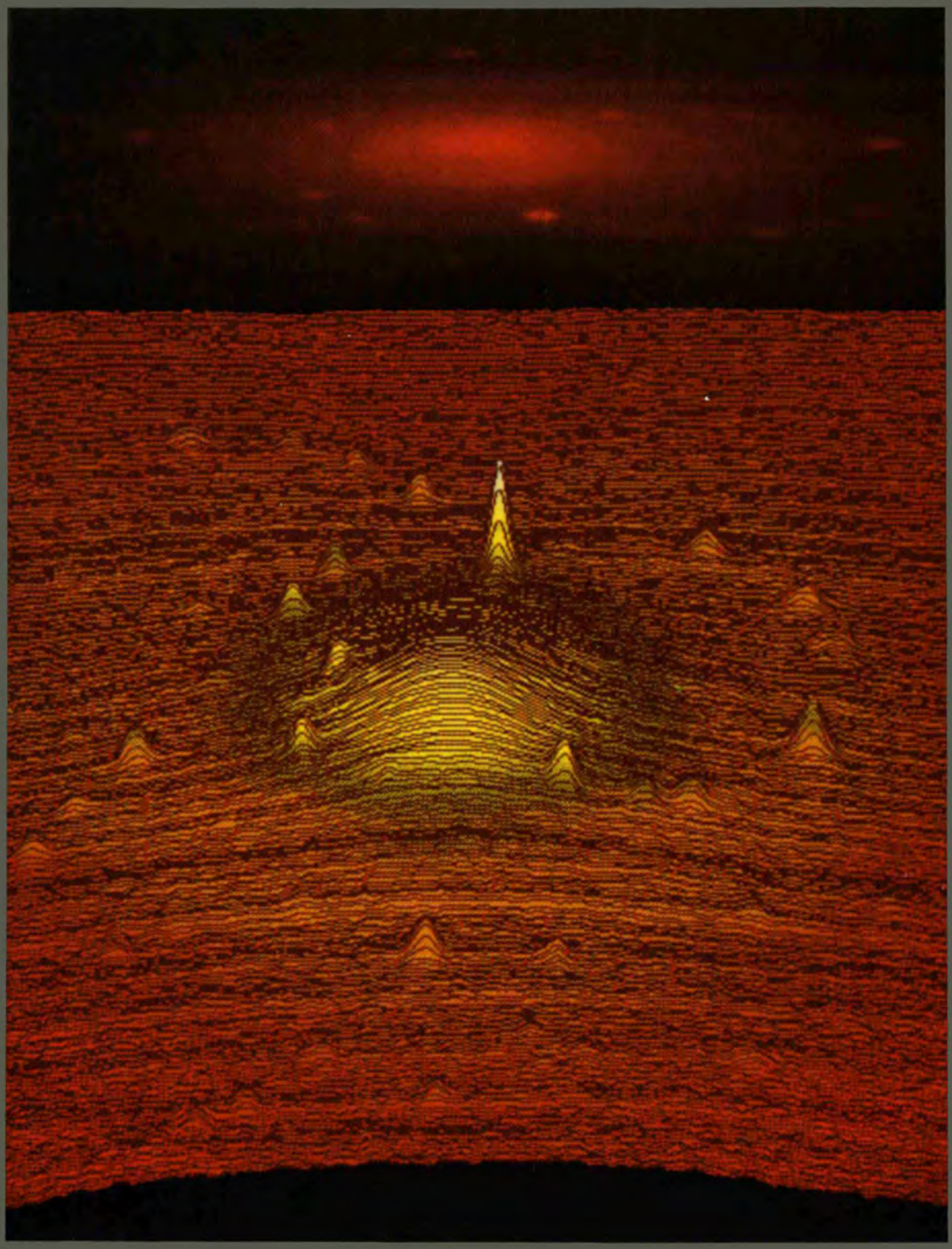

ANNUAL REPORT 1992

institut Max von Laue
Paul Langevin
Grenoble - France

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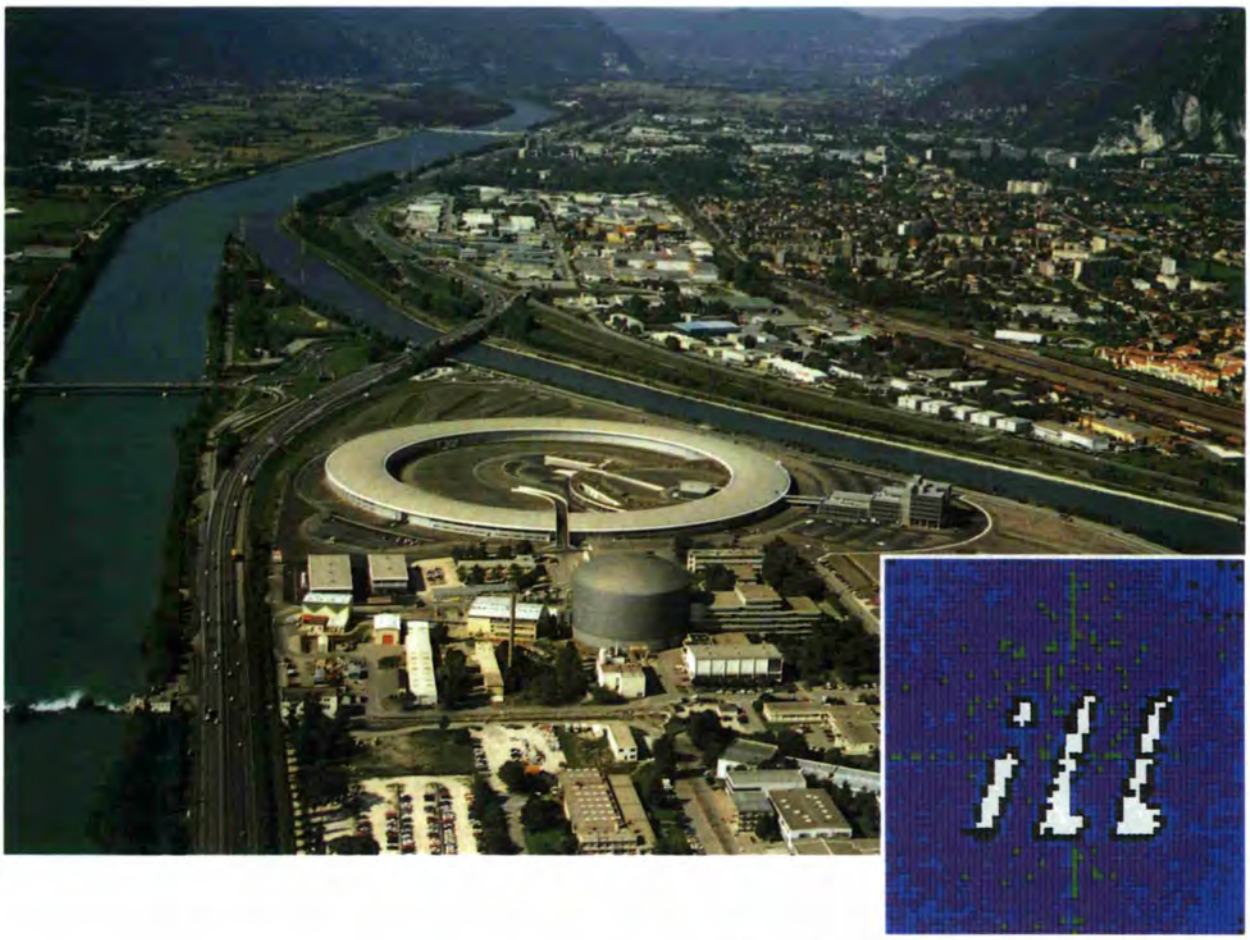


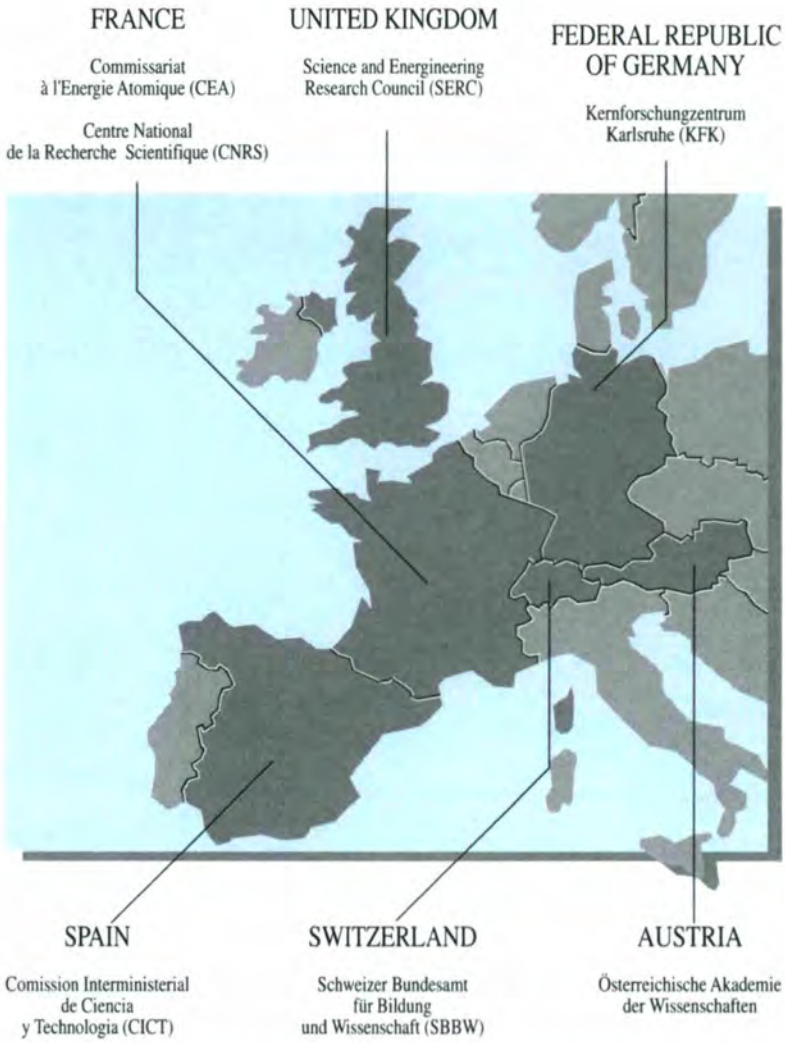
Neutron image taken with a microstrip gas detector, developped first at the ILL. The letters are made of neutron absorbing plastic material. The distance between point and line of the "i" is 2 mm. Since reactor neutrons are presently not available, the detector was irradiated by a collimated Am-Be source. The exposure time was 240 hours at a rate of 4 counts per second.

Front cover:

Laue diagram (shown in landscape mode) of a large crystal of triclinic hen egg-white lysozyme observed with a cold neutron beam (LLB-saclay). The recording device was an X-ray imaging plate equipped with a gadolinium oxide converter screen.

