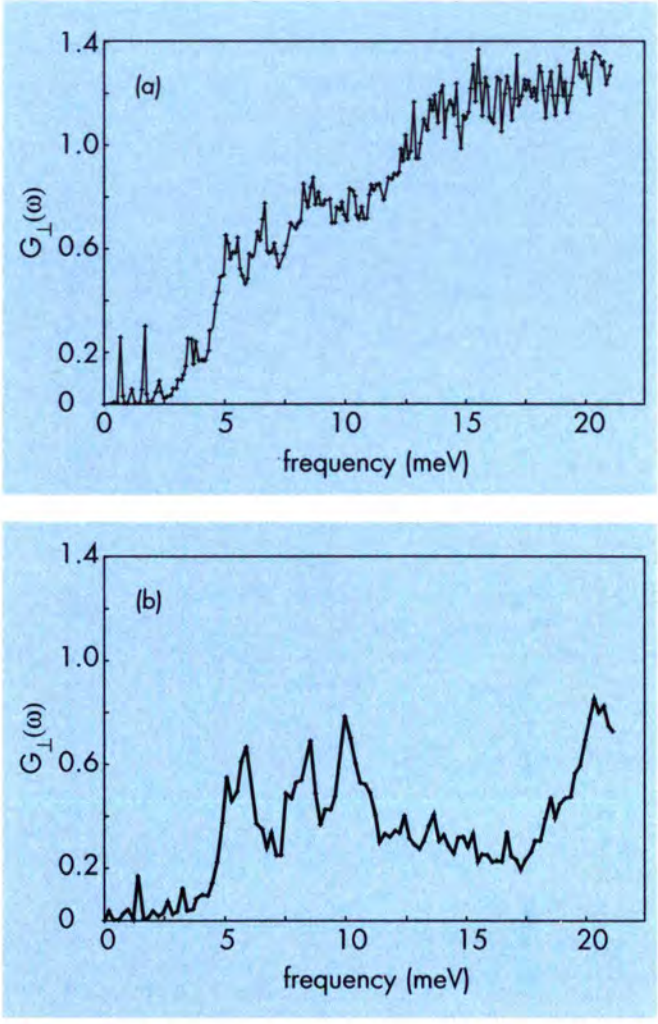

Fig. 3: Simulation-derived density of states in the direction perpendicular to the chain axes
a) trans-polyacetylene
b) Na-doped (12.5 at. %) trans-polyacetylene.

calculated from the simulations of the pure and doped systems. The simulations are decomposed to determine the contribution of rigid-body motions to the atomic trajectories. From these simulations there is an indication that the mean-squared displacements of the polyacetylene atoms become close to isotropic on doping. Experiments (performed with the instrument MIBEMOL at LLB) and simulations are in accord that doping results in a marked change in the vibrational density of states in the direction perpendicular to the chain axes, a broad minimum appearing at ~ 16 meV. This spectral region is dominated by intramolecular torsional displacements, see Figs. 3a and 3b.

Quasielastic scattering

Dynamics of urea inclusion compounds (ILL, University of Bordeaux)

Long chain hydrocarbon molecules such as n-alkanes are known to form inclusion adducts with urea. In urea inclusion

compounds, the hydrogen-bonded network of urea molecules (hereafter called the host) contains essentially "infinite" and parallel channels of approximate diameter 5.2 Å (at room temperature) in which the n-alkane chains (the guests) are trapped in an almost "all trans" conformation. The n-alkane/urea inclusion compounds are known to undergo a structural phase-transition from a low-temperature phase (LT) to a high-temperature phase (HT) at a temperature that depends on the length of the guest molecules. In general, the transition temperature increases with the length of the guest molecule. In the LT phase the host substructure is orthorhombic whilst it is hexagonal in

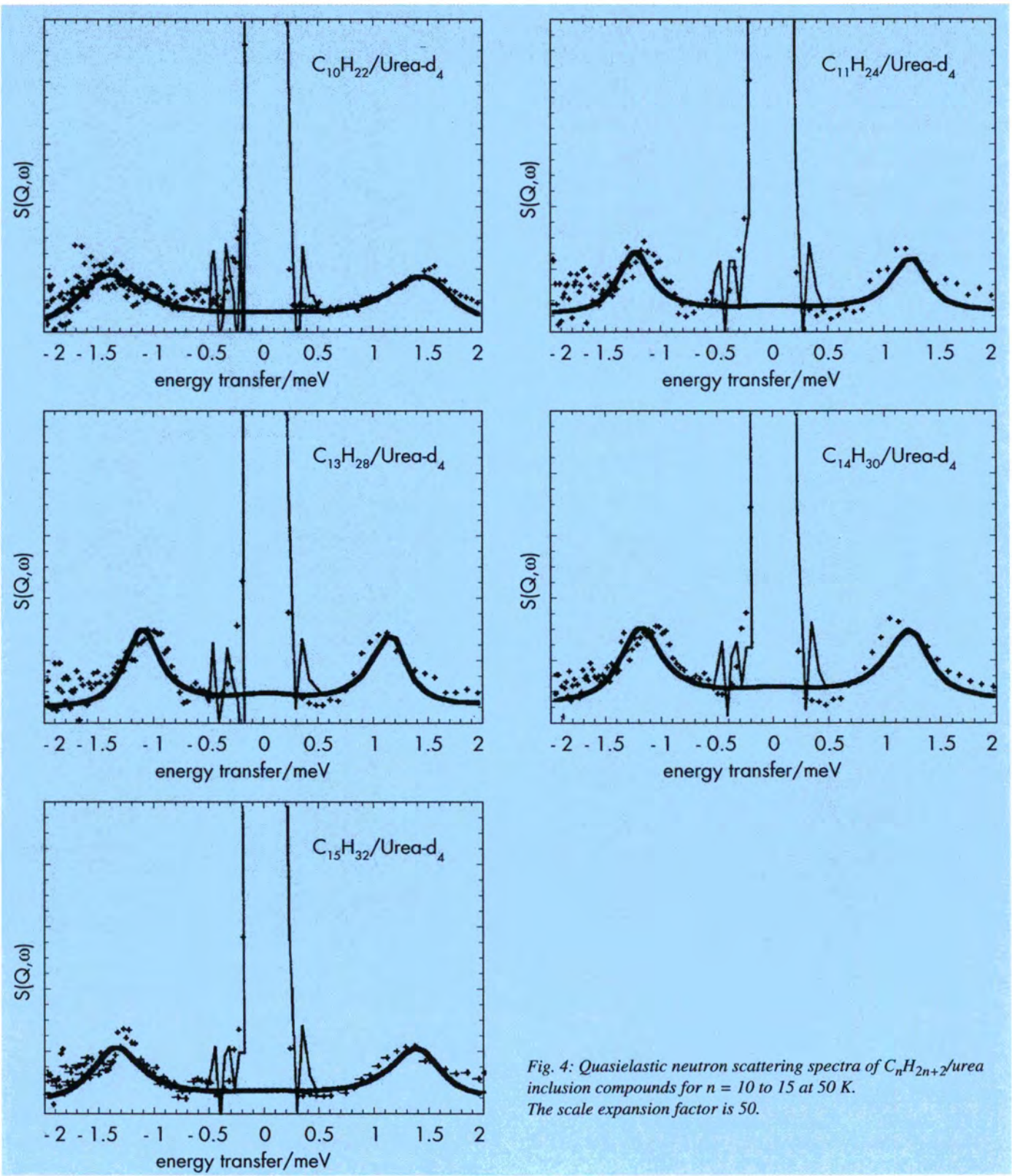

Fig. 4: Quasielastic neutron scattering spectra of C_nH_{2n+2}/urea inclusion compounds for n = 10 to 15 at 50 K. The scale expansion factor is 50.

the HT phase. The guest substructure is essentially characterized by its one dimensional packing with a periodic repeat distance c_g. An important property of urea inclusion compounds is that the ratio of c_g versus the host lattice-parameter c_h is not a rational number: urea inclusion compounds are therefore incommensurate composite structures in both their LT and HT phases. It should be noted that the hexagonal structure of urea is not stable without the guest component: the stable crystalline structure of pure urea is tetragonal and does not contain empty channels.

Pioneering ^{1}H-NMR works revealed that in the HT phases of the compounds, the n-alkane guest undergoes fast reorientations about the $\vec{C}$ axis of the urea channel. Although the existence of translational fluctuations was detected by X-ray diffraction, it is only very recently that the translational motions of the guest molecules along the channel axis could be analyzed precisely by means of incoherent quasielastic neutron scattering (IQNS) technique. These experiments, performed on the n-nonadecane $C_{19}H_{40}$/urea inclusion compound, have shown that within the characteristic time scale of the spectrometer, large amplitude diffusive reorientations of the guests were observed but could not be assigned to $2\pi/6$ jumps, as usually assumed regarding the hexagonal symmetry of the urea channels. In the LT phase of the samples, the reorientational motions were frozen-in and side-peaks assigned to low-frequency longitudinal oscillations of the hydrocarbon chains were observed at about 1.2 meV. Such low-frequency inelastic peaks were not observed in the crystalline phase of pure n-nonadecane samples and other related inclusion compounds. It must also be pointed out that these inelastic peaks cannot be assigned to any kind of intramolecular vibration of the n-alkane chains involving the longitudinal displacements of the hydrogen atoms, such vibrational modes (the longitudinal accordion "LAM" modes) being expected to be observed at about 12.5 meV for n-nonadecane. It is therefore expected that these low-energy excitations are characteristic of the one dimensional packing of the guest molecules within the urea channels so that the mean frequency of the oscillations should be a function of both the chain length of the n-alkane chain and also of the specific interactions between the urea host and the guest.

Incoherent quasielastic neutron scattering experiments were performed by using the spectrometer MIBEMOL of the LLB-Saclay on a series of urea inclusion compounds n-C_nH_{2n+2}/urea-d_4 with n = 5↔9. Using semi oriented samples, the spectra were recorded in two geometries, i.e. with the $\vec{Q}$ momentum transfer vector parallel ($Q_{//}$) and perpendicular ($Q\perp$) to the urea host tunnel axis. It was therefore possible to investigate separately reorientational and translational motions in both the low temperature (LT) and high temperature (HT) phases of the samples. The low-frequency excitations observed in the LT phase and only in the $Q_{//}$ geometry can be assigned to the "sliding mode" of one sublattice (the n-alkane guests) with respect to the other (the urea host). Fig. 4 shows that the mean frequency of this "sliding mode" does not follow a simple law with the chain length of the included alkane. It seems to depend upon the parameter c_g/c_h which characterizes these incommensurate composite structures [3]. The spectra have been quantitatively analyzed by means of a model of damped oscillator [4] and the results interpreted on the basis of the structural properties of these composite incommensurate systems. On the characteristic time scale of the experiments, reorientations of the n-alkane chains are effective only in the HT phases of the compounds. Fig. 5 shows the evolution with temperature of $C_{13}H_{28}$/urea inclusion compound and the fit with the model.

Diffusion of Ni^{2+} in $Ni_2Mo_6S_8$
(ILL, University of Kiel, TU Berlin)

Binary and ternary molybdenum cluster chalcogenides (Chevrel phases) of composition Mo_6X_8 and $A_xMo_6X_8$ show a manifold of chemical and physical properties depending on the nature of the chalcogen atom X, the nature of the ternary metal A, and the stoichiometry of the latter. They are able to undergo reversible topotactic redox reactions at ambient temperature via electron/ion transfer. Electrons are accepted by appropriate levels of the host-lattice conduction-band and the resulting negative excess charge is compensated by the simultaneous uptake of mobile cations A^+ or A^{2+} which occupy empty sites in the lattice channels.

Small cations, such as Li^+, Cu^+ or Ni^{2+}, form the so called Chevrel phases of type II where the rhombohedral unit-cell is compressed in direction of the threefold symmetry-axis. This leads to a squeezing of the X_8 cubes and in consequence to the formation of two times six potential lattice sites with distorted tetrahedral symmetry. These sites are arranged on two concentric rings around the unit-cell origin. The large number of possible lattice sites within the empty channels should facilitate the diffusion of the guest ions within the host lattice.

Fig. 6 shows a projection of the 3d-framework of inner and outer sites of $Ni_2Mo_6S_8$ around the unit-cell origin (Δ). Possible jump distances are indicated and vary between 1.2Å and 2.9Å. Electrochemical work gave evidence of fast long-range diffusion for e.g. $Li_3Mo_6S_8$ with $D_{(300K)} = 1.4 \times 10^{-9} cm^2/s$ or $Ni_2Mo_6S_8$ with $D_{(300K)} = 1.7 \times 10^{-9}$ cm^2/s. Quasielastic and inelastic neutron scattering experiments were performed on IN10 to study the motional behaviour of the intercalant Ni^{2+} in $Ni_2Mo_6S_8$ on a microscopic scale. T-dependent fixed-window scans revealed a motional broadening of the spectra above 250K. The inelastic spectra measured as a function of scattering vector and temperature contained a constant 20% of elastically scattered intensity [5]. This corresponds to the incoherent scattering cross-section of the immobile host lattice Mo_6S_8 and indicates the Ni^{2+} motion to be a long-range diffusion process.

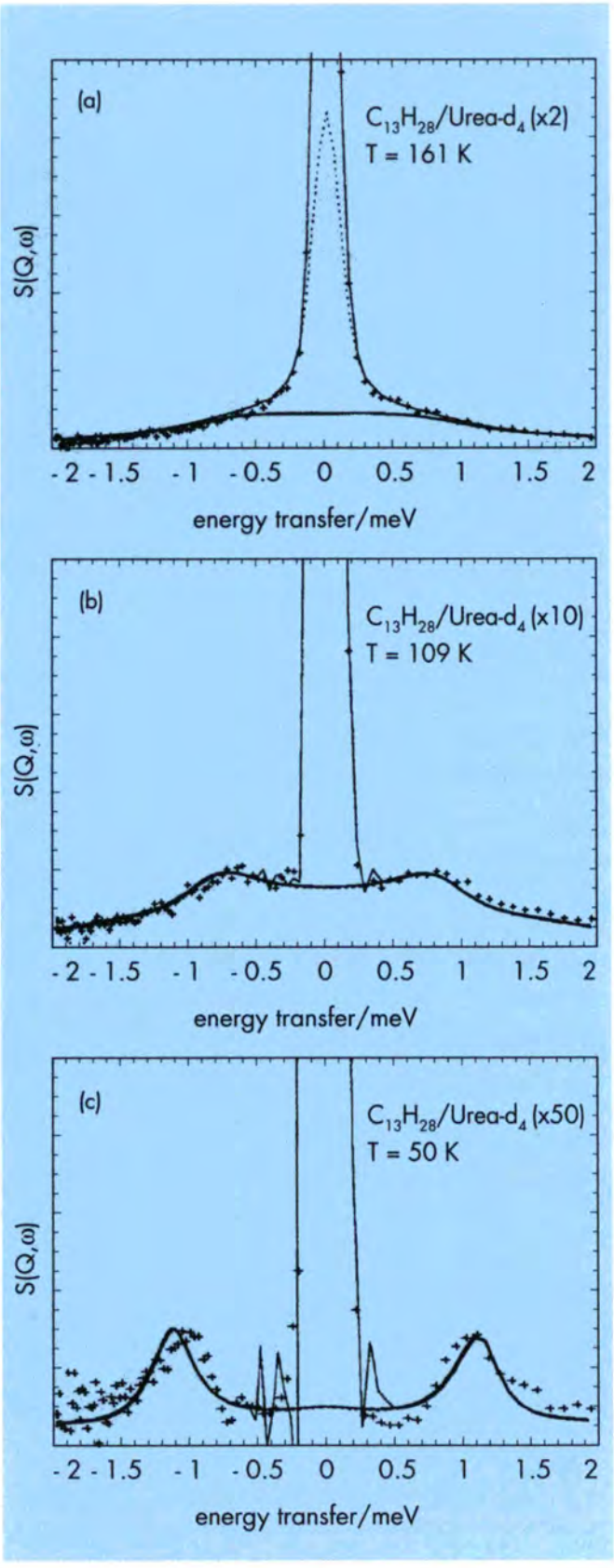

Fig. 5: Quasielastic neutron scattering spectra of $C_{13}H_{28}$/urea inclusion compound for 3 temperatures:
a) T = 50 K - expansion 50;
b) T = 109 K (below the transition temperature) - expansion 10;
c) T = 161 K (above the transition temperature) - expansion 2.

A simple jump-diffusion model fits the T- and Q-dependence of the inelastic spectra; $t_{co}=1.5 \times 10^{-12}$s, E_A=24kJ/mol. The jump vector amounts to 2.1 Å and can be correlated to the distances indicated in figure 6, assuming that thermal averaging merges the six inner sites into the unit-cell origin. A long-range diffusion process consists of intracluster jumps of 2.3Å and intercluster jumps of 2.1Å (Fig. 6). Most surprising is the high value of the diffusion coefficient which amounts to $D_{(300K)} = 3 \times 10^{-9}$cm^2/s. To our knowledge this is by far the highest value found by neutron scattering techniques for the diffusion of a transition metal within a solid compound at room temperature.

Quantum Rotations

Rotation/Precession of NH_3 groups in Hofmann Clathrates (ILL, CNRS, ANSTO, LLB, ISIS)

Although quantum rotation of molecular species is often regarded as an excellent example of a single-particle motion several recent studies have revealed pronounced coupling effects. The temperature dependence of the j=0↔j=1 transitions of the NH_3 rotor in $Ni(NH_3)_2Ni(CN)_4.2C_6D_6$ suggest these transitions become strongly coupled to diffusive motions of the NH_3 unit as the temperature is increased [6]. At temperatures below about 4K the j=0↔j=1 transitions give rise to sharp inelastic features but as the temperature is increased these peaks develop a Lorentzian shaped foot which steals intensity from the parent peak (Fig. 7). At around 30K the inelastic peaks are almost unshifted but appear completely Lorentzian with appreciable intensity spreading beyond 1meV. The rotational constant for NH_3 is about 0.67. Any inhomogeneous broadening of the j=0↔j=1 peaks does not extend beyond this value. These observations are difficult to understand within the

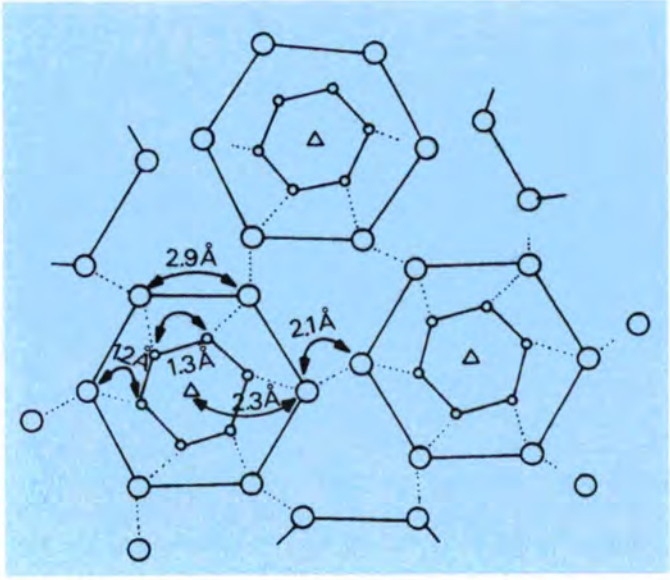

Fig. 6: Cluster of inner (o) and outer (O) Ni sites around the unit cell origin (Δ) in $Ni_2Mo_6S_8$.

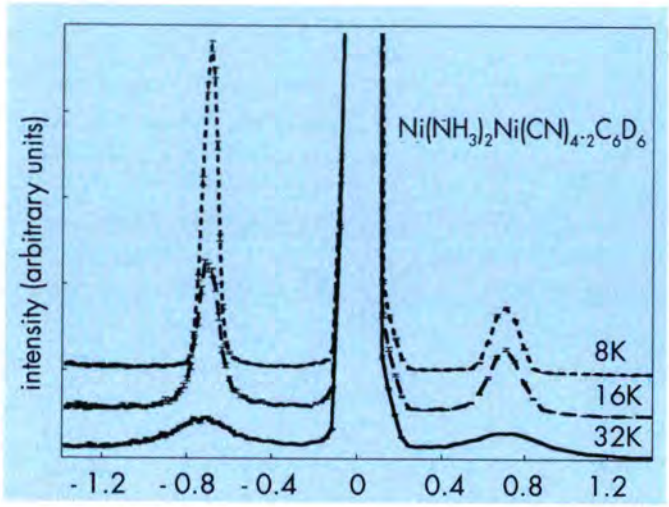

Fig. 7: Inelastic neutron spectra of the Ni_Ni Hofmann clathrate as a function of temperature recorded on the MIBEMOL spectrometer at LLB Saclay.

normal concept of free-rotation since the NH_3 rotor can only become hindered by interaction with the motions of its environment.

The low-temperature crystal structure has been redetermined [7] and the NH_3 groups occupy sites of time-averaged 4-fold symmetry due to dynamic rotational disorder. However, the INS vibrational spectrum at 20K reveals that the instantaneous NH_3 symmetry is no higher than C_s [8]. Again, this suggests considerable interaction with the environment.

A possible explanation for these inconsistencies is based on the rotation of a triangle within a square.

The sum the of the distances, r, between the three H-atoms and the four nearest neighbour atoms is constant regardless of the orientation of the NH_3 group. The total repulsive potential between the triangle of H-atoms and its 4 nearest neighbours (which form a square) can be reduced by allowing the centre of the triangle to move away from the centre of the square. During a $2\pi/3$ rotation of the H3 triangle, the position of the centre of the triangle corresponding to the minimum $\Sigma(1/r^3)$ describes a circle of radius 0.26Å around the centre of the square. Fig. 8 shows the trajectories of the three H-atoms, and the centre of the H_3 triangle, during the $2\pi/3$ rotation which follows the minimum-energy route.

All three H-atoms follow each other around the same trajectory - which now has four-fold rotational symmetry. The minima of this new rotational potential correspond to orientations where two H-atoms experience equal potentials whilst the third H-atom experiences a higher potential leading to an effective symmetry of C_s.

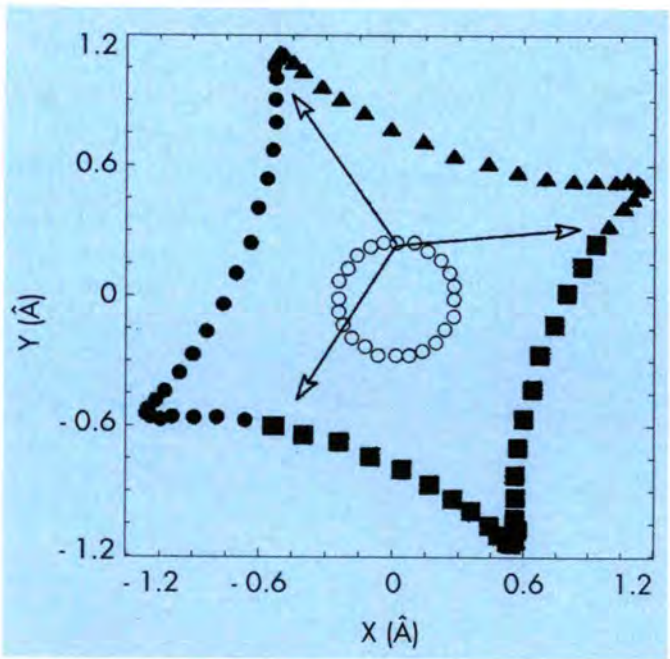

Fig. 8: Trajectories of the three H-atoms (square, triangle and filled circle) during a $2\pi/3$ rotation following the minimum energy path. The open circles show the corresponding trajectory of the centre of the H_3 triangle.

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Secretary: Gordon Kearley

Magnetic excitations in rare earth dimers. High-resolution inelastic neutron scattering

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Understanding the nature of magnetic interactions between neighbouring transition and rare-earth metal ions in insulating lattices is a prerequisite for understanding macroscopic magnetic phenomena and for the design of new magnetic materials. The area of "Molecular Magnetism" is presently very active [1]. The bridging geometry, connectivity, dimensionality, and the combination of magnetic building-blocks are systematically varied to produce compounds with novel magnetic properties. Dimers and higher clusters of magnetic ions can be considered as molecular models for a detailed study of the microscopic magnetic interactions. Co-operative phenomena arising from extended interactions do not complicate the situation in these systems, and an analysis in terms of simple molecular-models is possible.

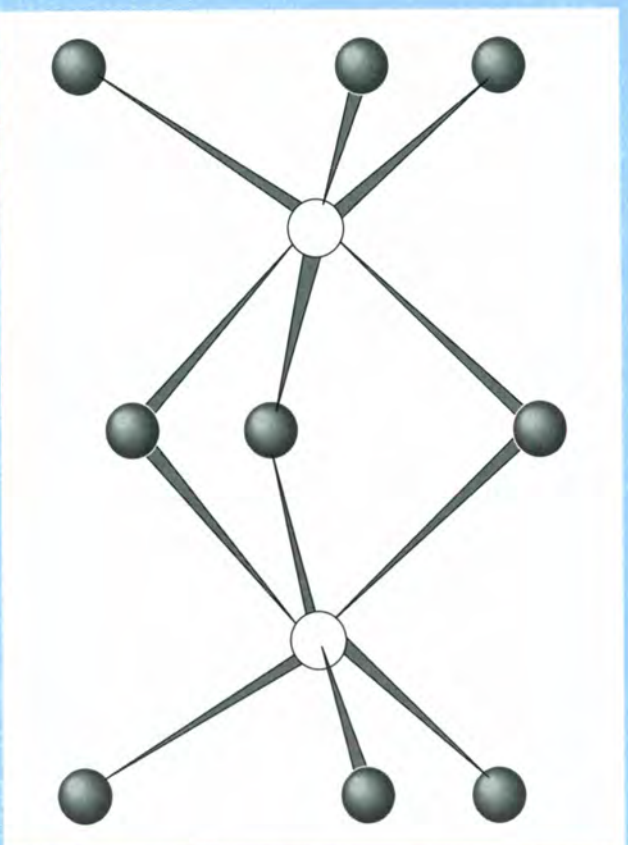

Fig. 1: Schematic illustration of the structure of the $R_2X_9^{3-}$ dimers.

We have combined high-resolution inelastic neutron scattering (INS) and optical spectroscopy to investigate transition-metal and rare-earth metal ion clusters in detail [2-6]. Here we illustrate the results obtained for rare-earth dimer systems over the past few years by presenting two selected examples. The family of compounds $Cs_3R_2X_9$ ($X = Cl^-$ Br^-; $R = Sm^{3+}$...Lu^{3+}, Y^{3+}) is ideal for such a study [7]. The $R_2X_9^{3-}$ dimers consist of two face-sharing octahedra, as shown in Figure 1. The compounds crystallize in space group $R\bar{3}c$, with the trigonal dimer-axis parallel to the crystal c axis. The compounds can be synthesized by the methods described in ref. [7]. We used the rare-earth oxides as starting materials and transformed them to halides either with HX or with NH_4X. Mixed crystals can be prepared, and by using $Cs_3Y_2X_9$ as a host, the single-ion properties of the R^{3+} ions can be studied for comparison. On the other hand, trivalent transition-metal ions T^{3+} can be incorporated into the structure, thus producing mixed R^{3+}-T^{3+} dimers.

Figure 2 shows INS spectra at 5.8K of polycrystalline $Cs_3Yb_2Cl_9$ and $Cs_3Yb_2Br_9$ measured on IN6 [6]. One prominent inelastic peak is observed for both compounds in energy loss and energy gain. The peak energies are 3.25(3) cm^{-1} and 3.00(3) cm^{-1} in the chloride and bromide, respectively. Since Yb^{3+} in an octahedral coordination has a well separated Kramers doublet ground state, the most simple theoretical model can be used for the intradimer exchange interaction: coupling of two Kramers doublets. Both a Heisenberg and an Ising

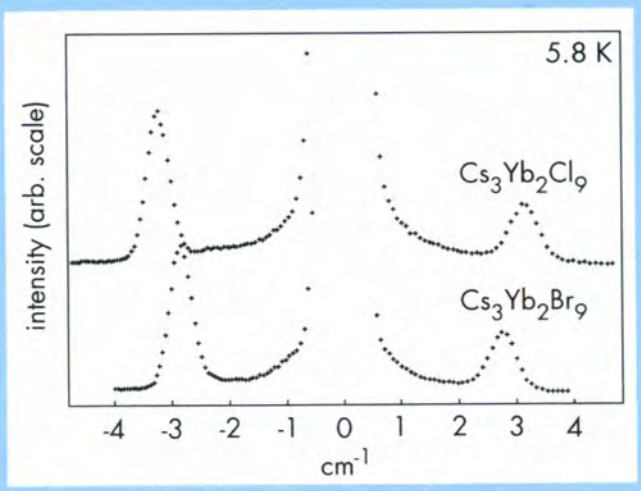

Fig. 2: Inelastic neutron scattering spectra of polycrystalline $Cs_3Yb_2Cl_9$ and $Cs_3Yb_2Br_9$ at 5.8 K. Conditions: instrument IN6, sum of all scattering angles, wavelength 5.9 Å. (From ref. 6).

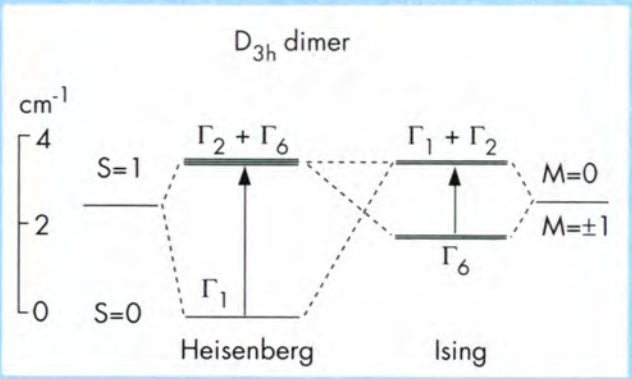

Fig. 3: Energy splitting of two exchange-coupled Kramers doublets according to eqs. (1) and (2). The dimer levels are designated in the D_{3h} dimer point group.

model split the ground state into two dimer levels, whereas an XY model produces three dimer levels with equidistant energies. The Heisenberg and Ising interactions for a dimer can be written as:

$$\text{Heisenberg: } \hat{H}_{ex} = -2J\vec{S}_1 \cdot \vec{S}_2 \quad (1)$$

$$\text{Ising: } \hat{H}_{ex} = -2J^z \hat{S}_1^z \cdot \hat{S}_2^z \quad (2)$$

The corresponding splitting pattern for antiferromagnetic coupling is shown in Figure 3 with the designation of dimer levels in D_{3h} notation. The arrows indicate the allowed INS transitions.

In order to distinguish between the Heisenberg and the Ising case we have to consider intensities, in particular their dependence on the scattering vector Q. It can be shown that the Q-dependence of the signal from the dimer excitation in the Heisenberg and Ising models is given by [6]:

$$\text{Heisenberg: } I(Q) \sim F^2(Q)\left[1 - \frac{\sin QR}{QR}\right] \quad (3)$$

$$\text{Ising: } I(Q) \sim F^2(Q) \quad (4)$$

F(Q) is the magnetic form-factor and the square bracket in eq. (3) represents a so-called interference term [8]. This factor is very typical of dimer excitations, and it reflects the separation R of the two magnetic ions in the dimer. Since this factor tends to zero as Q approaches zero, it is very important to measure intensities down to the lowest Q values. We used IN5 for these measurements. The experimental results are compared with the functions (3) and (4) in Figure 4. The intensity of the inelastic peak disappears as Q approaches zero, the behaviour expected for a S = 0 → S = 1 dimer excitation in the Heisenberg model (eq. 3). The size of the singlet-triplet exchange splitting is remarkable for a rare-earth system. Using the Hamiltonian (1) we get:

$2J = -3.25\ cm^{-1}$ for $Cs_3Yb_2Cl_9$

$2J = -3.00\ cm^{-1}$ for $Cs_3Yb_2Br_9$ (5)

We attribute these high values of the exchange parameters to the close proximity of the Yb^{3+} ions in the dimer, resulting in a relatively strong overlap of the relevant magnetic orbitals. The difference of approximately 10% between $Cs_3Yb_2Cl_9$ and $Cs_3Yb_2Br_9$ is reminiscent of exchange coupled transition-metal ion systems with face-sharing octahedra.

In the next example, $Cs_3Dy_2Br_9$, we investigate the exchange splitting of the lowest-energy crystal-field (CF) excitation [9]. Its energy is determined in the diluted $Cs_3Y_2Br_9$:10%Dy sample, and Figure 5a shows the corresponding region in the 1.5K INS spectrum

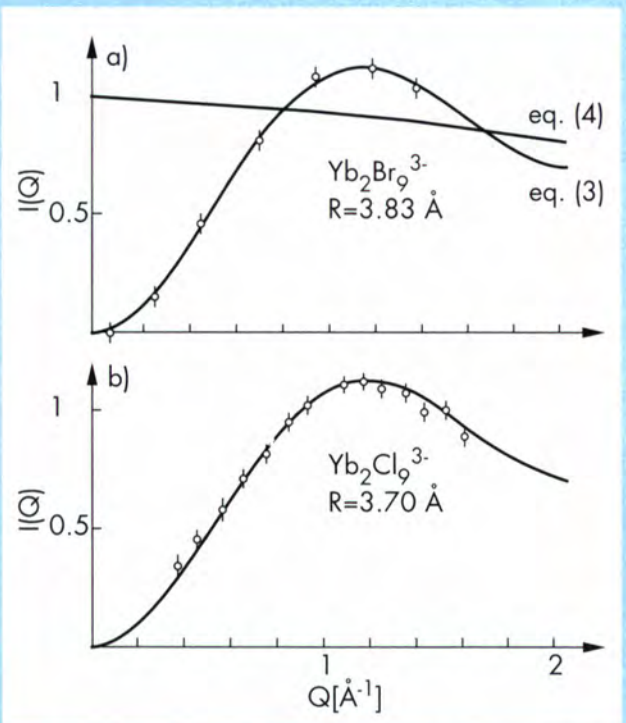

Fig. 4: Observed (circles with estimated error bars) and calculated (thin lines) INS intensity of the singlet-triplet excitation as a function of Q. The thick lines are fits of eq.(3) with a scaling factor as an adjustable parameter. The function 4 is included in (a) for comparison. (Adapted from ref. 6).

measured on IN5, with a single peak at 15 cm^{-1}. Figure 5b shows the same CF excitation in the undiluted $Cs_3Dy_2Br_9$. The effect is dramatic. Instead of a single line we observe a highly structured spectrum covering the energy-range from 10 cm^{-1} to 17 cm^{-1}. At least four components are resolved, and for a full analysis we need their temperature-dependence and their Q-dependence. Both the ground and the first excited CF states are split by exchange interactions. In addition to the transitions shown in Figure 5, we observed a transition between two exchange-split levels of the ground state at 0.65 cm^{-1}, exhibiting the same Q-dependence as the $Yb_2Br_9^{3-}$ excitation presented in Figure 4. Using all the observed INS data, supplemented by high-resolution optical spectra, we obtained the empirical energy-level scheme shown in Figure 6a. For an analysis of the relative INS intensities and their Q-dependence, the appropriate cross-section formulae were derived.[3]. The computed energy-level scheme shown in Figure 6b was obtained by diagonalizing the Hamiltonian:

$$\hat{H}_{Dimer} = \hat{H}^1_{CF} + \hat{H}^2_{CF} + \hat{H}_{ex} \quad (6)$$

where $\hat{H}^1_{CF}$ and $\hat{H}^2_{CF}$ describe the crystal-field splitting of the two Dy^{3+} ions and $\hat{H}_{ex}$ is a Heisenberg exchange operator with 2J = -0.05 cm^{-1}. The calculated energies and relative intensities are in good agreement with the data. It is not obvious that this splitting corresponds to the Heisenberg model. In the ground state we do not have a simple singlet-triplet splitting as in $Yb_2Br_9^{3-}$ because of the proximity of the other CF states. In the excited state we have a total of eight dimer-levels. The reason for this doubling with respect to the ground state that either of the two Dy^{3+} ions of the dimer can be in the excited CF state. The proper dimer wave-functions are thus given by:

$$\Psi \pm = \frac{1}{\sqrt{2}} \left(\Phi_1^{GS} \Phi_2^{ES} \pm \Phi_1^{ES} \Phi_2^{GS} \right) \quad (7)$$

The magnetic ordering in Dy^{3+} compounds with extended interactions can often be interpreted in terms of an Ising model [10]. This is usually attributed to a highly anisotropic g-tensor of Dy^{3+}. In our $Dy_2Br_9^{3-}$ dimer the observed behaviour cannot be reproduced by an Ising model. In the analogous $Ho_2Br_9^{3-}$ dimer, on the other

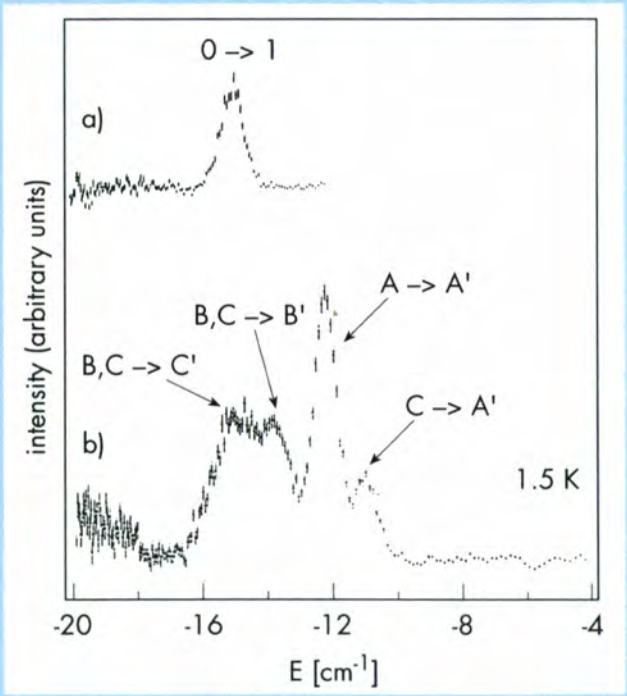

Fig: 5: Inelastic neutron scattering spectra of polycrystalline $Cs_3Y_2Br_9$ 10% Dy^{3+} (a) and $Cs_3Dy_2Br_9$: (b)) Instrument IN5, wavelength 4.8 Å.

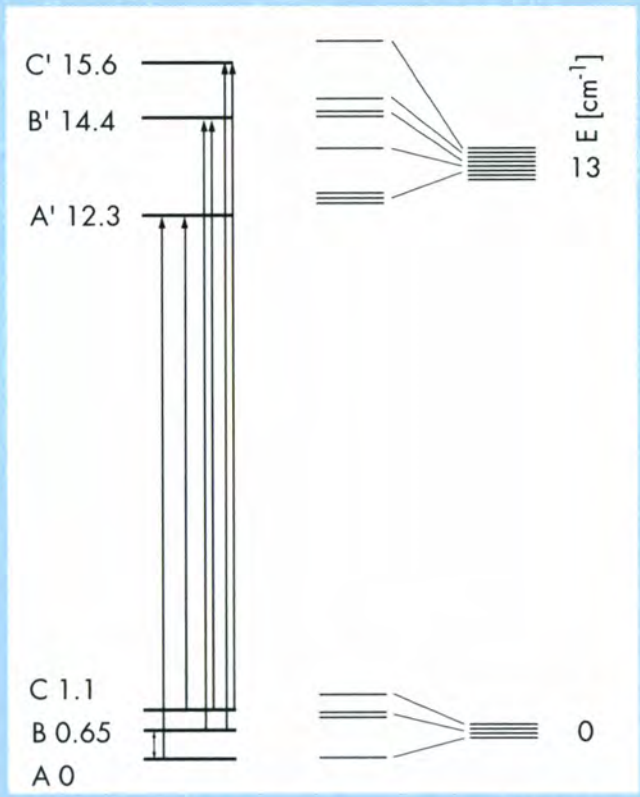

Fig. 6: Exchange splittings of the first two crystal-field levels in $Cs_3Dy_2Br_9$.

a) Experimentally determined splitting using INS. The arrows correspond to the observed transitions.

b) Calculated splitting using eq.(5) with a Heisenberg exchange Hamiltonian and 2J = -0.05 cm^{-1}.

hand, the Heisenberg model was found to be inadequate and a tensor formalism was used to account for the observed INS data [11].

The direct observation of exchange-splittings in the lowest CF states by high-resolution INS and optical spectroscopy of $Cs_3R_2X_9$ dimer compounds has led to a better understanding of the nature of the magnetic coupling between neighbouring rare-earth metal ions in insulating lattices. Accurate values for the exchange parameters can be directly derived from the data.

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Large molecules

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B. Farago
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C. Lartigue (CNRS)
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External members

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C. Poinsignon (UJF)
D. Quenard (CSTB)
P. Terech (CENG)

Scientific activities of some college members have continued outside the ILL in 1993. Bernhard Frick was on leave at NIST for 1 year where he did tests at the backscattering spectrometer and measurements with glasses using triple axis and TOF instruments; he returned to ILL in July 1993. During the last two years Bela Farago spent half of his time at LLB where he was putting into operation the neutron spin echo experiment; he is back since January 1994. Pierre Terech returned from a stay at NIST where he was working in the polymer division from August 1992 to February 1993; he left ILL in spring 1993 and took up a position at CENG. Peter Lindner did various SANS experiments at LLB Saclay and at Risø National Laboratory. Colette Lartigue who worked for two years at the University Joseph Fourier, Grenoble, came back to the ILL in January 1994.

Scientific Highlights

Cold neutron diffraction by volume phase holograms for the study of light-induced reactions in photopolymers

Photosensitized PMMA slices of 2 mm thickness were prepared from a fluid deuterated MMA ($C_5O_2D_8$) monomer, a thermal initiator and a photo-initiator. If the mixture is kept for 15-20 h at 50°, an uncompleted thermal polymerization takes place which supplies the three essential constituents of the polymeric material for the storage of volume phase holograms: about 90% of the polymer PMMA; 10% of the monomer MMA; and the photo-initiator.

So far, little direct evidence is available about the mechanism which results, upon illumination, in the modulation of the light-optical and the neutron-optical refractive indices. Our speculations are the following: the PMMA molecules can be considered as chains of monomer units linked by chemical bonds and forming a nearly static matrix. Within this matrix the free monomer molecules can move around. One chain unit has the same coherent scattering length as a free monomer molecule itself, because it consists of the same nuclei. The relevant difference between free monomer molecules and monomer units in the polymer chain is the fact that the first are mobile and the latter not. If some region of the block is illuminated, the photo-initiator is activated and starts the growth of polymer chains from the residual monomer molecules. This means that mobile scattering units, which come along by the random walk of the diffusion process, are trapped in illuminated regions. To support this process the samples are heated to temperatures of 50°C for several hours after illumination. The photo-induced polymerization obviously provokes a change in the number density of the scattering units [1].

All experiments have been executed using permanent holograms which have been prepared by using the holographic set-ups in Osnabrück. The installation of such a set-up at the sample position of D11 would allow us to follow up the structural changes during the writing process; and the decay of the density modulation in any photosensitive material as a function of a number of interesting physical parameters, as temperature, light- and UV-illumination, etc. A conceptual design of such an installation is in preparation.

Fig. 1 shows the diffraction probability for the 1st peak of diffraction versus angle of incidence of the neutron beam. The neutron wavelength was 1 nm, and the grating period was 249.2 nm. No changes in reflectivity could be detected after 6 weeks; after 4 months, however, the reflectivity was diminished by more than two orders of magnitude.

Our artificial thick gratings exhibit cold neutron diffraction properties which are comparable to those of monochromator crystals for thermal neutrons. One of the possible neutron-optical applications became already important in the context of the calibration of the new neutron small-angle camera at the HMI in spring 1993.

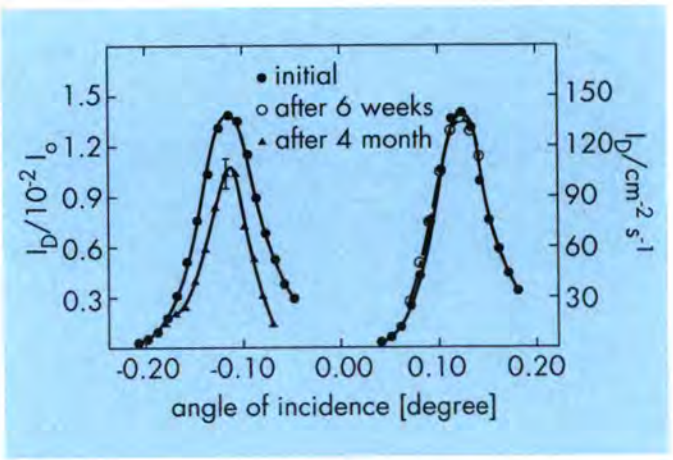

Fig. 1: Diffraction from a 1.8 mm thick sample of D-PMMA: DMDPE containing a Laser-generated hologram. I_D and I_0 are diffracted and incoming intensity, respectively.

Similar gratings were prepared in undeuterated PMMA. It has been shown in December 1993 that gratings of up to 1600 nm lattice constant can be used to calibrate the Bonse-Hart camera at ESRF [2].

2D-Melting of a Langmuir Monolayer investigated by Neutron Reflectivity

The melting and crystallization of monolayers of fatty alcohols at the air-water interface has recently been investigated using grazing incidence diffraction of synchrotron radiation. For the series of 1-alkanols ranging from $C_9H_{19}OH$ (T_{m2D}=2°C) to $C_{16}H_{31}OH$ (T_{m2D}=67°C). these experiments have provided detailed information on the 2D crystalline structures but nothing on the properties of the liquid phase which ought to be determined for a better comprehension of the thermodynamics of the 2D melting process.