Contents

Associates of the ILL



Countries with scientific membership

Steering Committee
(at its last meeting)

❍ Hansen (BMFT)	❍ Aymar (CEA)	❍ N.N. (SERC)
❍ Klose (KFK)	❍ Bouchard (CEA)	❍ Richards (Univ. Durham)
❍ Schunck (BMFT)	❍ Comès (CNRS)	❍ Voss (RAL)
❍ Steiner (Univ. Mainz)	❍ Sevin (CNRS)	❍ Wilkins (SERC)

Scientific Council

Plenary Session	Subcommittees
30 members	66 members

Status: November 1992

DIRECTORATE:

Director:
J. Charvolin

Co-directors:
P. Schofield, R. Scherm

DIVISION/DEPARTMENTS

REACTOR DIVISION
Head: E. Bauer

- Reactor Operation
- Operation of Sub-assemblies
- Site Security

INSTRUMENT OPERATION DEPARTMENT
Head: A. Heidemann

- Instrument Technicians Service
- Central Service: Support for Experiments
- Advanced Cryogenic Service
- Chemistry and Biology Labs.
- Site and Buildings Maintenance Service

INSTRUMENT AND METHODS DEPARTMENT
Head: J.C. Faudou

- Instruments and Methods
- Construction & Mechanical Maintenance
- Electronics
- Monochromators
- Multi-detectors
- Special Instruments
- Multilayer Laboratory

COMPUTING DEPARTMENT
Head: D. Rimmer

- Automation, Data Acquisition and Treatment
- Scientific Computing (DEC-1091)
- Telephone

ADMINISTRATION DEPARTMENT
Head: H.M. Spilker

- Personnel
- Finance & Purchasing
- Welfare & Staff Training
- Translation Office
- Secretariat of the Steering Committee

DIRECTORATE SERVICES

SCIENTIFIC COORDINATION & PUBLIC RELATIONS OFFICE
Head: B. Maier

- Coordination of the Experimental Programme
- Organisation of Workshops & Conferences
- Public Relations

DELEGUE FOR SAFETY, MEDICAL AND HEALTH PHYSICS GROUP
J.F. Veyrat

SAFETY ENGINEER
H. Sallé

LIBRARY
Head: C. Castets

SCIENTISTS' SECRETARIAT
Head: F. Parisot

SCIENTIFIC SECTORS

COLLEGES
CONVENORS: COLLEGE SECRETARIES

2 Theory
3 Fundamental and Nuclear Physics
4 Structural and Magnetic Excitations
5 Crystal and Magnetic Structures
6 Liquids, Disorder and Defects in Materials
8 Biology
9 Chemistry

PHYSICISTS' REPRESENTATIVES
Scientific Staff

- 66 Expermentalists
- 12 Theoreticians
- 30 Thesis students

INSTRUMENT GROUPS
Heads: Senior Scientists

- Fundamental and Nuclear Physic's Instruments
  Head: M. Pendlebuy
- Three-axis Spectrometers
  Head: B. Dorner
- TOF, High Resolution, SAS, Diffuse Scattering Instruments
  Head: C. Janot, J. Suck
- Diffraction Instruments
  Head: J. Brown

Status of 31/12/1992

The fence between the ILL and the ESRF, erected for the construction of the Synchrotron and the associated premises was removed on 4 May 1992, giving way to a common site for both institutes.

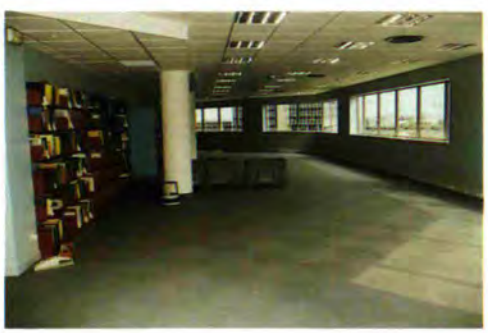
J. Charvolin, ILL Director (centre) pushes the gate open.

The Directors of both institutes are contemplating this important moment: R. Haensel (Director General of the ESRF), third from the left and J. Charvolin (ILL Director), fourth from the left.

The joint ILL-ESRF library was inaugurated in June 1992.

The new building for the joint library.

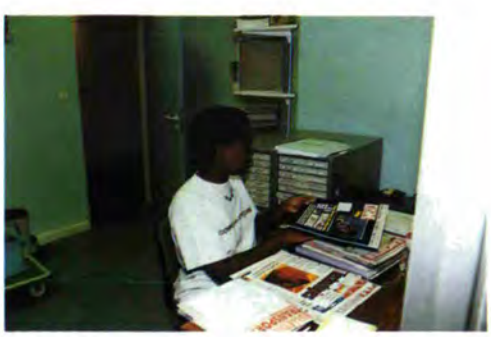
The removal of the books from the old library into the new building.



The hall of the new library prior to the installation of all shelves.

The shelves have got their place and fill the hall.

The readers' corner provides an agreable and wide space.



Danielle Marlin at work in her new office.

On 25 September 1992 Mr. Shozo Shimomura, President of the Japanese Atomic Energy Research Institute (JAERI) visited the ILL.

In the picture (second from left) he was welcomed by J. Charvolin, ILL Director, (second from right) and E. Bauer, Head of the Reactor Division (right).

In the picture, Mr. Shimomura is receiving explanations about the ILL-HFR by E. Bauer.

The Consul General of Germany in Lyon, Herr v. Hengstenberg, (second from right), visited the ILL on 20 October 1992. He and his wife were received by J. Charvolin, ILL Director, H.-M. Spilker (Head of Administration) and P. Armbruster (German Assistant Director (from left to right).

M. Rouvillois, Administrateur Général of the French Atomic Energy Commission CEA was guest of the ILL on 5 November 1992.

In the picture he (on the left) is welcomed by the ILL Director, J. Charvolin. On the right, M. Aude (Bureau des Relations Publiques et de la Communication du CEN-Grenoble).

M. Rouvillois visited the "niveau D" of the HFR. In the picture from left to right : M. Le Roux, Director of CEN-Grenoble, Mme. Antoni (Directrice de la Communication, CEA-Paris), M. Rouvillois, M. Bauer (Head of the ILL Reactor Division) and M. Barthélémy (Adjoint au Directeur, Président du Comité Central des Activités Sociales, CEA-Paris).

A very successful International Workshop on "Methods in the Determination of Partial Structure Factors of Disordered Matter by Neutron and Anomalous X-ray Diffraction" was held at the ILL from 10-11 September 1992. The picture shows the participants in front of the ILL building.

From 5-7 October a Workshop on "Applications of High Resolution Gamma Spectroscopy in Studies of Atomic Collisions and Nuclear Lifetimes" took place at the ILL. The picture shows some of the participants during animated discussions in front of the Chadwick Amphitheatre. In the centre, H. Börner, one of the scientific organizers discussing with P. Armbruster, Deputy Director of the ILL.

A "Journée des Polymères et des Colloïdes" was organized by P. Lindner and E. Geissler on 14 and 15 April 1992.

P. Lindner was the ILL organizer of the "2nd European workshop on neutron X-ray and light scattering as investigative tool for "soft" condensed matter" in Bombannes (France) from 31 May - 6 June 1992.

L'événement majeur de l'année a certainement été la réunion de printemps du Comité de Direction à Cadarache le 21 mai 1992, cette réunion a été décisive pour le futur de l'ILL en affirmant :

– la décision de remettre en état le réacteur suivant le projet proposé par l'Institut, le redémarrage est maintenant envisagé pour la mi-1994 et, le réacteur étant remonté à l'identique, on peut envisager un fonctionnement sans problème pendant vingt ans après cette date,

– le constat de l'accord des trois Gouvernements et des Associés sur le principe d'une prolongation de la Convention entre les trois partenaires pour une période d'au moins dix ans à partir du 1.1.1994 et l'intention d'établir un protocole sur ce point pour présentation aux Gouvernements pour signature.

Les conclusions de cette réunion expriment clairement la volonté des Associés de maintenir l'ILL dans son statut de laboratoire multinational et, en définissant le cadre de son fonctionnement futur, elles lui permettent d'envisager les directions à suivre pour préparer le retour en exploitation après le redémarrage.

Remise en état du réacteur

Le projet de remise en état a été lancé immédiatement après la réunion du Comité de Direction à Cadarache. Cette réaction immédiate a été rendue possible par un important travail préalable de préparation des actions techniques et administratives. On peut résumer l'ensemble du projet en le décomposant en trois actions : le démontage de l'ancien bidon réflecteur et son transfert hors de la piscine, la préparation de cette dernière pour recevoir le nouveau bidon, la fabrication et l'installation de ce nouveau bidon dans la piscine. La première de ces actions a été terminée la dernière semaine de novembre, elle a été entièrement conduite par les équipes de l'ILL dans les coûts et délais prévus et sans le moindre incident. Ce fut un moment très important pour l'Institut qui était juste à mi-chemin du long parcours devant le mener de l'arrêt du réacteur en mars 1991 à son redémarrage vers la mi-1994. L'accomplissement de cette action permet de mettre maintenant l'accent sur les actions concernant le remontage proprement dit et qui sont ressenties de façon nettement plus positive. La seconde action, la préparation de la piscine pour l'installation du nouveau bidon, vient de démarrer, elle est aussi assurée par les équipes de l'Institut. La première étape de la troisième action, la fabrication du nouveau bidon, est bien en cours maintenant, elle a été confiée à un industriel spécialiste des grandes structures en alliage d'aluminium et son suivi est assuré par l'Institut renforcé par un Architecte Industriel, elle se déroule de façon tout à fait satisfaisante.

Les procédures administratives aussi ont été lancées et, l'arrêt du réacteur dépassant deux ans, il sera nécessaire de déposer une demande de décret d'autorisation de remise en service. Les dossiers correspondants, aussi bien techniques qu'administratifs, sont en cours de préparation et les premiers seront bientôt présentés aux autorités compétentes. Ce sont là les démarches prévues en ce domaine et elles se développent normalement.

Pour conclure ce paragraphe, j'insisterai sur le fait que les coûts et délais des actions techniques ou administratives entreprises ont été respectés grâce aux compétences, engagement et coordination des différentes équipes de l'Institut qui ont participé à ces actions ; ceci concerne non seulement les équipes de la Division Réacteur et du Service de Protection Radiologique, mais aussi celles des Départements Exploitation des Expériences et Instruments et Méthodes qui ont démonté et déplacé les instruments pour libérer les accès au réacteur.

Projets instrumentaux

Pour assurer la réserve financière nécessaire à la remise en état du réacteur, l'Institut a dû réduire son budget normal de 24 % entre 1991 et 1993, cette réduction a touché tous les secteurs et en particulier celui des investissements. Dans ce cadre budgétaire nous ne pouvons envisager mener simultanément l'achèvement des projets instrumentaux et méthodes en cours, les actions d'entretien, le transfert du système informatique vers UNIX et le démarrage de certains projets instrumentaux du programme de modernisation. Nous avons décidé de donner la priorité à l'achèvement des travaux en cours et le démarrage du programme de modernisation dans son ensemble ne sera pas possible. Nous ne pourrons envisager de lancer que quelques projets limités mais nous n'avons pas encore pris de décision ferme pour ce dernier point car il nous manque des éléments d'information concernant certaines composantes du budget 1993.

L'Institut se retrouve donc dans une situation où certaines de ses activités de création en instrumentation, appareillage et méthodes vont être ralenties. Ces activités étaient un des éléments assurant la qualité et l'originalité des travaux scientifiques effectués à l'Institut, elles contribuaient aussi fortement à son rayonnement et les autres centres de neutronique s'en étaient souvent inspirés pour leur développement. Un ralentissement de ces activités ne peut être que temporaire, justifié par l'urgence de la remise en état du réacteur avec un budget limité, et leur rétablissement après le redémarrage devra être une priorité.

Directions pour le retour en exploitation

L'Institut a été très perturbé par l'annonce de la demande de l'Associé britannique de renégocier la Convention Intergouvernementale en vue de diminuer sa participation financière ; il craignait que ceci n'affecte profondément la collaboration entre les trois pays, collaboration équilibrée et fructueuse qui avait assuré son efficacité et son succès. Le fait que le principe d'une prolongation de la Convention entre les trois partenaires ait été réaffirmé a certainement dissipé les inquiétudes à ce sujet. Cependant, la nécessité de prendre en compte les difficultés financières actuelles, en particulier celles de la Grande Bretagne, impose à l'Institut d'envisager son retour en exploitation en 1994 dans un cadre budgétaire extrêmement contraignant. Compte tenu des contributions financières attendues des trois pays membres et de celles espérées de membres scientifiques actuels et potentiels, la diminution du budget par rapport aux années de fonctionnement normal précédentes pourraient

atteindre 15 %. Il est donc nécessaire de préparer dès maintenant l'Institut à un tel changement et d'adopter les mesures qui lui permettront d'assurer, outre le service aux utilisateurs et son activité scientifique, un programme minimal de développements en instrumentation et technologie neutronique, comme évoqué dans le paragraphe précédent.

Un minimum de 25 instruments programmés exploités pendant 5 cycles a été estimé compatible avec le budget envisagé. La liste de ces 25 instruments a été établie sur la base des discussions du "Users' meeting" du 17.10.1991, en utilisant des critères d'unicité et de complémentarité par rapport aux instruments des autres centres européens et après consultation des scientifiques de l'Institut. Cette liste a été présentée au Conseil Scientifique du 16.10.1992 et approuvée. (Les instruments retirés de la programmation pourraient être pris en charge par des "Collaborating Research Groups" (CRG) des pays membres, dans le cadre d'un contrat établi avec l'ILL).

L'Institut a reconsidéré ses structures et mode de fonctionnement et a élaboré une nouvelle organisation qui lui permette de travailler efficacement avec un effectif réduit. Les grandes lignes de cette réorganisation ont été approuvées par le Comité de Direction lors de sa réunion d'automne à Grenoble le 26 Novembre 1992. L'effectif minimal atteignable est de 400 personnes. Cette diminution d'effectif à 400 personnes apparaît aussi être le maximum possible, dans le cadre des budgets futurs, pour limiter la croissance du budget personnel et préserver un budget d'investissement qui permette les développements instrumentaux et d'appareillage souhaités. En fait l'Institut a dû définir un nouvel équilibre entre effectif et moyens de travail compatibles avec le nouveau budget.

Ce fut là une direction difficile à prendre, et douloureuse, car la réduction d'effectif impose à l'Institut de se séparer de certains de ses collaborateurs qui avaient contribué à son développement et à son succès pendant les vingt cinq années qui ont suivi sa fondation. En effet, la diminution de l'effectif, passant de 480 personnes avant l'arrêt du réacteur à 400 personnes, s'effectue en grande partie par des départs "naturels" (fin des contrats à durée déterminée, retraites à l'âge de 60 ans, départs volontaires) mais implique aussi les départs en pré-retraite d'un certain nombre d'agents dans le cadre d'une Convention d'Allocations Spéciales du Fonds National de l'Emploi (AS-FNE). Une proposition dans ce sens a été présentée au Comité de Direction d'automne qui en a approuvé le principe, les modalités de mise en place de ce plan sont actuellement à l'étude avec la Direction Départementale du Travail et de l'Emploi (DDTE).

Conclusion

Comme déjà dit plus haut, si les questions concernant la continuation de la coopération de trois pays membres sont maintenant sans objet, l'analyse de la situation actuelle et de son évolution probable fait apparaître d'autres inquiétudes quant à la façon suivant laquelle l'Institut pourra assurer un niveau de fonctionnement raisonnable pendant sa seconde période d'existence. Nous arriverons à maintenir l'Institut en activité pendant les deux années prochaines, mais à un prix très élevé : pertes de certaines compétences et mise en sommeil temporaire de développements technologiques et instrumentaux. L'effet des pertes de compétences se fera sentir dès le redémarrage, quand il faudra remonter les instruments car une bonne part de la mémoire les concernant risque d'être perdue suite aux départs de personnel et malgré nos efforts pour les organiser au mieux. D'autre part si l'Institut ne retrouve pas les moyens lui permettant de relancer un programme de développement technologique et instrumental raisonnable, il ne retrouvera pas le pouvoir attractif nécessaire pour remplacer son personnel touché par les retraites à venir par du personnel jeune de qualité. Pendant la seconde partie de son existence l'ILL, en tant que laboratoire multinational, doit pouvoir continuer à assurer le rôle qu'il a eu pendant ses vingt premières années et aussi l'élargir en donnant une place accrue aux membres scientifiques actuels, que nous remercions pour leur soutien pendant cette année, et futurs. Ayant mis en route la remise en état du réacteur, la Direction va tout mettre en oeuvre pour réaliser ce but malgré des conditions générales difficiles.

L'équipe de direction

P. Armbruster a quitté l'Institut le 31.10.1992 à la fin de son contrat pour retourner au GSI à Darmstadt. Nous le remercions pour son action à l'Institut et nous lui souhaitons tout le succès possible dans ses nouvelles activités. R. Scherm, venant du PTB à Braunschweig, a succédé à P. Armbruster le 01.12.1992. R. Scherm est bien connu à l'Institut, où il a participé aux développements de spectromètres trois axes et temps de vol et il connaît bien l'Institut. P. Schofield et moi-même sommes donc très heureux de le voir se joindre à nous pour participer à la direction pendant cette délicate période de changement.

L'année a été tristement marquée par le décès de trois collaborateurs très appréciés et respectés :

– M. Walter Mampe, scientifique renommé qui a été pendant de longues années un pilier dans notre secteur de physique fondamentale,

– M. George Iche, un membre très actif du groupe "Théorie" de l'ILL,

– M. Alain Schalk, collaborateur du Département Informatique.

Nous garderons un excellent souvenir de leur présence et de leur engagement au service de l'ILL.

J. Charvolin

The most important event of the year was certainly the Spring meeting of the Steering Committee at Cadarache on 21 May 1992. This meeting was decisive for the ILL's future with:

– the decision to refurbish the High Flux Reactor in accordance with the ILL's proposal, the restart being envisaged for mid-1994; as the reactor is being rebuilt on the same basis, its operation can be envisaged without any major problem for twenty years from that date,

– the agreement of the three governments and the Associates on the principle of prolongation of the Intergovernmental Agreement for a period of at least ten years from 1.1.94, and the intention of drawing up a protocol on this point to submit to the three governments for signature.

The conclusions of this meeting clearly express the will of the Associates to maintain the ILL's status as a multinational laboratory. By defining the future context of operation of the ILL, this makes it possible to envisage the directions to be followed in preparation for the return to operation after the restart.

Reactor refurbishment project

The refurbishment project was initiated immediately after the Cadarache meeting of the Steering Committee. This immediate reaction was made possible by the considerable prior preparation work by ILL on the technical and administrative steps necessary. The whole project can be summarised by dividing it into three operations: the dismantling of the old reactor vessel and its removal from the swimming-pool, the preparation of the pool to receive the new vessel, and the manufacture and installation of the new reactor vessel in the swimming-pool. The first of these operations was completed in the last week in November, and was carried out completely by ILL teams within the cost and time limits envisaged, and without the smallest incident. This was a very important date for the ILL, the half-way point on the long road from the reactor shutdown in March 1991 to its restart in mid-1994. The completion of this operation now makes it possible to emphasise the operations for the reinstallation proper, which are regarded much more positively. The second operation, the preparation of the swimming-pool for the installation of the new reactor vessel, has just started, and this is also being done by the ILL teams. The first stage of the third operation, the manufacture of the new vessel, is now well in progress; this contract has been placed with a company specialising in large aluminium alloy structures and is being monitored by the ILL, supported by an Industrial Architect. This is progressing to our complete satisfaction.

The administrative procedures have also been initiated, and as the reactor shutdown will exceed two years, it will be necessary to apply for a decree authorising the resumption of operation. The relevant dossiers, both technical and administrative, are in preparation and the former will shortly be submitted to the authorities concerned. These are the normal steps in such cases, and are progressing normally.

To conclude this paragraph, I wish to emphasise that the cost and the timetable for the technical and administrative operations undertaken have been respected due to the skill, commitment and coordination of the different ILL teams which have participated in these operations; this concerns not only the Reactor Division and Radiation Protection Unit teams, but also those of the Instrument Operation and Instruments & Methods Departments, which have dismantled and removed the instruments to provide access to the reactor.

Instrument projects

To ensure that the financial reserve necessary for the refurbishment of the reactor is available, the ILL has had to reduce its normal budget by 24% between 1991 and 1993, and this reduction has affected all sectors, in particular the investments. In this budgetary context we cannot envisage simultaneously completing current instrument and methods projects, maintenance operations, the transfer of the computer system to UNIX and the initiation of instrument projects under the Modernisation Programme. We have decided to give priority to the completion of work in progress, and that a start on the overall Modernisation Programme will not be possible. We can only envisage starting a few limited projects, but we have not yet taken a final decision on this last point, as we lack information on certain items in the 1993 budget.

The ILL is thus in a situation where certain of its creative activities in instrumentation, equipment and methods will be slowed down. These activities have been one of the elements in the quality and originality of the scientific work at the ILL, and also contributed considerably to its influence, and often inspired the development of other neutron centres. Slowing down of these activities can only be temporary, justified by the urgency of the reactor refurbishment with a limited budget, and after the restart priority must be given to their resumption.