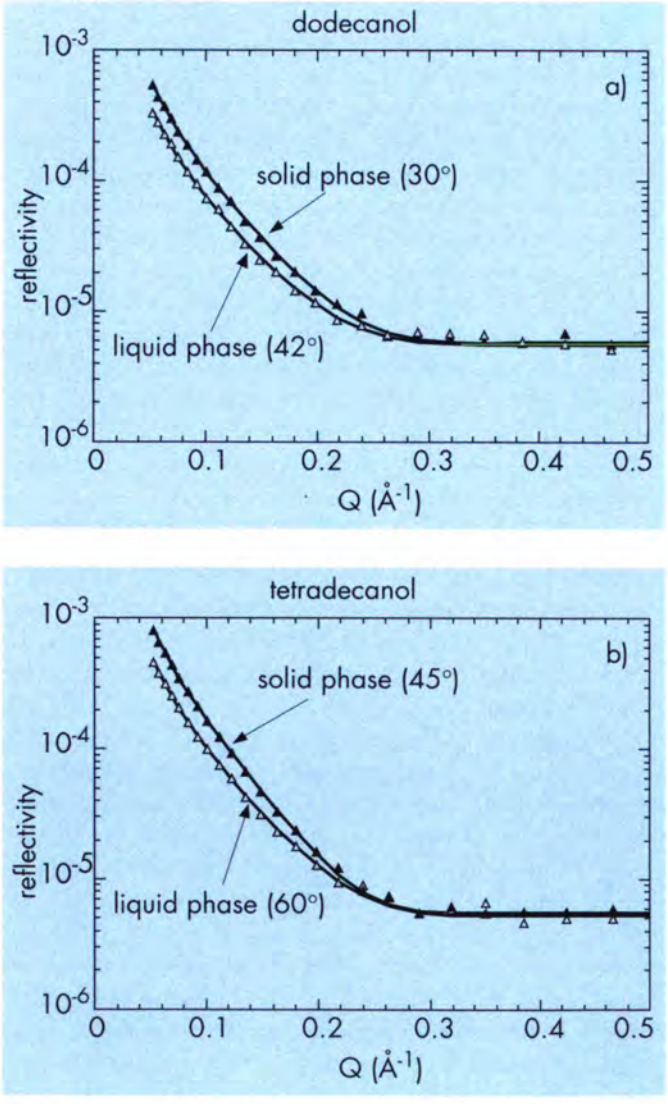

Fig. 2: Neutron reflectivity of monolayers of deuterated fatty alcohols at two temperatures on both sides of the 2D melting point (a) $C_{12}D_{25}OH$, (b) $C_{14}D_{29}OH$.

Spreading monolayers of perdeuterated 1-alcohols on top of null-reflecting water, their changes in thickness and density could be determined using the time-of-flight reflectometer CRISP at the neutron spallation source ISIS. Due to the relatively short length of these chain molecules, we have explored a Q-range up to 0.5 Å^{-1} (with an incidence angle of 1.5 deg).

Fig. 2 shows the changes in neutron reflectivity occuring at 39 °C for 1-dodecanol and at 55°C for 1-tetradecanol [3]. The fitted curves (solid lines) show that the surface area per molecule increases by about 30% at the melting temperature due to decreases of both the thickness and the density of the monolayer.

Local dynamics in polymer glasses

Side group and main chain deuterated and fully protonated *atactic polystyrene* of high molecular weight was investigated by time-of-flight and backscattering in a wide temperature range around the glass transition temperature (T_g=375K). In the glass an inelastic low frequency excess scattering over the Debye contribution is observed [4,5] which shows a weak effect on isotope substitution, i.e. is shifting towards lower frequencies for deuterated phenylrings. The dynamic response changes towards a more quasielastic spectrum at already 200K below the glass transition T_g. A partial deuteration of the samples allows the conclusion that the phenylring dynamics changes at these temperatures. This can be seen from Fig.3, where the calculated mean squared displacement is shown as a function of temperature. Clearly the fully protonated sample shows higher values of $\langle u^2 \rangle$ above about 150K. This has its correspondence in the low frequency scattering which is observed in this temperature regime below an energy

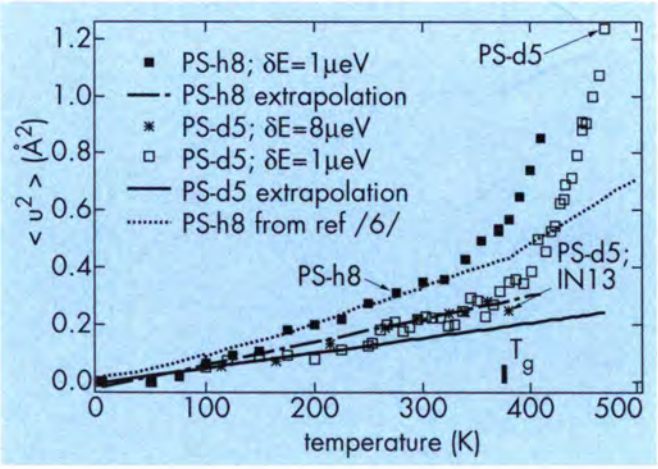

Fig. 3: Mean squared displacements for PS-d5 and PS-h8 calculated from the Q-dependence of the elastic scattering up to 2Å^{-1} and with 1μeV energy resolution from IN10 data. The two straight lines are low temperature extrapolations of the mean squared displacement. Data for PS-d5 measured on IN13 (*) are shown for comparison.

transfer of about 1.5 meV. If the temperature is increased further close to T_g, then the low frequency relaxation process, which is well known for very different types of glasses, is observed to set in very rapidly. Thus two different dynamic regimes are detected in polystyrene.

Another example where the side group dynamics of a polymer could be separated from the main chain dynamics using partially deuterated samples is polyisoprene. The dynamics of the methyl side group had been detected far below the glass transition applying the fixed window technique on IN10 and IN13 [6]. The first decrease of the elastic scattering shown in Fig.4 is ascribed to the methyle group dynamics and it levels off before, near the glass transition temperature, a second decrease appears which is related to the fast glass transition relaxation process. Model calculations for methyl group jump models reveal that only a distribution of relaxation times or activation energies, having its origin in the local disorder, can explain the relatively slow intensity decay with temperature.

Flow enhanced concentration fluctuations in sheared, semidilute polymer solutions

Using light scattering and SANS with various scattering geometries (different beam paths with respect to the shear gradient direction) and shear flow geometries (Couette or cone-and-plate), it has been observed by several groups that the scattering intensity of a *semidilute* polymer solution is strongly increased by shearing the system. Flow enhanced concentration fluctuations have been found to be either anisotropic with respect to the flow direction or to be isotropic. A debate is centred around the question whether shear induces a shift in the cloud point of the solution or whether the concentration fluctuations in the entangled polymer system are amplified and distorted by other mechanisms, *without* a shift in the critical temperature for phase separation.

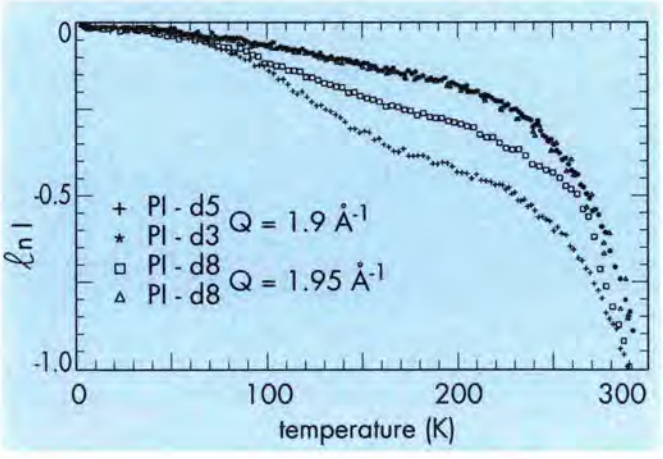

Fig. 4: Elastic scattering as a function of temperature as observed on IN10 for differently deuterated polyisoprenes. The first relaxation step corresponds to the rotational dynamics of the methyl groups and the second step corresponds to the onset of a fast dynamic process near the glass transition.

Figure 5 (page 140) shows one of the results of recent shear experiments performed at the SANS instrument PAXY at LLB [7] with a semidilute solution of perdeuterated polystyrene in the solvent di-octylphthalate (DOP) at a concentration 9% w/ w. DOP is a theta solvent for polystyrene at a temperature of T ≈ 22°C. These SANS experiments have been performed at different shear gradients $\dot{\gamma}$ in the "strong shear" regime (Weissenberg number $Wi = \dot{\gamma}\, t_c >> 1$, with t_c being the longest relaxation time of the system). Variation of the temperature, as a further parameter, allowed tuning of the solvent quality; hence, different regions of the phase diagram of the polymer solution were explored, ranging from poor solvent conditions at T=15°C in the vicinity of the phase boundary, across the theta region around T=22°C to the good solvent regime at T=50°C.

At rest, an azimuthally isotropic scattering pattern is observed. Under shear, the pattern (see Fig. 5) becomes slightly anisotropic at large momentum transfer q, with a long axis perpendicular to the flow direction. At low q, closer to the beamstop, a pronounced increase *parallel* to the flow direction leads to a double winged shape of the pattern which ressembles closely the "butterfly patterns", also observed in deformed gels, rubbers as well as in polymer melts. The effect is increasing with increasing shear. Compared to the measurements in the theta region, it is in the good solvent regime (T=50°C) smoother but still visible. At temperatures below T=22°C, however, when approaching the two phase region, a strong isotropic increase of the scattering intensity is observed which superimposes on the "butterfly" pattern.

Fig. 6 shows the radial intensity distribution, corresponding to the raw data shown in Fig. 5 in directions parallel and perpendicular with respect to the flow direction. In perpendicular direction, the differential scattering cross section $(d\Sigma/d\Omega)_\perp$ of the sheared *semidilute* solution remains within the statistical error identical to the isotropic scattering at rest ($(d\Sigma/d\Omega)_{iso}$), as being observed already with sheared *dilute* solutions and with melts. On the contrary, a pronounced increase of the differential scattering cross section in parallel direction, $(d\Sigma/d\Omega)_\parallel$ is observed at the lowest q values. In the theta regime at temperatures around T=22°C and in the good solvent regime at T=50°C (data not shown here), this increase in parallel direction can be approximated by a power law of $q^{-1.6}$. At larger values of the momentum transfer q, however, the intensity in parallel direction is lower than in perpendicular direction and at even higher q the anisotropy vanishes.

A possible theoretical explanation considers disinterpenetration of an assembly of regions of higher concentrations and regions of lower concentrations in the solution [8], as proposed for the description of percolation

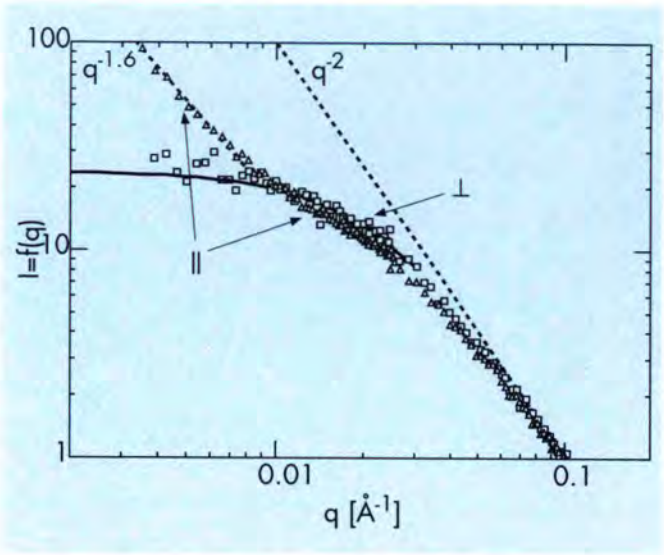

Fig. 6: Differential scattering cross section $d\Sigma/d\Omega=f(q)$ of polystyrene in sheared semidilute solution following from the raw data shown in Fig. 5. Evaluation in the directions perpendicular (⊥) and parallel (||) with respect to the flow direction. The continuous line corresponds to the scattering of the solution in the quiescent state.

clusters of regions of high crosslinking ratio after random crosslinking of a semidilute solution, which is well suited to predict the "butterfly" effect in uniaxially deformed swollen gels. The deformation in the parallel direction acts as a dilution of the high concentration regions (harder) inside the low concentration regions (softer). These regions may be highly "interpenetrated" in the *quiescent* state, i.e. their screening length ξ (observable by scattering) is much smaller than their maximum size. Dilution, as equivalent for instance to shear in || - direction, will increase the "visible" size of the clusters. However, the sheared semidilute solution is entangled but not crosslinked. This is similar to the case where free mobile labelled chains are embedded in a stretched matrix: "butterfly" effects are observed when the matrix is crosslinked, as well as when it is a melt of long chains, which are just entangled. In stretched gels a power law of $q^{-1.6}$ at low q is both observed and predicted; it is apparently observed also in the case of the sheared semidilute solution as described above.

Secretary: Peter Lindner

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– DIRECTORATE – SERVICE

Public Relations

During 1993 the ILL saw the visits of two outstanding personalities:

Professor Georges Charpak

The Nobel Prize winner, Professor Georges Charpak, spoke at the joint ILL-ESRF Colloquium on 31 March 1993. He received the prize in 1992 for his invention and development of detectors in the field of high-energy physics.

Professor Charpak has been a member of the Instrument Subcommittee of the ILL's Scientific Council.

Since 1959 he has worked at CERN where he invented the multiwire proportional chamber. This work was published in 1968 and led to the development of different kinds of multiwire detectors.

In parallel, a technology of 2-dimensional multidetectors for neutrons has been developed in collaboration by LETI-ILL (Patent, April 1968, R. Allemand, J. Jacobé, E. Roudaux) followed by industrial production.

A new improvement has been developed at the ILL by using a technique of micro-strips deposited on glass plates (Patent July 1986, A. Oed), which increases the counting capacity and the 2-dimensional spatial resolution of such detectors.

Dr. Gerhard Stoltenberg

On 15 September 1993, Dr. Gerhard Stoltenberg from the Auswärtiges Amt in Bonn, accompanied by Hans von Hengstenberg, Generalkonsul der Bundesrepublik Deutschland in Lyon, visited international research institutions with German collaboration in Grenoble: the ILL, ESRF, EMBL, IRAM and the High Field Magnet Laboratory.

Dr. Stoltenberg signed the first German/French Convention for the foundation of the ILL on 19 January 1967 in his then capacity as Bundesminister für Forschung und Wissenschaft.

Volker Knoerich, Ministerial-Dirigent in the BMFT/Germany, also took part in the guided tours.

The lunch in the ILL-ESRF joint restaurant provided the opportunity for G. Stoltenberg to meet personalities from Grenoble public life: Joël Gadbin, Préfet de l'Isère; Jean-Paul Watteau, Recteur de l'Académie de Grenoble, Chancelier des Universités; Alain Nemoz, Président de l'Université Joseph Fourier, Grenoble; François Gillet, Directeur du Pôle Européen Universitaire et Scientifique; Joël de Leiris, Maire-Adjoint de Grenoble, chargé des Relations Internationales, des Universités et de la Recherche.

During the press conference concluding his visit, G. Stoltenberg expressed his strong impressions on the effective and intense scientific collaboration between Germany and France and also at the European level in the Grenoble region. He noted that this fruitful collaboration merits greater support by the German and French Governments.

As in 1992, the ILL participated in "La Science en fête", initiated by the French Ministry of Education. Many research laboratories from the Grenoble region manned stands side by side in Place Victor Hugo in the centre of Grenoble for three days, 4 to 6 June. The ILL-ESRF joint stand was a great success. Directors, scientists and engineers explained in personal discussions the activities of the ILL to the public.

During the "Semaine Européenne de la Culture Scientifique" (basically organized by the ESRF) the ILL participated in the European Press Day on 23 November, on the ILL-ESRF-EMBL joint site. An international press conference was held in the morning followed by guided tours to the institutes in the afternoon. Several publications appeared afterwards.

Bernd Maier, Scientific Secretary, took early retirement in June 1993. Since the first activities of the ILL, he was responsible for scientific coordination of the users' programme and for public relations. Assisted by Gerry Briggs and later by Herma Büttner he created a well organized office. He produced many brochures and leaflets about the ILL and regularly promoted articles in the press

on the scientific achievements of the ILL. The ILL Annual Reports produced by B. Maier were of high professional standard and greatly appreciated by the readers. His heart was devoted to the well-being of the Institut.

Since July 1993, with the new organization, H. Büttner is head of the Scientific Support Group in the Science Division, which includes scientific coordination.

The public relation activities were taken over by B. Dorner for scientific matters. He remains a member of the TAS Group in DS and is instrument responsible for IN1. As far as technical aspects and relations with local public authorities are concerned J. F. Veyrat, head of the Safety, Medical and Health Physics Group, is in charge.

Bruno Dorner
Scientific Secretary

Safety, Medical and Health Physics Group

Health Physics

1993 has been another year during which the work of the Health Physics Service has been closely connected with the work in the reactor.

Individual Dosimetry monitoring, checking the radioactivity of all the equipment dismantled in the reactor, evaluation of the active items to the radioactive waste disposal.

Amongst this work, one operation has required the most effort from the Service.

- The cleaning and decontamination of the reactor swimming pool so as to provide satisfactory environmental conditions for personnel working on the new reactor vessel. The results were excellent, so that staff can work normal hours in the pool.

Safety

Various measures have been taken:

- To decrease the number of industrial accidents;
- To follow up the safety of the work on the reactor: preparation of safety plans;
- For the Safety Unit, a major project has been monitoring the external and internal painting of the Reactor Building;
- Training ILL staff on safety (fire extinguishers, handling, electricity, first aid practice, etc);
- As the Head of Safety, Medical, Health Physics and Environment (D.SPSE) is now also in charge of problems relating to the environment, efforts have been made to introduce a better system for collecting waste (used oils, metals, papers, etc.).

Joint Works Medical Service

In addition to medical surveillance of ESRF and ILL staff, the Joint Medical Service has directed its activities to an enquiry of staff working on computer screens and risks connected to conditions of work, particularly back problems.

The Joint Medical Service is fully operational in its new premises in ILL 17.

Jean-François Veyrat

– SCIENCE – DIVISION (DS)

How is science surviving in the third and last year of neutron drought? In normal conditions an ILL scientist often had to restrict his activities because as a local contact he had to deal also with the instrumental and technical aspects of an experiment. Now many have found the time to delve deeply again into scientific problems, to go back to previous experiments, to treat more complex data. Results were put in order and collated. Quite a number changed roles: they travelled as users to Orphée, ISIS, HMI, Prague, Brookhaven, NIST, Australia, and Japan and came home with new results. We express our gratitude to those research centres which welcomed our scientists for visits or even longer periods. A few scientists managed to escape their "neutrons-only" world and got acquainted with other research methods such as synchrotron radiation, muons or even material characterisation in an industrial environment. Some scientists replaced neutrons by computer simulations.

The sudden neutron drought was of course most dramatic of all for our thesis students. Without neutrons and with a supervisor who might have left for another continent they sometimes had to pass an independence test. They often found neutrons elsewhere and changed their subjects to some extent. I am happy to say they all made it.

Recently quite a few were busy tackling the n-body problem, whether the current reorganisation was a 1st or 2nd order phase transition, as it shows features of both: it needs energy but it exhibits critical fluctuations. In the new Science Division, the reorganisation mainly concerns the instrument groups which comprise all the experimental scientists and instrument technicians. These groups are responsible for further improvement of experimental methods and particularly the development, maintenance and operation of our instruments. Development of experimental techniques and instruments has always been one of the strong points of the Institut, a tradition which we want to keep alive in the future. This effort will be based on both the DPT and DS divisions. While major instrument projects are completely handled within DPT, the initiation of studies (PIAFE), smaller projects (Laue Detector and ^{3}He polariser) or even a bigger project like GAMS5 are dealt with in DS.

The attentive reader may note that the traditional separation of the annual report into reports from colleges and instrument groups has survived the reorganisation. The ILL's scientific life will continue to be organised with a minimum of regulations and a maximum of liberty within the colleges. Being in a one-to-one correspondence with the sub-committees, the colleges are also the natural connection to our user community.

Reinhard Scherm

Scientific Coordination Office

The office helped in the organisation of several workshops in 1993, which were held at the ILL. The list is as follows:

Workshop	Organisers
"Neutrons & X-rays in the Study of Magnetism" **Dates** 21-23 January 1993	G.H. Lander, (EITU Karlsruhe), W.G. Stirling, (Keele), C. Vettier (ESRF), J. Martinez (ILL/Madrid), P.J. Brown (ILL)
"Memorial Colloquium" Walter Mampe **Dates** 29 January 1993	M. Pendlebury
"Dynamics of Disordered Materials II" **Dates** 22-24 March 1993	A.J. Dianoux, W. Petry (ILL), D. Richter (Jülich)
"Quasicrystals" **Dates** 2-4 June 1993	C. Janot
"Progress in Gaseous Microstrip Proportional Chambers" **Dates** 21-23 June 1993	P. Geltenbort

Because of the reactor shutdown the ILL scientists and thesis students had to apply for beam time at other research centres. The ILL gave financial support to some 70 experimental visits to the following research centres: LLB Saclay (F), LURE Orsay (F), ISIS Didcot (GB), PSI Würenlingen (CH), HMI Berlin (D), GKSS Geesthacht (D), PTB Braunschweig (D), NIST Gaithersburg (USA), BNL Brookhaven (USA), Chalkriver (Canada), JAERI Tokai (Japan), KEK Tsukuba (Japan). The most frequently visited research institute was LLB Saclay.

Within a special agreement between JAERI (Japan) and the ILL, four ILL scientists were invited to work for several months at the JRR-3M reactor in Tokai. Travel and living expenses were covered by the JAERI Foreign Researcher Invitation Programme.

Joint ILL-ESRF Library

Librarian: Christine Castets

1993 Scientific Literature Budget: 1348.2 KFF, Excl. Taxes

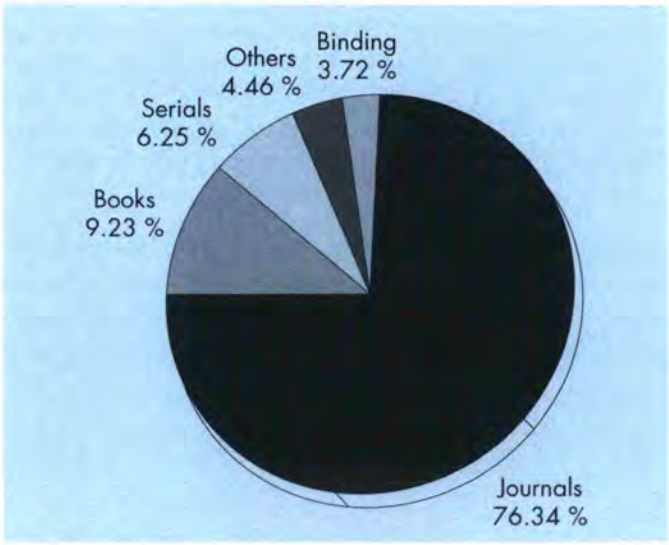
ILL Share : 57.5% = 775.2 KFF, Excl. Taxes

In 1993, the 10 % increase in literature budget as planned in the "Agreement for the Operation and Maintenance of a Joint ILL-ESRF Library" allowed the library to operate in good conditions and even to improve the service to users:

- It was possible to maintain the journals previously subscribed to, despite the continuing increase in their costs, and even to take out some new subscriptions.
- Book acquisition was increased by 10% compared with 1992
- Several CD-ROM data bases could be purchased and installed.

During 1993, the effort was concentrated on backlog cataloguing expected to be completed in July 1994: 3300 new entries were registered thanks to equal additional help from ILL and ESRF.

Allocation of literature costs in 1993.



- 1045 books were processed, of which 622 were additional copies of existing books:
  - 396 books for ESRF Departments or Divisions
  - 100 for ILL Departments or Divisions
  - 549 for the Joint Library (500 in 1992)
- 900 volumes of journals were bound.

A CD-ROM station "libre service" was installed in the reading room making it possible to load up to a total of 12 discs.

This is a major improvement in the service to users since scientists can now search directly and at any time the following data bases:

- INSPEC-On Disc Physics (Physics Abstracts), 1989-1993, 5 discs loaded permanently
- Medline, 1982-1993, 14 discs of which 6 loaded
- ISI Science Citation Index, 1993, one disc loaded

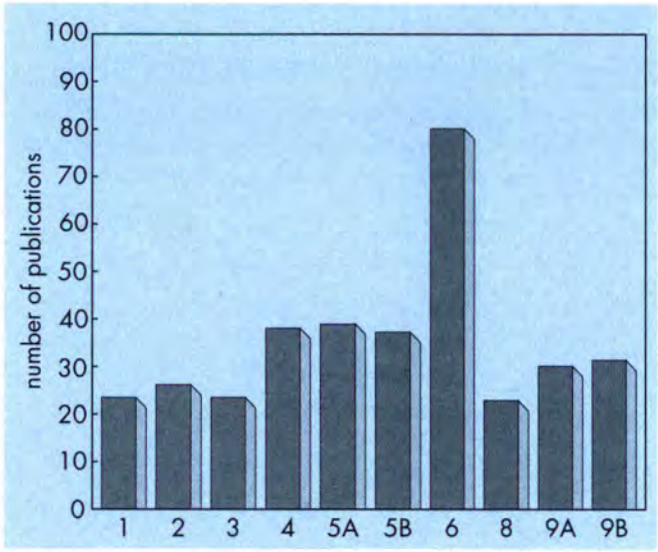
The most used is of course INSPEC.

Current Contents on Diskette with Abstracts (Physical, Chemical and Earth Sciences) installed on the network since 1992 remained a useful tool for current bibliographic searches.

Publication files of ILL and ESRF were transferred onto the LORIS/DORIS system of the library.

Publications:

For the ILL, 339 publications were received (compared with 600 in 1992).



Publications received in 1993 by subject:

1 - Instruments and Methods
2 - Theory
3 - Fundamental and Nuclear Physics
4 - Excitations
5a- Crystallographic Structures
5b- Magnetism
6 - Liquids, Disordered Materials
8 - Biology
9a- Chemistry- Small molecules
9b- Chemistry- Colloids and Polymers

Herma Büttner

Nuclear and fundamental physics (NFP) Group

PN1 Fission product separator LOHENGRIN on beam tube H9 (H.R. Faust, G. Fioni, I. Gartshore)

PN3 Curved and flat crystal spectrometers GAMS2/3, GAMS4, GAMS5 (project) on the through-tube H6 - H7 (H. Börner, A. Williams, R. Oliver)

PF1 Cold polarized beam at the end position of guide H53 (J. Last, U. Mayerhofer, R. Bender)

PF2 Ultra-cold neutron source and distribution system on level D using the vertical guide from the cold source and neutron turbine (W. Drexel, P. Geltenbort, H. Just)

PN1 Fission product separator

The installation of the reverse energy dispersion (RED) magnet, which will provide a substantial reduction of the background and an increase of up to a factor of 7 in the counting-rate of the Lohengrin spectrometer, was completed. The support frame was designed and manufactured. It was mounted on an air-pad system to provide easy positioning of the magnet and to give the possibility of having access to the old focal plane.

The exit section of the spectrometer was considerably modified: the beam tube was shortened by 25 cm, the vacuum valve replaced and two additional diaphragms were added. In the direction perpendicular to the Lohengrin parabola, the size of the beam can be varied (maximum opening 5 cm) with a rotating cylinder driven by an electric motor and remote-positioned by a PC. Thirteen shutters each of them about 3 cm wide and remote-pneumatically operated, give the possibility of sampling the 40 cm of the Lohengrin parabola. The combined use of both diaphragms is essential in the tests of the modified ion-optics of the spectrometer and for experiments requiring a very high-purity beam.

The experimental area and the data acquisition and control rooms underwent significant improvements: a false floor was laid down and a suspended ceiling was mounted to provide a better working environment. The electronics used to control the instrument was re-cabled to assure an easier maintenance.

PN3 Gamma ray spectrometers

The upgrade of the GAMS2/3 spectrometer (München-ILL collaboration) is nearly completed. The new optical interferometers are assembled and aligned with respect to the faces of a reference cube. The spectrometer is currently being reinstalled at its original site in level C of the reactor.

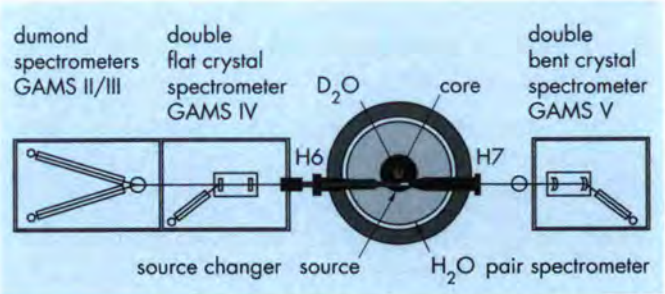


Fig. 1: Implantation of the γ-ray spectrometers GAMS2/3 and GAMS4 at the H6 and GAMS5 at the H7 side, respectively, of the throughgoing beam tube.

The 5.8 m DuMond spectrometer GAMS1 will be replaced by a two-axis focussing spectrometer of focal length ~17 m. This spectrometer, GAMS5, is currently under construction (see section "projects"). Fig. 1 shows schematically the intended implantation of the different spectrometer set-ups on either side of the through-tube. The high-resolution measurements can be complemented by measurement of primary γ-ray spectra using the former pair spectrometer PN4. This spectrometer has been offered as a CRG instrument.

The two-axis flat crystal spectrometer GAMS4 (NIST - ILL collaboration) is currently stored in the second guide hall (ILL22) where it is kept under running conditions. Currently a new antivibration system is being developed for this spectrometer at NIST.

PF1 Cold polarized beam facility

In December 1992 it was proposed to move PF1 from its old location at H14-2 to the end position of H53 in the new guide hall. This neutron beam had been used before in the n-$\bar{n}$ experiment. After the general layout had been designed this project was formally accepted in April 1993.

Since then, work has been done on infrastructure details of the installation. The new facility not only features an enlarged floor surface for experiments, but in addition, an area for experiment preparation and testing (Fig. 2). Future experimenters will also appreciate the separation of the experiment electronics from the physicist's cabin.

At its exit in the EVA cabin H53b has an integrated neutron capture flux of $1 \cdot 10^{10}$ n·cm^{-2}·s^{-1} and a cross section of 60x100 mm^2. This cross section will be maintained throughout a 4 m long ^{58}Ni extension guide between the EVA monochromator and the PF1 polarizer. We hope to have at least 80% of this flux available for PF1.

At present there are no supermirror polarizers available which can accept the full beam cross-section but it is hoped to be able to use two standard size polarizers on top of each other. In principle the use of a ^{3}He spin filter would be an elegant method of solving the problem of large area beam

polarization but the application of this technology to neutrons is still under development.

Work on a focussing device is also advancing. Some 100 silicon strips, each 5 mm wide and 70 mm long with a thickness of 0.25 mm, were coated with a non-polarizing supermirror. The sputtering was done in Würenlingen, Switzerland.

Currently, the second magnet of the former BILL spectrometer is being used at the old PF1 site to measure the ^{177}Lu ß-spectrum. Earlier runs revealed a halo of electrons of arbitrary energy which are scattered on the walls of the inner vacuum pipe and find their way into the detector. This leads to a significant electron background around and above the electron energy end point. To remedy this situation S. Schönert from the University of Munich has developed a new detector which adds a segmented silicon detector to the old wire chamber geometry. It is thus possible to measure the energy of an electron in coincidence with a wire chamber signal and to exclude events where the electron kinetic energy does not correspond to the magnet setting. At the time of writing, December 1993, the first data is being taken with the new detector and electronics set-up.

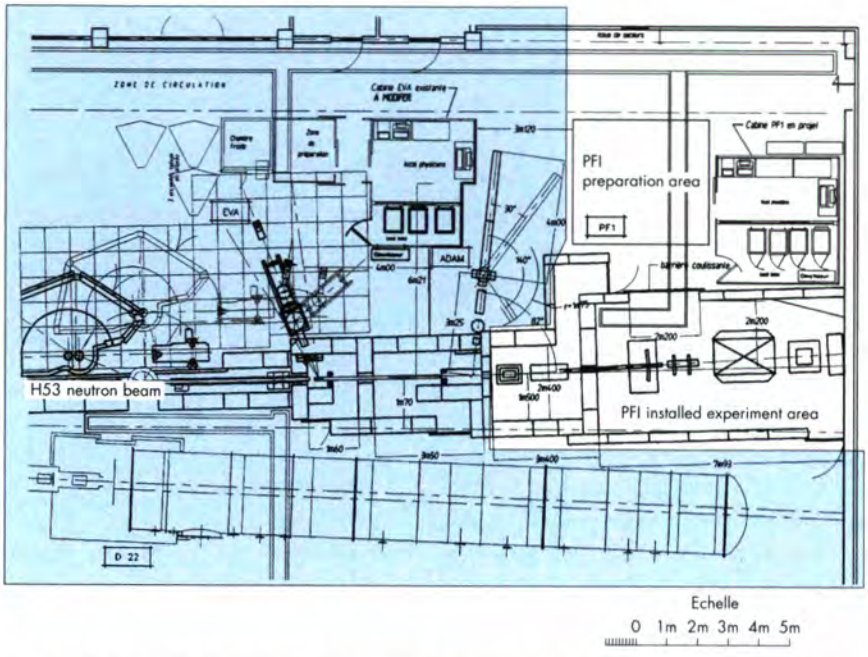


Fig. 2: The plan of a large part of the second neutron guide hall, ILL22. The unshaded areas at the end position of the H53 cold neutron guide show the region occupied by the new intense cold polarized beam facility for fundamental physics called PF1.

PF2 The source of very cold and ultracold neutrons

The source of very cold and ultracold neutrons (VCN/UCN) on level D was operated in the context of ILL's "Special Instruments" from its installation in 1985 until the reactor shut-down in 1991. Under the reorganization of the ILL in 1993 it became the instrument PF2 and is now one of the regularly scheduled instruments in the nuclear and fundamental physics group. Its applications range from experiments in particle physics (search for an electric dipole moment of the neutron, precise determination of the lifetime of the free neutron) through optical experiments (neutron microscopy, interferometry) to condensed matter physics for experiments with extremely high absolute resolution obtainable with UCN (neV). The high intensity is a result of the design of the source that can be seen in Fig. 3 (page 140): a neutron guide (TGV) made of metallic Ni dips with the Aluminium entry window into the deuterium of the vertical cold source and transmits neutrons within a velocity range from about 30 to 200 m/s to the experimental floor on level D. The beam is split into halves: one half supplies a beam of VCN to the experimental floor, the other half is guided to a neutron turbine. There, VCN are Doppler-shifted to become UCN by reflections on the preceding blades of the neutron turbine (690 cylindrical Ni mirror blades mounted on a wheel structure of 1.8 m diameter moving at a peripheral speed of 30 m/s). The measured intensities at the respective exit slits were:

VCN density: 0.25 cm^{-3} $(m/s)^{-3}$ at 50 m/s

UCN fluxes: $2.6 \cdot 10^4$ cm^{-2} s^{-1} up to $v_z = 6.2$ m/s

and $3.3 \cdot 10^4$ $cm^{-2}s^{-1}$ up to $v_z = 7$ m/s

These values show that PF2 is the strongest source of VCN and UCN worldwide. Available for external proposals are 1 beam of VCN, 3 high intensity beams of UCN in a switch mode and one permanent UCN side beam of lower intensity. For possible future needs a second beam of VCN and another permanent beam of UCN can be made available. This unique source has been described in detail in (1).

During the reactor shut-down the second, curved part of the above mentioned neutron guide has been renewed; it has been fabricated by the Technische Universität München (TUM) under the supervision of H. Nagel. It was assembled and leak tested successfully in autumn 1993 at the ILL and its installation is scheduled for May 1994.

Experiments with direct ILL involvement concern currently the neutron lifetime measurements and the neutron EDM measurements:

MAMBO II:

It was shown by the experiments of W. Mampe et al. (2) that UCN storage experiments can supply the most precise values for the lifetime of the free neutron. Such experiments

on the decay of the free neutron give essential information about the weak interaction coupling constants g_A, g_V. A detailed analysis of the former bottle experiment showed that it should be possible to improve the experimental precision from ±3 s to below ±1 s with a more advanced design. A new apparatus is therefore being constructed in a collaboration between the TUM and the ILL in the context of a doctoral thesis (3).

In bottle experiments UCN are stored in a trap of variable volume and one counts the number of remaining neutrons as a function of storage time. During storage, neutrons are lost by the decay of the free neutrons and by absorption or inelastic scattering on the trap walls. Assuming that the losses on the trap walls are proportional to the wall collision rate the neutron lifetime can be determined by an extrapolation to zero of the ratio of wall area to trap volume. Gravity enters as a correction, as wall elements at different heights contribute differently to those losses. Furthermore, it has been shown in the context of this doctoral thesis that there exist non-vanishing energy transfers during wall collisions - an effect that may not be explained fully by mechanical vibrations of the trap walls.

In the new experiment (MAMBO II - Mampe bottle II; see Fig. 4 (page 140) the storage volume is integrated in a larger surrounding pre-storage volume. This pre-storage volume allows the shaping of the energy-spectrum of the UCN before they are transferred into the storage trap. The design ensures furthermore that the UCN-spectra are independent of the trap volume at the time when the UCN are transferred into the storage volume. The construction of the experimental apparatus is nearly finished and experiments should begin immediately the reactor restarts.

Extensive analytical calculations have led to a detailed understanding of this experiment. A Monte Carlo program package has been developed in order to describe neutron trajectories for any geometry which allows the quantitative description of phenomena that cannot be treated satisfactorily by analytical methods.

It has been shown that with this new apparatus it should be possible to obtain a total error for the neutron lifetime of about ±0.8 s, or it may be only ±0.6 s - if the loss coefficient can be proven to be sufficiently temperature independent.

New neutron EDM apparatus:

After an interruption of 8 months, on-site development is now continuing. Concerning the built-in magnetometer using ^{199}Hg atoms, the f-number of the ultraviolet light optical systems has been improved and the Hg nuclear spin relaxation time in the polarizing vessel has been increased to more than 100 s by applying a dotriacontane wax surface coating. Following these changes, the aim of having an RMS noise of less than 2 nanogauss for the 3 minute machine cycle magnetic field strength measurements has now been achieved. The next task is to examine the behaviour of the magnetometer in strong electric fields.

The control of the EDM measuring instrument is being reorganized so that it employs two PCs running under LABVIEW.

References

(1) Steyerl A. et al., Phys. Lett. A 116 (1986) 347

(2) Mampe W. et al., Phys. Rev. Lett., 63(6) (1989) 593

(3) F. Schorr, Doktorarbeit, Technische Universität München, July 1993 also: V.V. Nesvizhevski, ILL report 93 VVNO02S

Very cold neutron beams at ILL

(Responsible: P. Ageron)

In recent years several different VCN beams have been used for fundamental physics experiments with the following guides on the cold neutron source (except for the former SN5).

	width [cm]	height [cm]	radius [m]	cut off λ [Å]	examples of use
SN5	7	7	9.8	69	reflectometry
H17	3	5	150	12	UCN production in He_{II} (λ=9 Å)
H18	3	20	25	28	neutron electric charge (λ = 20 Å)
TGV	7	7	13	60	interferometer
extraction	3,4	3x2,4	3.5	68	(λ = 100 Å)

Figure 5 shows the measured VCN spectra for the following guides:

SN5 max (on the garland side)

SN5 mean (over the whole section) [1]

H18 mean [2]

Entrance to the turbine, level D, on the garland side max at x = 0.2 cm mean at x = 3.7 cm [3]

From these measurements one sees that

- SN5, which is a thermal source, has brightness 50-100 times lower than the other guides which come from the cold source;
- the vertical guide (TGV to level D) which penetrates inside the cold source is clearly superior for the longest wavelengths (>50-100 Å);
- the H18 guide and, a fortiori, the other cold guides (H17, H14 or H 53) are superior for the shorter wavelengths (>10-20 Å).

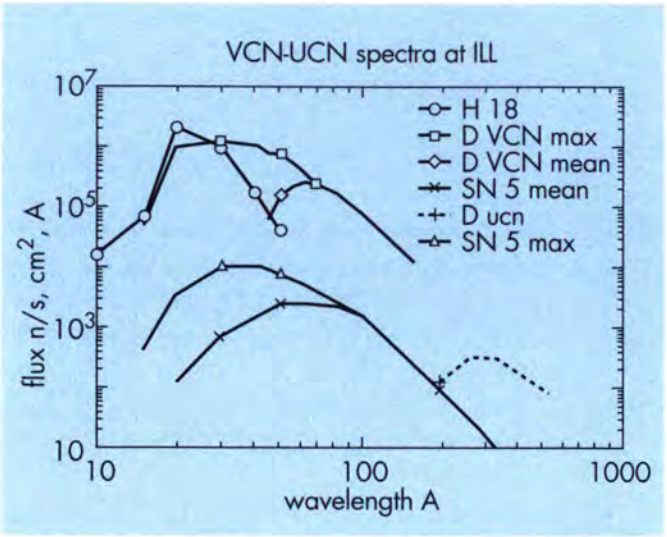


Fig. 5: VCN-UCN spectra at ILL. Shown are the measured UCN spectra for the following guides: SN5 max (on the garland side), SN5 mean (over the whole section), H18 mean, entrance to the turbine, level D, on the garland side max at x = 0.2 cm, mean at x = 3.7 cm.

To take VCN from these different cold guides in the future, side deviators would be necessary, because end positions are no longer available for VCN extraction. Options for consideration are:

- deviation, and monochromation with $\Delta\lambda/\lambda = 10\%$ by artificial crystals, i.e., a multilayer film with bilayer thickness $d \geq 2 \times 30$ Å or mica with d = 10 Å. The deviation $\alpha = 2\theta$ Bragg and the selected wavelength λ are related by $\lambda = 2d \sin(\alpha/2)$.

Their reflectivities at long wavelengths are still to be investigated;

- deviation with a cut off $\lambda_* = \gamma_*/1.7 \cdot 10^{-3}$ (for Ni) by multislit benders (with slit width w and length l).

The characteristic angle is given by:

$$\gamma_* = \sqrt{\frac{2\alpha}{l/w}}$$

They could be made like those of the feed guide in the magnetic storage ring NESTOR [5] with many thin glass sheets of thickness = 0.2 mm and length 300 mm bent to a radius as small as 200 mm, separating channels of width = 3 mm so that l/w = 100. Monte Carlo simulations for the case $\lambda = 60$ Å and deviation $\alpha = 30°$ have shown, for an incident solid angle of 10^{-2} steradian, an overall transmission of 60% for natural Nickel coating (R = 98%) and 90% for a supermirror coating (R = 95% in the SM region) where R is the reflectivity.

Larger l/w (about 1000) may be obtained if the neutrons propagate inside silicon wafers coated with nickel or supermirror, with a length of 100 mm and a thickness of 100μm; the reflectivity of 99% at the interface has been measured, but the inelastic scattering on silicon becomes too severe for long wavelengths ($\lambda > 20$ Å) [4].

One can summarize the possible wavelengths in Å selected by these different systems as a function of two choices for the deviation:

	bender: cut-off wavelength		crystal: selected wavelength	
deviation	multislit l/w = 100	multiwafer l/w = 1000	multilayer d = 60 Å	mica d = 10 Å
90°	100	33	85	14
30°	60	20	30	5

In conclusion, new Very Cold Neutron beams can be obtained:

- **for long wavelengths** ($\lambda > 50$ - 100 Å) with multislit deviators or multilayer monochromator, on the vertical guide at level D

- **for shorter wavelengths** ($10 < \lambda < 50$ Å) with multiwafer deviators or mica crystals on the present or modified horizontal cold guides H17, H18, H14 or H 53.

Hans G. Börner

References

[1] P. Ageron, R. Golub, M. Hetzelt, W. Mampe, J.M. Pendlebury, J. Robson and K.F. Smith, 1977, Proc. Int. Symp. on Neutron Inelastic Scattering, vol.1 (Vienna: IAEA), pp. 53-66.

[2] P. Ageron, unpublished.

[3] A. Steyerl, H. Nagel, F.-X. Schreiber, K.-A. Steinhauser, R. Gähler, W. Gläser, P. Ageron, J.M. Astruc, W. Drexel, R. Gervais and W. Mampe, Phys. Lett. A117 (1986), 347.

[4] U. Grüning, A. Magerl and D.F.R. Mildner, Nucl. Instrum. and Meth. A314 (1992) 171-177.

[5] Ein Injektionssystem für einen Neutronenspeicherring, K.T. Kügler, Bonn, IR.78.25.

Diffraction (DIFF) Group

D1A: (1/2 CRG) High resolution powder diffractometer (J. Rodriguez-Carvajal, A.W. Hewat, P. Cross)

D2B: Very high resolution powder diffractometer on thermal beam H11 (T. Vogt, A.W. Hewat, P. Cross)

D1B: (CRG) Two-axis diffractometer with multidetector on thermal guide H22 (C. Ritter, B. Ouladdiaf, K. Ben Saïdane)

D3B: Two-axis polarized neutron diffractometer with lifting counter on hot beam H4 (F. Tasset)

CRYOPAD: Cryogenic Polarization Analysis Device for Spherical Neutron Polarimetry on IN20 (F. Tasset, S. Pujol)

D4B: Disordered materials diffractometer sharing the hot beam H8 with IN1B (P. Chieux, P. Palleau)

D9: Four-circle diffractometer on the hot beam H3 (M.S. Lehmann, C. Ritter, J. Archer)

D10: Four-circle triple-axis spectrometer on thermal guide H24 (G.J. McIntyre, B. Ouladdiaf)

D15: (CRG) Two-axis diffractometer with lifting counter on the inclined thermal beam (CRG) IH4 (P.J. Brown, M. Reehuis, G. Schmid)

D19: Multidetector diffractometer for protein crystallography on the thermal beam H11 (S.A. Mason, J. Archer)

D20: High-flux multidetector on the thermal beam H11 (J. Pannetier, P. Convert, J. Torregrossa)

The new diffraction group is little changed from the old diffraction group, except that with the reduced ILL budget, instruments D1B, $^1/_2$D1A and D15 will be taken out of service and hopefully operated by Collaborating Research Groups (CRGs). These CRGs will be integrated so far as possible into the normal activities of the group, and CRG scientists will be given offices next to ILL scientists. However, D1B will continue to be be used for scheduled experiments until D20 is operational with its new detector. D1A, which is presently operational at Saclay, will return to ILL in July 1994, and D15 will be re-installed in the reactor before being handed over to a CRG.

Apart from the new D20 detector, other major improvements will include the new 2D position sensitive detector for D19 and the use of the former D19 detector on D10. New focussing monochromators will be available for D1A and D2B, the latter using the new bent wafer technique. D20 will also have a new pyrolytic graphite focussing monochromator to provide very high intensity for real-time experiments. Good progress has also been made with cryopad-II which will replace the original cryopad on D3, and with development of the ^{3}He polarisation filter (for details, see the chapter "Projects").

Shortly after the re-organisation in July 1993, the diffraction group moved from its somewhat isolated position in the computer building to the first floor of the main building. Space was also found on the first floor for the new scientific computing group of Jane Brown, with whom we expect to work closely. For the first time all diffraction group scientists were brought together in the same building, while instrument technicians were brought together in ILL20.