Directions for the return to operation

The ILL was very disturbed by the announcement of the British Associate's request to renegotiate the Intergovernmental Agreement with a view to reducing its financial contribution; it was feared that this would seriously affect the collaboration between the three countries, which has been balanced and fruitful, and has ensured the ILL's efficiency and success. The fact that the principle of an extension of the Agreement by the three partners has been reaffirmed has certainly dissipated the concern on this point. However the need to take account of the current financial difficulties, in particular those of the United Kingdom, requires ILL to envisage its return to operation in 1994 in an extremely restrictive budgetary context. In the light of the

financial contributions expected from the three member countries and those hoped for from current and potential scientific members, the reduction in the budget in comparison with the preceding years of normal operation could reach 15%. It is therefore necessary now to prepare the ILL for such a change, and to adopt measures ensuring that, apart from the service to users and its scientific activity, a minimum programme of developments in instrumentation and neutron technology will be maintained, as mentioned in the previous paragraph.

A minimum of 25 scheduled instruments operated for 5 cycles is considered compatible with the budget envisaged. The list of these 25 instruments was drawn up on the basis of the discussions at the users' meeting on 17.10.91, using criteria of uniqueness and complementarity in relation to instruments at other European centres, and after consultation with the ILL scientists. This list was submitted to the Scientific Council on 16.10.92 and was approved. (The instruments no longer scheduled could be taken over by Collaborating Research Groups (CRGs) from member countries, under a contract with ILL).

The ILL has re-examined its structures and mode of operation, and has worked out a new organisation to permit it to operate efficiently with a reduced staff. The broad lines of this reorganisation were approved by the Steering Committee at its Autumn meeting in Grenoble on 26 November 1992. The minimum staff attainable is 400 persons. This reduction of staff to 400 also appears to be the maximum possible, in the context of future budgets, to limit the growth of the staff costs budget and to conserve an investment budget permitting the instrument and equipment developments desired. ILL has in fact had to define a new equilibrium between personnel and means of work compatible with the new budget.

This was a difficult and painful step to take, as the reduction in staff requires the ILL to part with some of its staff who had contributed to its development and success during the twenty-five years from its foundation. The reduction in staff, from 480 before the reactor shutdown to 400 persons, is in fact taking place largely by 'natural' departures (end of limited-term contracts, retirement at age 60, voluntary departures) but also necessitates early retirement for a number of staff under a 'Fonds National de l'Emploi' Agreement. A proposal in this sense was submitted to the Autumn meeting of the Steering Committee, which approved the principle, and the practical implementation of this plan is currently being studied with the 'Direction Départementale du Travail et de l'Emploi' (local labour authority).

Conclusion

As stated above, although there are no longer any doubts on the continued cooperation of the three member countries, the analysis of the present situation and its probable development bring out other concerns as to how ILL will be able to ensure a reasonable level of operation for its second lease of life. We shall be able to maintain the operation of the ILL during the next two years, but at a very high price: loss of certain skills and temporary suspension of technological and instrument developments. The effect of the loss of skills will be felt at the restart, when it will be necessary to reinstall the instruments, as a considerable part of the collective memory of them is liable to be lost as a result of departure of staff, despite our efforts to organise these as well as possible. On the other hand if the ILL does not find again the means to enable it to restart a reasonable technological and instrument development programme, it will not recover the attractiveness necessary to replace its staff affected by the forthcoming retirements by young high quality personnel. During the second phase of its existence ILL, as a multinational laboratory, must be able to continue to play the part which it had during its first twenty years, and also to expand this by giving an enhanced place to the current scientific members, whom we thank for their support during the current year, and future scientific members. Having initiated the refurbishment of the reactor, the Management will do all in its power to achieve this aim, despite the present difficult conditions.

The Directorate

P. Armbruster left ILL on 31.10.92 at the end of his contract to return to the GSI at Darmstadt. We thank him for his work at the ILL and wish him all possible success in his new post. R. Scherm, coming from the PTB at Brunswick, succeeded P. Armbruster on 1.12.92. R. Scherm is well known at the ILL, where he took part in the development of three-axis spectrometers and time-of-flight instruments, and he knows the ILL well. P. Schofield and I are very happy to have him join us in the Directorate during this sensitive period of change.

During the year the ILL was saddened by the deaths of three much appreciated and respected colleagues:

– Walter Mampe, a well-known scientist who was for years a pillar of our fundamental physics sector,

– George Iche, a very active member of the ILL theory group,

– Alain Schalk, a member of the Computing Department staff.

We shall long remember their presence and their commitment in the service of the ILL.

J. Charvolin

Das wichtigste Ereignis des Jahres war sicherlich die Sitzung des Lenkungsausschusses in Cadarache am 21. Mai 1992. Diese Sitzung war für die Zukunft des ILL entscheidend:

– Es wurde beschlossen, den Reaktor gemäß dem Projektvorschlag des Instituts wieder instand zu setzen. Die Wiederaufnahme des Betriebs ist für Mitte 1994 vorgesehen. Mit einem unverändert wiederaufgebauten Reaktor wird ein problemloser Betrieb für etwa 20 Jahre - von diesem Datum gerechnet - erwartet.

– Weiterhin wurde die Vereinbarung der 3 Regierungen und der Gesellschafter zur Kenntnis genommen, sich prinzipiell auf eine Verlängerung des Vertrags zwischen den 3 ILL-Partnern für eine Periode von mindestens 10 Jahre ab 1.1.94 zu einigen und ein entsprechendes Protokoll zu verfassen, welches den jeweiligen Regierungen zur Unterschrift vorgelegt werden soll.

Die Beschlüsse dieser Sitzung bringen klar den Willen der Gesellschafter zum Ausdruck, das ILL in seiner Funktion als multinationales Forschungszentrum zu erhalten. Sie erlauben, anhand der Definition des zukünftigen Betriebs, die entsprechenden Maßnahmen zur Vorbereitung des Routinebetriebs nach dem Wiederanfahren des Reaktors zu treffen.

Wiederinstandsetzung des Reaktors

Das Projekt der Reaktorreparatur wurde unmittelbar nach der Sitzung des Lenkungsausschusses in Angriff genommen. Diese rasche Reaktion war durch die vorausgegangene, intensive Vorbereitung aller technischen und administrativen Schritte möglich geworden. Das gesamte Projekt unterteilt sich in drei Abschnitte: Die Demontage des alten Reflektortanks und seine Entfernung aus dem Schwimmbecken, die Aufbereitung dieses Beckens für den Einbau des neuen Tanks, sowie Herstellung des neuen Tanks und dessen Montage im Becken.

Der erste dieser Abschnitte wurde in der letzten Novemberwoche zu Ende geführt; er wurde ausschließlich von der Reaktormannschaft des ILL innerhalb der Kostenabschätzung und der vorgesehenen Termine ohne Zwischenfälle bewerkstelligt. Dies war ein äußerst wichtiger Moment für das ILL, das sich gegenwärtig auf der Hälfte der langen Strecke zwischen der Abschaltung des Reaktors im März 1991 und seiner Wiederinbetriebnahme gegen Mitte 1994 befindet. Die Beendigung dieses ersten Abschnitts erlaubt es jetzt, sich energisch um die Maßnahmen zur eigentlichen Wiederinstandsetzung zu kümmern, die von der Belegschaft wesentlich positiver empfunden werden.

Der 2. Schritt, die Vorbereitung des Reaktorbeckens zum Einbau des neuen Tanks, hat bereits begonnen und wird ebenso von der ILL-Reaktormannschaft bewerkstelligt. Die erste Etappe des 3. Abschnitts, die Herstellung des neuen Tanks, ist bereits ziemlich fortgeschritten und ist einem auf große Al-Legierungsstrukturen spezialisierten Industrieunternehmen anvertraut worden. Die Abwicklung wird durch das ILL überwacht, das hierbei durch einen Industriearchitekten unterstützt wird. Der Verlauf dieser ersten Etappe ist durchaus zufriedenstellend.

Da im Falle einer über 2 Jahre hinausgehenden Reaktorabschaltung eine Genehmigung zur Wiederinbetriebnahme erforderlich ist, wurden die notwendigen administrativen Schritte eingeleitet. Entsprechende technische und administrative Dossiers werden gegenwärtig erstellt; die ersten werden demnächst den zuständigen Behörden vorgelegt werden. Dies ist eine auf diesem Gebiet durchaus übliche Prozedur; sie läuft reibungslos ab.

Zum Abschluß dieses Kapitels möchte ich betonen, daß alle Kostenabschätzungen und Termine der technischen und administrativen Schritte dank der Kompetenz, dem Einsatz und der Koordination der verschiedenen beteiligten ILL-Teams eingehalten werden konnten. An den verschiedenen Aktionen waren nicht nur die Reaktorabteilung beteiligt, sondern auch die Strahlenschutz-Abteilung sowie die Abteilungen EDEX und DIM, die mit der Demontage und Entfernung der Instrumente beauftragt waren, um Zugang zum Reaktor zu schaffen.

Instrumentenprojekte

Um die notwendige Finanzreserve für die Wiederinstandsetzung des Reaktors sicherstellen zu können, war das ILL gezwungen, in den Jahren 1991-93 sein Normalbudget um 24% zu vermindern. Diese Kürzung berührte alle Bereiche, im besonderen die Investitionen. Im vorgegebenen Budgetrahmen ist es uns unmöglich, gleichzeitig die Fertigstellung der laufenden Projekte auf dem Gebiet der Instrumente und Messmethoden voranzutreiben, die nötigen Maßnahmen zum Unterhalt der Geräte zu treffen, die Umrüstung der Rechnersysteme auf UNIX vorzunehmen und mit der Verwirklichung gewisser Instrumentenprojekte im Rahmen des Modernisierungsprogramms zu beginnen. Deshalb haben wir uns entschlossen, der Vollendung laufender Arbeiten den Vorzug zu geben. Die Inangriffnahme des Modernisierungsprogramms in seiner Gänze wird sich nicht verwirklichen lassen. Wir werden nur in beschränktem Umfang einige Projekte beginnen können; wir haben jedoch diesbezüglich noch keine endgültige Entscheidung getroffen, da uns noch gewisse Informationen über die genaue Zusammensetzung des Budgets im Jahre 1993 fehlen.

Die Lage des ILL erfordert es also, die Entwicklung von Instrumenten, Geräten und Meßmethoden zu verlangsamen. Gerade diese Aktivitäten jedoch stellten bisher Qualität und Originalität der wissenschaftlichen Arbeiten des Instituts sicher. Sie waren auch Teil seiner Ausstrahlung. Von ihr ließen sich andere Neutronenzentren bei ihrer Entwicklung inspirieren. Eine Verzögerung dieser Aktivitäten kann deshalb nur vorübergehend sein und wird nur gerechtfertigt durch die Dringlichkeit der Reaktorinstandsetzung im Rahmen eines beschränkten Budgets. Ihre volle Wiederaufnahme nach dem Betriebsbeginn des Reaktors muß Priorität haben.

Richtlinien für die Rückkehr zum Routinebetrieb

Anläßlich der Ankündigung des britischen Gesellschafters, die zwischenstaatliche Abmachung mit Ziel der Reduzierung seines Beitrags neu zu verhandeln, war das ILL sehr besorgt; man fürchtete, daß dies nachhaltig die Zusammenarbeit der 3 Länder am ILL beeinträchtigen würde. Diese ausgeglichene und fruchtbare Zusammenarbeit war Garant für die Effizienz und den Erfolg des ILL. Die Tatsache, daß schließlich prinzipiell Einigung über eine Verlängerung der Abmachung erzielt worden ist, hat diese Besorgnisse zerstreut. Die Notwendigkeit jedoch, auf die gegenwärtigen finanziellen Schwierigkeiten, im besonderen des britischen Partners, Rücksicht zu nehmen, zwingen das

ILL, den für 1994 vorgesehenen Routinebetrieb in extrem eingeschränktem Budgetrahmen zu planen. Unter Berücksichtigung der zu erwartenden finanziellen Beiträge der drei Mitgliedsländer sowie derjenigen, die von den gegenwärtigen und zukünftigen wissenschaftlichen Mitgliedern erhofft werden, könnte die Budgetkürzung gegenüber den vergangenen, normalen Betriebsjahren 15% erreichen.

Schon jetzt ist es deshalb erforderlich, das ILL auf diese neue Situation vorzubereiten und Maßnahmen zu treffen, die es ihm erlauben werden, über den Nutzerservice und die wissenschaftliche Aktivität hinaus ein minimales Entwicklungsprogramm auf den Gebieten der Instrumentierung und der Neutronentechnik sicher zu stellen, wie im vorausgegangenen Abschnitt erwähnt.

Ein normaler Experimentierbetrieb mit mindestens 25 programmierten Instrumenten über 5 Reaktorzyklen sollte mit dem vorgesehenen Budget vereinbar sein. Die Liste dieser 25 Instrumente wurde auf der Basis des ILL Benutzer-Treffens vom 17.10.1991 zusammengestellt, wobei Kriterien wie Einzigartigkeit und Komplementarität mit Instrumenten anderer europäischer Zentren, sowie die Ratschläge der ILL Wissenschaftler berücksichtigt wurden. Diese Liste ist dem Wissenschaftlichen Rat am 16.10.1992 vorgelegt und von diesem gebilligt worden. (Die nicht mehr programmierten Instrumente könnten von sogenannten Collaborating Research Groups (CRG) aus den Mitgliedsländern im Rahmen eines mit dem ILL ausgearbeiteten Vertrags übernommen werden).

Das ILL hat seine Strukturen und seinen Betrieb neu überdacht und einen neuen Organisationsplan ausgearbeitet, der es ihm erlauben sollte, wirkungsvoll mit reduzierter Belegschaft zu arbeiten. Die prinzipiellen Strukturen dieser Umorganisation sind vom Lenkungsausschuß auf seiner letzten Herbstsitzung in Grenoble am 26.11.1992 gebilligt worden. Die Mindestbelegschaft umfaßt 400 Personen. Dieser Abbau auf 400 Personen erscheint gleichzeitig als das im zukünftigen Budgetrahmen mögliche Maximum, mit dem Ziel das Anwachsen des Personalbudgets zu begrenzen und ein Investitionsbudget zu erhalten, welches die Entwicklung erwünschter Instrumente und Geräte erlaubt. In der Tat mußte das ILL ein neues Gleichgewicht zwischen Personal und Arbeitsmittel, beide mit dem neuen Budget vereinbar, finden.

Dies war eine schwer zu treffende und schmerzhafte Entscheidung, da die Personalkürzungen das ILL zwingen, sich von mehreren Mitarbeitern zu trennen, die zu seiner Entwicklung und seinem Erfolg in den 25 Jahren seit seiner Gründung beigetragen haben. Tatsächlich ist ein großer Teil der Personalverminderung von 480 (vor der Reaktorabschaltung) auf 400 Personen auf "natürliche" Abgänge zurückzuführen (Vertragsende bei Zeitverträgen, Pensionierung im Alter von 60 Jahren, freiwillige Abgänge); diese beinhaltet aber auch die Versetzung in den Vorruhestand einer gewissen Anzahl von Mitarbeitern im Rahmen einer "Convention d'Allocations Spéciales du Fonds National de l'Emploi" (AS-FNE). Ein entsprechender Vorschlag ist dem Lenkungsausschuß auf seiner Herbstsitzung vorgelegt worden und wurde im Prinzip gebilligt. Die Verfahrensweise für die Umsetzung dieses Plans wird gegenwärtig bei der Direction Dép. du Travail de l'Emploi (DDTE) geprüft.

Schlußfolgerung

Wie bereits erwähnt sind nun alle Zweifel über die weitere Zusammenarbeit der drei Mitgliedsländer gegenstandslos geworden. Allerdings lässt eine Analyse der gegenwärtigen Situation sowie der vermutlichen weiteren Entwicklung neue Sorgen aufkommen, wie am Institut während seiner zweiten Lebenshälfte ein vernünftiger Betrieb gesichert werden kann. Sicher werden wir das ILL während der nächsten zwei Jahre aktiv halten können, allerdings zu einem sehr hohen Preis: Verlust mancher Kompetenzen und vorläufige Zurückstellung der technologischen und instrumentellen Entwicklungen. Die Auswirkungen der Kompetenzverluste werden bei der Wiederinbetriebnahme des Reaktors spürbar werden, wenn die Instrumente wieder aufgebaut werden müssen. Ein guter Teil des hierfür notwendigen "Gedächtnisses" könnte nämlich beim Ausscheiden von Personal, trotz unserer Anstrengungen, eine optimale Organisation zu gewährleisten, verlorengehen. Wenn andererseits das ILL nicht die Mittel finden sollte, wieder eine vernünftiges, technologisches und instrumentelles Entwicklungsprogramm anzufangen, wird es nicht wieder die nötige Anziehungskraft erreichen, um das in den Ruhestand versetzte Personal durch junge und qualifizierte Mitarbeiter zu ersetzen. In seinem zweiten Lebensabschnitt muß das ILL als multinationales Forschungszentrum weiterhin die Rolle spielen können, die es während seiner ersten zwanzig Jahre innehatte, ja diese sogar ausbauen, indem es den gegenwärtigen wissenschaftlichen Mitgliedsländern mehr Platz einräumt. Diesen gilt unser Dank für ihre Unterstützung in diesem Jahr sowie für die Zukunft. Nachdem die Direktion die Wiederinstandsetzung des Reaktors eingeleitet hat, wird sie nichts unversucht lassen, dieses Ziel trotz schwieriger, allgemeiner Bedingungen zu verwirklichen.

Der Stab der Direktion

P. Armbruster verließ das ILL am 31.10.1992 am Ende seiner Amtszeit, um an die GSI Darmstadt zurückzukehren. Wir danken ihm für seine Tätigkeit am ILL und wünschen ihm großen Erfolg bei seinen neuen Aufgaben. R. Scherm von der PTB-Braunschweig ist seit 1.12.1992 sein Nachfolger. Er ist bereits am ILL bekannt, wo er an der Entwicklung von 3-Achsen- und Flugzeitspektrometern beteiligt war und ist mit unserem Institut bestens vertraut. P. Schofield und ich sind daher sehr glücklich, daß er sich während dieser delikaten Übergangszeit zu uns in der Leitung des ILL gesellt.

Das Jahr war vom Tod dreier sehr geschätzter und respektierter Mitarbeiter überschattet:

– W. Mampe, renomierter Wissenschaftler, der jahrelang einer der Stützpfeiler der Gruppe "Grundlagenphysik" bildete,

– G. Iche, ein sehr aktiver Mitarbeiter der Gruppe "Theorie"

– A Schalk, Mitarbeiter der Informatikabteilung.

Wir werden sie und ihr Engagement für das ILL in besonderer Erinnerung behalten.

J. Charvolin

Collaboration with ESRF

During 1992 there were a number of important developments bringing about closer relations with our neighbours, the European Synchrotron Radiation Facility (ESRF). We now share a single common site, formally inaugurated by the two Directors on 4 May by the unlocking of the gate in the fence dividing it; the fence has now been removed. There is now a single site entrance with a new guardhouse to deal with the increased traffic; a computerised entry system for visitors is being introduced. A Joint Building was opened during the summer. It now houses the Joint Library, the theoreticians of both institutes and a restaurant and cafeteria. The latter is developing into a common meeting place for staff of both institutes. The old ILL cafeteria building in the ILLTON is currently being converted to accommodate the Common Medical Service. Plans to share laboratory facilities for chemistry and biology are going ahead.

At the scientific level there are many contacts with ESRF, both formal, through part or full-time attachment of ILL staff to ESRF, and informal. A number of joint ILL/ESRF workshops have been held including one on 'Determination of Partial Structure Factors in Disordered Materials' and more are planned for 1993. The two institutes from time to time together invite guest speakers for joint lectures.

During the reactor shutdown the ESRF has benefited from many of the technical services of the ILL, and technical staff released have been seconded to ESRF to help with their beam-line commissioning programme. A jointly sponsored project to demonstrate instrument control and data acquisition under Unix has been successfully completed.

Both ILL and ESRF managements continue to take an interest in the provision of international schooling in Grenoble and have maintained contact with the local education authorities on the contracts of foreign teachers and the improvements of conditions in the International Sections of the schools.

Our best wishes go with R. Haensel, the retiring Director-General of ESRF, and we welcome his successor, Y. Petroff.

P. Schofield

Theory

Members of the College

S. Brazovskii
B. Clements
B. Fourcade
G. Iche
E. Krotscheck
A. Levanyuk
C. Misbah
P. Nozières
J. Palmeri
Y. Saito
A. Schofield
N. Schopohl
A. Valance
J. Voit
M. Walker
J. Wheatley

Introduction

In 1992, the Theory College worked on condensed matter physics.

The life of the College was considerably affected by the reactor refurbishment programme and its concomitant budget restrictions implying the freeze of several posts and, more specifically, the (temporary) discontinuation of its activities in nuclear and fundamental physics. Another event greatly influencing its activities was the move to the Joint (ILL-ESRF) Building and its (geographical) merger with the new ESRF theory group - both through all kinds of inconvenience associated with the move as well as through the excitement caused by the close contacts with the young ESRF team.

The research in condensed matter physics was mainly in two major subfields: theory of correlated fermions and related quantum liquids, often in low dimensions, and models relevant for crystal growth and soft condensed matter (membranes, vesicles, etc.).

S. Brazovskii pursued work on the theory of low-dimensional electronic crystals. A description of dislocation arrays (soliton lattices) in the vicinity of an interface of a charge/spin density wave system or a conducting polymer and a metal has provided a detailed understanding of both static and kinetic phenomena. Various aspects have been studied in collaboration with N. Kirova and S. Matveenko (theory) and R. Currat and P. Monceau (experiments).