The first priority of the new diffraction group is of course the re-installation of the instruments; D1B and D10 in the guide hall (as well as D1A at Saclay) are already effectively operational. The instruments in the reactor hall will be replaced as soon as we have access to that area, with the major task being the re-installation of D19, D2B and D20 on the H11 beam tube. The re-installation of D3, D9 and D4 should be somewhat easier, except that in the case of D4, the only instrument responsible, Pierre Chieux is leaving under the early retirement plan. The absence of other staff on detachment means that there will be only one experienced scientist per instrument available for the re-installation of all of the diffractometers in the reactor.

A second priority has been the modernisation of the computer resources available to the group. All PDP-11 control computers are being replaced by (second hand) micro-vaxes to simplify maintenance. Under the Unix plan, three Silicon Graphics Indigo machines have already been purchased (one second hand), and by the time the reactor re-starts we will have similar Unix machines available to all of the diffractometers for data analysis. Instrument control will however, remain with the micro-vaxes for the present, with all computers communicating through ethernet, which will also eventually be the link to instrument electronics and make it easier to change instrument control computers.

The choice of Unix computers was determined by ease of operation - the Indigo has a graphic user interface similar to Windows-NT and Macintosh - and by the availability of software for diffraction data analysis. In particular we have purchased the CERIUS modelling package from the Cambridge (UK) company Molecular Simulations, and also make extensive use of the 3D data visualisation package Iris Explorer, for which there are local centres of excellence in Edinburgh and Oxford (NAG). Each of our Unix workstations operates at about 10 times the speed of the former central computer, which means that real-time data collection can now also be analysed in real-time, allowing the scientist to intervene more effectively in the experiment, rather than simply to collect data blindly.

As an example of the use of CERIUS, Fig. 1 on page 141 shows the structure of a small molecule inside a zeolite cage, together with the neutron powder diffraction pattern calculated for this structure. The molecule can be moved around within the structure and the diffraction pattern updated almost instantly to reflect the new geometry. Alternatively, the likely positions for the molecule can be calculated using the energy minimization module of CERIUS, and this can serve as a starting point for the Rietveld refinement module. The fast 3D graphics of the Indigo make it very easy to examine complicated structures and data.

Another example is shown in Fig. 2 on page 141. This is data from a 'real-time' experiment on D1B, where a diffraction pattern has been collected every minute as the sample undergoes a phase transition on cooling. Iris Explorer has been used to plot the diffraction surface in 3D, and this surface can be spun around with the mouse pointer to find the most interesting features. Other examples of the visualisation of 3D electron and magnetic spin densities, position-sensitive detector data etc are given in the College 5 report.

D1A High Resolution Powder Diffractometer on Thermal Guide H23

D1A was moved to Saclay as a complete working instrument soon after the start of the ILL reactor long shutdown, and will remain there until July 1994, shortly before the restart of the ILL reactor. At the same time, the D1A control computer was updated to a micro-vax running the MAD diffraction data collection software. At Saclay, D1A was installed on a cold neutron guide, the only suitable position available, and has been working near the guide cut-off of 2 Å. The intensity on the medium flux reactor is of course several factors lower than it was at ILL, but is still sufficient for many experiments, especially those on magnetic structures. In fact, a great many different visitors made use of D1A at Saclay under the guidance of Juan Rodriguez-Carjaval, a scientist detached from ILL, with the expert assistance of Peter Cross, an ILL technician. When D1A returns to ILL, a new 25-detector/collimator bank will be installed, and the machine will be half supported as a scheduled instrument and half operate as a CRG.

D1B High Efficiency PSD Powder Diffractometer on Thermal Guide H23

To bring D1B in line with most other ILL instruments as regards instrument control and data acquisition, the PDP11 computer was replaced by a MicroVax II computer running under VMS, and a direct ethernet connection has been installed. The ILL standard control program MAD has also been implemented.

Due to its great success in investigating magnetic structures, phase transitions, kinetic in situ reactions and texture studies, we think that the future of D1B will be assured as a CRG instrument with the same field of interest. However, D1B will operate as an ILL instrument until D20 is fully scheduled with its new PSD detector.

D2B High Resolution Powder Diffractor on Thermal Beam H11

The highest priority for D2B improvement is the construction of a new Ge monochromator that will improve the line shape in the high resolution geometry. The present monochromator is a composite of 30x10 mm slices of squashed germanium, focussing a 300 mm high beam onto a 30 mm high sample. This gives high intensity (10^7 n.cm^{-2}.sec^{-1}) at good resolution ($1.5x10^{-3}$), but in the high resolution mode (design limit $5x10^{-4}$) the peak shape is too broad and not sufficiently uniform. These defects are due to variations in both the mosaic spread of the squashed germanium and in the alignment of the individual slices. A new technique, developed at Brookhaven by Larry Passel and others with the help of Tom Vogt from ILL, uses stacks of thin wafers whose mosaic has been increased by bending rather than squashing.

The ILL is using a similar technique to produce the new D2B monochromator. However, instead of using commercial wafers, as produced for the electronic industry, the ILL is cutting the wafers from a large perfect crystal. The advantage is that our wafers will all be perfectly aligned with respect to each other, so that the stack of wafers will permit reflections from any [hhl] plane giving us the usual choice of wavelengths from the same monochromator. If the wafers are misaligned around their normal, then only the reflection corresponding to this normal can be used, with no choice of wavelength.

D3B Two-axis Polarised Neutron Diffractometer

As was mentioned briefly in the 1992 annual report, R. Papoular of the Laboratoire Leon Brillouin has made important progress dealing with Fourier inversion of 2-D single-crystal data of limited statistical accuracy and resolution. This has applications to high-Tc magnetization densities. In general, data collected on D3 with the normal beam geometry compatible with large cryomagnets is severely resolution limited in the vertical direction.

Recent developments of the Fourier inversion technique with the CEN-Grenoble Neutron Diffraction Group means that it is now possible to calculate the most probable 2-dimensional and 3-dimensional magnetization densities from such an hybrid set of data see Fig. 3 on page 141. This should offer our users a new systematic way of looking at D3 data. This calculation is intensive because it proceeds by iteration, but we have shown that with the new generation of RISC processors it takes only 30 minutes on the best table-top machine. E. Ressouche, a long term visitor from the CENG helping with the rebuilding of D3B, is working on this technique with the aim of having it operational at reactor restart.

Cryopad-II

Ordered in August 1992, the new cryostat for CRYOPAD was delivered in February 1993. Designed by Serge Pujol it has a liquid helium autonomy of one week and its most spectacular feature is the 19 cm diameter room temperature RT-bore, large enough to host most sample environments. The two niobium Meissner shields were ordered and delivered in July to be mounted and tested satisfactorily at low temperature in September. Using a sensitive Gaussmeter in the RT-bore we could verify for the first time the shielding efficiency of these opened cylinders against an axial magnetic field. We are happy to say that it matches the design calculations made in 1992 by Luc and Michel Thomas.

Further calculations were made this summer using ANSYS in order to establish the design for the precession coils which are to be installed in the annular space between the two shields. This original calculation of a magnetic coil confined in a Meissner shield environment, which imposes special limiting conditions for magnetic induction lines, has been the subject of a stage "Maitrise Sciences et Techniques" for Ivan Neyret. In the compromise made, the simplicity of the device and ease of use was given high priority, to little detriment of performance. The resulting superconducting coil was ordered in October and will be delivered in February 1994.

The Mu-metal shield needed to cancel the earth's field during cooling is being manufactured. In the mean time we are studying a new design for the magnetic guide-fields outside the cryostat (the so-called nutators) since they have to provide good magnetic confinement, a requirement due to their proximity with the vertical opening in the zero-field sample chamber.

We hope to have CRYOPAD-II ready for neutron tests and calibration by summer 1994 when the IN20 host spectrometer is back in operation.

D4 Disordered Materials and Liquids Diffractometer on hot beam H8

After the completion of the new position sensitive detectors on D19 and D20, the next priority is for a large angle PSD on D4. The choice of construction technique will depend on the results with D20, but already plans have been made for a modular PSD consisting of eight individual PSD elements. These future developements will have to await the new instrument responsible, since unfortunately Pierre Chieux, the father of liquids diffraction at ILL, is leaving under the early retirement plan. Because D4 time-shares a beam with IN1, and counts as only half an instrument, we can appoint only one scientist in this area. The change over of instrument responsible will therefore be difficult.

D9 Four-circle diffractometer on the hot beam H3

The instrument is scheduled to be ready for the start of the reactor, and the assembly is planned for late spring. During the complete reactor shut-down the instrument technician J. Archer, was employed at the Hahn-Meitner Institute, Berlin, and at his return late in the year the first preparations began. The instrument itself is at present located in the guide hall, while the monochromator housing and the electronic cabinets were kept near their original locations. A few parts of the equipment have been on loan, particularly the micro-Vax controlling the instrument and vacuum-shield furnace, but they will all be returned before March 1994. The only outstanding part of the preparation is then a recabling of the monochromator, which is now underway.

At the startup D9 will therefore be equipped with temperature control units going from 15 K to about 1100 K. It will also, as before, have a small 32 by 32 pixel position sensitive detector. The monochromator for the start-up phase will be the traditional Cu(220) in transmission, but it is planned as quickly as possible to continue the short-wavelength tests of a horizontally curved Be monochromator that were under way precisely at the time of the reactor shut-down.

D10 Four Circle 3-Axis Diffractometer on thermal guide H24

The main advantages of D10 for diffraction and spectroscopic studies are its excellent q resolution due to its location on a neutron guide and the small mosaic spread of the monochromator, its very low intrinsic background, full 3-D access in reciprocal space, temperatures from 1.6K to 900K, optional energy analysis, either to reduce the inelastic background or to study inelastic features (still with full 3-D access), the easy change of instrument configuration during an experiment, and strong sample table to support heavy furnaces and cryostats.

The typical applications are to studies of 'conventional' crystal and magnetic structures, of phase transitions, of incommensurate structures, of quasi-elastic scattering (Huang and critical scattering), of diffuse scattering, of novel materials such as quasi-crystals and multilayers, and of inelastic scattering.

During the reactor shutdown the new more-robust ω-rotation turntable has been installed. This turntable can support either the new offset open χ-circle, or the new fully automated tilt stage for heavy furnaces, pressure cryostats and cryomagnets. The ω-axis has direct encoding with an absolute error of less than 0.004°, small enough to take full advantage of the excellent resolution of D10. The crystal-orienting drives are now all equipped with five-phase stepper motors which are virtually resonance free and allow much faster and more accurate positioning. The automation of the double-tilt stage means that, if the furnace or cryostat permits it, several layers of reflections can be accessed under

computer control. The offset χ-circle can accommodate the new D10 four-circle dilution cryostat built by S. Pujol. Under 0.1K has been obtained routinely independently of the setting for χ. A very clear advantage afforded by this cryostat is that it can be used in the same manner as the previous ^{4}He cryostat at temperatures above 1.6 K. We eagerly look forward to using it in anger in 1994!

D10 is thus in very good shape to shoulder the load of the single-crystal diffraction experiments immediately after the start-up especially before D9 and D19 come back on-line. It is therefore not planned to make further changes to D10 until then. Eventually though, the present D19 position-sensitive detector will be installed on D10 to improve efficiency of structural data collection and measurement of diffuse scattering.

D15 Two Axis Diffractometer with Lifting Counter on inclined thermal beam IH4

D15 will become a CRG instrument from the restart of the reactor, but ILL will first re-assemble it and the platform on which it sits. D15 has been a unique instrument for the study of crystals at very low temperature; it is the only machine which can accommodate very large cryostats and magnets and still collect 3D data using its lifting detector. It is ironic that at the same time as D15 is being taken out of service, new instruments largely inspired by D15 are being constructed at other reactor centres such as Saclay. However, since several groups from all 3 associate nations showed strong interest in continuing to use D15, it is hoped that it will not be too difficult to support it as a CRG instrument.

D19 High flux multidetector diffractometer on the thermal beam H11

D19 is a four-circle single crystal diffractometer which at startup will incorporate a larger (64°x20°) position-sensitive detector (PSD). D19 works best in the wavelength range 1.2 to 2.4 Å and is most efficient for larger unit cells (>10 Å on edge), but even for single reflections will give improved intensity integration because of the detector's spatial resolution of 0.2°x0.2°.

As in the past, D19 will share the H11 beam with the powder diffractometers D2B and the upgraded D20, making the H11 beam without doubt the most productive at the ILL. D19 has the following features: high resolution due to a maximum monochromator take-off angle of 90°; a choice of up to four monochromators by rotation about a vertical axis of an ILL turret monochromator mount (being re-built so that it no longer interferes with D20's beam); vertical focussing of the beam for graphite and Ge monochromators; a C-shaped Huber Eulerian cradle on which a 2-stage 15K Displex cryorefrigerator is routinely mounted. A Munich mirror furnace has also been used by T. Vogt and Z. Mursic up to 2500K.

The old vertically-mounted high pressure (8 atm He) multiwire "banana" detector is set symmetrically about the equatorial plane, with the sample at the centre of vertical curvature. The detector rotates on a γ-arm ($\gamma=2\theta$ in the equatorial plane), on air cushions. The combination of an Eulerian cradle and a large position-sensitive detector allows data collection with a choice of geometries. Most experiments have been performed with normal beam geometry, and peak integration is usually by a learned volume minimum variance method. The availability of a wider PSD (20° rather than 4°) will further increase the range of single crystal diffraction experiments possible with thermal neutrons. Typical in the past were studies on phase transitions in multi-domain samples, human haemoglobin, organic molecules on the lysozyme surface, helium single crystals, acetylene polymers, liquid crystals, Vitamin B12, and a number of cyclodextrin complexes. In order to mount the detector on D19, substantial modifications are being made to the detector support, and new shielding is being built. This is necessary because the radius of vertical curvature of the new detector is 60 cm, compared with 115 cm before. For most experiments - all except those with very small unit cells, which would more logically be run on D9, D10 or D15 - the new PSD will give a real gain in efficiency of up to a factor of six. For the experiments for which D19 is primarily designed i.e. diffraction from single crystals (or fibres) with larger unit cells, the large gain in solid angle will lead to more extensive data sets in shorter times.

Electronics and software modifications to read the extra pixels (320 * 100, compared with 512 * 16 before) will be made for the 1994 start-up without change of philosophy. At present D19 is controlled by a dedicated Microvax. The diffraction data are displayed and analysed on a Vaxstation 3100 close to the instrument. Programs such as G.J. McIntyre's MULPLT for 3-d displays of raw data, and fairly complete program systems, such as that implemented at D19 for fibre diffraction by the University of Keele group, run comfortably on the Vax-station. The change from these computers (under VMS) to a Unix work-station will be made after the reactor restart with the benefit of experience from other diffraction group instruments. This will allow us to commission the new detector - and compare it with the old one - and gain extensive experience with it before changing computers.

D20 High flux multidetector on the thermal beam H11

(see the contributions of the Projects and Techniques Division to this Annual Report, partly under Construction of New Instruments, and partly under Multidetector Group)

The delay in the construction of the 160° Position Sensitive Detector is mainly due to the departure to the ESRF, at the end of 1992, of our technician M. Berneron, who had made most of the developments for the banana construction, and had the expertise for the realisation of some critical parts in the detector. He has been back at ILL

since October 1993. The detector is now ready to be mounted after some adjustments to suppress instability in the gas amplification.

The 52 pieces of the new HOPG monochromator are at ILL and have been tested with neutrons and X-rays. The mechanical support for the 4x13 elements of this focussing monochromator is currently under study and will be available in mid-1994.

The data acquisition system is complete and operational except for the synchronisation module. A Silicon Graphics computer has been purchased for the control and data analysis of D20.

The 1994 reactor cycles will be used for instrument tests and commissioning experiments. The diffractometer is expected to become available for external users in the first months of 1995.

Alan Hewat

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[2] R.J. Papoular, E. Ressouche, J. Schweizer and A. Zheludev (1992).

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Large Scale Structures (LSS) Group

D11 Small-Angle Scattering Diffractometer on the cold guide H16 (P. Lindner, L. Vuillard, K. Ibel, A. Polsak)

D16 Four-circle Diffractometer on cold guide H15 (J. Zaccai (IBS), V. Rodriguez)

D17 High Resolution Small-Angle Scattering diffractometer and Reflectometer on the cold guide H17 (H.-J. Lauter, P.Timmins)

DB21 Diffractometer for very large unit cells on cold guide H15 (E. Pebay-Peyroula (IBS), C. Wilkinson (EMBL))

D22 New Small-Angle Scattering Diffractometer on cold guide H512 (R. May, R. Oeser, K. Ibel, R. Gay)

Laue detector
Collaborative project with EMBL and Freie Universität, Berlin (M. Lehmann), see "Small Projects in DS

The Large Scale Structures group was created as part of the reorganisation of the ILL on July 1st 1993. It comprises the above listed instruments which cover a wide range of science from physics through materials science and chemistry to biology. The common theme is the study of particles or density fluctuations on a scale up to hundreds of nanometres.

We are particularly fortunate in the group in that none of the instruments has been dismantled for access to the reactor. We are therefore in a good position to provide working instruments immediately the reactor restarts. The past year has been taken up with small improvements to the instruments and their preparation for the start-up. Three developments are of particular note. The new small-angle scattering instrument D22 is in the final stages of completion and after a short commissioning period should be available for users in the second user cycle after the reactor start-up. During 1993 a project was initiated by J.-B. Suck for placing D16 and D17 on straightened versions of the guides H17 and H18. This is primarily to increase the flux of 3 - 10 Å neutrons on D17 and hence to facilitate its conversion into a reflectometer. Although it has not yet proven possible to fund this project, studies are continuing with a view to implementing it in the future. Finally, very important advances have been made by EMBL and ILL in the development of detectors for use in a future Laue-diffractometer. For details see the chapter "Projects".

As a first step in the conversion to UNIX the group purchased a Silicon Graphics Iris Indigo R50XZ computer accompanied by the graphics software "Explorer". A further UNIX machine will be purchased in 1994 in preparation for the restart of the experimental programme, ensuring that data treatment facilities will be available for some time under both VMS and UNIX.

We are all waiting anxiously for the reactor to restart and to be able to use and make available to outside users our range of new and improved instruments.

D11 Small-Angle Scattering Diffractometer on the cold guide H16

A major change at D11 in 1993 has been the replacement of the old CAMAC electronics by VME. The hardware has been successfully installed and tested, the instrument control program is currently being completely revised.

A further improvement is the motorisation of the 20m collimation guide section; all collimation sections at D11 are now operated by motors and are under computer control. Two more Cd sheets as attenuators have been installed directly after the selector position. D11 now has a choice of three attenuators, with attenuation factors of ≈ 1/300, 1/1100 and 1/2700 respectively. The process controller of the compressed air pistons which place the chosen attenuator into the beam is connected to the instrument computer via the VME system.

A common security system for the three D11 selectors (Adèle: $\Delta\lambda/\lambda$ = 40%, Brunhilde: $\Delta\lambda/\lambda$ = 9% and Constanze: $\Delta\lambda/\lambda$ = 10%) has been installed. The "standard" selector after the restart will be the new light weight 10% selector "Constanze" made from composite material. All selectors are now driven by AC motors which themselves are powered by a common, new REFU 317. Changing the selectors will become a rapid and smooth operation in the future as only one cable is used; each selector is identified by an individual plug to which the standard cable is connected. The selector speed will be changed by a control program which directly addresses the REFU amplifier.

The optical sample alignment system has been further improved by installing a compact small laser together with a halogen lamp. The light beam is reflected from a neutron transparent silicon wafer into the path of the primary neutron beam. It will be operated by a switch at the sample position thus avoiding opening of the collimation section in the chopper casemate.

Further improvements before the restart are in progress with respect to the sample environment. In particular, a new sample table with a motor driven lifting device and standard rack plates for common use on the sample changers of D11, D17 and D22 are under construction.

D16 Four-circle Diffractometer on cold guide H15

D16 is in the first group of ILL instruments to be scheduled when the reactor restarts next summer. It is still one of the very few neutron diffractometers in the world that allow very good Q-resolution over a wide Q-range for studies of crystalline or partially ordered systems with large

unit cells. By February 1994, the instrument will be in full running order. A number of small but important improvements have been carried out; a complete recabling of the instrument, checking and where necessary, replacing motors, an overhaul of the electronics and tuning of the multidetector. Work is in progress on the monochromator axis - a re-designed carriage mount will be aligned to facilitate wave-length changes during experiments.

D17 High Resolution Small-Angle Scattering Diffractometer and Reflectometer on the cold guide H17

D17 has undergone a series of small improvements in the past year in preparation for the reactor start. A new power supply has been installed for the velocity selector which will be under computer control. An improved alignment system is under construction and new attenuators, similar to those of D17, have been installed. The instrument will restart in the same configuration as it was at the reactor shutdown. Thus it will run as a small-angle spectrometer and as a reflectometer for experiments appropriate to its long wavelength. In the medium term, after the commissioning of D22, the instrument will be optimised and used predominantly for reflectometry. The first step in this direction is to make available the shorter wavelength "garland reflections" which are present in a narrow beam close to the wall of the guide. This will require an improvement of the translation of the whole instrument and the installation of a multilayer monochromator option. In a later phase it is foreseen to straighten the H17 and H18 guides in order to produce a greatly increased flux of 3 - 10Å neutrons.

DB21 Diffractometer for very large unit cells on cold guide H15

DB21 is a low resolution diffractometer used for experiments of biological interest. Biological macromolecules, i.e. proteins, assemblies of proteins with nucleic acids such as viruses or ribosomes, are objects of typical size varying from 50 to a few hundred Ångstroms. Low resolution for these experiments means less than 10 Å. A suitable wavelength of 7.53 Å is obtained with a potassium intercalated pyrolitic graphite monochromator. The previous monochromator was broken at the reactor shutdown. During 1993 new monochromators were made by P. Touzaint at the "Ecole d'electrochimie". A 2 mm thick HOPG was purchased from Union Carbide and then sliced in three parts. Two of them have been intercalated with Potassium (KC8 intercalation) and then pressed to reduce the mosaicity which increased during the intercalation process. The first one has been tested with neutrons at Siloe (P. Flores) and with gamma-rays at ILL (A. Escoffier), it showed a mosaicity of 1.7°. The second was pressed at a higher pressure and tests are currently underway at Saclay. The third monochromator will then be intercalated and pressed according to these results (a suitable mosaicity would be less than 1°).

In addition to the usual type of experiments, there is a demand for increasing the resolution to about 6 Å (determination of domains with intermediate degree of ordering). This would require another monochromator selecting a wavelength of 4.5 Å (standard HOPG). In order to change the wavelengths between two experiments easily without closing the neutron guide, an automatic monochromator changer has been designed and built (G. Schmidt). It will be installed as soon as the electronic work is ready.

The critical point of the instrument is the detector: for long counting times (typically one data set is collected in a week or longer), it is very important to have a good stability of the detector. This stability is becoming increasingly difficult to maintain due to the ageing of the photo-multipliers. For this reason a multiwire ^{3}He detector has been designed (J. Jacobé) having a similar resolution (1.8 x 1.8 mm) and an overall size of 20 x 20 cm. Preliminary tests at low He pressure have been carried out successfully and tests at nominal pressure will be carried out in the near future.

D22 New Small-Angle Scattering Diffractometer on the cold guide H512

1993 was a year of small, but important, steps forward for D22, which visibly turned into a usable instrument.

The 1 x 1 m detector with 16K pixels of 0.75 x 0.75 cm from CERCA, delivered just before the beginning of the year, was installed in D22's vacuum beam tube of 2.5 m diameter and 20 m length. It was subjected to first tests using an AmBe source which allowed us to define the axes in the memory and showed that all of the detector electrodes are counting. The final adjustment of the amplifier gains requires reactor neutrons. The pressure, humidity and temperature detectors in the rear of the detector were

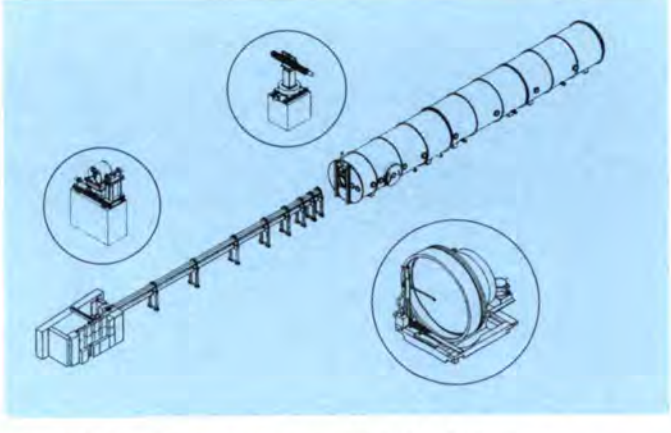

Fig. 1: Schematic view of the new Small-Angle Scattering instrument D22 showing details of the velocity selector, sample position and detector.

connected to a cabinet which was added to the already existing industrial process controller dealing with the collimation and vacuum-pump supervision.

The last mechanical items were mounted in the course of the year 1993. This concerns the attenuator disk, equipped with new mechanics and with 3 different attenuator plates, the box containing antiparasitic apertures of different size as well as the tube which connects the latter with the end of the collimation system and which carries the laser and halogen light serving for alignment. The attenuator plates have 88 holes each with 0.1 mm (in 0.25 mm Gd), 0.2 mm and 0.4 mm diameter (both in 1 mm Cd), and are expected to reduce the neutron flux about 5000, 1200 and 300 times, respectively. The sample table equipped with an electric piston, an XYΦ-table and the sample changer were installed in front of the detector entrance cone. Two prototype sample racks are under test.

The Dornier velocity selector, turning at a maximal speed of 28,300 rpm for neutrons of 4.5 Å at a resolution ($\Delta\lambda/\lambda$) of 10 % (FWHM), was installed on a translation and rotation table in its "casemate", where it was tested once more successfully, together with its independent vacuum pumps. Devices for monitoring its vacuum, vibrations and temperature were also connected to the industrial process control system.

All encoded movements were cabled to the VME data acquisition and shaft-control electronics by the ILL electronics group. With the exception of the four-pane entrance aperture, all of these movements can be controlled by the instrument computer, a Vaxstation 3200, which is interfaced with the process controller and with a PC compatible running the graphical supervision program InTouch (under Windows). The instrument control program SAS (compatible with that of D11 and D17) was further adapted to the needs of D22 by K. Wotschack before he left the ILL for early retirement in summer. First dummy experiments moving the detector in the tube and counting neutrons from the AmBe source were carried out and showed where small modifications to the control program are necessary. The instrument will be fully operational for the second scheduled user cycle after the start-up.

Chemistry and Biochemistry Laboratories

Since the reorganisation of the ILL the chemistry and biochemistry laboratories are under the responsibility of the Large Scale Structures Group.

Chemistry Laboratory
(P. Lindner, P. Chenavas, M. Romero)

The ILL maintains a main chemistry laboratory on the second floor of ILL20 as well as a smaller laboratory in the neutron guide hall next to the small angle scattering instrument D11. Whilst the facilities are foreseen mainly for visitors' sample preparation they are also used by in-house scientists. As well as an extensive range of chemicals and solvents, equipment such as glove boxes, furnaces, an I.R. spectrometer and a density meter are available. Full details of facilities may be obtained from the engineer-in-charge, Mlle P. Chenavas.

In 1993 the laboratory was also used by ESRF staff and discussions are taking place with a view to the ILL participating in the rather more extensive facilities being built up in the ESRF main building.

Biochemistry Laboratory
(L. Vuillard, P. Chenavas, P. Romero)

The ILL also maintains a small biochemistry laboratory on the second floor of ILL20, for visitors to carry out last minute sample preparation. It is also used by in-house scientists to support their own research. Standard equipment includes a UV spectrometer, a fluorimeter, gel filtration apparatus and chromatography equipment. More sophisticated equipment, such as analytical centrifuges, is available to ILL users in the EMBL laboratories. In 1993 the EMBL has been making plans to extend the ILL20 building to provide more laboratories which will be available to ILL and to ESRF biological users. The extension is expected to be completed in late 1994 or early 1995.

Peter Timmins

Three-Axis Spectrometers (TAS) Group

IN1, INFB 3-axis and Be-filter spectrometer on the hot source beam tube H8 (B. Dorner and P. Palleau)

IN8 3-axis spectrometer on the thermal beam tube H10 (J. Bossy and D. Puschner)

IN14 3-axis spectrometer on the cold guide H53 on the horizontal cold source (R. Currat, S. Bramwell and A. Brochier)

IN20 3-axis spectrometer for neutron polarization analysis and spin-echo option on the thermal beam tube H13 (J. Kulda, T. Baumbach and C.M.E. Zeyen)

The above instruments are all located in the reactor hall. Three out of four have been dismantled, between October 1991 and February 1992, in connection with the work on the reactor beam tubes. Most of the instrument parts were stored either in the reactor hall itself or in the new guide hall. The dismantling of the IN14 spectrometer, also located in the reactor hall but looking at the horizontal cold source, was under discussion for some time but eventually was avoided. The instrument, including its heavy primary shielding, was not affected by the work on the upstream guide and on the reactor structures. It will thus be ready for neutron tests at reactor start-up.

According to current plans, the reassembly of IN1 and IN8 is to take place in early spring, after the corresponding beam tubes have been remounted. Additional delays are foreseen in the case of IN20, following the decision to use the H13 beam tube as a reactor vessel vibration test site, during the second half of June.

A limited programme of instrument development and upgrading was pursued during the shutdown. The main items in the programme are listed below.

The upgrading of the control electronics on IN1 and IN8 was budgeted in 1992 and 1993. All parts have now been delivered but the completion date of the project has recently become uncertain due to technical manpower reductions compounded with the unexpected departure of R. Taffut, the electronics technician in charge of the project. Work will continue throughout the first half of 1994.

A modification of the IN14 monochromatic beam geometry, aimed at reducing the monochromator-to-sample distance, is proceeding satisfactorily. The secondary beam shutter and the Soller collimator (or polarising bender) support are now integrated into the primary protection. Mechanical assembly and electronic adjustments are planned for Jan/Feb. 1994.

The 3-axis spectrometer control program, the so-called TAS program, is being entirely rewritten on the basis of the MAD routines, a well-supported ILL standard system. The program includes a CAMAC electronic library to be used on IN14, IN20, IN3 and IN12 as well as a VME library for IN1 and IN8. The user interface and data file format will remain essentially unchanged. The first version of the new TASMAD program was produced by Ph. Blanchard in Dec. 1993 and is currently under test on the IN12 μVax computer. The departure without replacement of Ph. Blanchard at the end of 1993 introduces uncertainties and delays for the final completion date of this project.

Another long-overdue project is the replacement of the PDP11 instrument computers by more modern, network-compatible machines. The choice was made to install DEC-Alpha stations 3000-300L on IN1, IN8 and IN14. A more powerful version is foreseen for IN20, where additional computing capacity is required in the spin-echo mode of operation for on-line magnetic-field profile optimization. The new machines are expected to open new possibilities for on-line data evaluation and interactive optimization of the measurement parameters.

In addition to the four instruments in the reactor hall, two other three-axis spectrometers are located in the guide hall: IN3, on thermal guide H24 and IN12 on cold guide H142. Both are now included in the list of instruments proposed for CRG use. In preparation for the reactor start-up, a substantial amount of mechanical and electronic maintenance work was carried out on each of the two guide hall instruments. As a result, IN12 is now fully operational while additional electronic maintenance work is still required on IN3. With regard to radiological safety, both instruments have been re-equipped in order to meet the new ILL safety standards.

Problems have developed with the group's 6T cryomagnet during operation at LLB-Saclay. Systematic quenching is observed in the 4-6T range when the magnet is first cooled after a room temperature warm-up ("training"). The magnet is presently under test at ILL in order to identify the origin of the problem. A decision to send the magnet for repair, or to use it as it is, will follow shortly.

A number of projects or possible improvements have not been addressed due to manpower and budgetary constraints. One such project is the rebuild of the IN8 primary spectrometer, the design of which was dictated by existing space limitations at the time of construction. With the implementation of the H11 project in 1984, these limitations have been relaxed, and a simpler and more efficient spectrometer geometry will now be possible. A detailed design study has been included in the 1995 group budget requests.

Another important project is the redesign of the IN20 polarising Heusler monochromator, in order to extend the useful incident energy range of the instrument to higher energies. A preliminary study underlined the difficulties

associated with the very limited space available in the monochromator housing. Obviously, the project becomes much more costly if the primary protection has to be redesigned. On the other hand, the recent progress achieved with the ^{3}He polarising filter technique (see chapter "Projects"), indicates that this latter technique may become competitive in the not-so-distant future. When this occurs, the Heusler crystal may be replaced by a non-polarising crystal with good second-order discrimination and comparable lattice spacing , such as Ge(111) or Si(111).

Another area where important developments can be expected concerns the use of elastically bent perfect crystals (as opposed to plastically deformed mosaic crystals) as monochromator or analyser. J. Kulda has been active in this field for many years, in collaboration with groups at PTB Braunschweig, NPI Rez (Prague) and more recently at JAERI (Japan). His report on recent tests on a series of elastically bent silicon crystals is included below.

Elastically deformed perfect crystals and crystals with a lattice spacing gradient are generally recognized as suitable candidates for focussing monochromator or analyzer applications, thanks to the fact that the beam propagation in this case is deterministic (the beam trajectories can be calculated for known strain fields). Up to now the experimental as well as theoretical investigations in this direction have concentrated mostly on silicon which is available in perfect crystal quality for any required size and orientation and exhibits, thanks to its covalent bonding, an excellent long term mechanical stability under applied loads. Its main disadvantage is the rather low scattering length density, which can, however, be compensated for by increasing the diffracting volume, thanks to the low beam attenuation.

A series of test experiments has been performed at different neutron facilities (PTB Braunschweig, JAERI, NPI Rez near Prague) to assess the performance of elastically bent perfect Si monochromator crystals in comparison to the mosaic ones (PG, Cu, Ge) [1]. In most cases both direct neutron beam flux delivered at sample position and powder diffraction spectra with a suitable standard (Al_2O_3, Si) were recorded. Horizontal focussing was suppressed with Si crystals by rather tight collimation (20'), quite large bending radii (~15 m) and beam cross-sections of about 20x20 mm^2 at the sample position, in order to maintain equal conditions for both types of crystals. Typical results of a comparison between Si(331) and Cu(220) - both having $d_{hkl}\approx1.25$Å - and between Si(422), Si(511) and Ge(511) - $d_{hkl}\approx1.05$Å - are displayed in Fig.1 (a) and (b), respectively.

In general the presently available Si crystals provide fluxes a factor 2-3 lower than good Cu and PG monochromators (for reflections with similar d_{hkl}). As expected this disadvantage diminishes rapidly whenever focussing into a small volume in real and/or reciprocal space is required. Silicon also becomes a competitive candidate whenever $\lambda/2$ suppression is important: its performance is about equivalent to that of plastically deformed Ge crystals of the same thickness, while the excellent homogeneity and reproducibility of the elastic deformation and low cost of silicon single crystals should be an advantage. These tests are to be continued at ILL after the reactor restart.

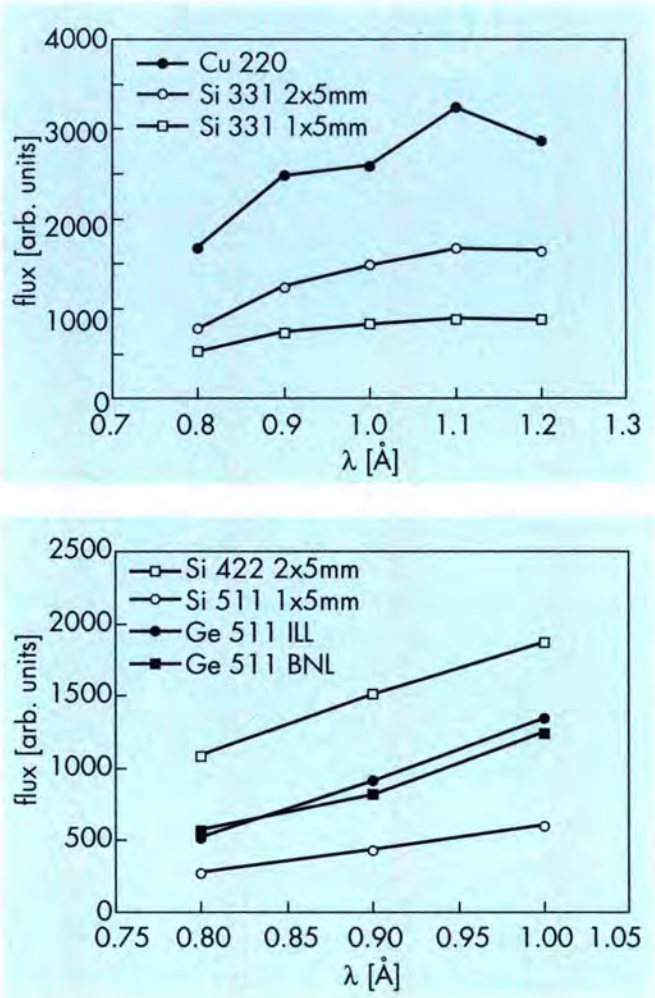

Fig.1: Directly measured output fluxes (scaled by cotθ to account for differences in wavelength resolution) of mosaic Cu, Ge and of elastically bent Si (5mm single plate and 2x5 mm sandwich) monochromator crystals with $d_{hkl}\approx1.25$Å (a) and with $d_{hkl}\approx1.05$Å (b).

Roland Currat

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Time-of-Flight and High Resolution (TOF/HR) Group

IN4C New TOF spectrometer with a Brillouin option on the thermal tube H12 (project) (H. Mutka)

IN5 Multichopper TOF spectrometer on the cold guide H16 (G. Kearley, S. Jenkins)

IN6 Focussing TOF spectrometer on the cold guide H15 (A. J. Dianoux, S. Jenkins)

IN10 Backscattering spectrometer on the cold guide H15 (J. Cook, P. Joubert)

IN11 Spin-Echo spectrometer on the cold guide H141 (B. Farago, E. Thaveron)

IN15 High resolution spin-echo spectrometer for long wavelengths on the cold guide H511 (project) (C. Lartigue (CNRS-Grenoble))

IN16 New backscattering spectrometer on the cold guide H53 (project) (B. Frick)

D7 Diffuse scattering instrument with polarization analysis on cold guide H15 (O. Schärpf, I. Anderson, A. Murani, R. Rebesco)
Group Engineer: J.F. Barthélémy

Several members of the Group have spent a sizeable part of their time at other laboratories: I. Anderson spent two months at PSI at the beginning of the year. Since the reorganization, his position is now in the Projects and Techniques Division, but he is still co-responsible of D7. B. Frick came back from NIST in August and B. Farago has been half the time seconded to LLB. J. Cook left on March 1st for NIST where he will spend a year.

The TOF/HR group has acquired a Silicon Graphics IRIS Indigo R4000 workstation as part of the UNIX plan. This workstation is under the supervision of G. Kearley. An extended-graphics option is included to enable rapid manipulation of 3D images. Some of the group's software has already been "unixed" and work is in hand to provide more powerful visualization facilities for users. In the first stage this workstation will form the main-stay of the group computing activities but will eventually be supplemented by other workstations providing similar service at the instruments.

Dr. D.S. Sivia from ISIS spent two weeks at the ILL to implement his programs for Bayesian analysis of inelastic and quasielastic TOF data. The necessary modifications were made to allow their operation under UNIX.

One instrument of the Group is being offered as a CRG-A operation: IN13, the backscattering spectrometer on the thermal guide H24.

IN4C New TOF spectrometer with Brillouin option on the thermal tube H12

Preparation of the site for receiving the new spectrometer has started, and preinstallation of the shielding elements is foreseen in January 1994. The definitive installation of the primary casemate will await the end of the reactor remounting. The Fermi-chopper and the two background choppers are to be delivered in the first half of 1994. The assembly of the double curvature monochromator with four faces is in progress in Italy (Istituto di Struttura della Materia, CNR, coordinator Prof. F. Sacchetti, Perugia). A central forward scattering detector will be constructed by the Italian partner according to a design by the ILL detector group.

Detector tubes for higher angles have been purchased by the Italian partner who is also in charge of the detector electronics. The control and acquisition electronics have been conceived by the ILL electronics group and the major part has been ordered.

Since the reorganization of the Institute the project has been attached to the new Projects and Techniques Division (see there for more information).

IN5 Multichopper TOF spectrometer on the cold guide H16

The chopper-suspension system has been damaged by a number of incidents since its installation 7 years ago. This system is a prototype. Results of running/repairs are generally unpredictable. So we have taken the opportunity of the long shutdown to address some of these problems.

The axles for the magnetic suspension were installed over the top of the original axles causing a rather flexible axis and serious assembly/disassembly problems. We have developed new stiffer axles which if successful will be fitted to other choppers as failure occurs. We have also improved assembly techniques within the bearing components since several failures were associated with parts becoming detached during normal operation.

The performance of the adsorbing Gd_2O_3/epoxy coating around the periphery of the IN5 chopper disks has been remarkable, since at other institutes smaller disks rotating at considerably lower speeds have experienced several failures of this coating. This is all the more remarkable since there was an error in the original calculations made more than 25 years ago and recent finite-element calculations show that the coating should fail at the actual operating chopper speed of 20,000 rpm. The greatest stress is on the *inner* edge of the Gd_2O_3/epoxy band and two choppers have had slight damage at this point for some time.

These disks should be repaired to eliminate background problems, but in addition, the background could be further reduced by coating both sides of all disks and filling in one of the two windows on each disk.

The calculated stress at the weak point is 19.6 N/mm^2 at 20,000 rpm and the best adhesion for epoxy resins found after tests with various surface treatments is 17.9 N/mm^2. This is in agreement with the manufacturer's claims. One disk was repaired regardless, but duly failed under test at 20,000 rpm. Disks run at up to 60°C and differential expansion between the disk and the coating provides an addition mechanism of failure.

We are now embarking on a test of a sputtered Gd_2O_3 coating on one disk in order to test the adhesion and machinability of this coating and to assess the consequences of any distortion of the disk.

IN6 Focussing TOF spectrometer for long wavelengths on the cold guide H15

The main improvement carried out has been the VME chopper control and a new data acquisition program. The mechanical operation of the triple monochromator has been tested before putting it back in place. The instrument should be fully operational at the beginning of 1994 and the testing of the detection and acquisition system will be carried out by using a neutron source. Several safety features have been added to eliminate all possible risks of human exposure to the neutron beam.

IN10 Backscattering spectrometer on the cold guide H15

The programme of modernization of the electronics is nearly completed. The new motors and coders can be directly controlled by the VME crate, thus permitting the removal of the CAMAC controller. This upgrading was necessary in order to be compatible with the new type of operation, with a temperature scan of the monochromator, called IN10B. The high temperature cryofurnace used for IN10B is being assembled and tests will be done early in 1994.

A new device permitting a fast exchange between the doppler drive (IN10A) and the cryofurnace (IN10B) has been put in place and is working satisfactorily. This has necessitated some changes in the heavy concrete housing.

During the first tests of IN10B it was noted that some electric noise was produced by the start-up of the motors which are driving the motion of the lead curtain. This problem has been fixed by using electronic static relays.

IN11 Spin-Echo spectrometer on the cold guide H141

The NSE spectrometer received its new coils which have a more precise winding and current connectors placed close together to minimize the magnetic perturbation of the cables. The marble was extended to allow an easy exchange of the secondary spectrometer for IN11C, the high angle multidetector extension. The cabling is being reorganized for the same purpose. The last big items for IN11C (detector protection, analyzer support) arrived in December 1993. The He flight box and the equivalent of the "Fresnel" coils should come in 1994. The main and analyzer magnets are already mounted on the supporting mechanics and can now be easily attached to the sample table axis. If the water cooling is installed and if we have enough supermirrors by the restart of the reactor, in principle neutron tests could be started. The electronics part is being slightly modified to handle the new configuration.

IN15 High Resolution Spin-echo Spectrometer for long wavelengths on the cold guide H511 (cooperation ILL-KFA-HMI)

New sample cells with quartz windows for small angle scattering in a temperature range of - 100° C to 300° C have been designed and realized.

The multidetector has been renewed: the entrance window deformation has been reduced from 7 to 3 mm, the gas has been changed and the rear cover has been sealed.

It has been decided to replace the 16.5 m long prepolarizing H511 neutron guide (FeCo coating on an antireflecting layer). About 9 m of the new guide will be coated with natural Ni while only 7.5 m will be coated with the FeCo magnetic layer.

For the focussing option, new flat samples were tested. First, samples similar to the first prototype: it is the substrate, zerodur glass, which is polished to a μ-roughness guaranteed less than 3 Å (rms) on the top of which a thin layer (≈ 800 Å) is evaporated or sputtered; Cu^{65}, Cu^{65} + Al (120 Å on the top of Cu), $Ni_{1-x}Mo_x$ and C coatings have been tested. A second type of mirror was also investigated: it is the Ni-"Kanigen" thick layer (on an aluminium substrate) which is polished to the same μ-roughness: ≈ 3 Å rms. The diffuse scattering at the reflected beam has been measured on the neutron reflectometer at BENSC-Berlin. A signal/noise ratio of larger than 10^4 has been observed for all these samples at $Q \geq 0.0015$ Å^{-1}. This was the sensitivity of the test in view of a 5.10^{-4} background level. The addition of a protective layer, Al-layer, does not produce any extra scattering. Surprisingly, the same quality is also achieved with the Ni-"Kanigen" coating.

For the time of flight option, the permanent installation of the 3 choppers in the vacuum container and the complete cabling of the safety devices have been carried out. The safety unit for the choppers, also for the velocity selector, has been connected and tested. The group of 4 rotors can be driven and controlled locally from a Macintosh. The software for the remote control is still under development: ILL and ZEL-KFA-Jülich collaboration. The vertical link between the master crate of IN15 and the crate for the TOF-unit is still to be solved.

IN16 New backscattering spectrometer on the cold guide H53

Highest energy resolution in backscattering of better than 1 μeV is not available presently anywhere in the world. So how should it be tested whether the IN16 monochromators and analyzers produce the desired energy resolution of about 0.2 μeV? A more tedious way than using a backscattering spectrometer was to modify a small angle instrument to a backscattering spectrometer (especially tedious to explain the long measuring times to SANS physicists). This is what has been attempted again in another improved setup on the 8m-SANS at the NIST, Gaithersburg (Frick, Gehring, Neumann).