B. Clements, in collaboration with E. Krotscheck and H. Lauter, has been using microscopic theories to study the growth of liquid ^{4}He films on weakly attractive substrates. Their work provides a detailed growth scenario: they have found that close to the substrate the helium film grows by formation of well defined liquid layers. Above a minimum stable coverage a liquid monolayer uniformly covers the surface. Increasing the coverage forces the liquid into a compressed state, and the population of a second liquid layer becomes energetically favourable. This layer begins to grow by the formation of two dimensional liquid "clusters". Above a certain coverage, the second layer moves out of vacuum/cluster coexistence, and the system regains the full planar symmetry. The scenario is repeated for a third liquid layer as well. Clements is presently extending the theory to include finite-temperature effects. Also in collaboration with E. Krotscheck and H. Lauter, he is actively developing a theory of excitations which can be applied to quantum-film systems. This work will provide theoretical interpretation of the remarkably rich and complicated neutron scattering data for helium on graphite, which was obtained at the ILL by H. Lauter and collaborators.

B. Fourcade continued work on the shape of lipid vesicles. He was able to work out precise conditions under which vesicle shapes whose energy is an absolute minimum can be observed in partially polymerized membranes. These predictions were successfully verified in a collaboration with M. Mutz and D. Bensimon from Paris. He also succeeded in establishing, through numerical simulation, a phase diagram for very high genus surfaces, and can predict topology as a function of surface tension and osmotic pressure in this limit.

G. Iche returned to the theory college after a ten year career as a computer scientist. (He had worked out his thesis on brownian motion at the ILL earlier). His project was the establishment of an interface between theorists and experimentalists both through numerical simulations and through improvement of existing and development of novel methods of data analysis. Clear structure of this project had emerged within a couple of months when Iche was struck by illness and died in July. In the long term a successor will have to be found for this important activity.

E. Krotscheck has studied, in close contact with the experimentalists at the ILL, in particular with H. Lauter, the growth and excitation mechanisms of adsorbed helium films. Two new insights originated from this research: (1) They found that the growth of a quantum liquid film on a substrate can occur in a number of steps which are individually separated by phase transitions between uniform surface coverages, and the formation of two dimensional "droplets". (2) The phase transitions are accompanied by the softening of the ripplon excitation at long and intermediate wavelengths. This "softening" has the consequence that the lowest lying collective excitation develops "abnormal" dispersion and can decay. It is predicted that the phase transition should be accompanied by a finite lifetime of the ripplon.

C. Misbah's research covered various problems pertinent to crystal growth. He worked out a theory of parity breaking in eutectic lamellar growth and was able to include kinetic effects, crystalline anisotropy and diffusion layers. He also studied the dynamics of a step growing from a vapour phase by using a Kuramoto-Sivashinsky type of equation and could include step-step interactions. The latter strongly affect the step dynamics. He collaborated at various times with R. Kassner, D. Temkin and A. Valance.

A. Levanyuk investigated in collaboration with J. Lajzerowicz fluctuation-induced interactions between domain walls. This problem is of importance for the understanding of commensurate-incommensurate phase

transitions as may occur in the charge density wave systems studied in other ILL colleges. He initiated a collaboration with M. Vallade on fluctuation-induced first order transitions in solids. More specifically, they are aiming at understanding the phase diagram of quartz.

P. Nozières invested much of his energy into his Collège de France lectures on "Anomalous behaviour of one-dimensional Fermi liquids". He emphasized both perturbative approaches based on bosonization of a field theory and exact results for lattice models obtained from Bethe's Ansatz. His care about details of the Bethe wavefunction generated new spinoffs for the Hubbard model: the recognition that the ground state energy is nonanalytic in interaction strength and magnetization, and that the deconfinement of spinons and holons is asymptotically limited to the vicinity of the Fermi surface. His research interests were centred both on the physics of crystal growth and interfaces, and on anomalous Fermi liquids. In the first field, he clarified some properties of crystalline steps important for an understanding of the Grinfeld instability. From a fourth order amplitude expansion he could show that the primary bifurcation is undercritical. The saturation mechanism remains, however, to be understood. The Grinfeld instability could perhaps explain the island formation observed in epitaxial layers.

P. Nozières was further interested in the problem of localization in a gas of heavy particles coupled to a thermostat of light ones. Together with Varma, Giamarchi, and Ruckenstein, he studied in detail a related though simpler model of a resonant impurity hybridized with the conduction electron gas which includes an on-site s-d interaction. They find an interesting power-law dependence of the resonance width on temperature which can lead either to Fermi liquid or to novel exotic behaviour, depending on the exponent.

J. Palmeri considered apparently unrelated - through structurally similar - problems governed by retarded or nonlocal effective actions. In collaboration with E. Guitter from Saclay, he developed a general method for such problems and applied it to the statistical properties of tethered or polymerized membranes. Such membranes with long range interactions can undergo a crumpling transition between a flat and a swollen phase. They worked out a phase diagram for self-avoiding manifolds which could help to understand numerical results implying the stability of the flat phase of a 2d membrane in three dimensions.

A dual problem, governed by long-range attractions, is posed by a test particle coupled to a bosonic bath, the generalized polaron problem. Palmeri was able to show that the generalized polaron exhibits, in specific parameter ranges, a localization transition (dual to crumpling). Both aspects taken together suggest a wide range of applicability for his method in quantum statistical mechanics.

Y. Saito collaborated with C. Misbah on the morphological stability of steps in crystal growth under molecular beam epitaxy. They were able to identify regimes with stable and unstable step morphology. From Monte Carlo simulations in the unstable limit, Saito could demonstrate chaotic spatio-temporal behaviour, and the step front then exhibits fractal structure. The effect of shot noise near the instability point is currently being investigated.

A. Schofield worked on the Hall effect in the gauge model for high-T_c superconductors. The electrons are represented here by (fermionic) spinons and (bosonic) holons, and a central issue is the combination laws of physical properties out of spinon and holon responses. In a second stage one has to inquire how these responses are affected by the gauge field representing the constraint of excluded double occupancies. Together with Wheatley, Schofield elaborated the combination law for the Hall conductivity by deriving a consistent action to third order in the applied field. Interestingly, they obtain temperature-independent Hall constants at low doping while near doping levels with charge conjugation symmetry, the Hall constant scales as the inverse temperature - not unlike certain experiments in the high-T_c cuprates.

N. Schopohl worked on superfluids and the Kondo problem. He pursued a collaboration with D. Waxman and G.E. Volovik on the motion of an interface between the superfluid A and B phases in ^{3}He. In the problem considered, the interface expands with uniform velocity into the undercooled A-phase. They obtained an essentially exact solution of the Gorkov equations for the fermions which scatter off the moving interface. Their distribution function has an essential singularity at zero velocity and translates rigidly only with a slowly moving interface. The possibility for experimental observation is currently under investigation.

He further collaborated with the group of R. Tournier (CRTBT-CNRS) on transport and magnetic properties of high-T_c superconductors. They indicated the possibility of intrinsic surface superconductivity along normal layers inside the samples.

Together with D. Förster, Schopohl developed an auxiliary fermion approach for the problem of several Kondo impurities interacting with a band of intinerant electrons. They come up with an effective action for fermions hopping along a semi-infinite chain which allows them to study a variety of interesting physical properties.

A. Valance continued work on interface instabilities in crystal and epitaxial growth. Together with C. Misbah he investigated both analytically and through simulation, the transition to chaos in directional solidification, the nonlinear evolution of a crystal step and questions related to eutectic lamellar growth.

The research activities of J. Voit have been centred around the consequences of charge-spin separation in one-dimensional fermion systems and specifically the spectral properties of Luttinger liquids. The Luttinger model is a paradigmatic theory for real quasi-1D metals and learned speculations seem to indicate its importance for high-T_c superconductors. It has been found that charge-spin separation and power law correlation dramatically modify the one-electron spectral function compared to the familiar Fermi liquid. Specifically there are power-law divergences at frequencies related to the charge and spin velocities if the interactions are weak. In a collaboration with experimentalists in Neuchâtel (Malterre, Baer) on photoemission spectoscopy of organic superconductors it emerged that the Luttinger liquid provides a consistent description of the spectra if, and only if, the interactions are assumed strong and of long range. Furthermore, Voit initiated a collaboration with J. Wheatley on the behaviour of two coupled Luttinger chains.

In another project, he studied the influence of electron-electron interactions in a simple model describing the polymer polyaniline. This model discusses in detail the influence of ring-torsional degrees of freedom on the physical properties. For a weak Hubbard interaction they found an enhancement of dimerization, similar to but stronger than in the prototypical polyacetylene. As a consequence of a (successfully identified) secondary order parameter, new unexpected behaviour and a very rich phase diagram is found in the Spin-Peierls limit $U \rightarrow \infty$: the dimerized ground state can break down both with respect to an ideal paramagnet or Heisenberg antiferromagnet, and within the Peierls phase various crossovers occur because the periodicity of the ring torsions effectively quenches a self-consistency condition. These results obtained in collaboration with D. Baranowski from Bayreuth, are used as input for a more general study examining under what conditions Peierls' theorem holds.

M. Walker has continued work on competing-interactions types of models appropriate for the study of structural phase transitions. Symmetry arguments are used to derive appropriate layer variables in terms of which to formulate the problem, and multiple phase transitions in BCCD (betaine calcium chloride dihydrate) are being studied in detail (in collaboration with Cornelia Kappler). Also, together with Bill Buyers, efforts are being made to better understand the ordering which occurs below 17.5K in the heavy-fermion superconductor URu_2Si_2. A variety of different possible types of order (each based on the ordering of a particular type of uranium ion multipole moment) have been described, and the characteristics of the neutron scattering which would identify each of the possible types of order have been determined.

J. Wheatley was investigating transport properties of strongly correlated electron systems with emphasis on the normal state of the high-T_c materials. In the lightly doped regime, the transport problem is best viewed as scattering of charge (holons) from spin fluctuations. Together with B. Douçot from CRTBT-CNRS, he investigated charge scattering from chiral spin fluctuations. If the chiral symmetry is unbroken, the holon scattering is equivalent to that from a random flux. This mechanism will add to any other source of current relaxation present. Wheatley and Douçot find that its contribution to the resistivity will scale linearly with temperature below a crossover scale and then saturate. The crossover scale is eventually observable in $La_{2-x}Sr_xCu0_4$ if their mechanism is important.

Wheatley also collaborated with A. Schofield in a project on the Hall effect of doped Mott insulators, described in more detail in Schofield's entry.

Secretary: J. Voït

Nuclear and Fundamental Physics

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Summary

In spite of the lack of neutrons due to the reactor shutdown College III has been able to maintain a high level of scientific activities.

At the beginning of the year no instrument of College III was running but at the end of the year several experiments have been started: the BILL magnet was being used for an experiment at the PN7 site. The detector system of the LOHENGRIN spectrometer was used for measurements of the nuclear charge distribution in spontaneous fission of ^{248}Cm. The special instrument S51-INAA was running during most of the year examining rock samples irradiated at SILOE(CENG). All the main instruments of College 3 were undergoing major upgrades or being refurbished.

Changes have occurred this year in the scheduled instruments used by the College. The PN2 electron spectrometer facility of level D was dismantled thus terminating a productive 18 year period of operation. Those instruments devoted mainly to fundamental physics will be called PF for physique fondamentale. The PN7 cold polarised beam facility has been renamed PF1 and the Ultra-cold neutron facility on level D has become a scheduled instrument called PF2.

The LOHENGRIN spectrometer PN1 was equipped with a new detection system and an energy - focussing magnet. Both parts are now installed and tested.

Studies have continued on the extraction of fission product nuclei for transport to the neighbouring accelerator SARA where they would be used for exotic beam experiments.

The BILL electron spectrometer from the former PN2 was installed in a modified version with a new source chamber and partly new electronics at the PF1 area. An experiment to search for a heavy mass neutrino in the beta decay of ^{177}Lu is in progress.

The GAMS spectrometer GAMS2/3 was upgraded with a new interferometer and a vibration suppression system; the test interferometer GAM5T has been designed and should be assembled in the first part of 1993.

During the year, two of the College 3 staff left the institute: A.P. Williams joined the ESRF to construct a three axis spectrometer in a two-year period, and S. Ulbig went to Darmstadt as editor at Physikalische Blätter.

A "Workshop on Applications of High Resolution Gamma spectroscopy in Studies of Atomic Collisions and Nuclear Lifetimes" was held at the ILL from 5-7. Oct. 1992. This workshop dealt with current and future applications of the GRID method.

The College was saddened by the decease of W. Mampe who was a vigorous and creative member of the ILL from its beginning. A symposium in memoriam to his widespread contributions to nuclear and fundamental physics will take place at the ILL on 29th January, 1993.

Scientific Highlights in 1992

At Lohengrin (PN1)

Installation of the new Focussing Magnet

The project for the installation of the focussing magnet on the LOHENGRIN spectrometer continued in 1992. As reported in the technical section the ion optical performance of the new focussing magnet was measured and found to be in agreement with the calculations [1]. Furthermore, the detector system of the LOHENGRIN spectrometer was used for measurements of the nuclear charge distribution in spontaneous fission of ^{248}Cm.

For a new detection system, R & D work had to be performed to design and test an ionization chamber which, besides ensuring the appropriate measurement of the nuclear charge distribution of fission products, has also to measure the angle of the incoming particles with respect to the spectrometer axis. The latter task was achieved by the measurement of the time delay of the electronic signals on the DE and E_R part of the anodes. An angular resolution of ±1.5 degrees was obtained using α-particles from a ^{241}Am source [2] (see the Instrument Development section).

Calculation of Ionic Charge Distribution of Fission Products

The measurements on the Lohengrin spectrometer before the reactor shutdown, revealed, for the very asymmetric part of nuclear fission, considerable structure on the ionic charge distribution of ions leaving the target with velocities around 1cm/ns. Fig. 1 shows an example, demonstrating the effect of strong influence of electronic shells of the highly ionized atom [3]. In the measurement shown, the Neon shell (10 electrons bound to the nucleus) stabilizes the abundance of charge state fractions. Cases requiring the removal of electrons from the L shell are strongly suppressed. In order to better understand this behaviour we performed calculations on the basis of a simple prescription which models the equilibrium ionic charge distribution of a highly ionized atom. The input in the calculation is threefold. In a first step, we performed Hartree-Fock calculations to establish the binding energies of the bound electrons and the energies of excited states of the ion in a given ionization state q. This calculation ensures that the shell structure in the following deduction of F(q) is correctly taken into account. The calculations are carried out for all ionization states of the ion, from $q=1^+$ to q=Z. The second step consists of the modelling of the probability of occupation of the electronic shells for a given velocity of the ion. For this purpose we apply a 2 parameter formula which assumes the occupation probability to have the shape of a Fermi distribution. The occupation probability of an electronic level is given by

$$P_i = \frac{1}{2} + \frac{1}{2}\frac{(v_i - v_0)}{\sqrt{(v_i - v_0)^2 + \Delta^2}}$$

where v_i is the velocity of the electron in orbit i, which is derived form the calculated binding energy and v_0 is a function of the ion velocity. The parameter Δ finally determines the smearing out of the distribution which ensures the proper variance for the charge state distribution and governs the weakening of the shell structure effects. From the given atomic model we calculate the charge state fraction F(q) by summing over all possible combinations where a total of q electrons is missing in the electronic shells of the ion. The result of our calculation reproduces the measured distributions of F(q) using the same parameter set for different elements (an example is shown in Fig. 2).

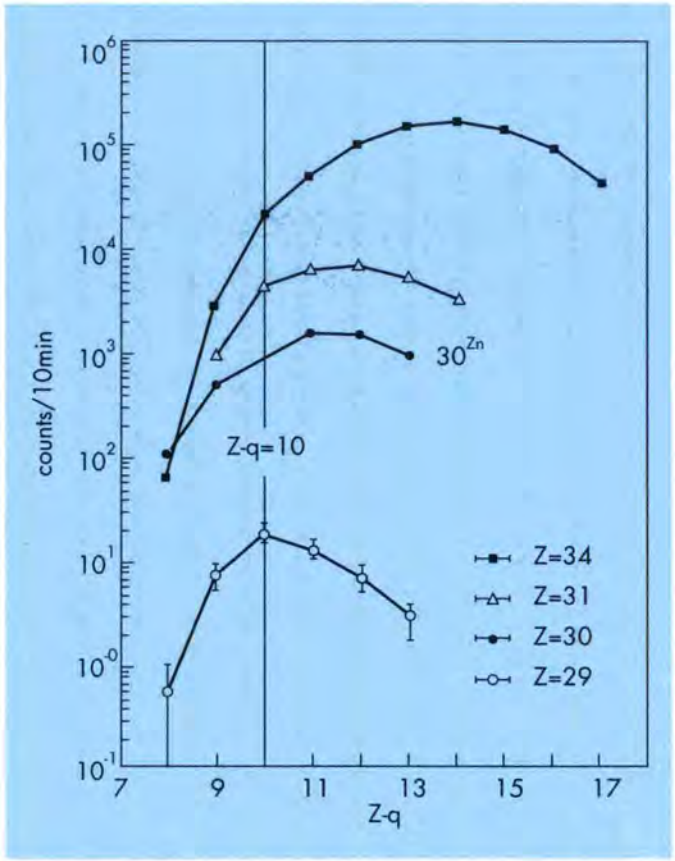


Fig. 1: Data of the ionic charge state fraction for copper, zinc, gallium and selenium, as measured in $^{239}Pu(n,f)$.

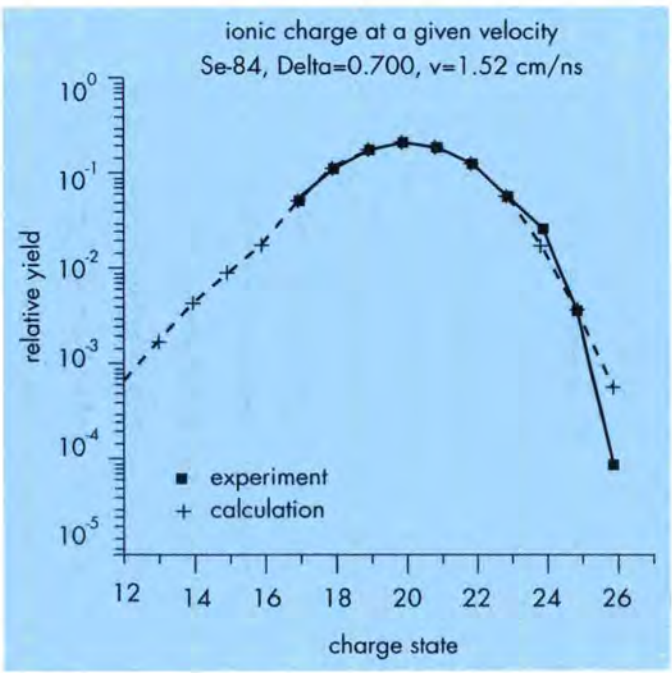


Fig. 2: Calculation of the charge state fractions F(q) for selenium 84 and comparison with experiment.

The very Asymmetric Fission of ^{250}Cf

Based on our experiment on the very asymmetric fission of ^{250}Cf following thermal neutron capture, the work on the LOHENGRIN data interpretation was continued. This far asymmetric region of fission activity shows strong structures in the fission fragment yield which have their origin in large proton and neutron odd-even effects [4]. It turned out that, correlating the data on the yield with the available Q-value of the reactions leads to an almost straight line, shown in Fig. 3. Here, all the data available for the asymmetric part are collected together, stretching over almost 6 orders of magnitude. A similar behaviour holds for the data set of ^{236}U for the same mass region. The correlation proves that, in these cases, the yield of a given isotope can be calculated with the 2 parameter formula

$$Y(Q) = e^{aQ+b}$$

The yield depends therefore only on the available Q-value, with no further dependence on the structure of nuclei involved or on the dynamics of the process. This is the first time that a clear correlation between Q-values and yield is established in nuclear fission. The correlation shows that for the fission region observed, proton and neutron odd-even effects are almost entirely explained by the respective gain in Q-value due to pairing. However, it does not mean that pairs will remain unbroken in the nuclear fission process. On the contrary, the correlation demonstrates that sufficient pair breaking has to take place to ensure also a proper yield of the unpaired fission products. The correlation observed demonstrates further that nuclear charge equilibration in this mass region is solely a consequence of the Q-value.

It turns out that the scatter of the data points in Fig. 3 is not correlated with specific fragments, and thus can not be accounted for by nucleon pairing or by nuclear structure effects. It appears, therefore, to be probably associated with the structure of wave functions involved, connecting the initial and final states of the compound nucleus and the fission product, respectively.

It should be mentioned that, especially for the data set of ^{236}U [5], we cannot exclude a curvature which would lead to a description of the data of the form

$$Y(Q) = e^{a\sqrt{Q}+b}$$

which, strikingly enough, prescribes the same dependence as the Geiger Nuttal rule for a-particle decay.

The established correlation allows the calculation of fission yields for a given isotope, if the Q-value for the mass split is known or can be estimated. Thus, for the production of the doubly magic nucleus ^{78}Ni in ^{249}Cf(n,f) we estimate from calculated Q-values a yield of 1.4×10^{-9} with an error of about a factor of 3.