The experimental setup is shown in Fig. 1. A good collimation was used for passing with a roughly monochromatic beam (from deflection by a graphite (002) crystal) through a perfect, flat Si(111) crystal (ø = 2 cm) mounted on a Mößbauer drive which was calibrated and optimized to achieve low vibrational amplitudes with an interferometer. The flat transmission crystal cuts an extremely narrow gap into the wavelength band of the incoming neutrons. Neutrons with wavelengths within the gap are then missing for the backreflection on the test object, the analyzer crystal. If the transmission crystal is moved then this gap is Doppler shifted. Thus one can scan the wavelength band of those neutrons which are backreflected from the analyzer to a detector of 50% efficiency. Of course this works only after a precise alignment.

Several crystals were tested: 1) a perfect, flat Si(111) single crystal, giving 0.18 ± 0.01 μeV, probably the resolution of our setup; 2) a spherical analyzer carrying flat, polished Si(111) hexagons, glued according to the "classic" IN10 technique, giving 0.39 ± 0.034 μeV and 3) a spherical analyzer of IN16, carrying smaller (4 x 4 mm^2) polished Si(111) crystals, glued with a new technique, giving 0.38 +- 0.026 μeV. Thus about the same energy resolution was measured for 2) and 3). For geometrical reasons one would expect a better resolution for the smaller IN16 crystals. However, the beam size might be the limiting factor and for intensity reasons it was impossible to reduce it further. Thus it is still an open question whether the deformation of the crystals prevents obtaining a better energy resolution.

Furthermore a whole set of purposely deformed crystals fixed with different glues was tested. The spherical deformation, i.e. the δd/d which is enlarged by deformation, should be tailored to get the desired instrumental resolution: about 1 μeV for the second analyzer set of IN16 and about 0.7 μeV for the NIST backscattering project. Clearly higher reflectivity and a wider linewidth were measured (0.6 μeV in the case of a polished deformed 0.7 mm thick Si(111) wafer). Further tests of the analyzer crystals and the technique to fix them onto the backing plates have been started at the Siloe reactor (Blanc, Frick, Magerl) and are very promising. A Bonse Hardt camera setup is used and it

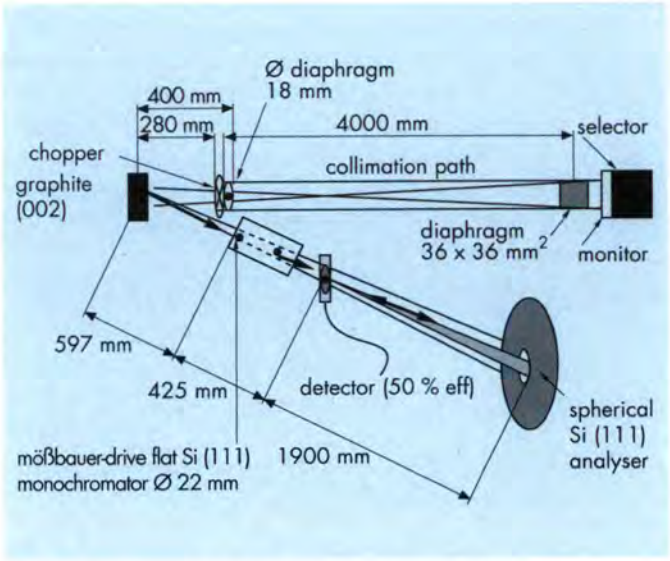

Fig. 1: Experimental setup used at NIST to test IN16 analyzers.

appears that with the higher flux available at Saclay, it should be possible to learn about the deformation using beam sizes down to 4 x 4 mm^2. This enables us to measure only one of the small single crystals on the analyzer plate. Such measurements are scheduled.

On the instrument itself several measures were undertaken to comply with the health physics regulations and to improve the background. The control programs and the electronics are currently being reviewed by the electronics and instrument computing group.

D7 Diffuse scattering instrument with polarization analysis on cold guide H15

D7 is waiting for neutrons. In the last year some money was spent on improving the safety of the instrument according to the new regulations. The shielding can now be closed by clamps on the front and rear. Also the doors at the entrance of the beam tube must now be closed to enable the shutter to be opened. In previous years it was easy to forget to close these doors, resulting in a higher background. The chopper has been equipped with a new drive and control unit and the polarizer within the shielding has been equipped with a step motor driven rotation table. This allows adjustment to be made from outside, thus satisfying safety regulations. We are now working with the new sputtering machine to get an improved polarizer, which has a higher transmission for the shorter wavelength of 0.31 nm. In this way we hope in the future to gain a factor of up to ten in intensity for this wavelength range.

Albert-José Dianoux

GAMS5 Project : Two-axis bent crystal spectrometer

Hans Börner

The promising progress which has been made in recent years in developing very high performance crystal bending devices has prompted the idea of using the ILL's reactor shutdown to build a new crystal spectrometer that will combine the outstanding resolving power which can be obtained with the GAMS4 flat crystal spectrometer, and the outstanding dynamic range obtained with the DuMond GAMS1,2/3 spectrometers.

Analogous to the two-axis flat crystal spectrometer, successive Bragg reflections on two crystals situated behind each other (with respect to the beam axis) eliminates direct imaging of the source geometry which will then be no longer critical in further improving the resolution.

The principle of operation of this new spectrometer may be inferred from Fig. 1. If γ-rays of a given wavelength λ are successively Bragg-reflected by the two crystals, the second crystal sees the γ-rays as if they originated from the virtual image produced by the first crystal. In this way the characteristics of the crystals (diffraction width θ_r, bending with θ_c) determine which portion of γ-rays emerging from the target is twice Bragg-reflected. And, as can be derived also from Fig. 1, the target width θ_s is no longer critical.

The basic layout of the GAMS5 spectrometer is very much an analogue of the GAMS4 two-axis flat crystal set-up. Likewise, it is equipped with high precision angle interferometers. The distance between the two crystals is 70 cm. The crystal bending devices allow us to vary the radius of curvature. All relevant interferometer parts which support the optics are made from glass ceramics, exploiting the extremely low thermal expansion coefficient of these materials.

The first version of this spectrometer will be equipped with the GAMS5T interferometer which has been built in the frame of a München -ILL collaboration and is currently being tested.

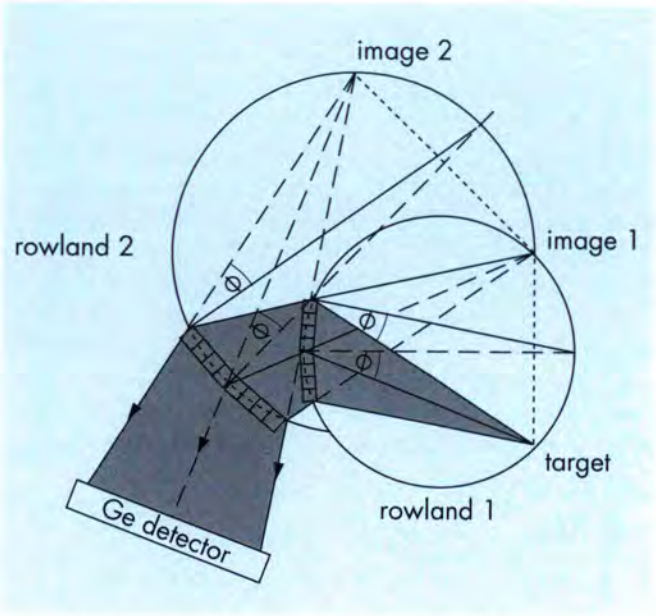

Fig. 1: Schematic diagram describing the principle of operation of the two- axis bent crystal spectrometer. The Bragg angle ϕ shown here is highly exaggerated. In realistic measurements ϕ is typically in the order of several minutes to degrees.

The PIAFE Project (Production, Ionisation et Accélération de Faisceaux Exotiques) Study on PN1

Herbert Faust

The PIAFE project was discussed by the Institut des Sciences Nucléaires (ISN) Grenoble and ILL scientists about three years ago. A collaboration has been established around ISN with several European countries which presently is working on a study. The aim is to use a thermal fission source implanted in the PN1 beamtube of the ILL reactor to provide neutron rich isotopes for transport via a beamline to the SARA accelerator complex at the ISN, which is some 400 m from the reactor. After delivery, the isotopes will be accelerated to energies which are sufficient to surmount the Coulomb barrier so that they can enter into nuclear reactions. For this project the LOHENGRIN facility would have to be modified. In addition, this would offer the possibility of studying very neutron rich exotic isotopes at a beam port in the ILL reactor hall. A feasibility study shows that with a neutron flux of 10^{14} n/cm^{2}s in an internal source arrangement, fission rates of 2.2 10^{14}/s can be expected in

a 6.3 kW source containing about 2g of enriched ^{235}U. The principles on the implantation of the thermal ion source have been defined in an internal report (1). Ionisation schemes, extraction and considerations on the isolator have been addressed in this report too. Furthermore, the radioactivity has been calculated. In follow-up work the beam optical system has been designed, including a periodic system of electrostatic einzellenses to confine the radioactive beam to the axis of the beam-tube, and a first mass separator with a deflection radius of 55°. Also the use of the BILL magnet as a high resolution mass spectrometer with $A/\Delta A \geq 5000$ has been discussed (Fig. 1). Scientific aspects are addressed in a report, which also reviews the possibilities provided by a 30 keV exotic beam port at the ILL site (2).

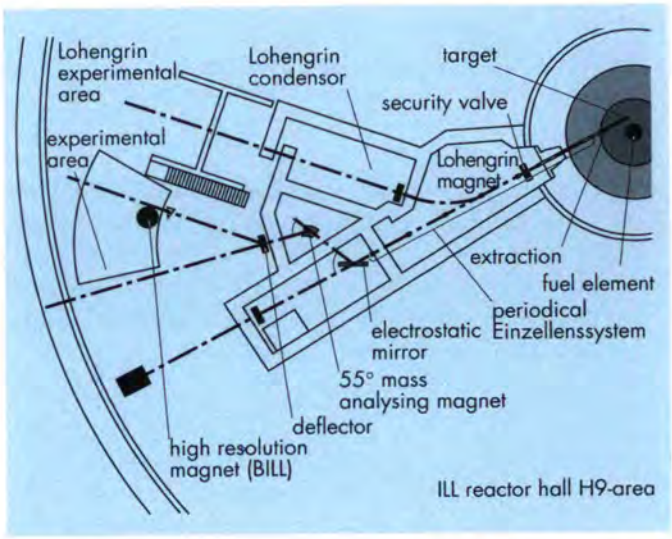

Fig. 1: Implantation study of the PIAFE project in the H9 area of the reactor hall. The beam is guided from the source near to the fuel element by electrostatic lenses to a mirror, a mass separator and the high resolution magnet BILL, which will be used as a mass spectrometer. For purpose of acceleration, the particles can be transported to the ISN.

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The ^{3}He Polariser Project

Francis Tasset

1993 has been another year of intense competition between the two possible routes (Hyperfine coupling of ^{3}He with optically pumped Rb/Direct pumping on metastable ^{3}He atoms followed by compression) toward the production of high density spin polarised gas. Although applications in fundamental physics (SLAC and MAMI) have up to now provided the strongest motivations and tend to concentrate the high level of expertise and funding required, several neutron scattering groups (Los Alamos, KEK, NIST, HMI) have begun significant investments into it.

At ILL, we have been following this development for several years. We started with a neutron test made on D3 before the reactor shutdown, on a Rb pumped cell in collaboration with the group of Professor T. Chupp. Despite the subsequent serious reduction in the scientific staff and the instrument development budget, the ^{3}He project remained funded at a reasonable level and we could continue to work on it.

At the beginning of 1993, an experiment was done by W. Heil et al. at MAMI, the Mainz Microtron, using polarised electrons scattered on a dense polarised ^{3}He target. A Toepler compressor was used successfully showing that the compression technique was possible, competitive and much cheaper than the Rb one being used at SLAC. Using funds from the European Community HCM programme allotted to this development, I was able to spend 3 months in Professor Otten's laboratory and work with R. Surkau and W. Heil on the new 2-stage amagnetic compressor made of large titanium pistons. The stay was very interesting and quite successful, culminating in a target being filled at 3 bars and 25 % polarisation.

A detailed estimate for a duplication of this glass-metal machine having shown that it is within the initial prevision for this project, I reported on the project at the ILL Scientific Council held in October with emphasis on the Mainz technique.

A further decisive step in this direction has been the arrival to Mainz, on 1 October, with the help of the HCM Network, of H. Humbot, a research associate, who gained experience in the field at Orsay in collaboration with M. Leduc at ENS. His first task is to build an optimized system for Neutron Spin Filters in Mainz. This system is the property of ILL and will be transported to Grenoble as soon as it becomes operational/useful for our polarised neutron programme here.

Owing to this favourable arrangement, things are now moving fast. Most of the optical parts, including the infrared LNA laser, were ordered in a few weeks and were delivered in 1993. We are now consulting prospective suppliers for the mechanical parts.

In the meantime, decisive progress has been made in the relaxation time in the high pressure cell. Being in Mainz just before Christmas, I was delighted to see the following:

a 150 cm^3 cell was filled with 2 bars of polarised gas in 37 min. and then closed. The polarisation was subsequently monitored every two hours by NMR. Two days later Christmas was coming and I had to leave: the signal was still strong showing a relaxation time of 43 hours!

It is true that hard work remains to be done in perfecting the second stage of the compressor in order to reach the high level of ^3He polarisation which we know is necessary to produce really intense polarised neutron beams. This is why it is very important that we clearly show our interest and needs to the people who are very skilled at it and probably able to reach such high polarisations.

On the other hand, in a relatively short time, decisive questions have been addressed with much success on several aspects of this system. In a very pleasant venture with atomic and fundamental physicists, the compact, transportable, neutron spin filter is becoming a reality for neutron scattering centres.

Laue-detectors

Mogens Lehmann

One of the instruments in the proposed modernization programme for the ILL was a diffractometer for the study of large unit cells. It was based on the use of the quasi-Laue method with cold neutrons and a limited wavelength range.

Although no modernization programme has started, the proposal has spurred a number of tests of new detector types. The reason for this is simple. No neutron diffraction instrument for macromolecular crystallography is of much use without a large position sensitive detector, and considering the eventual location of the instrument at an end-guide new types of detectors have been examined. These are combinations of neutron to light/γ-ray converters placed in front of suitable detectors.

Two approaches have been studied. In one case the detector was a position sensitive photomultiplier while in the other case image plate technology has been used.

For the photomultiplier (Hamamatsu R2487) a 1.5 mm thick Li glass scintillator was placed in front of the 4.5 by 5.5 cm^2 detector area. The 17 x 18 anode signals were converted into two pulses for each axis using a resistor chain. These four voltages were then recorded into a PC using a fast ADC converter and the position was calculated.

The detector was tested at the DN4 of the Siloë reactor in collaboration with staff from the EMBL and the CENG. It showed the method to be feasible. Counting rates of up to 10 kcounts/sec could be handled and the overall counting efficiency was 30 %.

The main difficulty seems at present to be the background. This is undoubtedly due to a mixture of fast neutrons and γ-rays, and more work is now underway to handle the discrimination against the latter.

Another more ambitious project is the construction of an image plate for neutrons, presently being undertaken at the EMBL outstation in Grenoble with support from the Freie Universität, Berlin.

Image plates are well-known to X-ray diffractionists. They are normally made from flexible plastic sheets containing BaFBr doped with Eu^{2+} ions. When irradiated with X-rays, electrons can be trapped in isolated, metastable states just below the conduction band. These states can be released by photo stimulation with visible radiation with the resultant emitted light lying in the blue region. The plate can thus be 'read' by scanning the plate with a laser while measuring the intensity and position of the emitted light. After cleaning with an intense light source the plate can be re-used.

Image plates for neutrons are obtained by adding Gd to the system, either as a thin plate in front or as a component of the plate. The high (n,γ) capture cross section for Gd ensures a good detection efficiency.

The prototype detector is a 40 cm long, 30 cm wide aluminium cylinder with the axis in the horizontal plane. The sample is placed in the middle of the cylinder, the beam is orthogonal to the axis and enters the detector through a small hole on one side. The diffracted neutrons pass through the aluminium to be detected by the image plate which is placed at the outside of the cylinder. After exposure this is read off much like one reads a phonograph. The pixel size is 0.25 by 0.25 mm^2, and the approximately 6 Mega pixels can be read in 5 min.

At present the detector has been assembled, and first tests are being done using X-rays. By the time of the reactor start-up it should be ready for testing with neutrons. Again an important part of the test will be to estimate the background sensitivity. To minimize this the detector tests should preferably be made at a location far from the reactor surface, and preliminary measurements are therefore planned to take place at the H142 position about 110 m from core. This is a cold beam with highest flux in the range from 3 to 6 Å, thus well-suited for the first Laue measurement tests. These can be done with the whole spectrum, while the detailed characterization is undoubtedly best done with a narrower wavelength range.

– PROJECTS – AND TECHNIQUES DIVISION (DPT)

The Projects and Techniques Division (DPT – Division Projets et Techniques) came into being on 1 July 1993. The purpose of the Division is to provide engineering services and project management support for all aspects of the experimental activities, including the computing infrastructure. It is responsible for improvements and innovation in the areas of beam distribution, neutron optics and detectors, sample environment and data acquisition. The Division was formed from the three previously existing Technical Departments – the Instrument Operation Department (EDEX), the Instruments and Methods Department (DIM) and the Computing Department (DI). Some of the activities of these Departments were moved to the Science Division (DS) and to the Administration Division (DA). From EDEX, the instrument technicians were transferred to the Instrument Groups in Science, and responsibility for the Chemistry and Biology Laboratories also passed to the Science Division; the Site and Building Maintenance Service moved to Administration. While the DIM remained within DPT, parts of the Computing Department dealing with administration and office computing, as well as Telecommunications, passed to Administration, while some staff members of the Department formed the nucleus of a new Scientific Computing Group in the Science Division.

The remaining parts of these Departments have been reorganized into two Branches: 'Instrumentation' and 'Development', and a Project Office. The Project Office acts also for the Science Division and helps to coordinate the activities of the two Divisions. It is the intention that, in the future, major instrument projects are managed from within the DPT in order to better coordinate the limited resources which will be available. Where necessary the scientist responsible will be detached to DPT from DS to act as project manager. Initially this arrangement covers developments of the neutron guide systems, the new time-of-flight spectrometer IN4C and the 'banana' detector of D20. Other existing instrument projects remain the responsibility of DS.

Although the DPT came into existence only in the middle of the year, it is appropriate that the Annual Report is presented in the new format of the new structure. Nevertheless it should be recorded that the old departmental structure survived until 30 June 1993, albeit with staff widely dispersed, both in helping the reactor refurbishment and on detachment to other organizations where their technical skills could be used in the absence of experimental activity at ILL. Some found the 'grass is greener on the other side of the fence' and will not return. We wish them a successful future.

The timing of the reorganization coincided with the first departures under the FNE Convention (see Director's Report). These included two of the Department Heads: J-C. Faudou and D. Rimmer, under whose leadership the DIM and the DI respectively had contributed so greatly to ILL's reputation in technical innovation and in service to the users. We are particularly grateful to both of them for working hard to the last minute to ensure a smooth transition to the new structure. A. Heidemann, previously Head of EDEX, now heads the Instrumentation Branch and C. Zeyen has taken charge of the Development Branch.

Despite the perturbations of 1993, progress has been achieved both in preparation for the reinstallation of instruments and in the various areas of technical development. This work, of course, all started under the old organization.

In this, my first and last contribution to the Annual Report as Head of Projects and Techniques Division, I wish to pay tribute to the skills, experience and dedication of all the staff, which I am sure will carry them well into the new life of the ILL after the reactor restart.

Peter Schofield

Project Office (W. Kaiser)

The purpose of the office in the new organization is to provide information, assistance and advice to all those concerned with the management of projects in the Science and the Projects and Techniques Divisions, on the allocation and control of the resources, personnel, facilities and finance of the various projects. The main activity was the update of the financial situation of spending for the instruments in 1993 and the preparation of the budget proposals for investment on the instruments in 1994 and 1995.

Neutron Guides (W. Kaiser)

H1-H2 Neutron Guides

As part of the refurbishment programme, 139 m of the in-pile guides, in the swimming pool and in the casemate, are being replaced. In addition, the opportunity is being taken to carry out work in these areas to enable further improvements of the neutron guides at a future date with minimum disruption to the scientific programme:

- The in-pile part of two new cold guides NG12 and NG13.
- The replacement of 11 m of H25 by a supermirror guide.

The guides of the in-pile part of the H1-H2 refurbishment have been delivered and the H2 guides are mounted in the mechanical support. The decision for the new guides NG12-NG13 was taken in April 1993. The new in-pile mechanical parts, allowing seven guides for cold neutrons, have been delivered and will be equipped with the guides before the end of the year (see Fig.1, page 142). The supermirror guide for H25 is being manufactured.

The replacement of the electrical control for the vacuum system of the H1-H2 guides has been finished.

H17-H18 Guides

The decision was taken to modify the geometry of these guides for a radius of 27,000 m to allow the installation of the diffractometer D16 on a new H17 guide and the small-angle spectrometer D17 on a new H18 guide. Therefore the H17 guide will not be refurbished in the out-of-pile part, and the H18 guide will not be available for the reactor restart. Major modification of the casemate of the H1-H2 guides is necessary. Preliminary studies are in progress.

H511 Neutron Guide

The present polarizing guide for the neutron spin-echo spectrometer IN15 has been coated with FeCo at HMI Berlin. After the decision to replace 16.5 m of this guide, a call for tender was prepared and the order will go out. 7.5 m of this guide will be coated again with FeCo at HMI.

IN4C Thermal Time-of-Flight Project (H. Mutka)

In the new organization of the Institut, the IN4C instrument project was attached to the Projects and Techniques Division. This reflects the main charge on the work, as roughly 4/5 of the manpower associated with the project belongs to this sector.

At ILL the main progress has concentrated on the choppers. For a while a rather uncertain situation prevailed concerning the availability of magnetic bearings for the new background chopper. Finally the initial idea of employing the old choppers adapted for a vertical rotation axis, with one new background chopper, was abandoned. A set of three new choppers was finally ordered and it is certain that this choice will be an advantage in the long term. The Fermi chopper and the two background choppers are to be delivered in the first half of 1994. The Italian partner (Istituto di Struttura della Materia, CNR-Frascati, coordinator Prof. F. Sacchetti) has concentrated on the mechanical design and fabrication of the curved monochromator assembly. A successful working prototype of a single row of eleven orientable elements has been produced. The full design of the four-face assembly with five of these rows on every face has been terminated and fabrication will be completed before the end of 1993

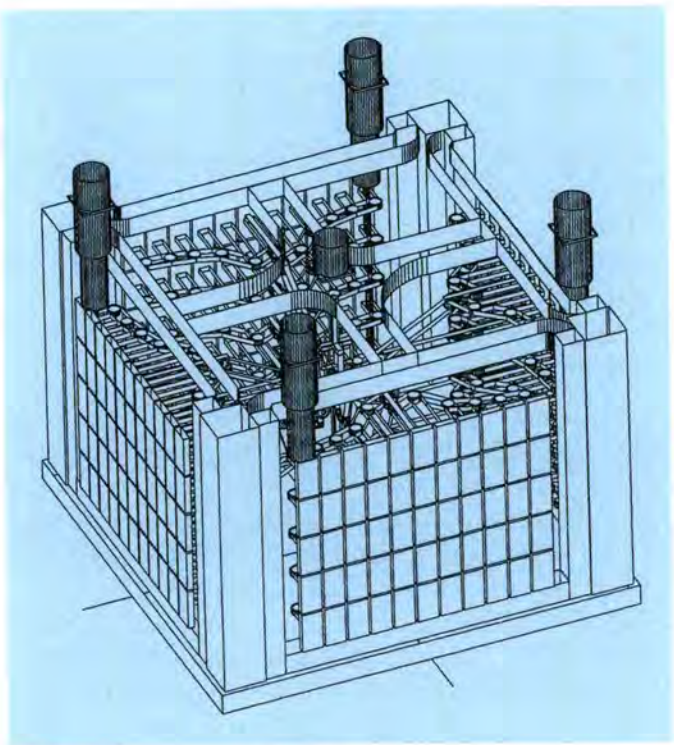


Fig. 2: IN4C thermal TOF spectrometer: a perspective view of the four-face monochromator exchanger under construction in Italy. Each face has 5x11 orientable elements for obtaining the double curvature.

(see Fig. 2). The graphite crystals for the monochromator have already been purchased and the Cu crystals are in production at the ILL. The assembly will be available for tests in the first half of 1994.

The Italian partner has received detector tubes which are being tested. Work has also started on the detector electronics according to the layout produced in the ILL Detector Laboratory. The cooperation on the central forward scattering detector is progressing, with some delay due to the unforeseen departure of the Head of the Drawing Office, who was in charge of the mechanical optimization. This detector will be constructed by the Italian partner according to a design established by the detector group of the ILL.

Preparation of the site for the installation of the new spectrometer has started, and pre-installation of the shielding elements is planned to start in January 1994. Definitive installation of the primary casemate will wait until the end of the reactor remounting.

The remaining design work consists of the details of the secondary flight box and sample environment, for which the concept already exists.

D20 High Flux Multidetector on the Thermal Beam H11 (P. Convert)

The construction of the powder diffractometer D20 has been dominated for many years by the realization of its fundamental part, the large linear Position Sensitive Detector, or Banana, covering 160° with 1600 cells (see Fig. 3 on page 142).

At the end of 1992, we were faced with the departure of our expert technician, M. Berneron, who had made most of the developments for the banana construction and had essential skills for the realization of some critical parts of the detector. Fortunately we were able to arrange his return to ILL in October.

1993 was used to carefully prepare the mounting of the detector:

- Realization of several frames or supports for the centring of the electrodes on their mechanical support, and their precise positioning on the mechanics of the detector;
- Construction of guard electrodes to improve the electrical field homogeneity at the ends of the detector zone;
- Cleaning of the cabin built for the dust-free assembly of the detector;
- Production of the 96-cell D20 prototype reproducing exactly the conditions of the large banana; the complete set of guard electrodes; gas filling of 3 bars ^3He + 1 bar CF_4; 3 modules of 32 amplifiers; 3 units of 32 logics; 3 VME data acquisition modules.

The 96-cell D20 prototype was successfully tested in March at LLB. The electrodes were found to operate perfectly: the electrode junctions have to be adjusted with a precision of 50 microns, the guard electrodes work well; the dedicated electronics are also working properly.

Following this, and after seven months of operation in the laboratory with a neutron source, another test was made in October-November at the Siloé reactor (CEN-G). This revealed an instability in the gas amplification of the electrodes. This question has now to be fully understood before the mounting of the large detector can take place. This will be completed as soon as the problem has been resolved.

All the pieces for the dedicated electronics are available (50 modules of 32 amplifiers, 50 units of 32 logics, power supplies). They will be assembled at the beginning of 1994.

The data acquisition system is complete, tested and operational, except for the synchronization module which has been designed but still has to be made.

1994 will be very busy in order to complete the instrument by the end of the year:

- Solving the problem of instability of the electrode amplification;
- Mounting of the banana;
- Assembly and test of the dedicated electronics;
- Mechanical modifications of the old diffractometer platform to receive the banana;
- Reinstallation of the H11 primary shielding;
- Shielding of the experimental area;
- Instrument control in VME standard (motors, encoders);
- Software for the D20 control with the Silicon Graphics dedicated computer;
- Production of the mechanical support for the HOPG monochromator, and adjustment of the 52 blades.

Instrumentation Branch

(A. Heidemann)

Introduction

As part of the new organization of the ILL the Instrumentation Branch was set up in the Projects and Techniques Division. This branch covers all activities concerning the construction and maintenance of the ILL instruments. It is responsible for the construction and installation of the instruments, for the delivery of neutrons to the instruments, for the design office and mechanical workshops (Central Workshop, Hall d'Essai), for instrument control and data acquisition, and for the computing infrastructure excluding Management Information Systems. The Instrumentation Branch consists of five Services:

- Neutron Distribution and Central Services.
- Mechanical Engineering.
- Electronics.
- Computing: Instruments and Network Infrastructure.
- Computing: Systems and Communications.

In addition the Branch has responsibility for managing two major projects: the refurbishment of the beam shutters and the programme for the reinstallation of instruments.

The Services have the following responsibilities:

Neutron Distribution and Central Services

- Systems for the supply of neutrons to the instruments (neutron guides, beam shutters, beam stops, safety loops).
- Operation and maintenance of the experimental halls.
- Vacuum systems.

Mechanical Engineering Service

- Finite element calculations for the layout of instruments.
- Mechanical design of instruments by the Drawing Office
- Preparation of new instruments by the 'Hall d'Essai' and the Central Workshop.

Electronics Service

- Design, construction, testing and maintenance of instrument control and data acquisition systems.

Instruments and Network Infrastructure Service

- Instrument computers and software for the four condensed matter instrument groups.
- Hardware of the scientific computing networks.
- Coordination of the networks on the site, including connections to ESRF, EMBL and externally.

Systems and Communications Service

- Administration and operation of central computing facilities and of workstations.
- Data base and archives.
- Software libraries.
- Electronic mail.
- Micro-computing (PCs, Macintoshes).
- Instrument control and computing for the Nuclear & Fundamental Physics Group.

It is hoped that despite the considerable reduction in staff, of the order of 25 to 30 % during 1993 and 1994 compared to the situation in 1991, we will still be able to provide reasonable technical support to the instruments. In the following section we present the activities of the Instrumentation Branch during the year 1993 in more detail.

Neutron Distribution and Central Services (R. Mathieu)

The main activities have been as follows:

- Contribution to the project for modernizing the beam shutters.
- Coordination of the work on the following instruments: EVA, PF1, GAMS5, and studies for the acquisition of the possible CRG instrument ADAM.
- Safety studies for certain nuclear physics experiments: ^{177}Lu and ^{198}Au on PF1.
- Work on the experimental halls ILL7 and ILL22: cleaning, painting, removal of old cables, etc.
- Contribution to the scheduling of the reinstallation of instruments.
- Assistance to the construction teams on the reactor: lifting, internal and external transport.
- Intervention work on instruments and the reactor.
- Production of poster boards to illustrate the function and purpose of the instruments, which will be installed next to the instruments after the restart.
- Assembly of an 'historical' exhibition in the old library in ILL4.
- Coordination of sales of sample environment equipment.

Mechanical Engineering (M. Thomas)

Although the ILL's scientific activity was reduced during the long reactor shutdown, the mechanical engineering group's workload has not diminished, owing to the work in progress for the ILL instruments and its contribution to the reactor refurbishment programme.

Assembly Hall and Workshop

The assembly hall, with the assistance of the Neutron Distribution and Central Services, undertook the project for rebuilding the mechanical parts of the beam shutters and

safety loops. Some of the more usual activities of the assembly hall have continued, such as the assembly and tests of the IN15 choppers, the D22 velocity selector and the rebuild of the controls of the D11 velocity selector. The workshop was able to assist with the reactor refurbishment by responding very quickly to the requirements of the project.

Drawing Office

Summer 1993 saw a change of engineer in charge (departure of A. Billington end of July and arrival of P. Malbert beginning of September) and a reduction of staff by early retirement and detachment. The main activity was concentrated on improvements for existing instruments and on new instruments.

Improvement of existing instruments

- GAMS2/3: completion of the rebuild.
- New secondary spectrometer for IN11 with a multidetector.
- Sample areas of the instruments D11, D17 and D22.
- Continuation of the study for the installation of the new multidetector for the instrument D20.
- Monochromators for D2B, D19 and D20.
- Multidetector modification for D19.

New instruments

- Gamma spectrometer GAMS5.
- Continuation of intensive studies for the TOF spectrometer IN4C.
- Study of the Brillouin spectrometer IID.

Preliminary projects

- Installation of instruments ADAM and PF1 on the H53 neutron guide.
- Installation of the instrument IN22 (previously IN20B) on the H25 guide.
- Modification of the H17/H18 guide area in view of the installation of the future reflectometer (rebuild of D17).

Calculation Laboratory

The most significant of the studies carried out were:

- Study of the static behaviour of the IN4C vacuum box.
- Stress and dynamics verification of the IN4C Fermi chopper.
- Optimization of the housing of the IN4C multidetector.
- Characterization of elastic behaviour of flexure-based rotation modules for the ultra-fine rotation stage of GAMS5.
- Non-linear contact analysis of elastic behaviour of the reactor flange clamping collars.
- Magnetostatic study of neutron precession coils with superconducting Meissner screens.
- Mechanical analysis of the anticlastic curvature effect induced by the bending of a thin rectangular plate.
- Study of the elastic behaviour of a bilayered material subjected to a transversal and time-dependent thermal gradient.
- Study of the IN5 chopper disks under the effect of rotation (see Fig. 4 on page 143).

Electronics (R. Klesse)

The activity of the Electronics Service was concentrated on the following topics:

Improvement of existing instruments

The three-axis spectrometers IN1 and IN8 are in the process of being equipped with VME electronics. The backscattering spectrometer IN10 is now fully VME controlled and has been recabled. D11 was changed from CAMAC to VME within three months, and the electronics were considerably reduced. T13C was mounted on a VME plus Macintosh base and has become an independent moveable device. The instrument was running satisfactorily for the whole of 1993 at Orphée (LLB).

Preparation of the new instruments

IN15, IN16 and D22 are ready for commissioning in 1994. On D22 all motors are connected and running. Data acquisition is done with a new VME-VSB histogramming device which can handle more than 10^6 events per second.

Restart and tests of all the instruments in the two neutron guide halls

Many problems have been encountered caused by the two-year shutdown. Most of them have been solved.

Technical assistance to other ILL services and external laboratories (HMI, ESRF, PSI, Thomson, etc.)

During the period of the reactor shutdown, staff have been detached to other institutions, and work has been carried out under contracts.

Computing: Instruments and Network Infrastructure (A. Barthélemy)

The main aims of the Instruments and Networks Service in 1993 were:

- To maintain the equipment correctly to facilitate the restart of the instruments.
- To restart and test the neutron guide instruments and to continue software developments on new instruments.
- To modernize and to standardize the older computing equipment.
- To prepare the local network for decentralization of computing.
- To maintain a high technological level.

Maintenance

The instrument computers have remained connected. In this way the number of breakdowns has been reduced, but some units have had to be changed.

Restart of the Instruments

All the computers of the instruments on the neutron guides are operational. With the replacement of certain electronics systems, software developments have been carried out. This change has made it possible to check the cabling.

Modernization of the Instrument Computers

The PDP11 computers have been or are being changed, except on D3, D7 and IN11. For D20 a Silicon Graphics workstation has been purchased, and for the three-axis machines a DECstation 3000-300L and a Hytec CAMAC controller have been delivered.

The acquisition and control programs for a large number of instruments have been modernized and standardized on the MAD program (IN5, IN6, IN10, IN16, D1B, IN3, IN12, D10, DB21, D16, D11, D17, D22).

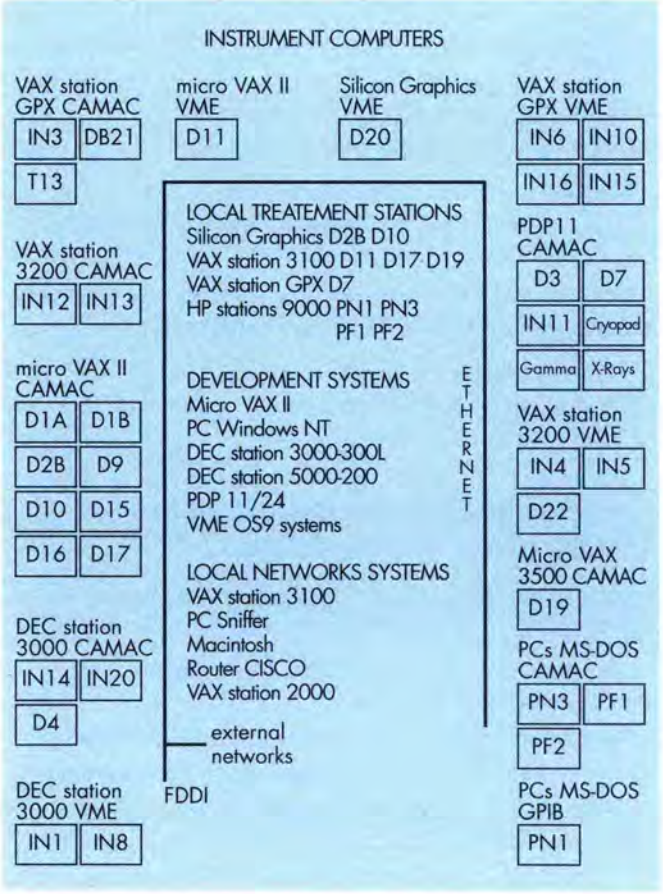


Fig. 5: Overview of the types of computers and electronics systems installed on the ILL instruments at the end of 1993.

Fig. 5 presents an overview of the types of computers and electronics systems installed on the ILL instruments at the end of 1993.

Changes in the Local Network

Considerable technical and financial efforts have been made on the ILL local network:

- An FDDI ring has been installed as part of the UNIX plan.
- A fibre optic Gigaswitch concentrator is operational; its two main aims are to permit rapid access to ILL servers with a possible evolution towards asynchronous transfer mode (ATM), and to prepare for changes in the computing centre.
- The asynchronous cabling has been updated with elimination of unused cables, and the installation of new terminal biprotocol servers and the gradual elimination of the line concentrators (MICOM, PDP11) are in progress.
- A computerized system for updating the cabling plans is operational.
- Studies are in progress for a joint program of the ILL, ESRF and EMBL networks towards RENATER planned for 1994.
- Monitoring of the network has been improved by way of the network management station and specific products on Macintoshes and PCs.

Technology Monitoring

The increasingly rapid development of computing makes it necessary to be extremely vigilant about future choices. A study of the possibilities of the Windows NT system for operation of the Microsoft instruments has been initiated.

The new technologies of the local networks have been studied in particular as the local, national and international network has become fundamental in the context of modern decentralized computing.

Computing: Systems and Communications (M. Le Sourne)

At the end of 1992 we submitted to the Steering Committee at its request the broad outlines of a UNIX plan providing for the progressive conversion of our computing applications to a UNIX environment. This plan was accepted as a whole, and an initial budget was provided for 1993. A considerable part of our activities has therefore involved the implementation of the investment plan and the establishment of a first platform to permit this work to start. The conversion to UNIX is a major operation, which will require time and effort from scientific and technical personnel, and it is clear that in the context of the reduction in staff this can only be implemented very gradually. For this reason we have also worked on the development of our central VAX system, so that for the immediate future we can maintain a VMS service appropriate to our needs

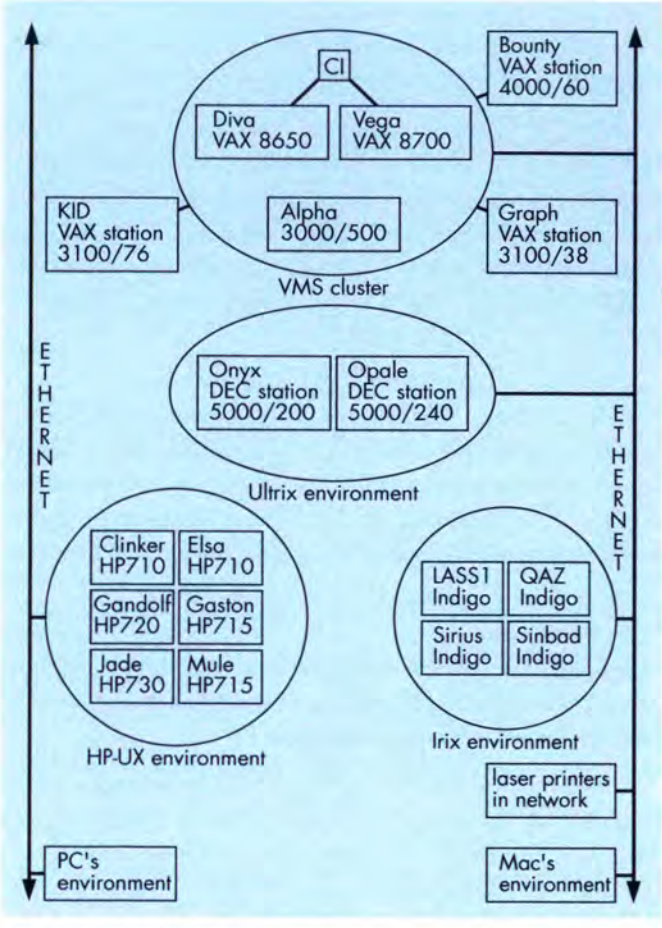


Fig. 6 : The stock of computing equipment available for scientific applications at the end of 1993 shown schematically.

and our financial means. Fig. 6 shows schematically the stock of computing equipment available for scientific applications at the end of 1993.

UNIX

The first investments have been for the purchase of workstations. To this end a study was carried out to compare the main equipment on the market; after considerable debate between the scientists and the computing staff, the choice was made of Silicon Graphics (SGI) and Hewlett-Packard (HP). Five instrument groups have received UNIX equipment:

- 2 HP stations for the Theoreticians.
- 2 SGI stations for the Diffraction Group.
- 1 SGI station for the Large Scale Structures Group.
- 1 SGI station for the Time-of-Flight and High Resolution Group.
- 1 HP station for the Nuclear Physics Group.

Reconfiguration has been carried out of one Dec 5000 station to act as server for X terminals and file server.

The graphics group initiated talks with the scientists to define the broad lines for graphics support and conversion to UNIX. This resulted in time investment in market standards such as X11, OSF/MOTIF, GKS, PHIGS, in evaluation of graphical packages such as KHOROS, AVS, etc., and in comparison of user interface builders (GUI's). In parallel we have introduced in this rather heterogeneous environment a few X terminals which were selected, after evaluation, from the Tektronix range.

During the whole of this period the members of the Service, with the aid of a number of training courses, have acquired considerable experience in the management of UNIX equipment and the organization of these systems for client/server. For day-to-day operation a procedure has been introduced to provide backups for these systems. A study is in progress for the choice of a product for saving and archiving in a heterogeneous environment.

VMS

There are several reasons, both financial and technical, why UNIX cannot be introduced immediately in its entirety:

- The investment cost of UNIX-based systems has to be spread over several years;
- The existing VAX **instrument** computers will continue to work at the reactor restart;
- There is an enormous investment in users' data treatment programs, written in older versions of VMS Fortran.

It was therefore found necessary to maintain a central processing service operating under VMS for the time being, in parallel with the installation of the UNIX computing facilities. The decision was accordingly taken to lease a DEC Alpha 3000 - 500 AXP computer which can run either VMS or UNIX environment. It will enable a smooth transition to be made at the time when a VMS central service is no longer required.

Data Base and Archive

The database has been renewed for integration in the UNIX environment. At present the VAX central system stores experimental data in binary format. In parallel a UNIX base will store the same experimental data in text mode. This will be maintained on a UNIX server with a tree structure permitting easy access to information. Some of the treatment tools, represented by a library of subroutines, have been made available to the users.

Software Libraries

One of the responsibilities of the Service is to provide libraries, compilers and development tools on the stations and servers.

- The Nag Fortran library has been installed on a UNIX server. With a view to ensuring continuity, we have set up the Harwell library for different types of stations.

• Fortran 90: a new version of this compiler has been installed and we have produced a document giving practical advice for the conversion of programs written in VAX Fortran. Fortran 90 compilers will be available from manufacturers during 1994.

Communications and E-mail

The ILL IP network is an Internet domain named ill.fr. Primary and secondary name servers have been installed on two existing DEC - 5000 stations. A mailing gateway has been defined, one of the functions of which is the distribution of mail to UNIX stations and also to Macintoshes and PC's. The service has also provided considerable assistance to users to enable them to make full use of the possibilities of Internet. The extension of our communications on this network has made it possible to eliminate the EARN link with Montpellier and the link with the HEPNET network.

Micro-computers

The stock of micros at ILL may be estimated at the end of 1993 at about 100 PC's and twice that number of Macintoshes. For all these Micro-computers, the Service has provided first level intervention work, which has made it possible to reduce maintenance costs considerably.

Macintoshes, extensively used for word-processing, are increasingly utilized in the scientific sector for various functions such as the presentation of documents, emulation of graphic terminals and X terminals, data treatment, electronic mail on IP network and access to Internet servers.

As regards PC's, these are more oriented towards specific tasks related to management applications and technical applications, and for the control of Nuclear Physics group instruments.

The aim has been to make these two environments as uniform as possible for the use of printers, exchange of documents, and their integration in the worlds of UNIX and VMS.

Support for the Nuclear and Fundamental Physics Group

On the basis of the timetable and forecasts produced in 1992, the group is firmly oriented towards the use and integration of PC's for control of the Nuclear Physics instruments PN1, PN3, PF1 and PF2.

The first few months were devoted to the overall study of PC's in the DOS and Windows 3.1 systems, and in the choice of software to be used both for experiment programs and for publishing and data treatment supports. The main direction is the choice of Microsoft software which, without being the most powerful, resolves the problem of compatibility between software, which goes in the direction of efficiency and reliability. The group is currently supporting the following software: DOS 6.0, Windows 3.1, Word 2.0C, Excel 4.0, Visual Basic Pro 3.0, Access 1.0, LAN Manager network and LABVIEW 3.0. For the calculations we have adopted Fortran 90 from LAHEY, which provides good compatibility with the VAX.

With a view to confirming the consistency of these ideas and their applications, we contributed to a considerable extent to the implementation of an experiment at ESRF, in collaboration with C. Vettier. This experiment operates very well in accordance with specifications: four coded movements and one acquisition system: monitor, timer, detector with scans and graphs.

We also incorporated a CAMAC driver in Windows 3.1 in order to connect the electronics which will not be changed in certain experiments (e.g. PF2). With the help of this driver we have produced an acquisition program skeleton based on object programming. In the context of the experiments we also restarted the magnet of the spectrometer BILL in collaboration with K. Schreckenbach (München).

Another aspect of our activities has been the renovation of the data acquisition system for the reactor (TCMS II), including design study, drafting of specifications, selection and ordering of hardware and software.

The aims for the coming year are: the restart of PF2, planned for February 1994, then PN1 for March, PN3 for August and finally PF1 in the last quarter of 1994.

Coordination of the Reinstallation of the Instruments (D.A. Wheeler)

The first objective, to have all the instruments in the guide halls operational by the end of 1993, is well in hand, although a few instruments will not achieve this due to technical difficulties.

The second objective, to have all of the 25 scheduled instruments operational in the middle of 1994, is dependent on the date of installation of the reactor block as work on the level C instruments cannot start until the reactor beam tubes are installed. The reinstallation of the instruments, which will mobilize more than 60 persons from the Science Division, the Administration Division and the Projects and Techniques Division, should in large part be achieved by the middle of 1994 as planned.

Beam Shutter Modernization (W. Kaiser)

The activity of the refurbishment of the beam-shutter system under **Quality Assurance** was concentrated on the H1-H2 neutron guides and the instruments in the ILL7 guide hall, which concerned 52 out of a total of 72 shutters. The shutter mechanism, the electro-pneumatic and electrical controls including supply of compressed air are completed. The new interlock system with keys for gate and shutter control is in place.

Development Branch

(C. Zeyen)

With this year's reorganization of the ILL the following activities were combined under the common label 'Development Branch': Monochromators, Detectors, Multilayers, Cryogenics, High Temperatures and Pressures. A new group 'Instrumental Techniques' was created, but its activities could not start because the entire staff had to help out in other areas of the ILL. The projected activity of this group (B. HAMELIN) will aim initially at a more efficient use of the reduced number of instruments as well as of the reduced number of cycles. The Development Branch staff had to show a great deal of flexibility this year since in many instances laboratory and project activities had to be done in parallel with help to other reactor or instrument-related activities.

Monochromator Laboratory (A. Magerl)

Immediately after the present shutdown in 1991 the Monochromator Group transferred one of its neutron diffractometers for crystal testing, T13C, to the neighbouring Siloé reactor. This proved extremely valuable for ongoing work of the group, and the long list of other users underlines the need for general purpose instruments. Nevertheless, the moderate beam quality and the limited availability of the beam made it desirable to transfer this year the complete second test diffractometer T13A to a beam position at a cold neutron guide at the LLB reactor at Saclay. The instrument is now installed with a fixed take-off angle of 90° for the primary diffractometer, but different monochromators such as HOPG, and Si 111, Si 113, and Si 115 made from oxygen-precipitated Czochralski crystals offer a good choice of wavelengths and resolutions with a very good beam quality. Monochromator components measured so far include Si crystals for applications in backscattering, HOPG for D20, Be-project, Ge for D2B, and Cu for IN4C and for LLB.

The present strong request for diffraction techniques other than neutrons puts a heavy demand on the group's X-ray and γ-ray diffractometers which have been heavily used throughout the year. However, parts of these facilities like the electronics and some mechanical components show serious signs of wear. For the near future improvements/ investments need to be envisaged if these experimental techniques are to be maintained, and alternative possibilities, as offered for example by the proximity of the ESRF, should be considered as well.

A new hot press for plastic deformation has been constructed and built in collaboration with the ILL high temperature laboratory. At present it is about to go into the test phase. This device is mechanically much more stable and precise than the old hot press, which has been in use for about 25 years, but which now lacks completely the mechanical precision and temperature homogeneity needed.

The work of the group was largely concentrated on the manufacture of monochromators for IN4C (Cu), D2B (Ge) and D20 (HOPG). These are three major and work-intensive projects. For example, the IN4C monochromator needs 110 individual Cu crystals! A significant support was also provided for IN16. The particular question here is how to cover the large spherical surfaces of 7 m^2 for the monochromator/analyser system with Si crystals which should either be stress free to achieve highest resolution or which should have well-defined stress conditions to obtain, say, a 5-10 times increased neutron flux.

In addition the group is occasionally asked for urgent assistance when installed monochromators fail. This year the IN3 graphite monochromator was broken when the instrument was modified, and the Ge monochromator of D1A was destroyed due to an imploding guide at LLB.

This year the Be-project came to a formal end. This project linked several major neutron scattering centres (PSI, Switzerland; HMI, Germany; BNL, USA, and Tohoku University, Japan) with the ILL and with the Max Planck Institut at Stuttgart in an attempt to grow Be crystals suitable for a neutron monochromator. It turned out that this goal was much more difficult to achieve than expected in the beginning. Nevertheless, there has been steady progress over the years concerning both the growth of high quality single crystals and the creation of an appropriate micro structure by plastic deformation. These studies have been continued both at Stuttgart and at the ILL within the framework of a diploma thesis. It has been possible to produce a suitable mosaicity for the required crystallographic plane with the correct anisotropy. Recent investigations with 1 mm-thick Be blades have shown that it is possible to approach for larger areas the reflecting power of Cu crystals. Further progress is expected from a continuation of the present studies in the form of a Ph. D. thesis project which is being carried out in collaboration with the TU Freiberg and the MPI Stuttgart.

Another research project in collaboration with the INPG, Grenoble, was continued successfully during this year. It concerns the synthesis of $Si_{1-x}Ge_x$ crystals by a low pressure CVD technique. The aim is to replace the mosaicity of monochromator crystals usually employed by a gradient in the lattice spacing for increased beam intensity. The diffraction properties have been calculated recently by a transfer matrix technique, and typical results are shown in Fig. 7. It needs to be noted that full reflectivity over an extended wavelength range can be built up in both Bragg and Laue diffraction geometry by a proper choice of the gradient of the lattice spacing. Some experimental results are shown in Figs. 8 and 9 (page 143). Fig. 8 shows a neutron diffractogram taken at the high resolution time-of-flight diffractometer of the TU München for a crystal with

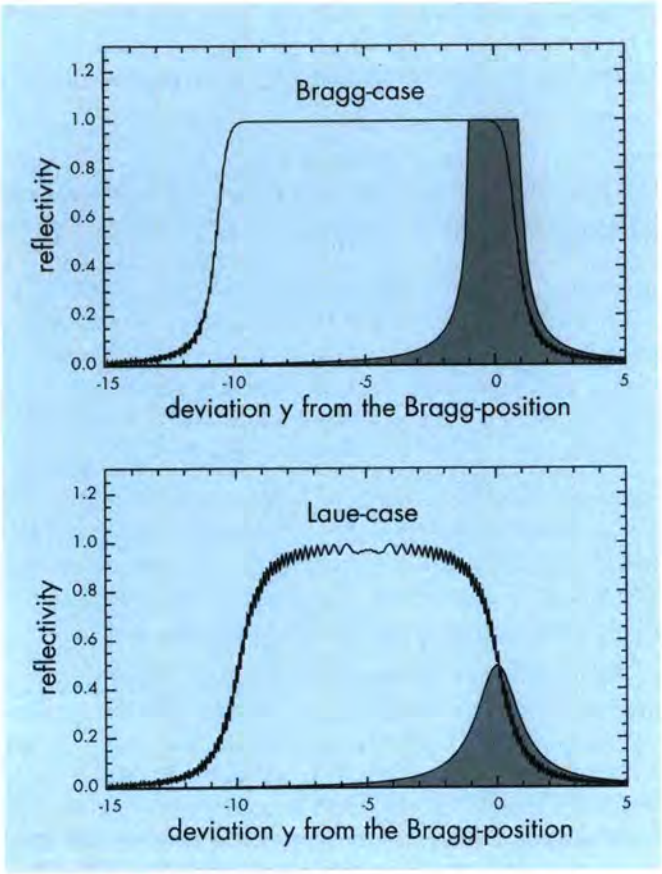


Fig. 7: Calculated diffraction profiles of $Si_{1-x}Ge_x$ crystals, which have a width of the reflection profiles five times larger than the Darwin widths of a perfect crystal, with optimized gradients in Bragg and Laue geometry, respectively. The curves presented are calculated for a crystal thickness of ten times the extinction length. The reflection profiles for perfect crystals of infinite thickness are shown in a deeper colour.

six $Si_{1-x}Ge_x$ layers with x = 0.08, 0.14, 0.19, 0.24, 0.29, and 0.32. The main peak originates from the thick Si substrate and the six additional maxima stem from the deposited epitaxial layers. Their reduced intensity and increased width is due to the fact that the thickness of the mixed layers of about 15 μm is only about half the extinction length. The peak position for x = 0.32 corresponds to a change of the lattice parameter of Δd/d = 1.3 %! Fig. 9 (page 143) shows a two-dimensional intensity plot in a colour code and its one-dimensional projection into a longitudinal diffraction scan of a $Si_{1-x}Ge_x$ crystal where the concentration was varied continuously during crystal growth between $0 \leq x \leq 0.03$. Such high energy X-ray diffraction data were taken at both HASYLAB at DESY, Germany, and NSLS at BNL, USA. Clearly the build-up of both mosaicity and gradient of the lattice spacing can be seen for this crystal whereas usual monochromator crystals after plastic deformation only show mosaicity.

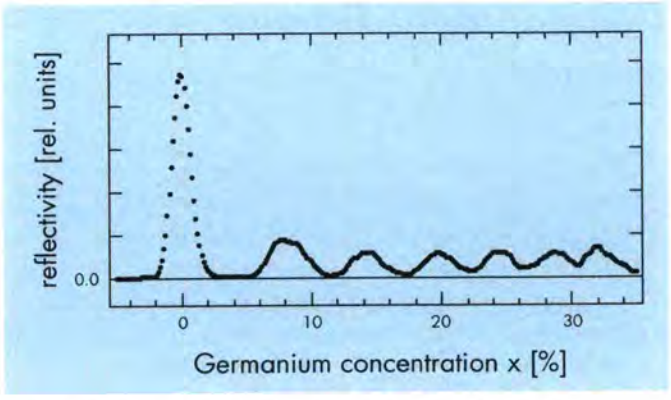


Fig. 8: Neutron diffraction scan of a $Si_{1-x}Ge_x$ with x = 0 (main peak from the Si substrate), and x = 0.08, 0.14, 0.19, 0.24, 0.29, and 0.32 (data taken at the high resolution time-of-flight diffractometer at the FRM, Munich).

Finally it should be noted that a Workshop on 'Focussing Bragg Optics' was organized jointly by the ILL and the Physikalisch-Technische Bundesanstalt Braunschweig in May. From all the contributions it became clear that there is still a large potential for improved neutron optics relating to new focussing principles and techniques to make optimized use of neutron beams.

Detector Laboratory (A. Oed)

The detector laboratory staff was reduced, in the course of the reorganization, from six to four. It was therefore not possible to continue with all the projects which were in progress. In particular, no further development of the new neutron microstrip gas detector technique could be undertaken. Nevertheless a large number of successful microstrip proportional counter (MSPC) applications in a variety of fields were reported at the MSPC-workshop (Report ILL 93 GE 048) held at the ILL this year.

A position-sensitive two-dimensional MSPC detector with charge division which was described in last year's report was successfully tested at the PSI reactor. For the moment the data acquisition rate is limited by the PC-based data system to about 7 kHz. A modification of the software, which is being implemented, will however allow data acquisition rates of up to 20 kHz.

The prototype of the D20 large MSPC was extensively tested, together with its VME electronics, at the Saclay reactor last March. Very high data rates at a perfectly constant detection probability over the entire detector surface were recorded. Further tests during the rest of the year were undertaken at the laboratory with a neutron source. The latter tests revealed a modification of the microstrip glass substrate, and hence of the detection signal amplitude, in the course of the last nine months. To avoid this problem in the future, a thin electronically conducting glass coating is envisaged. Promising tests have already been undertaken by the glass manufacturer. The general

future solution to this problem will be the regular use of electronically conducting glass substrates, instead of the ionic-conductor glass used in the D20 detector. The two-dimensional MSPC mentioned above is already equipped with electronically conducting glass substrates for the microstrips.

The ILL cryogenic laboratory has designed and delivered a ^{3}He distillation and purification unit which operates very satisfactorily (see Fig. 10 and Fig. 14 on page 144).

The detector group is also involved in the construction and further development of multiwire detectors. The following detectors were renewed or repaired: the gas charge of the IN15 multidetector had been polluted and was replaced. The opportunity was taken to pre-stress the entry window using a double-electron-beam weld technique in order to reduce its deformation. With the new filter gas (1 bar ^{3}He + 0.3 bar CF_4 instead of 1 bar ^{3}He + 0.5 bar C_3H_8) the window deformation is reduced from 7 to 3 mm.

The D15 multidetector has been reopened and two anode wires were found to be slack. All the anodes were rewired. After remounting and tests (D. FELTIN, Charactéristiques du multidétecteur de D15, DIM-93/022-DF) this detector was lent to HMI Berlin.

The Saclay multidetector was repaired at ILL (under guarantee). The 128 x 128 cell detector (1.5 mm spacing) had a deformed entry window and a cracked cathode glass plate.

Both this multidetector and the IN15 one have passed successful neutron tests and the detector casings are being closed by welding.

Multilayer Laboratory (I.S. Anderson, O. Schärpf)

Both evaporators have been used continuously throughout the year for the production of Co/Ti polarizers and Ni/Ti supermirrors. In addition to meeting in-house demands, polarizing benders were supplied to the National Institute of Standards and Technology, Washington D.C. and the Physikalisch Technische Bundesanstalt, Braunschweig. Supermirrors for a focussing device were also produced in collaboration with the Technical University, Munich.

Although it had been foreseen within the modernization programme to purchase a new sputtering facility, hopes to improve the multilayer quality were dashed when the modernization programme was stopped. Fortunately the ILL has signed a collaborative contract with the University of Evry, permitting the installation at ILL of a 'state of the art' sputtering facility recently developed for X-ray multilayers at the Laboratoire d'Électronique Philips (LEP).

The facility (see Fig. 11 on page 144), consisting of a UHV chamber with four RF sputtering positions, load lock module, on-line kinetic ellipsometry, quadrupole gas analysis and a multitude of ancillary equipment was dismantled by W. Graf together with the LEP staff and delivered to ILL at the end of April. The installation and commissioning of the primary functions: vacuum, water cooling, RF power, ellipsometry, were carried out during April and the first films deposited at the beginning of June (see Fig. 12 on page 144). In addition to significant improvements to the basic programs, notably simulation/fitting of ellipsometry traces (see Fig. 13) and PC-based control of the quadrupole gas analyzers, a number of technical modifications have been made to the facility to enable the deposition over 30 cm-long substrates.

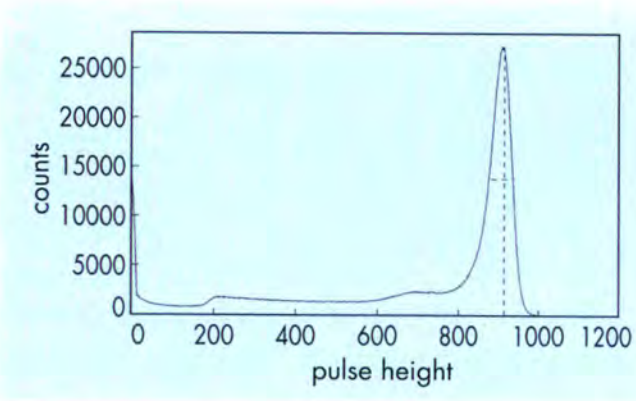


Fig. 10: Pulse height spectrum of the ^{3}He detection reaction measured in the laboratory with an Am-Be neutron source and ^{3}He gas recovered and purified using the new cryogenic unit.

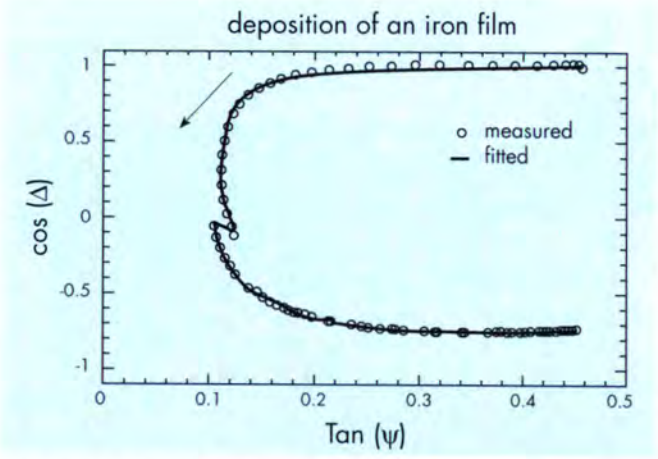


Fig. 13: On-line ellipsometry essentially determines the complex index of refraction of a film by evaluating the ellipsicity of polarized light after reflection. The variables ψ and Δ characterize the dielectric function of the deposited layer and its thickness. The figure shows the ellipsometry trajectory during the deposition of an iron film onto glass. The deposition follows the direction of the arrow, each point corresponding to a step of about 1.5Å. The first part of the curve can be simulated by an amorphous Fe film containing a 20% void fraction. At a thickness of 60Å a sudden step in the trajectory can be seen, corresponding to spontaneous crystallization of the film. After crystallization the trajectory can be well simulated by growth of a dense film with the refractive index of pure iron.

Presently the hardware is being adapted to cater for 20 cm-wide samples and the optimization of the uniformity shields is in progress.

Furthermore a series of ex-situ analysis techniques has been set up to characterize deposited films including mechanical profilometry, quartz thickness monitors, spectroscopic transmission and X-ray reflection. We are thus ready to achieve our aim: the production of significantly improved supermirrors for the neutron optics of ILL.

Cryogenics (D. Brochier)

Standard Cryogenics

The campaign for repair, modernization, and tests of standard ILL cryostats has been continued. The new model of sample holder, with a much shorter response time, is being generalized. Following previous development, a pneumatic cold valve has been perfected and is progressively installed on all standard cryostats. The assembly and testing of a special liquid nitrogen cryofurnace has been carried out. The Cryopad 2 (for neutron polarization analysis) has been assembled, tested and put into service (for the standard cryogenics part). Assistance has been provided for the drawings of the precession coils.

Assistance has been provided to other groups, for example:

- Construction, assembly and testing of a halogen mirror furnace;
- Welding for the Reactor Division;
- Preparation of experimental devices for the ESRF;
- Temporary secondment of a technician for the installation of the new beam shutters, and re-installation of fluids distribution on experimental areas;
- Assembly of an ultra vacuum bench for ^{3}He cells (neutron polarization by polarized ^{3}He project);
- Study, assembly, final testing of a cryogenic ^{3}He purifier for large quantities of ^{3}He, see Fig. 14 (page 144). After some assistance for the commissioning, the Detector Group routinely operates the system.

Very Low Temperatures

The SERC dilution insert has been repaired and re-tested.

The bottom section (heat exchangers, 1 K pot, still) of the 5 mK dilution fridge has been recently delivered by the CRTBT. It has been assembled with the thermometry. It is currently being tested.

The collaboration with A. Benoit (CRTBT) on the development of a new a-gravitational dilution technique has been continued, and has shown very interesting results:

- Bolometers for the TESTA GRIGIA telescope have been characterized, with N.E.P. of 10^{-16} watt Hertz$^{-1/2}$.
- The system can be operated starting from temperatures up to 10 K. This result is of great practical interest, as much for space applications as for use on 4-circle diffractometers. Studies are being carried out to extend the system by using standard cryo-coolers and thus saving liquid Helium.

Cryomagnets

- During a loan to the LLB, the TAS magnet has shown a permanent decrease of performance, from 6 T to 4 T. Up to now the reason for this failure has not been identified.
- The two TASSE magnets (spin-echo) have been tested satisfactorily, each for a period of one month. A system of data acquisition and alarms is being developed, in collaboration with the Instrumentation Branch.
- The Zeeman polarization cryomagnet has been commissioned. Due to a leak, the cryostat had to be returned to the factory (Oxford Instruments). The final performance accords with the specifications.
- The study of a small asymmetric split pair cryomagnet has been undertaken. A magnetic field of 2.5 T or 3 T is expected, in a useful diameter of 50 mm, and a useful gap of 40 mm $\pm$ 5° for the neutron beam divergency, the zero field point being out of the beam. This magnet would be mounted in a standard 'orange' cryostat. A call for tender has been issued. First replies give a clear indication of the feasibility at fairly low cost.

Temperature Measurement and Control

Development of the new ILLSEC (ILL Sample Environment Controller) has progressed. A prototype was delivered in the middle of 1993 and since then the software has been advancing steadily and hardware modifications made as problems or errors were encountered. Some manpower constraints mean that the projected delivery timetable may be retarded but every effort is being made to avoid this.

Contact has been made with the Laboratoire d'Automatique de Grenoble and it has been agreed that a newly qualified engineer will spend six months at the ILL to help develop an auto-adaptive control algorithm specifically designed around the ILLSEC. This will mean that the instrument will take advantage of 'state of the art' control theory.

High Temperature - High Pressure Laboratory

The activities of this group have been slowed down because the staff have been directly involved in the reactor refurbishment project.

Furnaces

The optical (quartz) furnace has been terminated and tested. A new 2000 K furnace has been developed, built and successfully tested. Three 2000 K furnaces together with spare resistors have been built and delivered to HMI and PSI. Several experiments with ILL furnaces have been performed at LLB, HMI and DESY. Each time the laboratory gave full technical support. A 1200 K furnace including a 3 tonne uni-axial pressure rig is under construction for the ILL Monochromator Group.

High Pressure Sample Environment

Pressure equipment has been lent to the Labor für Neutronenstreuung ETH Zurich, in particular pressure cells, a 15 kbar pump, an orange cryostat and a high pressure He gas generator. During 1993 this equipment has allowed former ILL users to perform experiments initially scheduled at ILL for summer 1991. One ILL technician and one engineer were on leave several times to PSI in order to assist with the use of the high pressure He gas generator. The results obtained have been published.

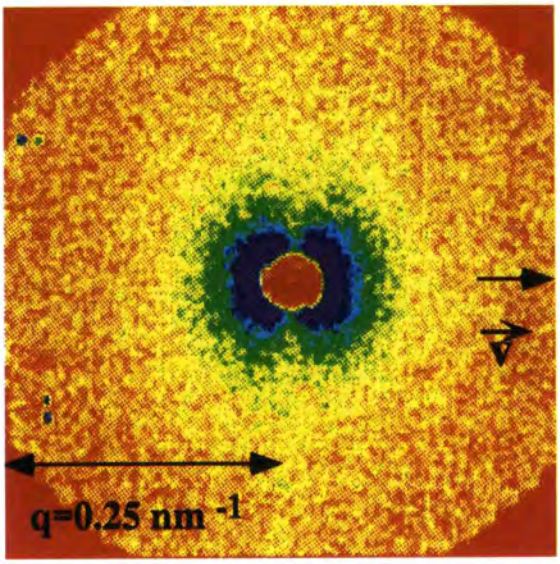
Instrumental Techniques (B. Hamelin)

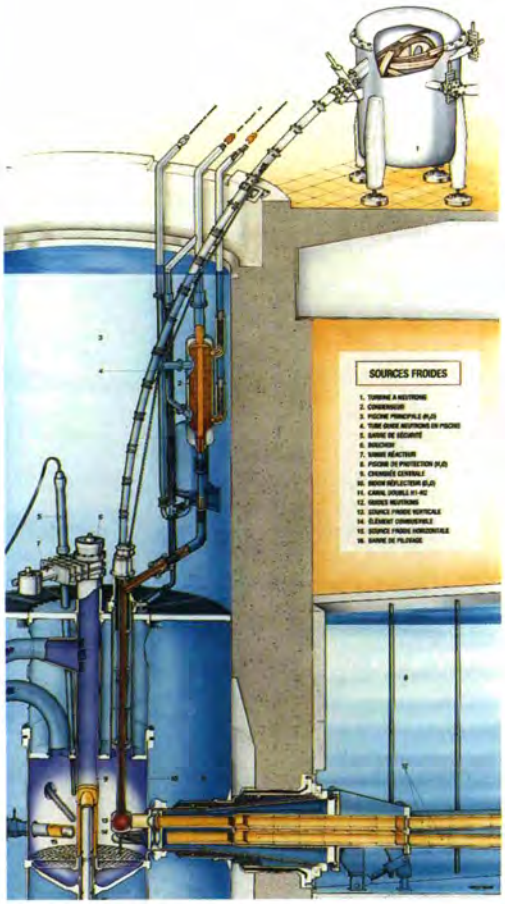
The aim of this group is to assess the efficiency of essential instrument components by simple diagnostic devices, to propose and design improvements of the instrument performance and of its user-friendliness. We identify a variety of actions to focus our attention on:

- Analysis and better knowledge of neutron beam divergence, spectrum and beam profiles;
- Improve sample-positioning techniques inside environment devices;
- More general use of neutron imaging techniques to ease aligning, sample quality checks by on-line topography;
- Use of a novel γ-ray imaging technique (patent Bastie, Hamelin) with a high-energy X-ray tube (200-400 keV) as a source. This allows quasi instantaneous volume characterization (mosaicity, parasitic grains) and easy sample alignment and orientation, even inside a cryostat or furnace. It will also prove valuable for the quick alignment or checking of composite monochromators;
- More generalized use of modern robotics on our instruments.

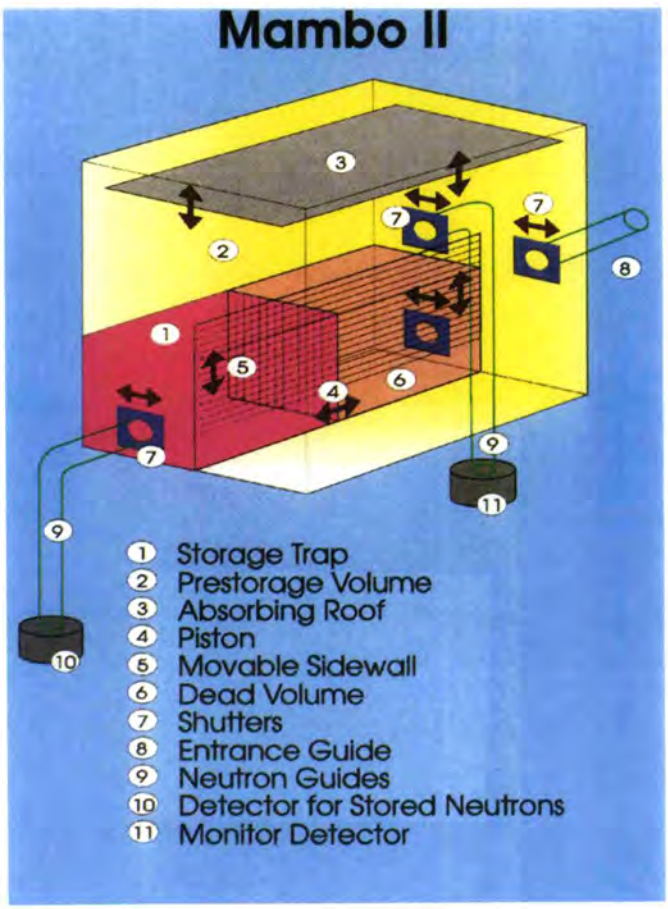
The Instrumental Techniques Group offers help to all instrument scientists to improve the performance and to optimize the use of beam-time of the instruments.

Coll. 9b - Fig. 5: SANS pattern (raw data) of a semidilute polymer solution (polystyrene, M_w=514000 g/mole, solvent Di-octylphthalate, concentration 9% w/w, temperature T=25°C), measured at PAXY, LLB. Solution in laminar shear flow at a gradient of $\dot{\gamma}$ =300 s^{-1} (the light spot in the middle of the detector is due to the primary neutron beam stop).
See report p. 98.

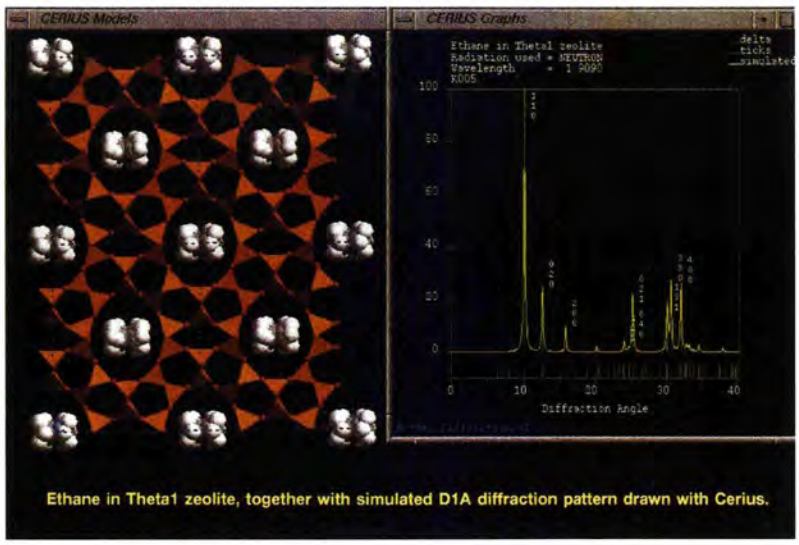




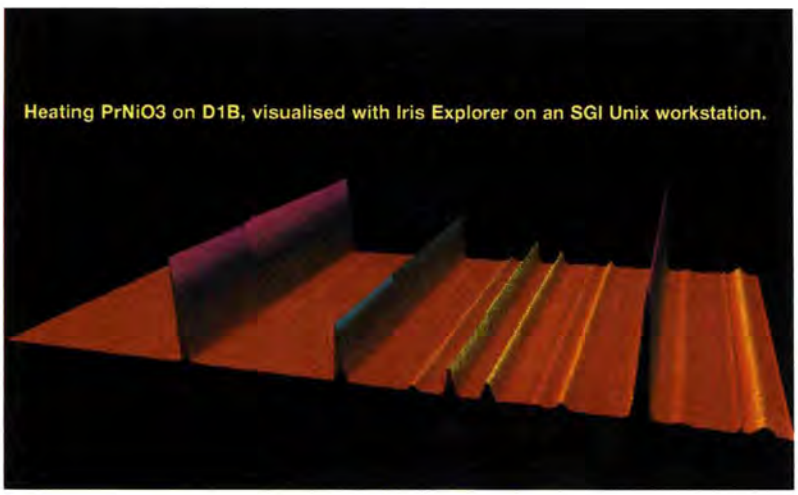
–DS– NFP - Fig. 3: The UCN source.
See report p. 107.



–DS– NFP - Fig. 4: Schematic view of MAMBO II.
See report p. 108.



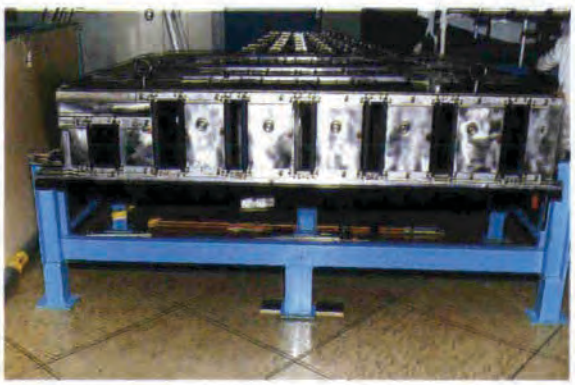
–DS– DIFF - Fig. 1: Ethane molecule inside a zeolite cage visualised with the CERIUS crystallographic software on one of the Diffraction Group Silcon Graphics Unix workstations. See report p. 111.



–DS– DIFF - Fig. 2: Data from a 'real-time' experiment on D1B, where a diffraction pattern has been collected every minute as the sample undergoes a subtle phase transition on heating, as visualised in by Iris Explorer. See report p. 111.

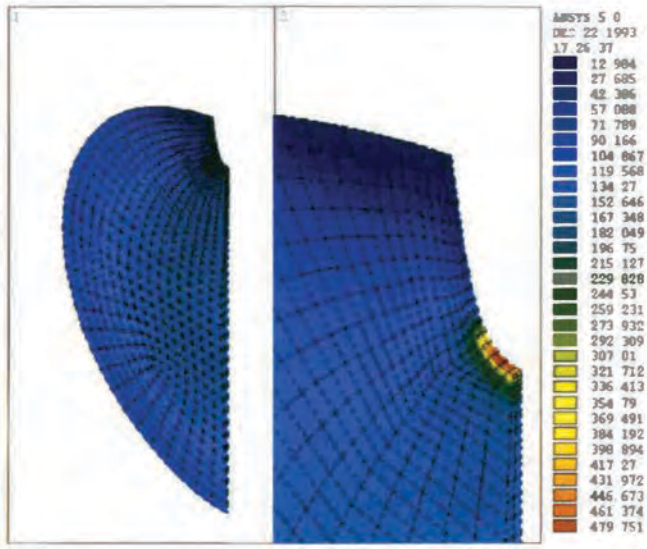
–DS– DIFF - Fig. 3: Iris Explorer maps of the unpaired electron distribution in $K_3(MnO_4)_2$ from polarized neutron diffraction data: the maximum entropy re-construction (fig. b) eliminates the spurious oscillations in the standard Fourier inversion (fig. a). See report p. 111.

DPT - Fig. 1A: Family photograph of the neutron guides team. From left to right: P. Ageron, W. Kaiser, J.L. Coquin, A. Cumin, R. Gandelli, P. Labonne (CILAS), S. Machicoisne (CILAS).
See report p. 128.

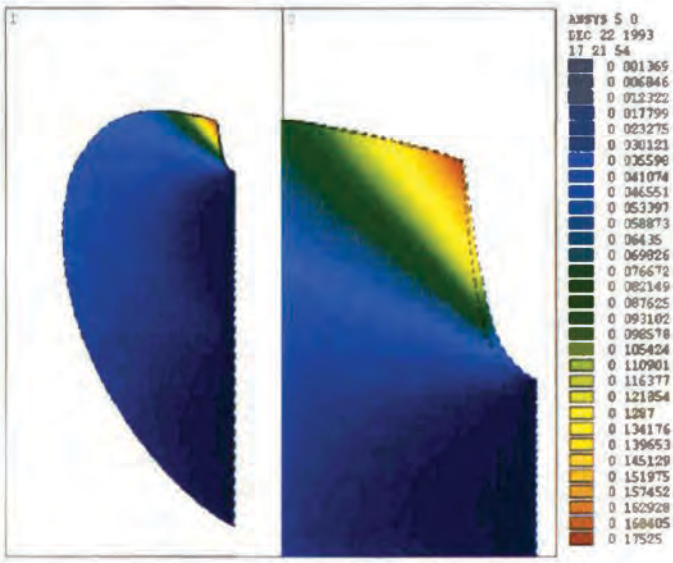


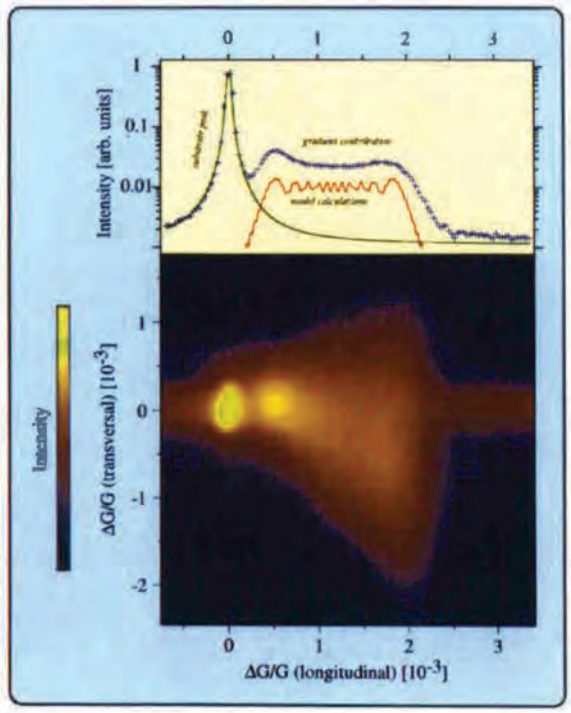
DPT - 1B: Photograph of the new mechanical support with the seven H1 guides. The two new cold neutron guides NG12 and NG13 are on the left hand side.
See report p. 128.

DPT - Fig. 3: The housing of the D20 banana multidetector opens in two pieces: Michel Berneron stands at the side of the front part on the final aluminium support which will be used at D20 on a 'Tanzboden'; the back part is mounted on a special strong support (yellow) used during the construction phase for the mounting of the 50 glass plates composing the 1600 cells, for their precise adjustment and for the operation of closing the housing.
See report p. 129.

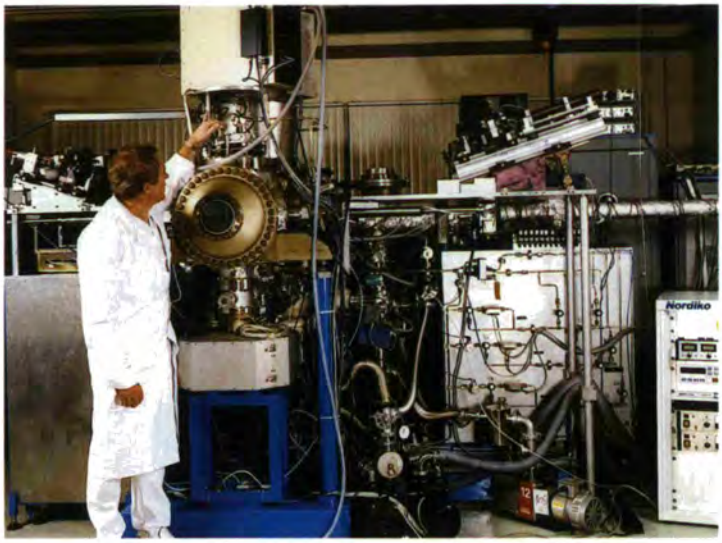


DPT - Fig. 4: Results of finite element calculations of the chopper disk of the TOF spectrometer IN5: disk rotating at 20,000 r.p.m. with a window at the periphery. Fig. 4a shows the stress distribution. Fig. 4b shows the deformations. The window opens under the effect of rotation by 0.18 mm which is unacceptable for the IN5 resolution. *See report p. 131.*



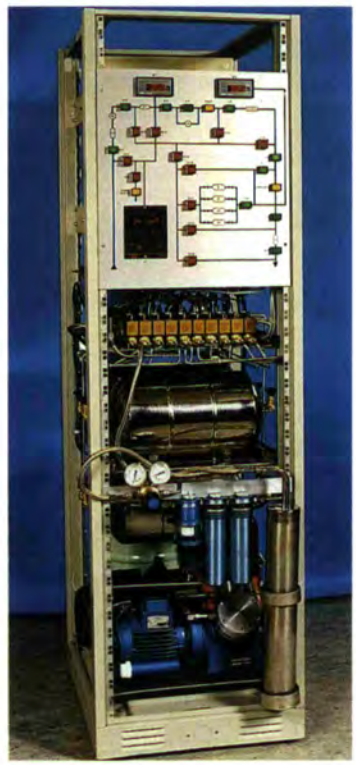


DPT - Fig. 9: 2D diffraction profile (bottom) and 1D projection (top) taken by high energy X-ray diffraction of a $Si_{1-x}Ge_x$ gradient crystal with $0 \leq x \leq 0.03$. G is the reciprocal lattice vector. The green line is a Lorentzian fit to the instrumental resolution function. The red model calculation has an arbitrary vertical scale factor. *See report p. 136.*

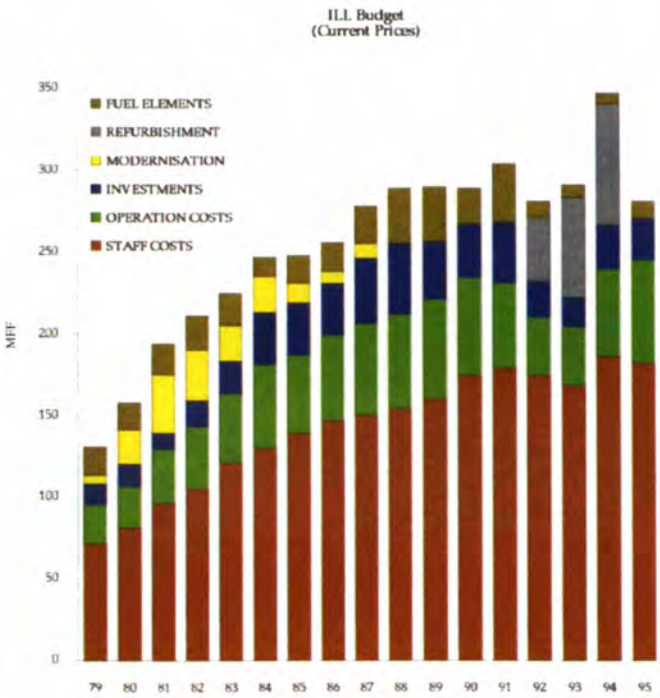


DPT - Fig. 11: Werner Graf in front of the new sputtering facility operated in collaboration with the University of Evry. *See report p. 137.*

DPT - Fig. 12: A view inside the deposition chamber with an Argon plasma illuminating the substrate carrier. *See report p. 137.*



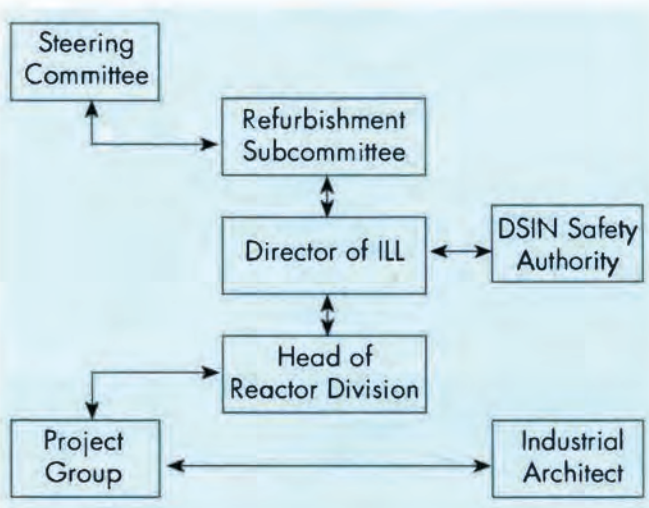
DPT - Fig. 14: Cryogenic ^{3}He purifier for large quantities of ^{3}He. *See report p. 138.*



DA - Table 1: The ILL Budget 1979-1995. *See report p. 155.*

– REACTOR DIVISION – (DR)

The organisation of the DR remains essentially the same as last year. In the following the main emphasis is on the reactor refurbishment. The Project Group acts as client for the project and reports to the Head of the Reactor Division. The complete structure is defined by the following organisation chart.



Dismantling

Conditioning of the reactor block

The reactor block was removed from the reactor swimming pool on 24 November 1992 (Fig. 1) and placed on the cutting machine platform. Conditioning started in position with the cutting off of the upper structure tubes with the aid of special tools. This work continued during the

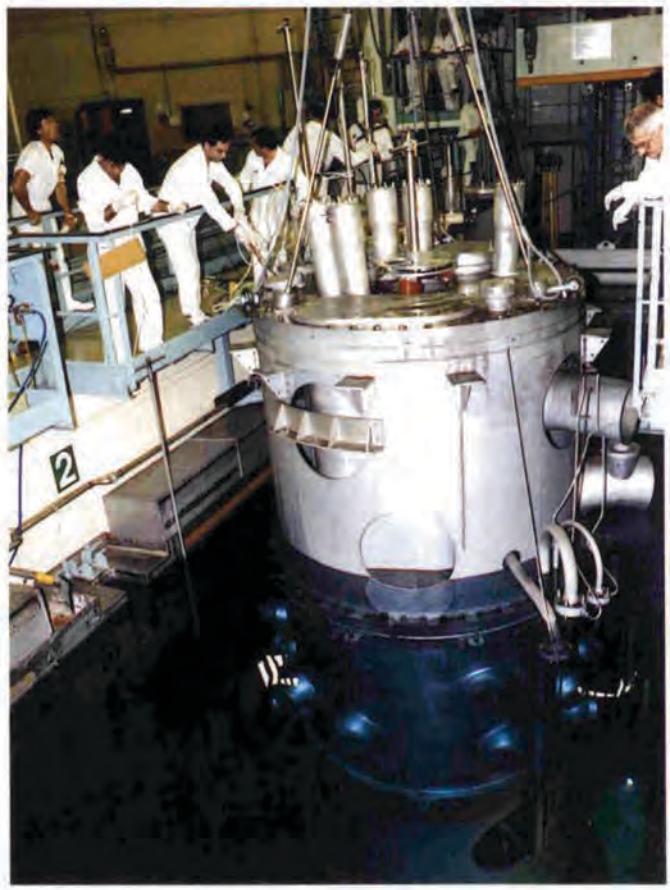


Fig. 1: Transfer of the old reactor vessel to the storage pool with assistance of G. Bonnet, A. Rimet, E. Mannino, J. Correard, M. Selva, J. Fayard, M. Mollier.

whole of 1993. Fig. 2 shows the support which was located in the storage pool. The upper part of the machine was delivered and assembled during the first half of April and the cutting work on the reactor block started on 19.4.93 (Fig. 3). The cutting up continued satisfactorily (Fig. 4), and was completed on 16.12.93 by the removal from the storage pool of the base flange of the reactor block (Fig. 5). At present there remains only the conical base of the reactor vessel, which will be positioned on a new platform and dealt with in the storage pool early in 1994 (Fig. 6).

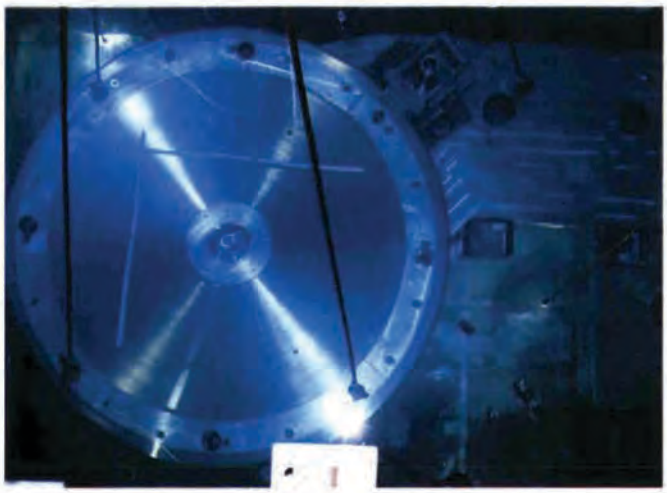


Fig. 2: The big turntable in the storage pool before the old reactor vessel was placed on it for cutting up.

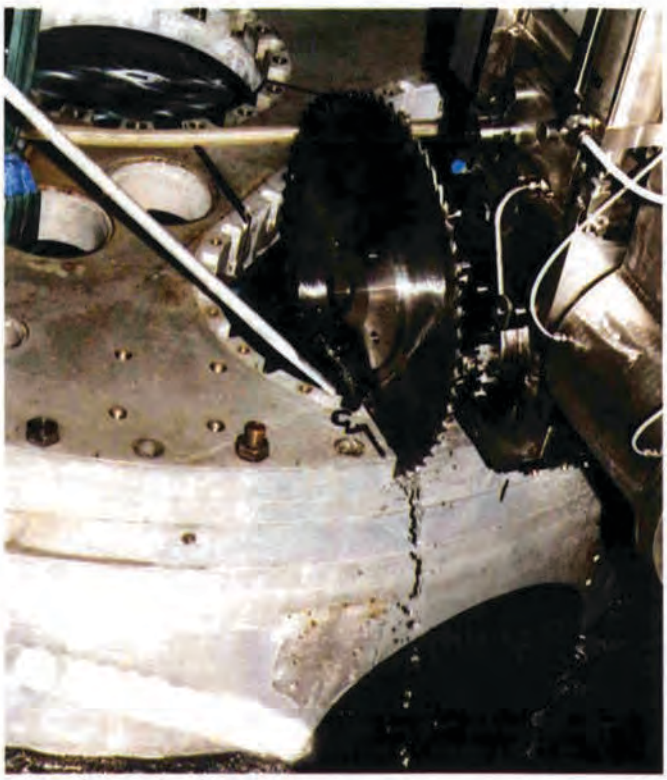
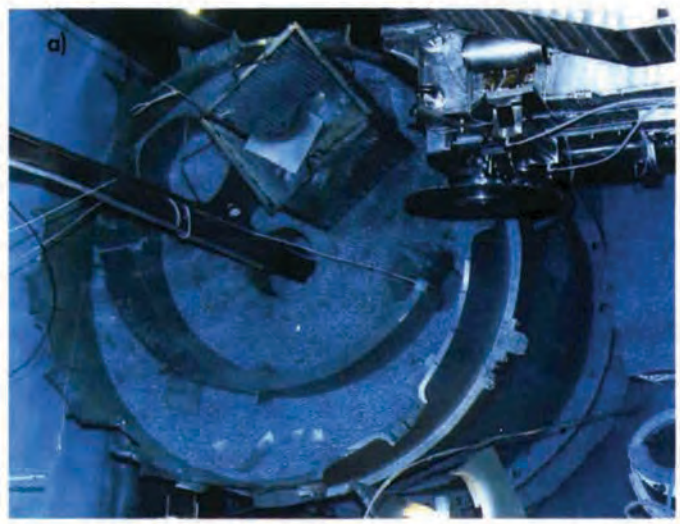


Fig. 3: The cutting machine attacks the upper part of the reactor vessel.

Waterproofing sleeves

The stainless steel sleeves which cross the reactor swimming pool, separating heavy from light water, were removed after cutting up the bellows.

When the structures of the reactor block were removed, geometrical readings were taken of the position of the different items, waterproofing sleeve axis for the control rod, centre of waterproofing sleeves for the chimney and the cold and hot sources. These records are necessary at the reinstallation stage to ensure the immediate identification of the geometrical tolerances in relation to the previous system of axes.



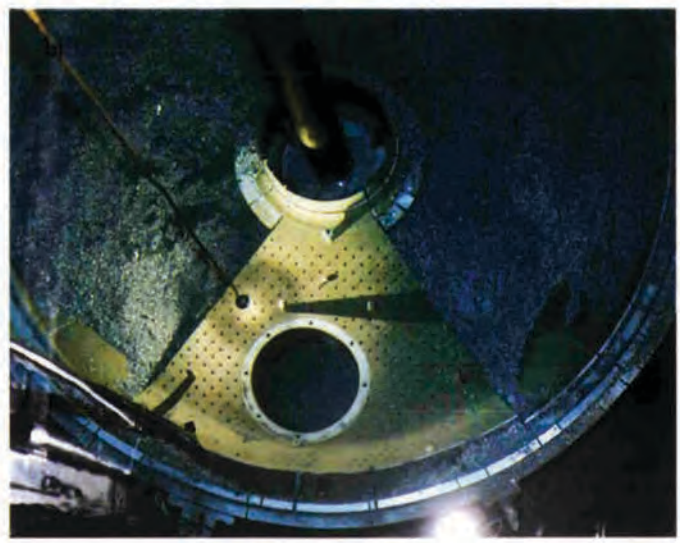


Fig. 4: The cutting process in a very advanced state.
a) The upper anti-turbulence grid covered with sawdust.
b) The lower anti-turbulence grid, last piece to be removed.

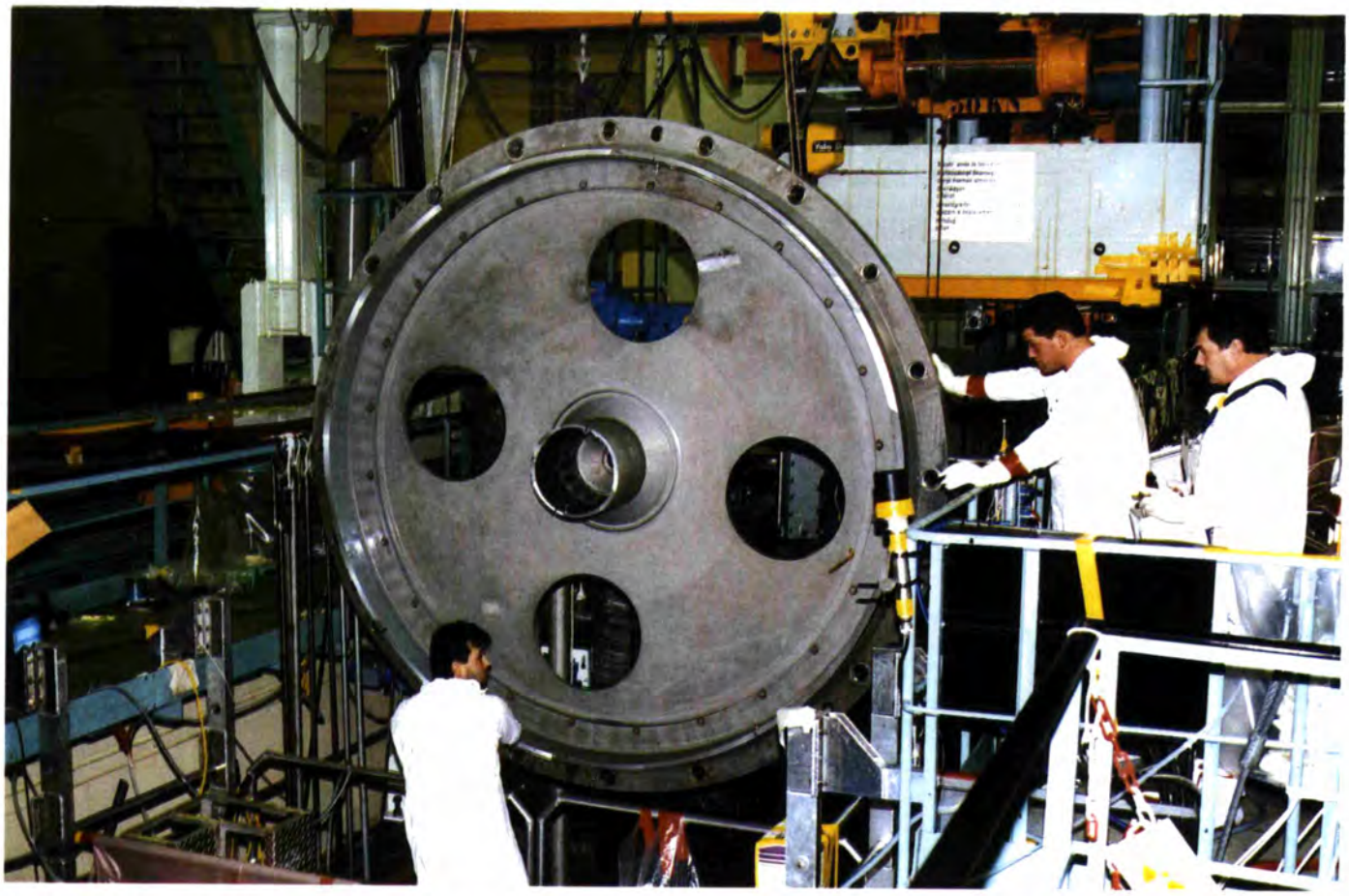


Fig. 5: The bottom flange of the old reactor vessel was taken out in one piece. C. Sevos, G. Matouillot, J.L. Beguet (from left to right).

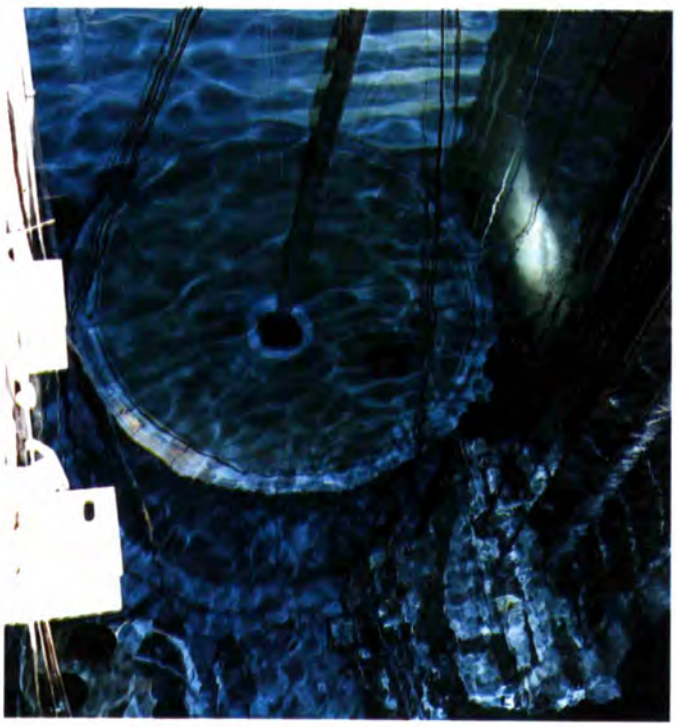


Fig. 6: The conical part of the reactor vessel.

Assistance and radiological records

Wherever there was a radiological risk, health physics staff gave continuous assistance in the operations. It may be noted that at all points involved in the work on the reactor the human factor has been very important in obtaining positive results.

Waste disposal

All the radioactive parts coming from the reactor zone which are not intended for reutilisation are treated as radioactive waste. Optimisation of the waste from cutting up and from processing of chips resulting from the cutting up is an everyday concern which requires intensive work and reflection in order to obtain satisfactory results.

Radiological results

The doses for the operators were low, corresponding to a small fraction of the legal limits.

Reconstruction

In parallel to the work of removing the reactor structures, 1993 was characterized by the work of reconstruction and renovation. The most important work concerned the reactor block and the swimming pool.

Reactor block

The different parts of the reactor vessel are being assembled to form the reactor block, which will be delivered to ILL early in 1994. Over the year 1993 the reactor block was taking shape, identical to its predecessor, see front cover.

All the work took approximately 40 000 man-hours during 1993.

Turned-down grid

The hydraulic studies necessary to define a new anti-turbulence grid for the heavy water came up with a new 'turned-down grid' design with the advantage of the possibility of easy replacement by removing it from the reactor through a tube in the upper structure. This new grid (Fig. 7) was installed in the reactor vessel during construction together with the fuel element support.

Beam tube thimbles

The reconstruction of the beam tube thimbles (Fig. 8) is based on recovery and re-machining in the ILL workshops (Fig. 9) of the rear parts recovered on dismantling and the welding of the front parts (Fig. 10) as new replacements. This operation started again in April 1993, and finished in November 1993, and covered the production of 10 beam tube thimbles. For the remaining positions existing beam tube thimbles will be utilised.

Fig. 7: The turned-down grid for the new vessel.

Fig. 8: A beam tube thimble under leak test. J.F. Garin-Cuchet, J. Pellegrino, J.P. Gonella, C. Yoccoz.

Fig. 9: Marc Locatelli in the ILL workshop reshaping a beamtube thimble.

Coupling sleeves

The coupling sleeves are the link between the structure of the reactor vessel and the external flange system. After numerous forming, welding and tensile tests on formed convolutions and after metallurgical structure examinations, ordering and manufacture of the bellows have been completed. All the bellows have now been delivered. The manufacturing processes and the welding procedures have been qualified and the initial deliveries are expected early in 1994.

Fig. 10a: J.P. Gonella and his colleague J.F. Garin-Cuchet welding a beamtube thimble.

Fig. 10b: Close-up of the welding procedure.

Fig. 11: The swimming pool lining under inspection.

Fig. 12: J.P. Gontier-Maurin, J. Gangi, L. Melesi, E. Stropiano, C. Yoccoz and B. Poclet at the bottom of the reactor swimming pool after cleaning. Beamholes can be seen in the background.

Reactor swimming pool

As a preliminary to any work in the reactor swimming pool, the lining has been decontaminated (see Fig. 11), the ambient radioactivity being now very low, such that manual work can be carried out without any particular radiological protection.

The lining was inspected in February/ March 1993, and no significant defect was found in its structure (Fig. 12).

Beam tube H1/H2

The coupling sleeve, internal shielding and beam tube thimble were tested on a trial installation (Figs 13 and 14), followed by a hydraulic test of the H1/H2 swimming pool. The coupling sleeve is currently at the final machining stage for length adjustment. The beam tube thimble is with the manufacturer for verification of leaktightness.

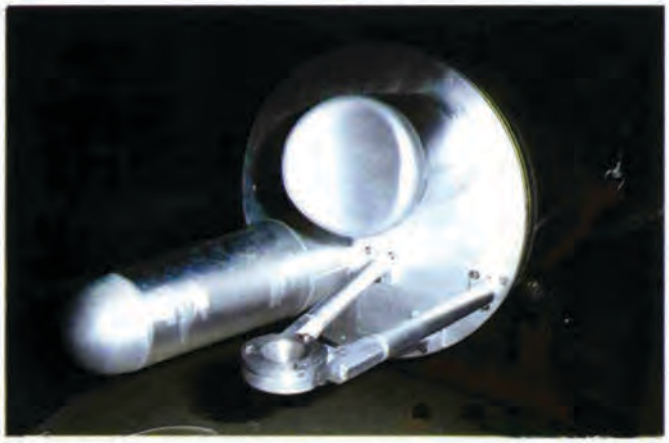


Fig. 13: Inner end of the H1/H2 beam tube.

A new housing for the in-pile guides permitting the installation of two additional cold neutron guides was built (see also the contribution in the chapter on the DPT, page 128).

Chimney

The manufacture of the new chimney is progressing normally. The stainless steel part is currently at the ultrasonic inspection stage, and the timetable and analytical requirements have been respected. The zirconium part will be delivered in accordance with the overall timetable for reinstallation.

Stainless steel waterproofing sleeves

The waterproofing sleeves which ensure leaktightness between the reactor swimming pool tank and the external flange system have been cut up (Fig. 15), in order to change the stainless steel bellows. The rear part has been recovered and the nose flange welded and machined in the swimming pool (Figs 16 and 17).

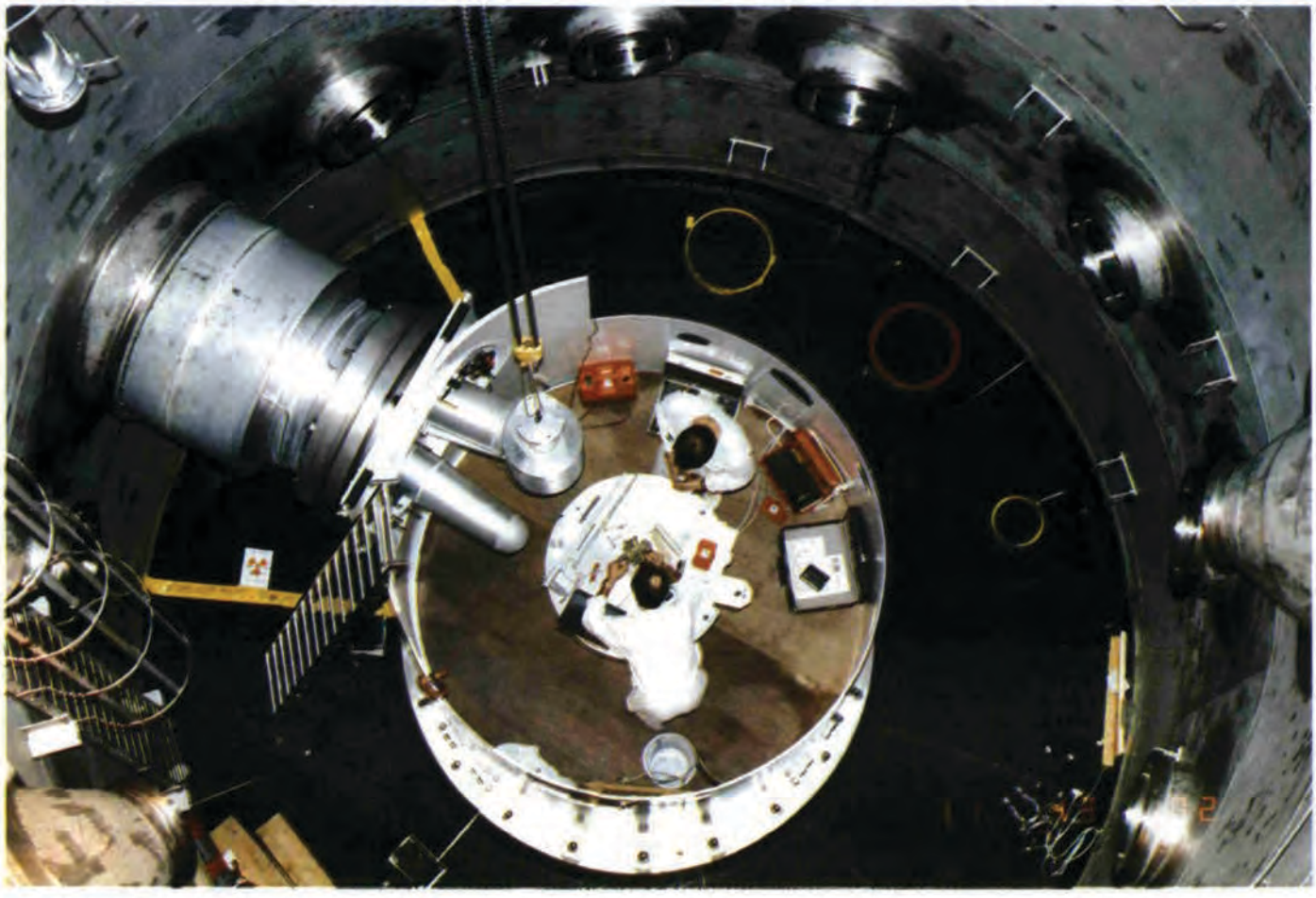


Fig. 14: J.L. Durieu and F. Saint Suplice verify the dimensions of H1/H2 relative to a model of the reactor vessel.

Work was completed in September 1993 with the replacement of the boral shielding on the noses and the hydraulic test of the swimming pool, which was completely satisfactory.

Painting of the reactor shell

Between August and November the metal shell changed its appearance (Fig. 18). The sanding and the three coats of paint on the external and internal parts were completed. Final acceptance of the work and pressurisation of the annular space took place in mid-December 1993.

Fig. 15: A new stainless steel bellows is welded to the outer part of the beam tube by S. Müller and F. Müller.

Fig. 18: Repainting of the reactor shell.

Fig. 16: P. Massafra welding the inner part of a new stainless steel bellows from the swimming pool side.

Fig. 17: F. Müller verifying the dimensions of a beam tube in the reactor swimming pool.

Mechanical maintenance

In parallel with the replacement of the central reactor structures, maintenance work on other parts of the installation, such as circuits, handling systems, safety devices and controls were carried out in 1993.

Electricity, electronics

The long reactor shutdown has been utilised for carrying out in depth maintenance on all the electrical and electronic installations in the reactor.

A new electrical control installation for primary and secondary beam shutters has been installed for the neutron beams on guides H1, H2 and H5. The racks for safety circuits, safety rod controls and high power safety circuits have been reorganised and renovated.

Work is well advanced on a network to improve fire detection and extinction in the reactor building and the associated facilities.

Studies and Metrology

Studies of metal seals

The parameters necessary to obtain leaktightness by compression of metal seals (Fig. 19) have been determined and tried out, and the tightening procedures are now known, ILL having carried out these tests.

Modelling studies

Models of the hot and cold sources and patterns for the fuel element and safety rods have been built: these are used for the geometrical verification of the equipment of the new vessel.

Metrology

The geometrical checks on the beam tubes (Fig. 20) and of the reactor block support made it possible to go back to the original tolerances with very satisfactory results. The equipment used made it possible to transfer the coordinates of the swimming pool site to the supplier of the new reactor block for the machining and assembly of the reactor block (Fig. 21) before its despatch.

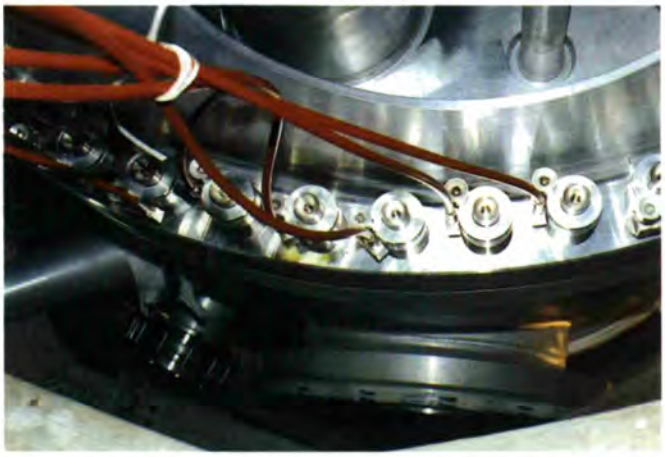


Fig. 19: Hydraulic tightening devices used to close the top of the new reactor vessel.

Fig. 20: Geometrical checks on the beam tubes by F. Saint Suplice and G. Signoretti.

Fig. 21: F. Saint Suplice and A. Rimet verifying dimensions inside the new reactor vessel.

Budget and Timetable

The budget approved by the Steering Committee for the reactor refurbishment project is still unchanged.

The timetable has been respected as a whole, and all the major steps for the year 1993 were respected. A minor delay is anticipated for the delivery of the reactor block. The timetable for the restart of the reactor remains as originally planned at the date of July 1994.

– ADMINISTRATION – DIVISION (DA)

Following the general development of the Institut, there was a change in priorities for the Administration. Support for the refurbishment of the reactor remained the main task, but during the year emphasis shifted to measures preparing the resumption of the normal scientific programme with the reactor restart, in particular the implementation of personnel policy measures and the reorganisation of the Institut.

A new staff complement target of approximately 400 has been accepted as the minimum necessary for normal operation, and as the maximum possible within expected contributions to the budget. Measures to reach this goal included - for the first time in the Institut's history - a limited number of redundancies for economic reasons for staff above a certain age level (56 years and 2 months) combined with an early retirement scheme. This step enabled the Institut to proceed with the necessary recruitments, in particular in the scientific sector, which has decreased considerably in numbers under the non-recruitment policy introduced during the reactor refurbishment.

The reorganisation of the Institut on 1.7.93 affected all sectors. Reorganisation took place in the middle of a running budget year. While maintaining the old budget structure for the whole year 1993, responsibilities for expenditure authorisations were redefined for the period between 1.7. - 31.12.93, taking account of the reorganisation. This procedure proved to be effective.

In the course of the reorganisation the Administration Division was augmented by a number of technical services (Telecommunications, Management Information Systems, Building and Site Maintenance). They were integrated into the Division, which henceforth will be organised in four services:

– Finance and Management Information Systems (MIS): the MIS Group has been combined with the former Finance Group (budget, accounting).

– Purchasing: this sector which is also responsible for the stores, transport and customs, has now been organised as a separate service.

– Personnel and Human Resources: in addition to its previous tasks, this service will now also be responsible for Telecommunications (telephone, fax).

– Building and Site Maintenance: this infrastructure service has been transferred without affecting its internal structure and purpose.

The Administration now comprises in addition to the areas of personnel and finance all the technical support functions of a general character. Within the future total staff complement target of the Institut the Division will consist of 63 staff.

The Division provided the secretariat for the two meetings of the Steering Committee on 1/2 June 1993 in Abingdon (UK) and on 24/25 November 1993 in Grenoble. The Subcommittee on Personnel Questions met on 7 April 1993 and the Subcommittee on Reactor Refurbishment had three meetings (4 March, 24 June, 18 October 1993).

The Head of the Administration continues to meet regularly with the Director of Administration of ESRF to settle questions of common interest. There were also several meetings with EMBL representatives to prepare the extension of the ILL/EMBL building (ILL20), as planned by EMBL. The legal instruments for the extension have been finalised. Construction will start in 1994 and result in 800 to 900 m^2 of additional laboratory and office space for the use of EMBL. ILL and ESRF staff and users will have possibility of access.

Finance and Management Information Systems

Implementation of the 1993 Budget

The first priority of the 1993 budget was the successful continuation of the refurbishment of the reactor. The other activities of the Institut aimed at maintaining the existing scientific and instrument potential of the ILL, completing of instrument projects and preparing for the restart, in particular as regards the reinstallation of instruments. Total expenditure is expected to amount to 323.8 MF, comprising a normal budget of 229.2 MF and the setting up of a reactor reserve of 94.6 MF, which alone represents 29 % of the total budget. It is assumed that 60.7 MF of this reserve will be spent in 1993, thus leaving a balance in the reserve of 33.9 MF at the end of 1993.

The following table shows the changes in expenditure between 1992 and 1993:

	Expenditure 1992		Estimated expenditure 1993		Change 92/93
	MF	%	MF	%	%
1. Staff costs	**173 759**	**56.2**	**167 561**	**51.7**	**-3.6**
2. Fuel elements	**9 926**	**3.2**	**7 700**	**2.4**	**-22.4**
Consumables	15 739	5.1	15 455	4.8	-1.8
Long term supplies and services	6 929	2.2	6 906	2.1	-0.3
Short term supplies and services	7 048	2.3	7 798	2.4	10.6
Travel	2 038	0.7	1 797	0.6	-11.8
Miscellaneous adm. costs	2 874	0.9	2 765	0.9	-3.8
Taxes and fees	945	0.3	1 374	0.4	45.4
3. Operation	**35 573**	**11.5**	**36 095**	**11.2**	**1.5**
Buildings	2 950	0.9	0	0.0	-100.0
Equipment	2 133	0.7	1 695	0.5	-20.5
Instruments	11 761	3.8	10 889	3.4	-7.4
Other investments	4 937	1.6	5 297	1.6	7.3
4. Total Investments	**21 781**	**7.0**	**17 881**	**5.5**	**-17.9**
5. Normal Budget (1-4)	**241 039**	**77.9**	**229 237**	**70.8**	**-4.9**
Reactor refurbishment:					
6. Setting-up of reserve	**(65 400)**	**21.1**	**(94 600)**	**29.2**	**44.6**
7. Expenditure	**38 728**		**60 700**		
8. Balance of reserve at end of year	**26 672**		**33 900**		
9. Additional reserve	**2 943**	**1.0**		**-**	**NC**
10. Total expenditure (5 + 7 + 8 + 9)	**309 382**	**100.0**	**323 837**	**100.0**	**4.7**

The normal budget decreased from 241.0 MF in 1992 by about 5 % to 229.2 MF in 1993. This decrease affected particularly staff costs, fuel elements and investments, whereas operation costs increased slightly.

Staff costs diminished by 3.6 % compared to 1992 as a direct consequence of the personnel policy initiated by the Management in order to adjust to the particular situation during the refurbishment and to prepare for the resumption of normal scientific work after the reactor restart in 1994 (cf. section on personnel management and human resources below). The total staff in post decreased from 421 at the end of 1992 to 382 at the end of 1993.

Fuel costs were reduced by 22.4 % compared to 1992, because there was less expenditure for the interim storage of the 18 irradiated fuel elements at Cadarache (where major expenditure on storage facilities had occurred in 1992). Fuel element production remained at 1 element per year. As in 1992 there were no new uranium purchases, nor expenditure for reprocessing.

Taking account of the reactor shutdown and the absence of scientific experiments, operation costs remained essentially at the same level as in 1992. The slight increase of approx. 1.5 % compared to 1992 can be explained by an increase in taxes and additional expenditure for the reinstallation of instruments.

Investments within the normal budget decreased by 17.9 % compared to 1992. This decrease is due to a large extent to the building sector where after the completion of the guardpost and the joint ILL/ESRF building in 1992 no new projects were undertaken. Scientific investments were reduced by 7.4 % to 10.9 MF; main investment projects were IN4C, PN2 (GAMS5), beamlines H1/H2 and the development of the polarized ^{3}He filter. The increase of 7.3 % in the sector of "other investments" is due mainly to the UNIX conversion programme in computing.

As planned, the implementation of the 1993 budget permitted the setting-up of a reserve of 94.6 MF for the refurbishment of the reactor of which 60.7 MF will be spent in 1993, thus leaving 33.9 MF at the end of the year to be carried forward. The Management expects that the anticipated overall external expenditure of 173.1 MF for the refurbishment of the reactor will be respected. The project will be finished in 1994. Expenditure in 1994 is fully financed by the carry-forward of the reactor reserve remaining from the years 1991, 1992 and 1993.

Income - Comparison of 1992 and 1993 Budgets

Income	Income 1992		Estimated Income 1993		Change
	MF	%	MF	%	%
Collaboration with ESRF	1 469	0.5	1 450	0.4	- 1.3
ILL's own income	11 687	3.8	3 093	1.0	- 73.5
Spanish contribution	4 650	1.5	4 859	1.5	+ 4.5
Swiss contribution	4 650	1.5	0	0.0	NC
Austrian contribution	1 550	0.5	1 620	0.5	+ 4.5
Associates' contributions	287 250	92.8	304 062	93.9	+ 5.8
Carry forward 92/93			2 943	0.9	NC
Utilization of interest			3 936	1.2	NC
Additional carry forward 92/93	- 1 874	- 0.6	1 874	0.6	-
Total	**309 382**	**100.0**	**323 837**	**100.0**	**+ 4.7**

The contributions of the Associates amounted to 304 MF which represented approx. 94 % of the ILL income. Among the scientific members, Switzerland did not prolong its contract with the ILL in 1993, due to the reactor shutdown. Negotiations for a new contractual basis with scientific members - Austria, Spain and Switzerland - after 1.1.94 have been held in 1993 and the respective contracts are expected to be signed soon.

As regards other sources of income, the 73.5 % reduction in "ILL's own income" resulted from the request of the Associates - following the practice at ESRF - to distribute interest earned by the Institut to the Associates, unless the Steering Committee decides to allocate them to the annual budget. The Associates, however, allow interest earned on particular funds (e.g. reactor reserve) to be credited to the respective fund, and in 1993 they also agreed that 3.9 MF of interest should be used to finance additional expenditure for the early retirement plan within the normal budget.

Forward look

The year 1994 is characterized by the completion of the reactor refurbishment project, the preparation for the resumption of the normal scientific programme, including reinstallation of instruments, the actual restart of the reactor in the middle of 1994 and the pursuit of the personnel policy, including the early retirement programme and a major recruitment effort in the scientific sector. The 1994 budget adopted by the Steering Committee on 25 November 1993 with a total of 346,6 MF comprises a normal budget of 264,0 MF and expenditure for the refurbishment of the reactor of 73,7 MF.

Overall survey: the ILL Budget 1979 - 1995

Table 1 (page 144) gives a survey of the development of the ILL budget between 1979 and 1995 at current prices, according to categories of expenditure. For 1994 the approved budget and for 1995 the proposed draft outline budget have been used. The survey shows in particular how expenditure in the normal budget (staff costs, investments, operation and fuel) has been reduced since 1991 to facilitate the financing of the refurbishment of the reactor.

Management Information Systems

In the framework of the reorganisation on 1.7.93 the Management Information Systems Group was transferred from the former Computing Department to the Administration Division where it is part of the Finance and Management Information Systems Service.

On the technical side, the continued implementation of the UNIX plan in the context of the client-server architecture led to the installation of a new HP/UX server, the shutdown of the MISSILL system (based on an old PDP11), the introduction of an increasing number of PCs, incorporating word processing functions and access to data bases, while the stock of Macintoshes remained almost unchanged.

As regards applications, the interest of the "site" base led to an increase in the number of access points (ILL and ESRF) and the gradual connection of dependent applications, particularly in the fields of personnel management, medical surveillance and scientific work. Other developments have been implemented using PC software such as Excel, Paradox, Access, etc.

In the future a major task of the Management Information Systems Group will consist in the introduction of a new software system package for the finance/budget/ purchasing sector. Preparatory work for this programme will start in 1994.

Purchasing

The Purchasing Service was involved in all commercial aspects of the reactor refurbishment project, and negotiated a number of other purchases mainly in the scientific and technical sectors.

Reactor Refurbishment

Purchasing continues to cooperate closely with the Project Group for the reactor refurbishment. In March, two major orders for the coupling sleeves of the reactor were placed; one half with ROLLS ROYCE THOMPSON (GB) and the other half with NEYRPIC FRAMATOME MECANIQUE (F). The bellows which will be fitted to the coupling sleeves have been ordered from WITZENMANN (D).

The last major orders for the refurbishment of the reactor were approved by the Subcommittee Refurbishment in June 1992. These three orders were placed as follows:

– WORMALD (GB) for the fire protection system,

– FORWARD INDUSTRIES (GB) for the central chimney,

– BARRIER (GB) for painting of the reactor building.

Several orders of smaller value were placed, notably, the nuts and bolts for the reactor block have been ordered from AUBERT et DUVAL (F). The contract for the manufacture of the folded-down grid and its diffuser was awarded to GIROD SISA (F); the grid was sent to ZEPPELIN (D) for assembly into the reactor block.

Other purchases

Other major purchases for the Reactor Division were financed from the normal budget; NOELL (D) were awarded the contract to refurbish the rail of the overhead crane in level D of the reactor building. The control system of the reactor will be completely replaced; BULL (F) were selected for supply of the computer system and SIEMENS (D) for the programmable controllers.

The in-pile mechanical parts of the neutron guides H1 - H2 will be replaced before the re-start of the reactor. PINK ENGINEERING (GB) was selected for the manufacture of these parts.

For the instruments, the most notable purchases were for the high priority "time of flight" neutron spectrometer IN4C. GLACIER (GB) won the order for the magnetic bearing suspension systems for IN4C neutron choppers, whereas the motors for these choppers are being supplied by AUXILEC (F).

In the Computing area, the acquistion of a DEC - alpha machine was most significant. By stopping the maintenance contract on the VAX 8700 the resulting savings are being used to lease the DEC - alpha computer thereby maintaining the central computer services' capacity for VAX-VMS processing and allowing a smooth transition to UNIX.

Distribution of purchases in the member states

Whenever possible, for major purchases, an international call for tenders was carried out; offers were compared on an ex works basis so as not to disadvantage British and German firms compared with local suppliers. This, together with negotiation of discounts from regular suppliers for routine purchases, enabled us to achieve considerable savings.

The distribution of ILL purchases (orders exceeding 50 KF) in the first 10 months of 1993 is shown below. The figure includes purchases for which a free choice of suppliers was possible excluding therefore the fuel cycle, electricity and small purchases less than 50 KF. To enable a comparison, the relevant figures for 1992 are also indicated. The fluctuations between 1992 and 1993 can be explained by major purchases for the refurbishment project.

Distribution of ILL purchases (orders > 50 KF)

	1992		1993	
	MF	%	MF	%
France	33.2	35	18.3	46
Germany	44.2	47	4.1	10
United Kingdom	14.8	16	15.0	38
Others	1.8	2	2.0	6
Total	94.0	100	39.4	100

Transport and Customs

The Single European Market came into force on 1st January 1993 thus removing customs controls at the borders within the EEC. This has allowed a freer movement of goods within the Community, but companies now have to do monthly declarations of all their arrivals and despatches on a standard form which is submitted to the customs authorities. After some teething problems, the system works very well, and we are now considering installing a computerised system for these monthly declarations.

Stores

A new and more efficient system for the supply of office stationery was introduced in 1993. Suppliers now deliver the goods directly to the secretaries' offices every fortnight; consequently there is now virtually no stationery held on stock in the stores.

During 1993 ESRF has set up its own store and therefore no longer relies on ILL's general store. ESRF does, however, continue to use ILL's raw material store with its special cutting equipment.

Personnel and Human Resources

The Personnel and Human Resources Service consists of three groups, Personnel Management, Human Resources and - since the reorganisation of 1.7.93 - Telecommunications and General Services.

Personnel policy

Personnel policy was determined by the aims of supporting the refurbishment of the reactor, delevoping scientific expertise and controlling the staff costs budget. In 1993 the emphasis moved to measures preparing for normal operation after the reactor restart.

The Institut continued to involve its staff as far as possible in the refurbishment of the reactor. This concerned in particular the staff of the Reactor Division, but in many instances also staff from other Divisions. In addition 24 staff were transferred internally to support the refurbishment or perform other important in-house tasks. These measures helped to retain staff, to enhance motivation and to control the external refurbishment costs.

Concerning the development of technical expertise the Management encouraged the secondment or detachment of scientists and technicians to other research centres (in particular ESRF, CNRS, LLB, HMI, NIST) and in some cases to industry (e.g. SGS-Thomson, Pechiney). Overall there were 38 cases of detachment or secondment which also helped to make considerable budgetary savings.

Since the beginning of the refurbishment project the Management had initiated a policy of facilitating natural departures to control staff costs. This policy was also confirmed by the consideration that the Institut, in view of the expected contributions after the reactor restart in 1994, is obliged to aim at a new staff complement target of approximately 400 (compared to 483 staff in post at the end of 1990). As a final step within a whole range of measures to achieve this target and to ensure a balanced composition of staff to operate the Institut, the Management proposed a plan for a limited number of redundancies for economic reasons together with an early retirement plan ("Convention FNE - Fonds National pour l'Emploi"). This plan was approved by the Steering Committee on 2 June 1993 and the Convention with the Labour Authorities was signed on 23 June 1993. During 1993 14 staff members aged between 56 years 2 months and 60 left the Institut under this scheme, and further departures are planned for 1994. A further 8 employees between 55 and 60, who had done shift work, took early retirement according to specific rules in 1993.

The resulting overall staff changes and the situation on 31.12.93 are given in the tables 2 and 3. Recruitment in 1994 and 1995 is essentially aimed at the scientific sector.

Staff complement situation at 31.12.1993

Staff movements in 1993 have slightly changed the breakdown by nationalities (numbers in brackets indicate the situation in 1992):

French	:	64.8 %	(63.2 %)
German	:	15.5 %	(16.4 %)
British	:	12.8 %	(14.7 %)
Others	:	6.9 %	(5.7 %)

For a comprehensive survey see Table 3.

Average age

The average age at ILL on 31.12.93 was 44.7 years. Table 4 shows the breakdown by age and staff category.

Salaries

A salary agreement was signed by the Management with the SA-ILL and FO unions on 4 May 1993 providing for general salary increases in 1993 as follows:

1 % on 1 May 1993

1.6 % on 1 December 1993

A meeting of the signatories will be held at the beginning of 1994 to review the application of this agreement. An adjustment may be made as a function of the general economic trends and the situation of the ILL.

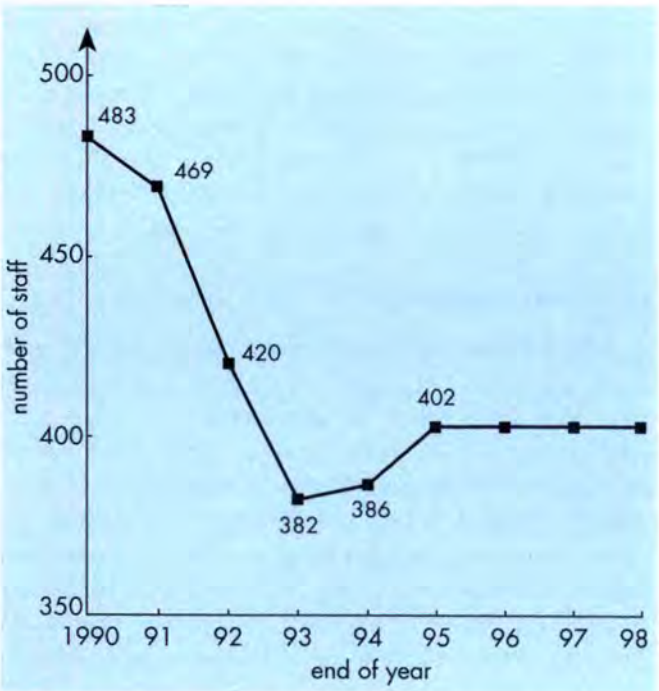


Table 2: Staff movements.

	CADRES						THESIS STUDENTS						NON-CADRES						TOTAL					
	G	B	F	O	T	Average Age	G	B	F	O	T	Average Age	G	B	F	O	T	Average Age	G	B	F	O	T	Average Age
DIRECTOR'S SERVICES			4		4	51.2							1	1	11		13	42.4	1	1	15	0	17	44.5
SCIENCE DIVISION	26	8	13	13	60	44.2	1	3		1	5	25.6	7	6	13	1.5	27.5	45.6	34	17	26	15.5	92.5	43.5
PROJECTS & TECHNNIQUES DIVISION	8	4	14	1	27	51.4					0		5	9	65	3	82	46.2	13	13	79	4	109	47.1
REACTOR DIVISION	2		6		8	49.4					0		3	12	72	3	90	43.8	5	12	78	3	98	44.3
ADMINISTRATION DIVISION	2	2	8		12	47.1					0		4	4	41.5	4	53.5	42.4	6	6	49.5	4	65.5	43.2
TOTAL	38	14	45	14	111	46.9	1	3	0	1	5	25.6	20	32	202.5	12	266	44.3	59	49	247.5	26.5	382	44.7
Staff at 31.12.92	39	19	46	11	115		6	5	3	1	15		24	38	217	12	291		69	62	266	24	421	
DIFFERENCE 92/93	-1	-5	-1	3	-4		-5	-2	-3	0	-10		-4	-6	-14.5	-1	-25		-10	-13	-19	3	-39	

G: German, B: British, F: French, O: Others, T: Total

Table 3: Staff complement situation at 31.12.1993

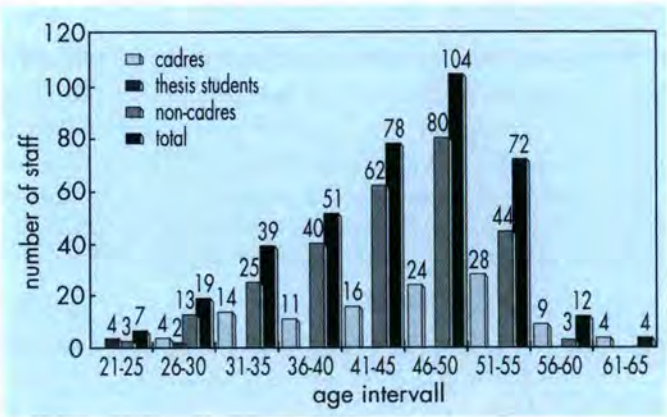


Table 4: Breakdown by age and category at 31.12.1993

Professional training

French legislation requires employers to assist in financing professional training, and 1.5 % of the payroll must be devoted to training costs. Part of this percentage is paid directly to the State as a contribution to the organisation of courses for young people and also to finance the system of leave for training. The majority of training provided in this context for ILL staff consisted of language and technical courses. In 1993 the conversion to the UNIX system required a specific training effort for computing staff and users. In 1993, 205 staff attended training courses.

International schooling

Schooling for children continues to be an essential point in the integration of families. ILL and the other employers concerned in Grenoble, including ESRF, have set up an Association (Association pour le Développement de l'Enseignement International dans la Région Grenobloise - ADEIRG) to develop and improve the system of 'international sections' set up by the French Ministry of Education. The purpose of this Association is to be a single representative spokesperson vis-à-vis the Education Authorities, and to permit a frank dialogue on individual cases and questions such as the contracts of the teachers in this system.

Communication

There have been two issues of the magazine 'La Boîte à Neutrons' in 1993. The subjects covered are connected with research, know-how and other subjects of general interest at ILL.

Telecommunications and General Services

The Joint Telephone Service continued to provide ILL and ESRF with telephone lines. The ILL radiotelecommunication systems have been modernised to give users a better and more efficient service.This group also provides a number of general services to facilitate the work of all staff as regards post, reprographics, photocopiers, errands in town, etc.

Building and Site Maintenance

The Building and Site Maintenance Service is in charge of the maintenance and modifications of the ILL site, buildings, technical installations (except the reactor) and experimental positions. Its purpose is to provide the necessary technical support in this field to all sectors of the Institut. Under the new management structure implemented on 1.7.93 the Service is attached to the Administration Division.

Maintenance, Repairs and Improvements

The areas concerned are: ILL site (roads and car parks, fences, drainage system and open spaces), buildings (structure and fittings, waterproofing) and technical installations (electricity, plumbing, heating, ventilation, air conditioning, handling) associated with buildings and experiments. Systematic maintenance is planned to prevent breakdowns, repairs are executed to minimize "down time" and improvements are made to increase reliability. The interventions are carried out by the group's workshops or by external contractors.

The Service also supervises the cleaning of buildings and open spaces, the clearing of snow and waste removal, the supply of furniture. Due to the reorganisation it had to organise and carry out many transfers of offices.

Constructions and Modifications

The Service designs and follows up the construction, renovation and modification of buildings, offices, laboratories and technical installations. In 1993 the Service was strongly engaged in the work for the refurbishment of the reactor. It supervised the repainting of the interior and the exterior of the steel shell of the reactor. It also managed the renovation of rails and structures of the main crane in the level D of the reactor building. The workshops of the Service, in particular the main sheet metal workshop, are continuously carrying out specific tasks for the refurbishment project.

To prepare the restart of the scientific programme, the Service installed new safety barriers around the experimental positions, carried out a renovation of the electrical distribution on these positions and constructed shielding for IN4C, EVA, ADAM and PF1. The Service will continue to participate in the reinstallation of instruments.

Another important project was the installation of the new premises for the joint ILL/ESRF Medical Service.

– COMMUNICATIONS –

Seminars

College 2

Theory

"Quasiparticle currents in one dimensional Peierls and Hubbard models".
S. MATVEENKO, Landau Institute, Moscow, Russia.

"Quantum localization transitions in generalized polaron models".
J. PALMERI, ILL, Grenoble, France.

"Liquid helium films: structure, growth and dynamics".
B. CLEMENTS, ILL, Grenoble, France.

"Electrons in magnetic fields".
I. VAGNER, SNCI, CNRS, Grenoble, France.

"Théorie de gap de spin dans les supraconducteurs à haute T_c : discussion des expériences de diffraction neutronique et de RMN".
M. LAVAGNA, DRFMC/MDN, CEN-Grenoble, France.

"Unified approach to the charge/spin density waves electrodynamics".
S. BRAZOVSKII, Landau Institute, Moscow, Russia.

"Treatment of recoil in neutron scattering from classical systems".
G.R. KNELLER, DBCM-SBPM, CEA-Saclay, France.

"Order by disorder and spin origami in strongly fluctuating magnetic systems".
E. SHENDER, University of Ottawa, Ontario, Canada.

"Spin supercurrents in ^{3}He B under an electric field".
V.P. MINEEV, Landau Institute, Moscow, Russia.

"Ondes de densité de charge bipolaroniques".
P. QUEMERAIS, ILL, Grenoble, France.

"Enroulement et localisation d'une chaîne polymère: influence des interactions chirales".
B. HOUCHMANDZADEH, Spectrométrie Physique, Université Joseph Fourier, Saint-Martin-d'Hères, France.

"Crossover from BCS superconductivity to Bose-Einstein condensation".
R. HAUSSMANN, Univ. München, Germany.

"Superconductivity and superfluidity in Fermi systems with repulsive interactions".
M. KAGAN, Kapitza Institute, Moscow.

"First principle theory in alloy surfaces".
A. PASTUREL, Maison des Magistères, Grenoble, France.

"Vérifications expérimentales des états polaroniques".
J. RANNINGER, CRTBT, CNRS, Grenoble, France.

"Two dimensional crystallization of organic molecules at the water surface".
B. BERGE, Spectrométrie Physique, Université Joseph Fourier, Saint-Martin-d'Hères Cedex, France.

"Sum rules and angular dependence in photoemission".
B. THOLE, Univ. de Groningen, Germany, and ESRF, Grenoble, France.

"Finite size magnetization and scaling behaviour in 2D x-y magnets".
P. HOLDSWORTH, ENS, Lyon, France.

"Reversible plasticity and surface phenomena in perfect crystals".
A.F. ANDREEV, Kapitza Institute, Moscow, Russia.

"X-ray dichroism: more sum rules".
P. CARRA, ESRF, Grenoble, France.

"Exact map of Kondo impurities onto a semi infinite chain".
N. SCHOPOHL, CRTBT, CNRS, Grenoble, France.

"Metals in a high magnetic field: a new universality class of marginal Fermi liquids".
V. YAKOVENKO, Rutgers University, New Brunswick, NJ, USA.

"Negative U extended Hubbard model for doped barium bismuthates".
A. TARAPHDER, NEC + LEPES, CNRS Grenoble, France.

"Modèle de Hubbard avec intégrale de saut dépendant de l'occupation des sites".
M. AVIGNON, LEPES, CNRS, Grenoble, France.

"Superconductivity in incommensurate crystals".
V.P. MINEEV, Landau Institute, Moscow
and CEN-Grenoble, France.

"Singularités dans les écoulements incompressibles".
T. DOMBRE, CRTBT, CNRS, Grenoble, France.

"Renormalization effects of vortex fluctuations in layered superconductors".
S. SCHEIDL, Univ. München, Germany.

"Vortex bidimensionnels et lignes de vortex dans les supraconducteurs lamellaires".
D. FEINBERG, LEPES, CNRS, Grenoble, France.

"Conductivity peaks broadening in the quantum Hall regime".
B. SHKLOVSKI, Univ. of Minnesota, USA.

"Hydrodynamics of density wave crystals".
S. BRAZOVSKII, Landau Institute, Moscow and ILL, Grenoble, France.

"Achille, la tortue et la croissance des cristaux".
J. VILLAIN, DRFMC/SPSMS/MDN, CEN-Grenoble, France.

"Pinning phenomena in superconductors".
A. LARKIN, Landau Institute, Moscow and CRTBT, CNRS, Grenoble, France.

"Statistics of conductance fluctuations in quantum dots".
K. EFETOV, M.P.I. Stuttgart, Germany.

"Liquides de spin sur le cactus de Husimi".
B. DOUÇOT, CRTBT, CNRS, Grenoble, France.

"Nearly ideal 2D Fermi gas in a magnetic field".
Y. BYCHKOV, Landau Institute, Moscow, Russia.

"Le mouvement Brownien retrouvé, ou, comment calculer correctement le coefficient de friction hydrodynamique".
J.P. HANSEN, ENS, Lyon, France.

"Paired electron crystal in the low density electron limit".
K. MOULOPOULOS, LEPES, CNRS, Grenoble, France.

"Breakdown of Fermi liquid beyond 1 dimension".
P.A. BARES, ILL, Grenoble, France.

"Points de Néel et ondes spirales dans un cristal liquide".
P. COULLET, Institut Non Linéaire, Nice, France.

"The s-wave, d-wave controversy in high temperature superconductors".
C.M. VARMA, A.T. and T. Bell Laboratories, Murray Hill, NJ, USA.

"Ab initio molecular dynamics studies of fullerenes and fullerides".
W. ANDREONI, IBM, Zurich, Switzerland.

"Light vs electrons: a survey of multiple scattering transport".
B. van TIGGELEN, Maison des Magistères, Grenoble, France.

"Ising simulations and nucleation in cellular automata".
G. GOMBOS, Res. inst. for Techn. Physics, Budapest, Hungary.

"Formation de structures organisées à l'état solide en métallurgie physique: exemples et nouvelles approches".
Y. BRECHET, LTPCM, Grenoble, France.

"Le modèle de Hubbard à 2D à faible remplissage de bande".
Anne-Marie DARÉ, Univ. de Sherbrooke, Canada.

College 3

Fundamental and Nuclear Physics

"Recent experiences in preparing to dismantle a nuclear reactor".
C. BATES, University of Liverpool and Manchester, UK.

"Ultra-cold neutron projects at pulsed sources".
A.V. STRELKOV, J.I.N.R., Dubna, Russia.

"Production of defects by neutrino recoil observed by perturbed angular correlation".
R. SIELEMANN, HMI, Berlin, Germany.

"Space and time reversal symmetry violation and polarized eV neutrons".
Yasuhiro MASUDA, KEK, Japan.

"Progress report on the implementation of a thermal ion source at the ILL (PIAFE)".
H. FAUST, ILL, Grenoble, France.

"Instrument neutron activation analysis at S51".
R. OLIVER, ILL, Grenoble, France.

"Antiprotonic X-rays as a probe of the hadronic interaction".
G. BORCHERT, KFA Jülich, Germany.

"Error assessment for future neutron lifetime measurements with MAMBO II".
V. NESVIZHEVSKY, PNPI, Saint-Petersburg, Russia.

"A simple phenomenology of pre-collective nuclei".
N.V. ZAMFIR, Brookhaven Nat. Laboratory, Upton, LI, USA.

"Probing low-energy collective nuclear modes with the inelastic neutron scattering reaction".
S.W. YATES, University of Lexington, Kentucky, USA.

"A future for electron spectroscopy at the ILL".
W.D. HAMILTON, University of Sussex, UK.

"Ion beam mixing of metal/metal and metal/Nitride layers - New perspectives".
K.P. LIEB, Univ. Göttingen, Germany.

"A tuneable monochromatic γ-ray source at the Gent Linac".
J. JOLIE, Univ. de Fribourg, Suisse.

"Recoil-ion momentum spectroscopy: a new tool to probe collision induced atomic reactions".
J. ULRICH, GSI Darmstadt, Germany.

"Multilayer mirror interferometer for cold neutrons".
Y. OTAKE-TAKAHARA, Kyoto Univ. Japan.

"Quality and availability of highly enriched actinide isotopes at VNIIEF".
S. VESNOVSKI, All Russia Scient. Res. Inst. for Exp. Phys. Arzamas-16 (VNIIEF) Russia.

"The capability of the high flux pulse reactor BIGR (Arzamas - 16) for high density UCN production.
V. SHVETSOV, A. STRELKOV, JINR Laboratory of Neutron Physics, Dubna, Russia.

College 4

Structural and Magnetic Excitations

"On the valence of Praseodymium in Pr-Ba-Cu-O".
V. NEKVASIL, Czechoslovak Acad. of Sciences, Prague, Czechoslovakia.

"Investigation of phonons in Cr_2O_3 on the PRISMA neutron T-O-F spectrometer".
T. MAY, Univ. Regensburg, Germany.

"Statics and dynamics in a model for modulated phases in A_2BX_4 systems".
T. JANSSEN, Univ. of Nijmegen, The Netherlands.

"Fast convolution in four dimensions: a new method for the interpretation of neutron scattering data".
W. SCHMIDT, ISIS, Rutherford Appleton Laboratory, UK.

The problem of the convolution of the Lorentzian and the Lorentzian squared with the resolution function.
J.E. LORENZO, Brookhaven Nat. Lab., USA.

"Neutron scattering study of $CsFeCl_3$ and $CsFeBr_3$ in external magnetic fields".
B. SCHMIDT, ILL, Grenoble, France.

"A Monte-Carlo study of magnetic phase transitions on an $Fe_xMg_{1-x}Cl_2$ model. From pure metamagnet to random field behaviour".
Laura HERNANDEZ, Inst. Nat. Sci. Appliquées, Toulouse, France.

"Phase transitions in disordered Perovskite-like single crystals".
S. VAKHRUSHEV, A.F. Ioffe Physico-Technical Institute, St. Petersburg, Russia.

"Some structural and electronic properties of monomolecular organic layers on semiconductors".
B.A. NESTERENKO, Acad.of Sci. of Ukrainia, Kiev, Russia.

Lattice dynamics and Fermi surfaces in metals and alloys investigated by neutron inelastic scattering".
A. IVANOV, Kurchatov Institute, Moscow, Russia.

"Recent advances in lattice dynamics".
D. STRAUCH, Universität Regensburg, Germany.

"X-ray and neutron diffraction analysis of dislocation structures in polycrystals".
P. KLIMANEK, TU Mining Academy Freiberg, Germany.

"Antiferromagnetic rare-earth ordering in the high-T_c superconductors $Rba_2Cu_3O_x$ (R = Yb, Ho), $RBa_2Cu_4O_8$ (R = Ho, Dy) and spin-wave excitations in Bi_2CuO_4".
B. ROESSLI, Paul Scherrer Institut, Villigen, Suisse.

"Investigation des verres protoniques $Rb_{1-x}(NH_4)_x H_2PO_4$ avec Tl^{2+} par résonance magnétique électronique".
V. IZOTOV, Univ. de Kazan, Tatarstan, Russie.

"Influence of dilution on the critical behaviour in the frustrated 3D Heisenberg system $CdCr_{2(1-x)}In_{2xS4}$".
Stéphanie POUGET, ILL, Grenoble, France.

"Magnetic ordering and excitations in quantum antiferromagnets".
A. HARRISON, Univ. of Edinburgh, UK.

College 5

Crystal and Magnetic Structures

"The first steps in a new dimension: an introduction to the silicon graphics workstation of the diffraction group".
A. HEWAT, ILL; G. McINTYRE, ILL; A. FITCH, ESRF; F. TASSET, ILL, Grenoble, France.

"Incommensurate magnetic systems: a quantitative analysis".
D. SCHMITT, Laboratoire de Magnétisme Louis Néel, CNRS, Grenoble, France.

"Flashes of Science" (I):
"The magnetic phase transitions of $MnWO_4$".
G. LAUTENSCHLÄGER, ILL, Grenoble, France.

"The investigation of the surface superconducting region in lead films using polarized neutron reflectivity".
M. NUTLEY, ILL, Grenoble, France.

"X-ray diffuse scattering from rough surfaces, interfaces and volume defects".
V. HOLY, The Masaryk University, Czechoslovakia.

"Neutron backscattering from vibrating silicon crystals".
R. HOCK, Univ. of Würzburg, Germany.

"Flashes of Science" (II):
"Magnetic structures of R_2BaNiO_5 compounds (R = rare earth)".
E. GARCIA-MATRES, ILL, Grenoble, France.

"Etude du magnétisme des composés $Ce_2Fe_{17}H_x$ (x = 0:5) and $Ce_2Fe_{17}N_3$".
O. ISNARD, ILL, Grenoble, France.

"X-ray scattering from epitaxial multilayers and surface gratings".
G.T. BAUMBACH, ILL, Grenoble, France.

"X-ray and neutron scattering studies of oxygen ordering in $YBA_2Cu_20_{6+x}$".
V. PLAKHTY, PNPI-CEN-Grenoble and St. Petersburg Nuclear Physics Institute, Russia.

"Electron and nuclear densities from maximum entropy method analyses of X-ray and neutron diffraction data".
C. HOWARD, ANSTO Lucas Heights Research Laboratories, Australia.

"Quantum theory of giant magnetoresistance in multilayered structures".
A. VEDYAYEV, DRF, CEN-Grenoble, France, and Moscow University, Russia.

"Magnetic properties of ternary phosphides with $ThCr_2Si_2$ - and $Zr_2Fe_{12}P_7$ - type structure".
M. REEHUIS, Hahn-Meitner-Institut Berlin, Germany and ILL, Grenoble, France.

"Neutron scattering from cubic ZrO_2".
D.N. ARGYRIOU, Australian Nucl. Sci. and Tech. Organisation, Menai, Australia.

"Symmetry analysis of magnetic structures of R_2CuO_4 (R = rare earth)".
I.M. VITEBSKY, Inst. for Single Crystals, Ukrainia Acad. of Science, Russia.

"How I spent my summer holidays - part I":
"Straight from the Seoul", A. HEWAT.
"Nipponese neutrons". C. ZEYEN.
"Neutron optics with bent perfect crystals".
J. KULDA, ILL, Grenoble, France.

"Surface anisotropies in epitaxial thin iron (110) films".
O.Mc GRATH, Lab. Louis Néel, CNRS, Grenoble.

"Numerical methods in micromagnetics: determination of the magnetic structure in ferromagnets".
D.V. BERKOV, Inst. of Chem. Phys. Chernogolovka, Russia.

"Applications of non-contact ultrasound".
S.P. PALMER, Univ. Warwick, UK.

College 6

Liquids, Disordered Materials and Metal Physics

"Density expansion spectroscopy: light and neutron scattering".
F. BAROCCHI, Univ. di Firenze, Italy.

"Structural studies of highly corrugated surfaces with He-beam diffraction".
E. KIRSTEN, MPI für Strömungsforschung, Berlin, Germany.

"Lattice dynamics of three dimensional quasicrystals".
P. GALLO, Univ. dell'Aquila, Italy.

"μSR studies of hydrogen in metals".
F.N. GYGAX, ETH Zurich and PSI Villigen, Switzerland.

"Relaxation in glycerol:
Do neutrons and light see the same ?"
J. WUTTKE, TU München, Garching, Germany.

"Progress Report on Be".
C. MAY, ILL, Grenoble, France.

College 8

Biological Structures and Dynamics

"Protein structure: analysis, prediction and design".
J.M. THORNTON, Univ. College London, UK.

"Une nouvelle famille de protéines riches en cystéines: structure et modélisation".
F. BAUD, ILL-IBS, Grenoble, France.

College 9

Chemistry

"Neutron reflectivity and surface tension study of a diblock copolymer at the surface of a selective solvent".
B.J. FACTOR, Institut Curie, Paris, France.

"Microstructure and rheology of soft matter - Investigations using neutron scattering and other techniques".
J.D.F. RAMSAY, Institut de Recherches sur la Catalyse, CNRS, Villeurbanne, France.

"On the application of polymer theory to giant worm-like lecithin microemulsions".
P. SCHURTENBERGER, ETH Zürich, Switzerland.

"Weakly charged polyelectrolytes".
F. SCHOSSELER, Université Louis Pasteur, Strasbourg, France.

"Fullerene intercalation chemistry and superconductivity".
M.J. ROSSEINSKY, Inorganic Chemistry Laboratory, Univ. of Oxford, UK.

"Laminar and turbulent flow behaviour of viscoelastic surfactant solutions".
H.W. BEWERSDORFF, Swiss Federal Institute of Technology, Zürich, Suisse.

"Structural and spectroscopic studies of rare earth oxy compounds".
J. HÖLSÄ, University of Turku, Finland.

"SANS and neutron reflectivity studies of grafted copolymers".
W. DOZIER, Argonne Nat. laboratory, USA.

"Rotational tunnelling of ammonia molecules".
M. HAVIGHORST, IFF, KFA, Jülich, Germany.

"Inelastic neutron scattering studies of the proton transfer dynamic in high region bonds".
F. FILLIAUX, LASIR-CNRS, Thiais, France.

"An introduction to Bayesian model selection".
D. SIVIA, RAL, Didcot, UK.

Thursday colloquium

"L'organisation spontanée dans les plantes vers des structures cristallines particulières".
S. DOUDAY, E.N.S. Paris, France.

"Modèles statistiques de l'évolution Darwinienne".
L. PELITI, Institut Curie, Paris, France.

"Physical properties of ultra thin films investigated by X-ray reflectivity".
J.J. BENATTAR, SPEC, CE Saclay, Gif-sur-Yvette, France.

"Nuclear magnetic ordering in metals".
F. POBELL, Univ. Bayreuth, Germany.

"The complex Ginzburg Landau approach to nonequilibrium pattern formation".
Wim van SAARLOOS, Leiden University, The Netherlands.

"High-T_c superconductors: Present status of applications".
H. RIETSCHEL, Kernforschungszentrum, Karlsruhe, Germany.

"Fluids in space".
D. BEYSENS, SPEC, CE Saclay, Gif-sur-Yvette, France.

"Giant, micelles, fluid membranes and reversibly connected networks: towards a unified view of amphiphilic polymorphism".
G. PORTE, USTL, Montpellier, France.

"High-resolution electron microscopy and its application to high-temperature superconductors".
K. URBAN, Inst. für Festkörperforschung, Forschungszentrum, Jülich, Germany.

"Morphogenesis of unicellular algae".
P. PELCE, Université de Provence - St. Jérome, Marseille, France.

"The human genome project (HGP)".
V. NOWOTNY, Washington Univ. School of Medicine, Missouri, USA.

"Liquid helium seen with neutrons".
R. SCHERM, ILL, Grenoble, France.

"Future neutron sources: reactors or spallation ?"
F. MEZEI, Hahn-Meitner Institut/BENSC, Berlin, Germany.

"Scars and isospectra: experiments in quantum chaos and mathematics".
S. SRIDHAR, Northeastern University, Boston, USA.

"Hydrodynamics of quasicrystals".
P. KALUGIN, Landau Institute, Moscow, Russia.

"Recent applications of muon-spin-resonance-spectroscopy to the study of magnetic properties of heavy fermion compounds".
A. SCHENCK, ETH Zürich and Paul Scherrer Institute, Zürich, Switzerland.

"Fluctuations in the C60 fullerene: aspects of rotational and translational fluidity".
N. ASHCROFT, Cornell University, Ithaca, NY, USA.

"The onset of superfluidity in thin ^{4}He films adsorbed on graphite".
P. CROWELL, Cornell University, Ithaca, NY, USA.

"High pressure effects on 1-D transition metal chalcogenides, fullerenes and high-temperature superconductors".
M. NUÑEZ-REGUEIRO, CRTBT, CNRS, Grenoble, France.

Workshops organized or sponsored by the ILL in 1993

Braunschweig, Germany, May 10-11, 1993.
Workshop on Focusing Crystal Optics.
Organizers: MAGERL A., WAGNER V.

La Grande-Motte, France, May 17-19, 1993.
Journées de la Diffusion Neutronique
Organizers: CHIEUX P., FRIES E.

Grenoble (ILL), France, January 21-23, 1993.
International Workshop on the Use of Neutrons and X-rays in the Study of Magnetism.
Organizers: BROWN P.J., LANDER G.H., MARTINEZ J., STIRLING W.G., VETTIER C.

Grenoble (ILL), France, January 29, 1993.
Colloquium in memory of Walter Mampe.
Organizers: PENDLEBURY M., BOERNER H.

Grenoble (ILL), France, March 22-24, 1993.
International Workshop of the Institut Laue-Langevin (ILL) and the Institut fuer Festkoerperforschung (IFF) der KFA Juelich on Dynamics of Disordered Materials II.
Organizers: PETRY W., RICHTER D., DIANOUX A.J.

Grenoble (ILL) , France, June 2-4, 1993.
Réunion Annuelle du Groupe Français d'Etude des Quasicristaux. (Livre de Résumés 1 - 2)
Organizer: JANOT C.

Grenoble, France, June 21-23 ,1993.
Workshop on Progress in Gaseous Microstrip Proportional Chambers.
Organizer: GELTENBORT P.

Stockholm, Sweden, May 13-17 ,1993.
Euroconference on Neutrons in Surface Science and at Interfaces.
Organizers: BERMEJO F.J., COSTA M.M.R.R., DAHLBORG U., FONTANA M., GAMARI-SEALE H., SCHERM R., LOVESEY S.W., DAHLBORG M.

Book Published

BARUCHEL J., HODEAU J.L., LEHMANN M., REGNARD J.R., SCHLENKER C. [Editors]
Neutron and Synchrotron Radiation for Condensed Matter Studies. Volume 1. Theory, Instruments and Methods.
(HERCULES: Higher European Course for Users of Large Experimental Systems)
(Springer Verlag, Berlin/Les Editions de Physique, Paris, 1993) ISBN 286883-185-0.

Conference Proceedings Published as Books or Journal Issues

Proceedings of the International Workshop on Dynamics of Disordered Materials II.
DIANOUX A.J., PETRY W., RICHTER D. [Editors]
PHYSICA A 201 n° 1-3 (1993).

Proceedings of the ILL/ESRF Workshop on Methods in the Determination of Partial Structure Factors of Disordered Matter by Neutron and Anomalous X-ray Diffraction.
SUCK J.B., RAOUX D., CHIEUX P., RIEKEL C. [Editors]
(World Scientific Publishing, Singapore, 1993)
ISBN 981-02-1463-4.

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LANDER G.H., STIRLING W.G. [Editors]
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Theses

BOUDARD M.
Structure et propriétés dynamiques de la phase icosaédrique AlPdMn.
Thèse, Institut National Polytechnique de Grenoble, Grenoble le 30 mars 1993.

EDER K.J.
Das Superpendel - Ein neues System zur Schwingungsisolierung fuer die Neutronenoptik.
Inaugurat Dissertation, Leopold-Franzens-Universitaet Innsbruck, Mai 1993.

GUTSMIEDL E.
Erzeugung und Aufwaertsstreuung von ultrakalten Neutronen in superfluessigem Helium.
Dissertation, Technische Universität München, 1993.

LAUTENSCHLAEGER G.
Untersuchung der magnetischen Phasenuebergaenge des Manganwolframats, $MnWO_4$.
Inaugurat Dissertation, Technische Hochschule Darmstadt, 1993.

NOELDEKE C.
Anordnung und Anregungen des Ammoniaks in Ytterbiumhexaammin.
Inaugurat Dissertation, Christian-Albrechts-Universitaet, Kiel, 1993.

SCHMID B.
Inelastische magnetische Neutronenstreuung an den quasi-eindimensionalen Singulettgrundzustandssystemen $CsFeCl_3$ und $CsFeBr_3$ unter dem Einfluss eines aeusseren Magnetfeldes.
Inaugurat Dissertation, Universitaet Regensburg, 1993.

STUHR U.
Neutronenspektrokopische Untersuchungen der Diffusion und der optischen Schwingungsmoden von Wasserstoff in Metall-Wasserstoff-Systemen.
Dissertation, Technische Hochschule Darmstadt, 1993.

TORRELLES ALBAREDA J.
Estudio de la relajacion estructural inducida termicamente en aleaciones vitreas del sistema Ge-Se mediante diffraccion de neutrones.
Memoria para optar al grado de Doctor en Ciencias Fisicas Universitat Autonoma de Barcelona, Febrero 1993.

WEBER M.
Untersuchungen zur Vibrationsdaempfung an den hochaufloesenden Gammaspektrometern GAMS 2/3 und GAMS 4 am ILL Grenoble. Kernspektroskopie an ^{177}Tm und ^{177}Lu.
Inaugurat Dissertation, Technische Universitaet Muenchen, 1993.

Conference Contributions

ABINGDON, UK: ICANS-XII International Collaboration on Advanced Neutron Sources - 1993/05/24-28

ANDERSON I., BOENI P., BUFFAT P., ELSENHAUS O., FRIEDLI H.P., GRIMMER H., HAUERT R., LEIFER K., MENELLE A., PENFOLD J., SOECHTIG J. Recent progress in supermirrors at PSI. (Contributed paper)

ALICANTE, Spain: 2nd International Discussion Meeting on Relaxations in Complex Systems - 1993/06/28-07/08

DIANOUX A.J., SAUVAJOL J.L., SMITH J., KNELLER G.R. Dynamics of cis- and trans-polyacetylene: a combined inelastic neutron scattering and computer simulation analysis. (Invited talk)

FRICK B., RICHTER D., ZORN R., FETTERS L.J. The fast relaxation process near the glass transition in amorphous polymers with different microstructure. (Contributed paper)

ANTIBES/JUAN-LES-PINS, France: 9th International Colloquium on Plasma Processes - 1993/06/6-11

ANDERSON I., ELSENHAUS O., BOENI P., BUFFAT P., FRIEDLI H.P., GRIMMER H., HAUERT R., LEIFER K., SOECHTIG J. Artificial multilayer supermirrors for neutron optics. (Contributed paper)

ASCONA, Switzerland: 2nd International Conference on Magnetoelectric Interaction Phenomena in Crystals (MEIPIC - 2) - 1993/09/13-18

MCINTYRE G.J., VISSER D., COLDWELL T.R., GRAF H., WEISS L., ZEISKE TH., PLUMER M.L. Magnetic ordering in the stacked triangular antiferromagnet $CsMnBr_3$ in the presence of an electric field. (Talk)

BEIDAIHE, China: Neutron Scattering Satellite Meeting, NSS-93 - 1993/08/17-19

CHATTOPADHYAY T. Modulated magnetic phases. (Invited talk)

KULDA J., LUKAS P., MIKULA P., VRANA M. High-resolution neutron diffraction study of internal stresses. (Poster)

KULDA J., STRAUCH D., ISHII Y. Experimental study of inelastic structure factors in silicon. (Poster)

MCINTYRE G.J. Geometrical aspects of single-crystal diffractometry with position-sensitive detectors. (Poster)

MCINTYRE G.J., PTASIEWICZ-BAK H. Phases of magnetic structure factors of non-centrosymmetric magnetised crystals by polarised-neutron diffraction. (Poster)

MIKULA P., KULDA J., LUKAS P., VRANA M., WAGNER V., SCHERM R. Recent developments of the neutron monochromators based on bent perfect crystals. (Invited talk)

MIKULA P., LUKAS P., KULDA J., STRUNZ P., SAROUN J., VRANA M., WAGNER V., ALEFELD B. Applications of curved crystals in many-crystal settings. (Poster)

BEIJING, China: XVIth International Congress of Crystallography - 1993/08/21-29

BAUMBACH G.T., GAILHANOU M., MARTI U., SILVA P., BESSIERE M., REINHART F.K., ILEGEMS M. Characterization of quantum well wires and surface gratings by X-ray diffraction reciprocal space mapping.

CHATTOPADHYAY T., BROWN P.J. Sudden disappearance of three-dimensional magnetic ordering in Gd_2CuO_4. (Poster)

LEHMANN M.S. Protein diffraction around the sulfur K-absorption edge using 5 Å X-rays from a storage ring. (Talk)

LEHMANN M.S., CIPRIANI F., DAUVERGNE F., GABRIEL A., WILKINSON C. An image plate detector for quasi-Laue neutron diffractometry. (Poster)

LEHMANN M.S., WILKINSON C., GABRIEL A., ALLIBON J., DAUVERGNE F. Position sensitive photomultiplier tube neutron detector. (Poster)

MCINTYRE G.J. Empirical and calculated thermal-diffuse-scattering corrections for single-crystal diffraction data collected with a two-dimensional position-sensitive detector. (Poster)

MCINTYRE G.J., OLOVSSON I., PTASIEWICZ-BAK H. Chemical bonding and temperature effects in the charge and spin densities of $NiSO_{4.6}H_2O$ and $NiSO_{4.7}H_2O$. (Poster)

REEHUIS M., OULADDIAF B., VOMHOF T., JEITSCHKO W. Magnetic order in the phosphides $Ho_2Fe_{12}P_7$, $Nd_2Co_{12}P_7$ and $Ho_2Co_{12}P_7$. (Talk)

BEIJING, China: XVIth International Congress of Crystallography. Synchrotron Radiation Satellite Meeting - 1993/08/31-09/03

LEHMANN M.S. Protein crystallographic measurement on the Troika undulator beam line of the ESRF. (Talk)

BENEDIKTBEUREN, Germany: BMFT Verbundtreffen Neutronen - 1993/10/18-20

DORNER B. Magnetische Anregungen in den quasi 1-D Systemen $CsFeCl_3$ und $CsFeBr_3$ im Magnetfeld parallel und senkrecht zur Kettenrichtung. (Talk)

LISS K.D., MAGERL A., SPRINGER T. Beugungseigenschaften von $Si_{1-x}Ge_x$ Gradientenkristallen. (Poster)

MAGERL A., ZULEHNER W. Optimierte Sauerstoffpraezipitation in Silizium: ein Beitrag der Neutronenstreuung zum Gigabit Bauelement. (Talk)

MAY R.P. D22, ein neues Instrument fuer Neutronenkleinwinkelstreuung am ILL. (Poster)

RITTER C., MONDAL S., CYWINSKI R., KILCOYNE S.H., RAINFORD B.D. A study of the transition between intrinsic and induced Mn moment in the system $Dy_{1-x}Y_xMn_2$. (Poster)

STOELKEN S., BARTSCH E., SILLESCU H., LINDNER P., ANTONIETTI M. Kugelffoermige Polymermikronetzwerke - neuartige Materialien als Bindeglied zwischen Polymeren und Kolloiden. (Poster)

BRAUNSCHWEIG, Germany: Workshop on Focusing Bragg Optics - 1993/05/10-11

DORNER B. Comparison of gradient and mosaic crystals by means of k-distributions in reciprocal space. (Talk)

KULDA J., WAGNER V., MIKULA P., SAROUN J. Comparative tests of neutron monochromators using elastically bent silicon and mosaic crystals. (Talk)

LISS K.D., MAGERL A. Can a gradient crystal compete with a mosaic crystal as a monochromator in neutron- or X-ray diffraction? (Talk)

MAGERL A., LISS K.D., DOLL C., MADAR R., STEICHELE E. Will gradient crystals become available for neutron diffraction? (Contributed paper)

MIKULA P., KULDA J., LUKAS P., VRANA M., WAGNER V., SCHERM R. Bent perfect crystals in asymmetric diffraction geometry in neutron scattering experiments. (Talk)

MUTKA H. Coupled time and space focusing for time-of-flight inelastic scattering. (Talk)

BRISTOL, UK: VIIth ECIS Conference - 1993/09

TERECH P. Surfactant aggregation in organic solvents: physical gels and living polymers. (Poster)

BUDAPEST, Hungary: Workshop on the International Use of Centres of Excellence and Joint Projects - 1993/03/26-27

HEIDEMANN A. The ILL: An international neutron research center. (Poster)

CARGESE, France: NATO-ARW on Hydrogen Bond Networks - 1993/08/16-22

DIANOUX A.J., HARRIS K.D.M., GUILLAUME F. Molecular motions in urea inclusion compounds. (Contributed paper)

CARRY-LE-ROUET, France: International Workshop on Electron Crystals - 1993/06/02-04

CURRAT R., LORENZO-DIAZ J.E. Neutron study of phase transitions and low-frequency excitations in $(MSe_4)_nI$ compounds. (Invited talk)

COMO, Italy: NATO Advanced Study Institute "Modern Aspects of Small-Angle Scattering" - 1993/05/12-22

LINDNER P. Polymers in solution. Flow techniques. (Invited talk).

MAY R.P. Small-angle neutron scattering of biological macromolecular complexes consisting of proteins and nucleic acids. (Poster & Talk)

DRESDEN, Germany: Workshop on High-Resolution Spectroscopy of Fission Fragments, Neutrons and γ-Rays - 1993/03

GELTENBORT P., MOELLER A., GOENNENWEIN F., KAUFMANN J., PETROV G., DUERING I., MAERTEN H., RUBEN A., OED A. Cold fission studies using a double-ionization chamber. (Contributed paper)

DUBNA, Russia: 3rd International Conference on Surface X-ray and Neutron Scattering - 1993/06/24-29

BAUMBACH G.T., HOLY V. Umweganregung excited by specular internal reflection and strong asymmetric X-ray diffraction.

BAUMBACH G.T., HOLY V., PIETSCH U., GAILHANOU M. The influence of specular interface reflection on grazing incidence diffraction and diffuse scattering from superlattices.

SCHAERPF O. Surfaces and interfaces and their role in supermirrors. (Invited talk)

EUGENE, USA: 20th International Conference on Low Temperature Physics - 1993/08/04-11

MARTINEZ J.L., GARCIA-MATRES E., GARCIA-MUNOZ J.L., RODRIGUEZ J. Magnetic properties of R_2BaNiO_5 oxides. (Poster)

FLORENCE, Italy: 2nd Liquid Matter Conference - 1993/09/18-22

SUCK J.-B., CHIEUX P., DUPUY-PHILON J., JAL J.-F., MORKEL C.

Collective atomic dynamics in mixtures of liquid metals and molten salts. (Contributed paper)

FRIBOURG, Switzerland: 8th International Symposium on Capture Gamma-Ray Spectroscopy and Related Topics - 1993/09/20-24

BOERNER H.G., PENDLEBURY J.M. New developments for the nuclear and fundamental physics facilities at the high flux reactor of the ILL Grenoble. (Invited talk)

DRISSI S., DÉLÈZE M., GARRETT P.E., JOLIE J., KERN J., MANNANAL S.J., TERCIER P.A., VORLET J.P., WARR N., MOUZE G., YTHIER CH., BOERNER H.G., JUDGE S., SCHRECKENBACH K., WILLIAMS A. Complete level structure of ^{112}Cd and the SU(5) dynamical symmetry. (Invited talk & Contributed paper)

JUNGCLAUS A. The gamma-ray induced Doppler (GRID) broadening method: a status report. (Invited talk)

GAITHERSBURG, USA: The Eighth International Meeting on Ferroelectricity - 1993/08/08-13

KAMBA S., PETZELT J., ZELEZNY V., SMUTNY F., DVORAK V., HLINKA J., QUILICHINI M., VOLKOV A.A., GORSHUNOV B.P., KOZLOV G.V., CURRAT R., LEGRAND J.F. Dynamical studies of fully deuterated BCCD. (Contributed paper)

GARCHY, France: Rhéophysique des Suspensions Colloïdales - 1993/12/15-17

TERECH P. Polymères vivants en milieu organique, exemple d'un complexe organométallique dans le cyclohexane.

GIF-SUR-YVETTE, France: Formation Jeunes Chercheurs "Frustration Géométrique en Matière Condensée" - 1993/12

CHARVOLIN J. Films d'amphiphiles. (Invited talk)

GLASGOW, Scotland: IXth International Conference of Virology - 1993/08/08-13

TIMMINS P.A. The architecture of tomato bushy stunt virus: Distribution of RNA and protein. (Contributed paper)

TIMMINS P.A. A decapsidation mechanism for turnip yellow mosaic virus. (Poster)

GRENOBLE, France: International Workshop on the Use of Neutrons and X-rays in the Study of Magnetism - 1993/01/21-23

KULDA J. On the cross-section of the thermal neutron coherent inelastic scattering. (Poster)

MCINTYRE G.J., PTASIEWICZ-BAK H., OLOVSSON I. Chemical bonding and covalency in $NiSO_4.6H_2O$ by measurement of charge and spin densities. (Poster)

OULADDIAF B., BALLOU R., LEKIEVRE-BERNA E. Magnetic phase diagram of $TbMn_2$. (Poster)

RITTER C., CYWINSKI R., KILCOYNE S.H., MONDAL S., RAINFORD B.D. Volume anomalies and thermal expansion in the system $Dy_{1-x}Y_xMn_2$. (Poster)

SCHAERPF O. Use of a multidetector in neutron polarization analysis of magnetic scattering. (Poster)

SCHAERPF O. Absolute cross-section determination of magnetic scattering from a La_2CuO_4 single crystal above T_N. (Poster)

GRENOBLE, France: HERCULES Course - 1993/02/14-04/02

LEHMANN M.S. Neutron crystallography of biological molecules. (Invited talk)

TIMMINS P.A. Virus structure. (Invited talk)

GRENOBLE, France: Workshop on "Dynamics in Disordered Materials II" - 1993/03/22-24

BUCHENAU U., LINDER K., FRICK B. Debye-Waller factors in amorphous polymers. (Poster & Contributed paper)

DUVAL E., ACHIBAT T., BOUKENTER A., FRICK B., GARCIA N., SERUGHETTI J. Comparison between light and neutron inelastic scatterings. The frequency linear behaviour of the light-vibration coupling coefficient. (Contributed paper)

FERRAND M. Thermal motions and function of bacteriorhodopsin in purple membranes: effects of temperature and hydration studied by neutron scattering. (Poster)

FERRAND M., DIANOUX A.J., PETRY W., ZACCAÏ G. Dynamical transition of bacteriorhodopsin in purple membranes revealed by neutron scattering: a relation between structure, dynamics and function. (Contributed paper)

FRICK B., RICHTER D., TREVINO S. Inelastic fast relaxation in a weakly fragile polymer glass near T_g. (Contributed paper)

ZORN R., RICHTER D., FRICK B., FARAGO B. Neutron scattering experiments on the glass transition of polymers. (Invited talk & Contributed paper)

GRENOBLE, France: IAEA Interregional Training Course on Nuclear Methods in Materials Research - 1993/05/10-21

ANDERSON I. Multilayer design and production for neutron optics. (Talk)

CONVERT P. Thermal neutron detection. (Talk)

HEWAT A.W. High T_c superconductors studied by neutron powder diffraction. (Talk)

KEARLEY G. Molecular spectroscopy and catalysis. (Talk)

LINDNER P. Polymers in solution. Flow techniques. (Talk)

PANNETIER J. Studying chemical reactions by neutron powder diffraction. (Talk)

RITTER C. Materials research on D1B. (Talk)

GRENOBLE, France: BEST, INPG, ENSPG Summer Course "Neutrons and Synchrotron Radiation" - 1993/09/14-24

DORNER B. Inelastic neutron scattering. (Invited talk)

TIMMINS P.A. Neutrons in biology. (Invited talk)

HELSINKI, Finland: Nordic Structural Chemistry Meeting - 1993/01/11-13

MCINTYRE G.J., OLOVSSON I., PTASIEWICZ-BAK H. Spin and charge density in $NiSO_4.6H_2O$. Bonding deformation and superposition effects. (Poster)

JUELICH, Germany: Neutron Scattering Seminar - 1993/10/11-12

TRAMPENAU J., DUBOS O., HENNION B., PETRY W. Strongly anharmonic phonons in monoatomic bcc phases. (Invited talk)

KOCHI, Japan: Meeting of the Japanese Physical Society Section on Elementary Particles - 1993/10/04-06

PENDLEBURY J.M. Electric dipole moments and CP violation. (Invited talk)

LA GRANDE-MOTTE, France: Secondes Journées de la Diffusion Neutronique - 1993/05/17-19

BALLOU R., DEPORTES J., OULADDIAF B. Effets de substitutions de Tb et Al sur l'hélimagnétisme à longue période dans le composé YMn_2. (Poster)

BALLOU R., DEPORTES T., OULADDIAF B. Dimorphisme structural, instabilité magnétique et frustration topologique dans la série $(Dy_{1-x}La_x)Mn_2$. (Poster)

CURRAT R. Etude par diffusion de neutrons des transitions de phase dans les composés quasi-unidimensionnels $(TaSe_4)_2I$ et $(NbSe_4)_3I$. (Poster)

DIANOUX A.J., KNELLER G.R., SAUVAJOL J.L., SMITH J.C. Densité d'états vibrationnels du polyacétylène: simulations de dynamique moléculaire et comparaison avec les résultats de diffusion des neutrons. (Poster)

MUTKA H. Diffusion Brillouin aux neutrons. Instrument inélastique aux petits angles. (Poster)

MUTKA H., ECCLESTON R., MOLINIE P., PAYEN C. Effet de la température sur la dynamique de spins de la chaîne antiferromagnétique de Heisenberg S=1: étude par la diffusion inélastique des neutrons de $AgVP_2S_6$. (Poster)

LONDON, UK: Third London Conference on Position-Sensitive Detectors - 1993/09/6-10

GELTENBORT P., OED A. MicroStrip gas chambers at the Institute Laue-Langevin. (Talk)

LOUVAIN-LA-NEUVE, Belgium: Workshop on Symmetries in Semi-leptonic and Leptonic Weak Interactions - 1993/06/4-7

LAST J. Cold, ultracold and polarised neutrons. (Invited talk)

PENDLEBURY J.M. Improving the neutron electric dipole moment measurements. (Invited talk)

LUNTEREN, Holland: European Research Conference on Dynamical Properties of Solids - 1993/09/26-30

CURRAT R. Neutron study of phase transitions and low-frequency excitations in modulated crystals. (Invited talk)

SUCK J.-B. Collective excitations in topologically disordered systems studied by neutron inelastic scattering. (Invited talk)

MAINZ, Germany: Spring Meeting of the German Physical Society, Section Hadrons and Nuclei - 1993/03/21-26

ABELE H., HELM G., KANIA U., SCHMIDT C., LAST J., DUBBERS D.
Verlustfreie Messung von ^{35}S und ^{63}Ni β-Spektren, und der Ursprung der 17 keV Neutrino-Signale. (Talk)

FIONI G., HESSE M., FAUST H. Eine neue Ionisationskammer fuer das erweiterte Massenspektrometer LOHENGRIN am ILL Grenoble. (Poster)

GELTENBORT P, OED A. Features of micro strip proportional counters (group report). (Talk)

MINNEAPOLIS, USA: 38th Annual Conference on Magnetism and Magnetic Materials - 1993/11/15-18

BRAMWELL S.T. Order by disorder in an anisotropic pyrochlore antiferromagnet. (Talk)

BRAMWELL S.T. Weak ferromagnetism in a Kagome lattice antiferromagnet. (Talk)

CHATTOPADHYAY T., BROWN P.J., ROESSLI B. Disappearance of three-dimensional magnetic ordering in Gd_2CuO_4. (Talk)

CHATTOPADHYAY T., ROSOV N., LYNN J.W., KAESTNER J., WASSERMANN E.F., BACH H. Temperature dependence of the magnetic excitations in ordered and disordered Fe_3Pt. (Talk)

ISNARD O., MIRAGLIA S., GUILLOT M., FRUCHART D. High field magnetization measurements of Sm_2Fe_{17}, $Sm_2Fe_{17}N_3$, $Sm_2Fe_{17}D_5$ and Pr_2Fe_{17}, $Pr_2Fe_{17}N_3$. (Invited talk)

MITO, Japan: 5th International Symposium on Advanced Nuclear Energy Research - 1993/03

DORNER B. Inelastic neutron scattering and polarized neutrons. (Panel contribution)

KULDA J., STRAUCH D., ISHII Y. Refinement of phonon eigenvector phases from intensities of neutron inelastic scattering in Si. (Contributed paper)

MONTE VERITA, Switzerland: 2nd International Conference on Magnetoelectric Interaction Phenomena in Crystals (MEIPIC - 2) - 1993/09/13-18

MCINTYRE G.J., VISSER D., COLDWELL T.R., GRAF H., WEISS L., ZEISKE T., PLUMER M.L. Magnetic ordering in the stacked triangular antiferromagnet $CsMnBr_3$ in the presence of an electric field. (Talk)

MONTERREY, USA: 20th RERC - 1993/08

MARTINEZ J.L., SAEZ PUCHO R., HERNANDEZ J., RODRIGUEZ J., GARCIA MATRES E. Magnetic properties of novel R_2BaCoO_5.

MONTPELLIER, France: Journée de Biochimie Structurale - 1993/12/02

TIMMINS P.A. Etudes structurales de macromolécules biologiques par diffusion des neutrons. (Invited talk)

NATHIAGALI, Pakistan: Seventeenth International Workshop on Condensed Matter Theories - 1993/06/18-24

CLEMENTS B.E. Dynamic excitations in Bose liquid films. (Invited talk)

NEW LONDON, USA: Gordon Conference on X-ray Physics - 1993/08/09-13

LEHMANN M.S. Protein crystallography with soft X-ray near the K-absorption edge of sulfur. (Talk)

OAK RIDGE, USA: Workshop on Fundamental Physics at the Advanced Neutron Source - 1993/11/09-10

BOERNER H.G. Precision gamma ray measurements: a review. (Invited talk)

PENDLEBURY J.M. Ultracold neutrons: a review. (Invited talk)

OKAYAMA, Japan: Meeting of the Japanese Physical Society Section on Atoms and Molecules - 1993/10/11-13

PENDLEBURY J.M. Fundamental physics with ultracold neutrons. (Invited talk)

PREDEAL, Romania: NATO Advanced Study Institute "Frontier Topics in Nuclear Physics" - 1993/08/24-09/04

JUNGCLAUS A., BOERNER H.G., JOLIE J., LIEB K.P., ULBIG S. Lifetime measurements with the gamma ray induced doppler (GRID) broadening method. (Talk)

REGENSBURG, Germany: 13th General Conference of the Condensed Matter Division. European Physical Society - 1993/03/29-04/02

BAUMBACH G.T., PIETSCH U. Grazing incidence X-ray diffaction and its interdependence on the specular X-ray reflectivity in the case of a semiconductor superlattice. (Abstract)

DIANOUX A.J., GUILLAUME F., EL BAGHDADI A. Dynamics of alkyl-type chains in crystals. (Contributed paper)

LISS K.D., MAGERL A., SPRINGER T., MADAR R. Fabrication and diffraction properties of $Si_{1-x}Ge_x$ gradient crystals. (Poster)

SCHAERPF O. A neutron multidetector with spin analysis applied to measure absolute magnetic cross-sections on high T_c materials. (Talk)

VOIT J. Charge-spin separation and the spectral properties of Luttinger liquids. (Talk)

VOIT J., BARANOWSKI D., BUETTNER H. Electronic correlations and electron-libron coupling in polyaniline. (Abstract)

RISØ, Denmark: Users' Meeting - 1993/01/08-09

LINDNER P. Semidilute polymer solutions under shear. (Poster)

MAY R.P. D22, the new small-angle neutron scattering facility at the ILL. (Poster)

ROSKILDE, Denmark: RITA Workshop - 1993/08/28

KULDA J. Elastically deformed versus mosaic monochromators. (Talk)

ROUEN, France: Réunion Annuelle du Groupe Défauts Ponctuels - 1993/06/24-25

RANDL O. Lacunes, phonons et diffusion atomique dans des alliages intermétalliques. (Talk)

SACLAY, France: Conference on Membrane Structure, Dynamics and Interactions via Neutron and X-ray Scattering - 1993/04

CHARVOLIN J. Membranes in chloroplasts and etioplasts. (Invited talk)

SACLAY, France: IXth International Conference on Small Angle Scattering - 1993/04/27-30

LINDNER P. Semidilute polymer solutions under shear. (Poster)

MAY R.P. D22, the new small-angle neutron scattering facility at the ILL. (Poster)

MAY R.P. Geometrical optimisation of neutron small-angle scattering instruments. (Poster & Talk)

TIMMINS P.A. Small angle neutron scattering from solutions and crystals of biological macromolecules. (Invited talk)

SACLAY-LLB, France: Réunion Thématique "Dynamique et Spectres de Phonons" - 1993/03/11-12

SUCK J.-B. Generalized vibrational density of states and total dynamic structure factor of icosahedral alloys. (Invited talk)

SAN DIEGO, USA: Fifth International Conference on the Crystallization of Biological Macromolecules - 1993/08/08-13

TIMMINS P.A. The organisation of detergents in solution and in crystals of membrane proteins. (Invited talk & Abstract)

SAN SEBASTIAN, Spain: QUENS'93 Quasielastic Neutron Scattering - 1993/09/27-28

DIANOUX A.J., EL BAGHDADI A., GUILLAUME F., BOYSEN H., CODDENS G. Translational and rotational motions of n-alkane molecules within the channels of urea inclusion compounds. (Contributed paper)

HEIDEMANN A. Directions in instrumentation for quasielastic neutron scattering. (Invited talk)

MUTKA H. Energy-resolved small-angle thermal neutron scattering: a challenge for instrumentation. (Talk)

SAN SEBASTIAN, Spain: NATO Advanced Research Workshop - "The Physics and Mathematical Physics of the Hubbard Model" - 1993/10/3-8

VOIT J. Charge-spin separation and the spectral properties of Luttinger liquids. (Invited talk)

SANDBJERG CASTLE, Denmark: Nordic School on the Application of X-ray Synchrotron Radiation - 1993/06/25-07/03

LEHMANN M.S.
Anomalous scattering in biology. (Talk)

LEHMANN M.S.
The noble art of proposal writing. (Talk)

SEATTLE, USA: American Institute of Physics Spring Meeting - 1993/03/22-26

BRAMWELL S.T. Critical properties of ultrathin films. (Talk)

BROWN P.J. Magnetic correlations in $La_{2-x}Sr_xNiO_4$. (Invited talk)

CHATTOPADHYAY T., SUMARLIN I.W., LYNN J.W., BARILO S.N., ZHIGUNOV D.I. Magnetic excitons of Pr in Pr_2CuO_4. (Talk)

NEUMANN D.A., KAMITAKAHARA W.A., FRICK B. Neutron scattering from vibrational modes in carbon solids. (Contributed paper)

NGAI K., FRICK B., TREVINO S.F., RICHTER D. Excitations in glassy polymers. (Contributed paper)

SHEFFIELD, UK: UK Neutron Beam Users Meeting - 1993/09/01-02

TIMMINS P.A. Neutrons in biology. (Invited talk)

STRASBOURG, France: E-MRS 1993 Spring Meeting - 1993/05/4-7

BAUMBACH G.T., GAILHANOU M., FISCHER H., MARTI U., SILVA P.C., REINHART F.K., ILEGEMS M. X-ray diffraction reciprocal space mapping of III-V gratings.

TRIESTE, Italy: Workshop on "The Liquid State of Matter: Opportunities from New Radiation Sources" - 1993/07

CHIEUX P., DAMAY P. Accuracy in neutron scattering determination of the structure of disordered materials. (Invited talk)

CHIEUX P., DAMAY P. Is neutron small angle scattering an appropriate tool for the study of criticality ? (Invited talk)

TROIS-RIVIERES, QUEBEC, Canada: Sixth International Conference on Organized Molecular Films - 1993/07/04-09

LEGRAND J.F. X-ray grazing incidence studies of the 2-D crystallization of monolayers of 1-alcohols at the air-water interface. (Poster)

ULM, Germany: 28th Europhysics Conference on "Transitions in Oligomer and Polymer Systems" - 1993/09/27-10/1

FRICK B., BUCHENAU U. Boson peak and fast relaxation process near the glass transition in polystyrene. (Contributed paper)

VELDHOVEN, Holland: Europhysics Industrial Workshop EIW-9 - "Nanometer-scale Methods in X-ray Technology" - 1993/10/11-13

BAUMBACH G.T., GAILHANOU M. X-ray diffraction from simple and epitaxial multilayered surface gratings.

BAUMBACH G.T., HOLY V. X-ray reflection from rough periodical multilayers.

VILLEURBANNE, France: Colloque S.F.M.E. - 1993/04

CHEYNET M.C., SOLAS D., ANTONIADIS A., BERRUYER J., FILHOL A. Microanalyse des ségrégrations en soluté dans les PFZ formés aux joints de grain d'un alliage Al-Zn-Mg. (Contributed paper)

WARSAW, Poland: Polish Academy of Sciences Course on Structural Biology - 1993/01/21-24

TIMMINS P.A. Neutron scattering for the study of biological macromolecules. (Invited talk)

TIMMINS P.A. Virus structure. (Invited talk)

WINDSOR, UK: Conference on Quantum Molecular Tunneling in Solids - 1993/07/12-15

HEIDEMANN A. New methods in neutron spectroscopy. (Invited talk)

ZUOZ, Switzerland: Summerschool on Neutron Scattering - 1993/08/15-21

DORNER B. Structural excitations. (Invited talk)

TIMMINS P.A. Neutron scattering in biology. (Invited talk)

Publications – ILL-Reports 1993

This list groups publications received during 1993 resulting from the research at the ILL.
ILL-Reports are listed first. They are followed by the list of publications in journals, conference proceedings, books with ILL authors and co-authors and by publications related to experimental work performed by visiting scientists at the ILL but without ILL co-authors.

ILL-Reports

(Code number 1 to 9)

93CO01G
COOK J.C. Monte Carlo simulation of the energy resolution function of the backscattering spectrometer IN10.
ILL-Report.

93PA02T
PAPOULAR R.J., RESSOUCHE E., TASSET F.
Comparison on various computers and workstations: runtime necessary to compute a crystallographic inverse Fourier transform using maximum entropy.
ILL-Report.

93MA03T
MAYERHOFER U. User's manual: a short guide and introduction to the hp9000/710 of college III.
ILL-Report.

93NE04T
NESVIZHEVSKY V.V. Error assessment for neutron lifetime measurement with MAMBO-2.
ILL-Report.

93PE05T
PENDLEBURY M., BOERNER H. Colloquium in memory of Walter Mampe. Grenoble (ILL), France, January 29,1993.
ILL-Report.

93GE06T
GELTENBORT P. Workshop on Progress in Gaseous Microstrip Proportional Chambers. Grenoble (France), June 21-23 1993.
ILL-Report.

93JA07T
JANOT C. Réunion annuelle du Groupe Français d'Etude des Quasicristaux. Grenoble (France), 2-4 Juin 1993. (Livre de résumés 1- 2)
ILL-Report.

93JA08T
JANOT C. Conférence Quasicristaux. Commande de travaux sur mémoire MS/SC n°92-1552/A000/DRET/DS/SR. Fiche de synthèse, Ministère de la Défense - Direction des Recherches Etudes et Techniques.
ILL-Report.

93FA09T
FAUST H., AGERON P., FOGELBERG B., JACOBSON L., PINSTON J.A., BENABED A., LIATARD E., PIAFE COLLABORATION. Principles on the implantation of a thermal ion source in the H9 beam tube of the ILL. Progress report.
ILL-Report.

Papers published in Scientific periodicals, Books and Conference Proceedings:

1. With ILL authors & Co-authors (Code number 101 to 400).

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FERNANDEZ-DIAZ M.T., MARTINEZ J.L., RODRIGUEZ-CARVAJAL J., BEILLE J., MARTINEZ B., OBRADORS X., ODIER P.
Metamagnetism in single-crystal Pr_2NiO_4.
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Physical Review B 47, 7584-7587 (1993).

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Europhysics Letters 21, 623-628 (1993).

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Surface Science 280, 197-207 (1993).

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Macromolecules 26, 795-804 (1993).

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Finite segments, "free spins" and random exchange in spin S=1 quasi one-dimensional antiferromagnets.
Solid State Communications 85, 597-599 (1993).

93BO112
BOUDARD M., BOISSIEU M. DE, JANOT C., HEGER G., BEELI C., NISSEN H.U., VINCENT H., AUDIER M., DUBOIS J.M. Atomic structure of the Al-Pd-Mn icosahedral phase.
Journal of Non-Crystalline Solids 153-154, 5-9 (1993).

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BOISSIEU M. DE, BOUDARD M., MOUDDEN H., QUILICHINI M., BELLISSENT R., HENNION B., CURRAT R., GOLDMAN A., JANOT C.
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Journal of Non-Crystalline Solids 153-154, 573-577 (1993).

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Zeitschrift fuer Kristallographie 203, 183-197 (1993).

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Author Index

Publications
and ILL-Reports 1993

ABELE H. 93AB171
ACHIBAT T. 93AC398
ADELMANN P. 93RE320
93RE321
ADRIAN M. 93WI342
AEBERSOLD M.A. 93AE388
AEPPLI G. 93AE1021
AGERON P. 93FA09T
AGTERBERG D.F. 93AG303
93AG322
AIBOUT A. 93JO253
AL ULSAT K. 93DO266
ALEGRIA A. 93AR135
ALEXEEV D. 93LA370
ALLAN D.R. 93LO1004
ALLENSPACH P. 93ME154
93ME164
93ME246
93RO203
93ST193
ALONSO J.A. 93MA387
93GA134
93GA309
ALS-NIELSEN J. 93AL310
93LE349
ALVAREZ F. 93AR135
AMADOR U. 93BL364
ANDERSON I.S. 93SC391
93BO248
93LE268
ANDONOV P. 93AN340
93AN369
ANDREJTSCHEFF W. 93PE124
ANNE M. 93BO225
AOUIZERAT-ELARBY A. 93DU158
APFELSTEDT I. 93KO288
ARBE A. 93AR135
ARCHE A.G. 93AR260
ARMBRUSTER P. 93FI199
ARNAUDAS J.I. 93MO142
ASGHAR M. 93AS386
ASMUSSEN B. 93AS123
93PR263
AUDIER M. 93BO112
93ME314
AYACHE C. 93AY251
BAER Y. 93DA368
BALDO CEOLIN M. 93BA120
BALLAUFF M. 93MA196
BALLOU R. 93LE337
93OD336
BALTA CALLEJA F.J. 93AR260
93BA258
BARANOWSKI D. 93BA205
93BA298
BARILO S.N. 93ST289
BARJ M. 93FA400
BARKALOV O.I. 93KO308
BARNES P. 93TU157
BAROCCHI F. 93BA170
93BA186
93BA218
BARON M.H. 93FI334
BARTLETT P. 93BA1013
93BA1017
BARTSCH E. 93BA129
93BA397
93WU206
BASTIDE J. 93BA136
93BA189
93ME1024
BATALLAN F. 93AR260
93BA258
BATESON R.D. 93BA191
BATLLE X. 93BA361
BAUD F. 93BA345
BAUM E.M. 93JU271
BAUMBACH T. 93GA353
BAYERL T. 93PF275
BEAUFILS J.P. 93BE106
BECUCCI M. 93WI330
BEELI C. 93BO112
BEHRENS R.K. 93ZE357
BEILLE J. 93FE101
BEINERT G. 93BA189
BELASH I.T. 93KO308
BELGYA T. 93JU271
BELLISSENT R. 93BO113
93BO312
93DE354
93KU339
BENA I. 93BE187
BENABED A. 93FA09T
BENETTI P. 93BA120
BERGE B. 93RE187
BERMEJO F.J. 93BE219
93BE220
93CH152
93CH217
93MA387
93MO384
BERNHOEFT N. 93BE1001
BERNSTEIN E. 93BE179
BERTAGNOLLI H. 93BA129
BERTHOLD H.J. 93BE119
BERTRAND C. 93LE1007
BEST S. 93BE1022
BISMAYER U. 93HE237
BLAISE A. 93PA145
BLANCHIN M.G. 93BE179
BLANCO J.A. 93GO242
BLAND J.A.C 93BA191
93PA190
BLANK H. 93AE388
93AS123
93BL208
93LA146
93PR263
BLESA M.C. 93BL364
BOBISUT F. 93BA120
BOEHM A. 93LA238
BOEHMER R. 93FE304
BOENI P. 93BO248
BOERNER H.G. 93BO324
93PE05T
93BO166
93BO371
93HA316
93JU102
93KL239
BOERSIG B. 93GO178
BOIREAU A. 93BO278
93BO283
BOISSIEU M. DE 93BO112
93BO113
93BO185
93BO312
93JA232
93JA259
93ME314
BONNET M. 93LA238
BONNETE F. 93BO255
BORDAS S. 93TO204
BORNEMANN H.J. 93RE320
93RE321
BOUCHENEB N. 93AS386
BOUCHERLE J.X. 93BO291
BOUDARD M. 93BO112
93BO113
93BO185
93BO312
93JA232
93ME314
BOUDJADA N. 93BO225
BOUE F. 93BA136
93BA189
93ME1024
BOUILLOT J. 93CR213
93LE1007
BOUKENTER A. 93AC398
BOUQUIERE J.P. 93BO161
93BO347
BOWDEN Z.A. 93MU294
93MU297
BOYSEN H. 93HE237
BRAMWELL S.T. 93AL310
93BR156
93BR174
93BR245
93BR301
93VI244
BRANT S. 93PE124
BRAUNE M. 93FE304
BRENTANO P. V. 93JU102
BRIAT B. 93FA400
BRIQUEU L. 93VA274
BRISSOT R. 93WA162
BROWN P.J. 93BR228
93BR230
93BR290
93KE223
93PA145

BRUECKEL T. 93RE235, 93ST289, 93BR380, 93KO288, 93MA241
BRUSON A. 93PL287, 93HO243
BUCHENAU U. 93HO352, 93BU356, 93KO308
BUCHER B. 93LI395, 93RO203
BUETTNER Helmut 93BA205, 93BA298
BUFFAT P. 93BO248
BUNE A.V. 93BU281
BURGER J.P. 93SC391
BURKHARDT N. 93VA332
BURLET P. 93PA145, 93PL287
BUSCHOW K.H.J. 93IS376, 93LE374
BUSSIERE A. 93BU300
BUTERA R. 93RI107
BUYERS W.J.L. 93WA299
BUZIER M. 93BA136, 93BA189, 93ME1024

CABANE B. 93DU1002
CAIGNAERT V. 93LO1004
CAMPBELL C.E. 93CL344
CANDAU S. 93CH350
CANNON R.D. 93JA207
CAPELLMANN H. 93SC150
CARLILE C.J. 93FI317, 93LA146, 93PR263
CASTEN R.F. 93JU102
CAVATORTA F. 93DE222
CELINSKI Z. 93BA191
CENDRIN F. 93CE394
CHABRE Y. 93RI257
CHAHID A. 93BE219, 93BE220, 93CH152, 93CH217
CHAN K.C. 93KA307
CHARVOLIN J. 93CH341, 93CH350
CHATTOPADHYAY T. 93CH256, 93SC128, 93ST289
CHEONG S.W. 93AE1021
CHEVRIER J. 93CH200
CHIEUX P. 93AN340, 93AN369, 93BA129, 93BA170, 93BA186, 93BA218, 93CH381, 93DU158, 93HO192
CHISHTI A.A. 93KA307
CHRISTENSEN A.N. 93CH346
CHROBOCZEK J. 93CE394
CLAPPERTON R.M. 93CL1018
CLARKE S.J. 93CL226
CLAUSEN K.N. 93AE1021
CLAVAGUERA N. 93TO204
CLAVAGUERA-MORA M.T. 93TO204
CLEMENTS B.E. 93CL116, 93CL343, 93CL344, 93SA359
COCKCROFT J.K. 93LU1012, 93SC118, 93WI250, 93CL226, 93FI117, 93VO144
CODDENS G. 93KE282
COHEN-ADDAD C. 93BA345
COLES B.R. 93KE223
COLMENERO J. 93AR135
CONVERT P. 93ZA198
COOK J.C. 93CO01G
COQUET E. 93CR213
CORBETT J.D. 93CO335
COULOMB J.P. 93LL234
COWLAM N. 93ZA198
CRETTEZ J.M. 93CR213
CRIADO A. 93BE219, 93CH217
CUBITT R. 93PA1020
CULLEN J. 93MO142
CURRAT R. 93AY251, 93BO113, 93BO312, 93CU252, 93LO183
CUTRONI M. 93NE167
CYROT-LACKMANN F. 93KL114
D'ASSEZA G. 93KR392
D'HONDT P. 93WA162
DARDEL B. 93DA368
DAVID A. 93BA129
DAY P. 93DA141
DE KRUIF C.G. 93WO331
DELAPLANE R.G. 93KE147
DELEZE M. 93DE315
DELFS C.D. 93DA141
DELMAS C. 93BO283
DEN BROEDER F.J.A. 93PA190
DEPORTES J. 93IS376, 93LE337, 93OD336
DERIU A. 93DE222
DESCOTES L. 93DE354
DESMOULINS C. 93TO363
DEVILLE A. 93ST289
DI COLA D. 93DE222
DIANOUX A.J. 93BU356, 93DE354, 93DE355, 93DI284, 93DI325, 93DU158, 93FE231, 93GU375, 93NE167, 93SA122
DIPRETE P. 93JU271
DJURADO D. 93SA122
DOENNI A. 93DO109, 93KR240
DOERFFEL M. 93FE304
DONG C. 93JA232
DORE J.C. 93ST197
DORNER B. 93DO295, 93PL287, 93SC215, 93SC319, 93ST214
DOSCH H. 93DO266
DREXEL W. 93DO266
DRISSI S. 93DE315
DRUYTS S. 93DR172
DUBBERS D. 93AB171
DUBOIS J.M. 93BO112, 93JA232, 93MA202
DUBOIS M. 93DU1002
DUERING I. 93MO333
DUPUY J. 93DU158
DURAND M. 93JA232
DUVAL E. 93AC398
EASTOE J. 93ST197
EBEL C. 93BO255
ECKERT J. 93CO335, 93EC1005
EGIDY T.VON 93PE124, 93KL239
EISENBERG H. 93BO255, 93CE394
EL BAGHDADI A. 93GU375
ELSENHANS O. 93BO248
ENCISO E. 93CH152
ENDOH Y. 93KR240
EPSTEIN J.L. 93CL343
ESPESO J.I. 93GO242
ESSER A. 93ES393
ETCHEBEST C. 93FE163
EWEN B. 93EW137, 93RI107, 93RI138
EZQUERRA T.A. 93BA258
FAGAN A. 93TO363
FAK B. 93MO384, 93SC385
FANJAT N. 93FA108, 93FA400

FARAGO B. 93EW137
93FA221
93RI107
93RI138
93RI377
93ZO399
FAUST H.R. 93FA09T
93GO178
93FI199
93HE318
FEHST I. 93FE304
FERNANDEZ-DIAZ M.T 93FE365
93FE101
93FE326
93GA327
FERRAND M. 93DE355
93FE163
93FE231
FETTERS L.J. 93FA221
93RI107
93RI138
93RI377
FIGGIS B.N. 93DA141
FIGLARZ M. 93BO225
93SE272
FILHOL A. 93MA267
FILLAUX F. 93FI317
93FI334
93KE282
FILLION G. 93ST289
FINNEMORE D.K. 93SC128
FINNEY J.L. 93BO161
93BO347
FIONI G. 93FI199
93HE318
FISCHER E.W. 93MA196
FISCHER J.E. 93SA122
FISCHER K. 93KO288
FISCHER P. 93DO109
93FI133
93KR240
93RO203
FISK Z. 93AE1021
FITCH A.N. 93CL226
93FI117
93VO144
93WI250
FLEGER H.W. 93LA146
FOGELBERG B. 93FA09T
FONTAINE J.P. 93FI334
FORD G.W. 93BA191
93FO195
FORGAN E.M. 93PA1020
FORSYTH J.B. 93BE1022
93BR230
FORSYTH V.T. 93FO121
93FO366
93LA103
93LA370
FOURCAUDOT G. 93KL114
FREEDMAN S.J. 93KA307
FREY F. 93PR209
FRICK B. 93AC398
93AR135
93AR260
93BA258
93FR311
93FR396
93JA259
93KO308
93LI395
93ZO399
FRIDKIN V.M. 93BU281
FRIEDLI H.P. 93BO248
FRUCHART D. 93IS376
93LE374
93TO363
FUESS H. 93HO125
93LA238
93MI210
FUJARA F. 93WU206
93BA397
FULLER W. 93FO121
93FO366
93LA103
93LA370
FURRER A. 93AE388
93DO109
93ME154
93ME164
93ME246
93RO203
93ST193
93WI348
GABRIEL A. 93GA353
GAILHANOU M. 93ST289
GAILLARD B. 93GA261
GALERA GOMEZ P. 93GA262
93LE337
GALERA R.M. 93AC398
GARCIA N. 93BE219
GARCIA-HERNANDEZ M. 93BE220
93CH152
93CH217
93MA387
93MO384
GARCIA-MATRES E. 93FE326
93GA110
93GA134
93GA309
93GA327
GARCIA-MUNOZ J.L. 93FE326
93GA327
GARRETT J.D. 93WA299
GAST A.P. 93FA221
GAY J.M. 93PA190
GEHRING P.M. 93MO142
GEIBEL C. 93KR240
GEIL B. 93BA397
GELTENBORT P. 93AS386
93DR172
93GE06T
93GE280
93GO178
93MO333
GEORGII R. 93KL239
GEYER A. DE 93GA261
93GE358
93PE360
GIAMARCHI T. 93GI211
GIBIN D. 93BA120
GILBERT R.G. 93MI1016
GINRAS M.J.P. 93BR301
GIRARD B. 93ME1024
GLAESER W. 93LI296
93WI1008
GODFRIN H. 93GO236
GOEMANS P. 93VA274
GOENNENWEIN F. 93FI199
93GO178
93HE318
93MO333
GOLDMAN A. 93BO113
93BO312
GOLDMANN M. 93RE187
GOLOSOVSKY I. 93PL287
GOMEZ-SAL J.C. 93GO242
GOMPF F. 93RE320
93RE321
GONZALEZ ARCHE A. 93BA258
GRAVEREAU P. 93BO278
GREENBERG J.S. 93KA307
GRILLET Y. 93LL234
GRIMMER H. 93BO248
GRINTER R. 93JA207
GRIONI M. 93DA368
GRIVOT P. 93BU300
GROSS M. 93FI199
93HE318
GRUEBEL G. 93LE349
GUCKELSBERGER K. 93SC385
GUEDEL H.U. 93AE388
GUETHOFF F. 93GU182
GUGLIELMI A. 93BA120
GUILLAUME F. 93GU375
GUKASOV A. 93PL287
GULIK-KRZYWICKI T. 93DU1002
GUYOT P. 93ME314
HARDER A. 93HA184
93HA316
HARRISON D.H. 93HA149
HARTMANN R.A. 93TE383
HAUERT R. 93BO248
HAUSER A. 93AE388
HAUSSUEHL S. 93FE304
HAYASHI S. 93HO173
HAYDEN S.M. 93AE1021
93DO109
HAZELL R.G. 93NO346
HEGER G. 93BO112
HEID C. 93KN382
HEID R. 93RE320
93RE321
HEIDEMANN A. 93HO173
HEIMING A. 93GU182
93RE321

HEINRICH B. 93BA191
HELLMANN E.H. 93HE139
HELLMANN G.P. 93HE139
HELM G. 93AB171
HENNION B. 93AY251
93BO113
93BO312
93CU252
93GU182
93LO183
93SH351
HENRY J.Y. 93BO291
HENSEL F. 93WI1008
93WI1019
HENSLER J. 93HE237
HERZIG C. 93GU182
93PE254
93TR169
HESSE M. 93FI199
93HE318
HEWAT A.W. 93FI133
HIGHMORE R.J. 93ZA198
HILFRICH K. 93HI151
93HI306
HOCK R. 93HO125
93LA238
HOFFMANN H. 93PI131
HOFMANN S. 93PI131
HOHLWEG G. 93HO373
HOLDSWORTH P.C.W. 93BR156
93BR245
93BR301
HOLZER B. 93HO373
HOPPE U. 93HO192
HORSEWILL A.J. 93HO173
93JO253
HOUSSAINI S. 93HO243
93HO352
93VE104
HUANG J.S. 93FA221
93RI107
93RI138
93RI377
HUENECKE J. 93VO273
HULLIGER F. 93DO109
HUTCHINGS M.T. 93AL310
HUTTON S.L. 93FE304
HYUN O.B. 93SC128
IBARRA M.R. 93RI155
IBBERSON R.M. 93RI155
IBEL K. 93ST197
ILEGEMS M. 93GA353
INGRAM B.T. 93CL1018
ISNARD O. 93IS376
93LE374
93TO363
JACOBS T.H. 93LE374
JACOBSON L. 93FA09T
JAL J.F. 93DU158
JANOT C. 93BO112
93BO113
93BO185
93BO312
93JA07T
93JA08T
93JA194
93JA232
93JA233
93JA259
93JA313
93ME314
JANSSEN E. 93PA190
JAYASOORIYA U.A. 93CO335
93JA207
JEANDEY C. 93OD336
JEITSCHKO W. 93RE235
93ZE357
JERICHA E. 93TE168
JEROME D. 93DA368
JILEK E. 93FI133
93RO203
JOHNSON E.L. 93JU271
JOHNSON M.R. 93JO253
JOHNSON M.T. 93PA190
JOLIE J. 93BO166
93BO324
93BO371
93JU102
93KL239
JONES S.L. 93TU157
JOVEN E. 93MO142
JUDGE S. 93DE315
93KL239
JUENEMANN R. 93VA332
JUNGCLAUS A. 93BO371
93HA316
93JU102
93JU271
KAHN R. 93AE388
KALDIS E. 93FI133
93LO1004
93RO203
KALOSKAMIS N.I. 93KA307
KALUS J. 93PI131
KANIA U. 93AB171
KAPPLER C. 93KA302
KARPINSKI J. 93FI133
93LO1004
93RO203
KAUFMANN J. 93MO333
KEARLEY G.J. 93BL208
93CO335
93FI317
93FI334
93JA207
93KE224
93KE282
KEEN D.A. 93PR209
KELLER F. 93VA274
KELLERSOHN T. 93KE147
KENCONO A.W. 93PI131
KENNEDY S.J. 93KE223
KERN J. 93DE315
KHITROV V.A. 93KL239
KIEBEL M. 93BA397
93WU206
KILPATRICK J.M. 93PE1010
KIMURA S. 93AN340
93AN369
KITA K. 93KR240
KLAUMUENZER S. 93KL372
KLEIN T. 93KL114
KLORA J. 93KL239
KNELL U. 93KN265
93KN382
KNELLER G.R. 93DI284
KNOEZINGER E. 93LA146
KOEBLER U. 93KO288
KOELKER W. 93HI151
KOENIG S. 93PF275
KOLESNIKOV A.I. 93KO308
KOMATSUBARA T. 93KR240
KOSSAKOWSKI R. 93BU300
KRAUSE D. 93BU356
KRIMMEL A. 93KR240
KROTSCHECK E. 93CL116
93CL343
93CL344
93SA359
KRUEGER J.K. 93KR392
KRUSCHE B. 93KL239
KUBAS J. 93EC1005
KUGLER J. 93MA196
KUGLER S. 93KU339
KUHS W.F. 93MC175
KULDA J. 93HO125
KUSMARTSEV F.V. 93SA359
LAMPARTER P. 93NU1006
LANDER G.H. 93MA241
93PA145
93LA1023
93LA1025
LANGAN P. 93FO121
93FO366
93LA103
93LA370
LANGEL W. 93LA146
93PR263
LARTIGUE C. 93BA136
93BA189
93LI264
LASJAUNIAS J.C. 93CH200
93KO308
LAST J. 93AB171
93KA307
LAUGIER J. 93MA267
LAUTENSCHLAEGER G. 93LA238
LAUTER H.J. 93LL234
93BA191
93CL116
93KN265
93KN382
93LA146
93PA190
LE CAER G. 93LE374
LE FLEM G. 93BO278

	93BO283
LE ROY J.	93CR213
	93LE1007
LEE S.L.	93PA1020
LEGRAND J.F.	93BU281
	93DU158
	93KR392
	93LE349
	93LE390
	93PF275
	93RE187
LEHMANN M.S.	93BA345
	93BO161
	93BO347
	93LE188
	93LE349
	93NO346
	93WI348
LEIFER K.	93BO248
LEISURE R.G.	93LE268
LELIEVRE-BERNA E.	93LE337
LEROUX B.	93AS386
LEVY F.	93CU252
	93LO183
LI J.C.	93LI264
LIATARD E.	93FA09T
LIAUD P.	93BU300
LIBMAN V.A.	93KL239
LIEB K.P.	93HA184
	93HA316
	93JU102
LIED A.	93DO266
LINDER K.	93LI395
LINDGARD P.A.	93LI323
LINDLEY P.F.	93BO161
LINDNER H.	93KL239
LINDNER P.	93BA136
	93MA196
	93PI131
	93RA389
LISS K.D.	93LI296
LISTER C.J.	93KA307
LITVINSKY L.L.	93KL239
LLEWELLYN P.L.	93LL234
LOEHNEYSEN H.V.	93KO288
	93ST126
LOEWENHAUPT M.	93ST126
LOIDL A.	93FE304
	93KR240
LOPAC V.	93PE124
LOPEZ CABARCOS E.	93AR260
	93BA258
	93GA261
	93GA262
LORENZO J.E.	93LO183
LORENZO-DIAZ J.E.	93CU252
LOVEDAY J.S.	93LO1004
LUCAZEAU G.	93FA108
	93FA400
LUTZ H.D.	93LU1012
	93SC118
MACDIARMID A.G.	93SA122
MAERTEN H.	93MO333
MAERZ K.	93MA196
MAGERL A.	93HO125
	93JA259
	93LI296
MAGLI R.	93BA170
	93BA186
	93BA218
MAHENDRASINGAM A.	93FO121
	93FO366
	93LA103
	93LA370
MALAMAN B.	93LE374
MALTERRE D.	93DA368
MALUGANI J.P.	93RO159
	93RO160
MANGIN P.	93HO352
	93VE104
MARCHAL G.	93HO243
	93HO352
	93VE104
MARET M.	93MA202
MARMEGGI J.C.	93MA241
	93MA267
MARSHALL W.G.	93MU297
MARTI U.	93GA353
MARTIN-MARERO D.	93BE220
	93MO384
MARTINEZ B.	93FE101
MARTINEZ J.L.	93BE219
	93BE220
	93CH152
	93CH217
	93EW181
	93FE101
	93FE326
	93FE365
	93GA110
	93GA134
	93GA309
	93GA327
	93MA387
	93MO384
MASCHKE U.	93EW137
MASON S.A.	93FO121
	93FO366
	93LA103
	93LA370
MASON T.E.	93AE1021
MATTIOLI F.	93BA120
MAY R.P.	93HA149
	93VA332
	93WO331
MAYERHOFER U.	93KL239
	93MA03T
	93PE124
MCDONALD I.	93ST197
MCEWEN K.A.	93EW181
MCGRATH C.A.	93JU271
MCGREEVY R.L.	93NI338
MCINTYRE G.J.	93AL310
	93FE304
	93KE147
	93MC305
	93OL140
	93PT148
MCMAHON M.I.	93MC175
	93NE1003
	93LO1004
MEDARDE M.	93BA361
	93FE326
	93GA327
MEDKOUR G.	93AS386
MENDES E.	93BA136
	93BA189
	93ME1024
MENENDEZ N.	93BL364
MENGUY N.	93ME314
MENOVSKY A.A.	93WA299
MENTZEN B.F.	93SA1009
MERCIER R.	93RO159
	93RO160
MESOT J.	93ME154
	93ME164
	93ME246
	93RO203
	93ST193
MEVARECH M.	93CE394
MEYERS S.	93KR392
MEZZETTO M.	93BA120
MICHAELSEN S.	93HA184
	93HA316
MIDDENDORF H.D.	93DE222
MIEHE G.	93MI210
MIGLIORI A.	93LE268
MILLS M.F.	93MI1016
MIRAGLIA S.	93IS376
	93TO363
MISBAH C.	93BE187
MOELLER A.	93MO333
MOELLER M.H.	93RE235
MOLINIE P.	93AY251
	93MU105
	93MU111
MOMPEAN F.J.	93BE219
	93BE220
	93MA387
	93MO384
MONCEAU P.	93CU252
	93LO183
MONKENBUSCH M.	93FA221
MOOK H.A.	93AE1021
	93PA1020
MOORE P.B.	93HA149
MORAL A. DEL	93MO142
MORAN E.	93BL364
MORKEL C.	93WI1008
MORON M.C.	93MO247
	93MO362
MOUDDEN H.	93BO113
MUELLER H.H.	93LE188
MUELLER U.	93MI210
MUENZENBERG G.	93FI199
MURANI A.P.	93MU294

	93MU297
MURSIC Z.	93HO125
MURZIN A.V.	93KL239
MUTKA H.	93ME154
	93ME164
	93ME246
	93MU105
	93MU111
	93MU212
	93RO203
	93ST193
MUTTERER M.	93GO178
NAPPER D.H.	93MI1016
NARZ T.	93FE304
NAST-LINKE U.	93GO178
NE F.	93WI348
NEDER R.B.	93PR209
NEEDHAM L.M.	93NE167
	93NE229
NELMES R.J.	93LO1004
	93MC175
	93NE1003
NEMBACH E.	93HI151
	93HI306
NESVIZHEVSKY V.V.	93NE04T
NEUMAIER S.	93GO178
NIELD V.M.	93NI338
NIELSEN M.	93NO346
NIERHAUS K.H.	93VA332
NINA M.	93FE163
NISSEN H.U.	93BO112
NOELDEKE C.	93RI286
	93RI367
NORMAN C.J.	93TU157
NOZIERES P.	93GI211
	93NO132
NUDING M.	93NU1006
NUECKER N.	93BU356
NUETZEL K.	93SC215
O'CONNELL R.F.	93FO195
OBRADORS X.	93BA361
	93FE101
ODANI S.	93BA345
ODDOU J.L.	93OD336
ODIER P.	93FE101
OED A.	93GE280
	93MO333
OESER R.	93BA136
	93BA189
OLAZCUAGA R.	93BO278
	93BO283
OLIVER R.A.	93VA274
OLOVSSON I.	93KE147
	93OL140
	93PT148
OSBORN R.	93ME164
	93MU294
	93MU297
OTSUKA T.	93DE315
OTTEWILL R.H.	93BA1013
	93BA1017
	93CL1018
	93MI1016
	93OT1014
	93OT1015
OULADDIAF B.	93LE337
	93OD336
PAALME T.	93VA332
PAAR V.	93PE124
PAASCH M.	93FE304
PACCARD D.	93LE1007
PACCARD L.	93LE1007
PAIXAO J.A.	93PA145
PALACIO F.	93MO247
	93MO362
PANNETIER J.	93CR213
	93PA269
	93RI257
	93SE272
PAPOULAR R.J.	93PA02T
	93BO291
PARES G.	93KL114
PASYUK V.V.	93PA190
PATARIN J.	93LL234
PAUL D.MCK	93PA1020
PAULSEN C.	93BR380
PAULUS W.	93PA165
PAYEN C.	93MU105
	93MU111
PAYER A.	93PA165
PEBAY-PEYROULA E.	93BA345
PEISL J.	93DO266
PENDLEBURY J.M.	93PE293
	93BO324
	93PE05T
PENFOLD J.	93BO248
PEREZ-VILLAR V.	93PE360
PERKINS S.J.	93PE1010
	93PE1011
PERNET M.	93BA361
PERRING T.G.	93AE1021
PETKOV P.	93PE124
PETRENKO A.V.	93PA190
PETROV G.	93MO333
PETRY W.	93BA397
	93DE355
	93FE231
	93GU182
	93HI151
	93HO373
	93KL372
	93PE254
	93TR169
	93VO273
	93WU206
PFEIFFER W.	93PF275
PFEUTY P.	93DE354
PFITZNER A.	93LU1012
PIAFE COLLABORATION	93FA09T
PICOT C.	93ME1024
PIGRAM W.J.	93LA103
PILGRIM C.	93WI1008
	93WI1019
PILSL H.	93PI131
PILTZ R.O.	93MC175
	93NE1003
PINSTON J.A.	93FA09T
PLAKHTY V.	93PL287
POETTGEN R.	93ZE357
POINSIGNON C.	93RI257
POMME S.	93DR172
PONYATOVSKY E.G.	93KO308
PRAGER M.	93AS123
	93LA146
	93PR263
PRANDL W.	93BR380
PRECHTL M.	93KR392
PRESS W.	93AS123
	93RI286
	93RI367
PREVEL B.	93DU158
PROFFEN T.	93PR209
PTASIEWICZ-BAK H.	93OL140
	93PT148
PUGLIERIN G.	93BA120
PUSZTAI L.	93KU339
QUE W.	93AG303
	93WA299
QUILICHINI M.	93BO113
	93BO312
RAMSAY J.D.F.	93RA389
RANDL O.G.	93VO273
RAVEAU B.	93LO1004
RAVELLE-CHAPUIS R.	93BE179
REATTO L.	93BA170
	93BA186
REEHUIS M.	93RE235
	93ZE357
REICHARDT W.	93RE321
REICHERT H.	93LL234
REINHART F.K.	93GA353
RENAULT A.	93RE187
RENKER B.	93RE320
	93RE321
RENNIE A.R.	93CL1018
	93HE139
	93MI1016
RESSOUCHE E.	93PA02T
REYNOLDS P.A.	93DA141
RICHTER D.	93EW137
	93FA221
	93FR311
	93FR396
	93PF275
	93RI107
	93RI138
	93RI377
	93ZO399
RIETSCHEL H.	93RE321
RIKOVSKA J.	93DE315
RIPERT M.	93RI257
RISTIG M.	93MO384
	93BE220
RITTER C.	93MO142
	93PA165
	93RI155

	93RI286
	93RI367
	93TU157
ROBINSON B.H.	93ST197
ROBINSON S.J.	93KL239
	93PE124
RODRIGUEZ FERNANDEZ J.	93GO242
RODRIGUEZ-CARVAJAL J.	93BA361
	93BE179
	93BL364
	93BO225
	93FE101
	93GO242
	93FE326
	93FE365
	93GA110
	93GA134
	93GA309
	93GA327
	93MO247
	93MO362
	93RO292
ROESSLI B.	93KR240
	93RO203
ROSENBERG H.M.	93NE167
ROSS D.K.	93LI264
ROSSAT-MIGNOD J.	93BO291
ROSTA L.	93KU339
ROTH G.	93RE321
ROUQUEROL J.	93LL234
ROUSSELOT C.	93RO159
	93RO160
ROUX B.	93FE163
ROUX D.	93CH350
RUBEN A.	93MO333
RUCKENSTEIN A.E.	93GI211
RUEHL M.	93VA332
RUSH J.J.	93KN265
	93KN382
RUSIECKI S.	93FI133
RYTZ D.	93AE1021
SAARELA M.	93CL343
	93SA359
SACERDOTE-PERONNET M.	93SA1009
SACKMANN E.	93PF275
SAEZ-PUCHE R.	93GA110
	93GA134
	93GA309
SAINTIGNON P. DE	93BU300
SAITO Y.	93SA180
	93UW177
	93UW279
SALAMON M.B.	93MO142
SALAS A.G.	93VA274
SALINAS-SANCHEZ A.	93GA110
	93GA134
	93GA309
SANTA CRUZ C.	93BA258
SATO N.	93KR240
SAUVAJOL J.L.	93DI284
	93SA122
SAVAGE H.F.J.	93BO161
SCHAERPF O.	93FA400
	93HI151
	93HI306
	93SC128
	93SC150
SCHEER E.	93KO288
SCHERM R.	93SC385
SCHERR E.M.	93SA122
SCHLAPBACH L.	93SC391
SCHLICHENMAIER R.	93SC127
SCHMAHL W.W.	93VO153
SCHMID B.	93LI323
SCHMIDT C.	93AB171
SCHMITT D.	93LE1007
SCHNAUSS W.	93BA397
SCHNEIDER M.	93SC118
SCHOBER H.	93RE320
	93RE321
	93SC215
	93SC216
	93SC319
	93KO308
SCHOELLHORN R.	93PA165
	93RI286
	93RI367
SCHOPOHL N.	93SC277
SCHRECKENBACH K.	93BU300
SCHROEDER A.	93ST126
SCHUMACHER G.	93KL372
SCHWARZ R.B.	93LE268
SCHWEDA E.	93SC127
SCHWEIZER J.	93BO291
SCONZA A.	93BA120
SEGUIN L.	93SE272
SEKI S.	93SA180
SENGER G.	93BE220
	93MO384
SERUGHETTI J.	93AC398
SEVERING A.	93ST126
SHAPIRO S.M.	93SH351
SILLESCU H.	93BA129
	93BA397
	93WU206
SILVA P.C.	93GA353
SIM R.B.	93PE1010
	93PE1011
SLEIGHT A.W.	93PA269
SMIRNOV O.	93PL287
SMITH J.A.	93CL344
SMITH J.C.	93DI284
	93FE163
SMITH K.F.	93PE1010
	93PE1011
SOECHTIG J.	93BO248
SOMEKH R.E.	93ZA198
SOUBEYROUX J.L.	93BO278
	93BO283
	93IS376
	93LE1007
	93LE374
	93TO363
STACHEL D.	93HO192
STASSIS C.	93GU182
STAUB U.	93ME154
	93ME164
	93ME246
	93RO203
	93ST193
STEEB S.	93NU1006
STEGE U.	93RI286
STEGLICH F.	93KR240
STEIGENBERGER U.	93EW181
STEPANOV A.A.	93ST289
STEYTLER D.C.	93ST197
STIRLING W.G.	93PA145
STRAEHLE J.	93SC127
STRAUCH D.	93SC215
	93SC216
	93SC319
	93ST214
STRIDE J.A.	93JA207
STROBL G.	93HO373
STROKA B.	93ST126
STUEHN B.	93HO373
STUHRMANN H.B.	93LE188
SUCK J.B.	93CH200
	93KL114
	93SU115
	93SU201
	93SU378
SUKHOVOJ A.M.	93KL239
SUZUKI T.	93DO109
SVARE I.	93LE268
SVENSSON E.C.	93SH351
SZPRYNGER A.	93SC385
TACHEZ M.	93RO159
	93RO160
TANG C.C.	93PA145
TARLING S.E.	93TU157
TASSET F.	93BO291
	93BR230
	93DA141
	93PA02T
TAU M.	93BA170
	93BA186
TAYLOR A.D.	93ME164
	93AE1021
	93MU294
	93MU297
	93NE229
TEN HAKEN B.	93TE383
TEN KATE H.H.J.	93TE383
TERBURG B.P.	93TE168
TERCIER P.A.	93DE315
TERECH P.	93TE276
THEOBALD J.P.	93GO178
THIELENS N.M.	93ES393
TIMMINS P.A.	93WI342
TOMEY E.	93TO363
TOMKINSON J.	93FI334
	93KE282
TORGESON D.R.	93LE268
TORNERO J.D.	93BL364
TORRELLES X.	93TO204

TRAMPENAU J. 93GU182
93PE254
93TR169
TRANQUI D. 93PA269
TRAPPMANN T. 93ST126
TRAUTVETTER H.P. 93DR172
TREGENNA-PIGGOTT P.L. 93BE1022
TREVINO S. 93FR396
TRIEB H. 93KL239
TROUNOV V. 93FI133
TROUW F. 93KE224
TUN Z. 93WA299
TURRILLAS X. 93TU157
UDOVIC T.J. 93KN265
93KN382
UIMIN G. 93BO291
ULBIG S. 93BO371
93JU102
ULBRICHT W. 93PI131
URBAN G. 93MA196
UWAHA M. 93SA180
93UW176
93UW177
93UW279
VALANCE A. 93BE187
VALLET-REGI M. 93BA361
VAN DE KLUNDERT L.J.M. 93TE383
VAN DER ENDE P. 93NI338
VANATALU K. 93VA332
VARMA C.M. 93GI211
VATIN-PERIGNON N. 93VA274
VAZQUEZ-IGLESIAS M.E. 93PE360
VERGNAT M. 93HO243
93HO352
93VE104
VERKERK P. 93NI338
93TE168
VERKHOVSKAYA K.A. 93BU281
VETTIER C. 93HO243
93HO352
93SH351
93VE104
VILLANI M. 93JU271
VILU R. 93VA332
VINCENT H. 93BO112
93JA232
VISENTIN L. 93BA120
VISSER D. 93AL310
93VI244
VITEBSKY I.M. 93ST289
VOGL G. 93VO273
VOGT O. 93PA145
VOGT T. 93BE119
93HE237
93HO125
93LA238
93MI210
93SC127
93VO144
93VO153
VOIT J. 93BA205
93BA298
93DA368
93VO130
93VO227
93VO285
VOLANAKIS J.E. 93PE1010
VOMHOF T. 93RE235
VONHOLDT E. 93BE119
VORLET J.P. 93DE315
WADZACK J. 93VA332
WAGEMANS C. 93DR172
93WA162
WALKER M.B. 93AG303
93AG322
93KA302
93WA299
WARTCHOW R. 93BE119
WASEDA Y. 93AN369
WAXMAN D. 93SC277
WEBER H.W. 93SC128
WEGENER W. 93KE282
WEIBEL P. 93DA368
WEISS L. 93BR380
WEITZEL H. 93LA238
WHITE R.P. 93CO335
93JA207
WILKINSON C. 93WI348
WILLIAMS A.P. 93HA184
93DE315
93HA316
WILLIAMS J.H. 93BR174
93WI143
93WI249
93WI250
93JO253
93WI328
93WI330
WILLIAMS W.G. 93NE229
WILLNER L. 93RI377
WINTER R. 93WI1008
93WI1019
WIPF H. 93KN265
93KN382
WITTMANN J.C. 93KR392
WITZ J. 93WI342
WOLANSKI M. 93KA307
WOSNITZA J. 93KO288
WOUTERSEN A.T.J.M. 93WO331
WRIGHT N.G. 93MC175
93NE1003
WUTTKE J. 93BA397
93WU206
WYDER P. 93ST289
YATES S.W. 93JU271
YETHIRAJ M. 93PA1020
ZACCAI G. 93BO255
93CE394
93DE355
93ES393
93FE163
93FE231
ZAMFIR N.V. 93JU102
93JU271
ZARBAKHSH A. 93ZA198
ZAWISKY M. 93TE168
ZEMB T. 93WI348
ZEPPENFELD K. 93ZE357
ZEYEN C.M.E. 93PR209
93TE383
ZHANG J. 93CO335
ZHIGUNOV D.I. 93ST289
ZIELINSKI F. 93BA136
93BA189
ZINN W. 93KO288
ZIRKEL A. 93RI377
ZOLLIKER M. 93RO203
ZORN R. 93ZO399

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