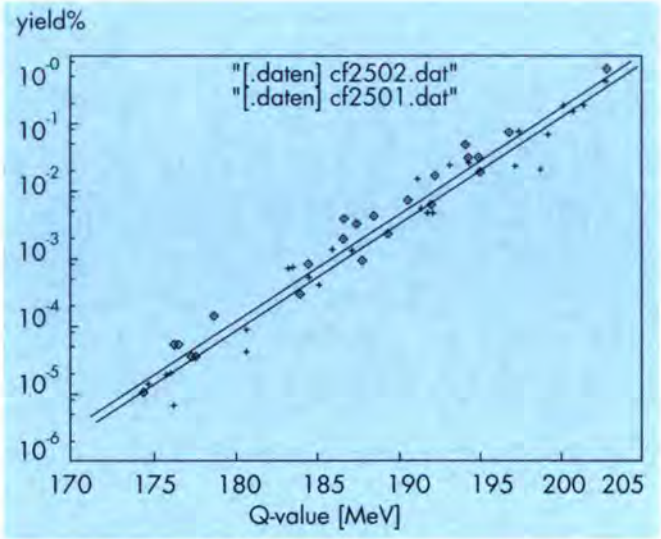


Fig. 3: Correlation plot of the log yield against the Q-value for the reaction ^{249}Cf(n_{th},f). The straight line is a fit to the data.

Nuclear Charge Determination in Spontaneous Fission of ^{248}Cm

A classical domain of study on nuclear fission at the ILL is the determination of nuclear charge distributions in the process. During the last few years proton odd-even effects in charge distributions have been established in ^{230}Th, ^{234,236}U, ^{240}Pu, and ^{250}Cf using thermal neutron induced fission at the LOHENGRIN spectrometer. In these measurements a correlation between the fissility parameter and the magnitude of the proton odd-even effect was established. From earlier mass distribution measurements in spontaneous fission decay evidence was however found that this correlation should undergo a breakdown for fission of the Cm-isotopes [6].

In order to verify this evidence it was decided to measure spontaneous fission of ^{248}Cm with the techniques used so far at the ILL for neutron induced reactions. For this purpose the ionization chamber from the Lohengrin spectrometer was modified to reject α-particles, which constitute the overwhelming background, by insertion of a third anode. This anode allows, via the strongly different ranges of fission fragments and α-particles, a discrimination and a strong inhibition for the α pile up. In a first run, coincidences between fission products and X-ray production have been measured which should allow for the calibration of the nuclear charge measurements. The coincident fission X-ray spectrum is shown in Fig. 4. The nuclear charge measurements proper have just started. Fig. 5 shows the calculated nuclear charge separation which can be expected applying our experimental method. It demonstrates that, if a considerable proton odd-even effect were to exist, we should be able to detect it. The difficulties of the measurement lie in the low fission countrate, the high α-background and the fact that we operate at the limit of the nuclear charge resolving power of our ionization chamber.

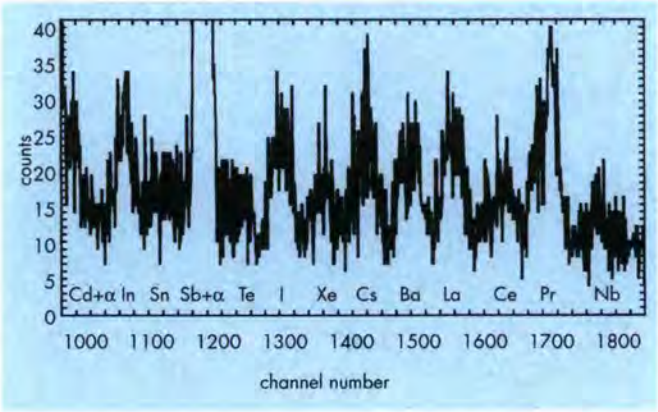


Fig. 4: X-ray coincidence spectrum for $^{248}Cm(sf)$.

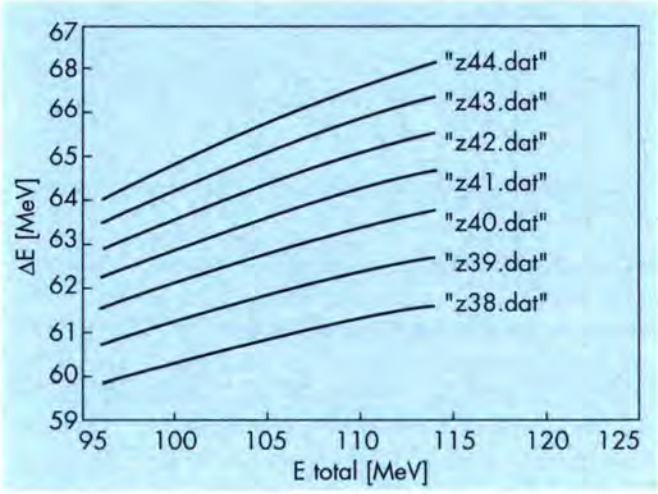


Fig. 5: Expected charge resolution for the spontaneous fission reaction of ^{248}Cf.

At PN3
GRID measurements

The GRID technique involves the measurement of the Doppler broadening of γ-rays emitted when a nucleus decays in-flight following recoil induced by the emission of prior γ-rays. To measure the very slight broadening requires the ultra-high resolution two-axis flat crystal ILL spectrometer GAMS4, which can measure γ-rays in the MeV region with a FWHM dE/E of ≈ 2ppm. The observed Doppler profile depends on the lifetime of the decaying state, the recoil velocity distribution which is determined by the feeding paths to a given level, and the slowing down in the target.

^{114}Cd

The nucleus ^{114}Cd has long been of pivotal importance in the study of vibrational excitations of spherical nuclei and of the coexistence and mixing of vibrational and intruder levels. The experimental underpinnings for this are some low lying states reminiscent of a near-harmonic vibrator, amidst others that cannot be easily understood. For example, in the 2-phonon vibrational triplet region, near 1200 keV, a compact quintuplet of states contains extra 0^+ and 2^+ states. While these states are often described as 2p-2h proton intruder excitations (leading to 2p-4h proton states) which mix thoroughly with the vibrational states, other interpretations have involved mixed symmetry modes and 3-phonon structures in a highly anharmonic vibrator.

The unique capabilities of the GRID technique have been exploited to measure lifetimes in ^{114}Cd (Brookhaven, Worcester, Notre Dame, ILL collaboration), shedding light on whether multi-phonon states can exist or if they are fragmented by Pauli effects and mixing: lifetime measurement of levels near 2 MeV in ^{114}Cd gave quantitative evidence for collective 3-phonon vibrational states [7].

148-152Sm

The transition from spherical to quadrupole prolate shapes in the Sm isotopic chain, that occurs near N=88,90, has attracted much attention both from experimental and theoretical investigators. Absolute transition rates, in particular of E1 transitions from the decay of low-lying negative parity states, are sensitive quantities which show a dramatic change in the nuclear structure across the transition region and are therefore a decisive test for the reliability of different models. In particular the Interacting Boson Model (IBM) was proved to be a versatile model, capable of explaining this transitional region simply. The E1 absolute transition rates and branching ratios were successfully explained in the framework of the sdf-IBM by introducing additional two-body terms in the operator. To date, the comparison between model predictions and experiment was restricted to branching ratios and $B(E1;1^- \rightarrow 0^+)$, due to the lack of empirical absolute transition rates for the decay of 3^- states. The purpose of the investigation was therefore to observe lifetime values of the 3^- and 1^- levels in ^{148,150,152}Sm employing the GRID technique. The experiments were done using the same sample of natural Sm_2O_3 for all isotopes. This was convenient since the isotopic composition of natural Sm allowed for the simultaneous investigation of the three different isotopes: whereas ^{148,150}Sm was produced via the classical (n,γ) reaction, ^{152}Sm was obtained via successive neutron captures starting from ^{150}Sm (^{150}Sm is unstable but has a large capture cross section of 15000 b).

The $B(E1;3^-\rightarrow 2^+)$ transition rates obtained were compared with the corresponding $B(E1;1^-\rightarrow 0^+)$ values and interpreted in the framework of the IBA-sdf model. It was found that, whereas the qualitative behaviour of these absolute transition rates can already be described considering only the one-body part in the E1 transition operator, a more complex form including two-body terms has to be employed to explain simultaneously all available experimental data (e.g. branching ratios).

Interpretation of GRID profiles

First principles Molecular Dynamic (MD) simulations were employed to describe GRID profiles (Helsinki-ILL collaboration). This technique is a new technique in the analysis of GRID lifetimes and demonstrates the interplay between the nuclear physics and solid state physics necessary for reliable results. Compared to the lifetime values obtained with the mean free path approach (MFPA) used in the previous analysis of GRID data, one obtains an overall reduction of ≈30% in lifetime values for the cases studied e.g. GRID profiles from transitions in ^{36}Cl, ^{49}Ti, ^{54}Cr, ^{57}Fe, ^{59}Ni and ^{61}Ni. The difference is mainly due to the velocity distribution (MD, see Fig. 6) and mean velocity (MFPA) description of the slowing down.

At the Cold Polarized Neutron Beam Facility PF1(PN7)

BILL at PF1 - Search for a 17 keV heavy neutrino

At the beginning of the repair of the reactor, the second magnet of the high resolution electron spectrometer BILL spectrometer was removed from the reactor platform and reinstalled at the end of the neutron guide PF1. New applications of the spectrometer are possible in this position. A special feature will be the feasibility of coincidence experiments in combination with the neutron guide facility.

In 1985 J.Simpson observed an anomaly in the β-spectrum of ^{3}H. He explained this anomaly with the admixture of a heavy neutrino with a mass of 17 keV/c^2 to the electron. Since then a controversial debate about the existence of this heavy neutrino has been going on.

The great interest in finding neutrino masses is stimulated by the desire to identify short-comings of the standard model of the electroweak interaction as a first step towards a new more unifying theory. A neutrino with a mass of 17 keV is not reconcilable within the standard model of the electroweak interaction and the standard model of cosmology. Recently, strong efforts went into developing models beyond the standard model which try to include a 17 keV neutrino in a consistent way. Simpson's first observation of a 17 keV neutrino, which emerged as a kink in the shape of the β-spectrum of ^{3}H, was questioned by other experimental groups. They did not observe any comparable kink-like destortion in their spectra. In 1991 A. Hime published new data of the b-spectra of ^{35}S and ^{63}Ni, which he claimed supported strongly the existence of the 17 keV neutrino with an admixture of $\sin^2\Theta \approx 0.008$. Owing to the high significance of his results, it was considered as the strongest indication of a 17 keV neutrino. A few other positive findings of the 17 keV neutrino were reported but with less significance.

At the same time no evidence for a 17 keV neutrino was observed in a first ^{177}Lu experiment with the BILL spectrometer at the ILL. Due to background uncertainties in the inpile configuration, the sensitivity of this experiment

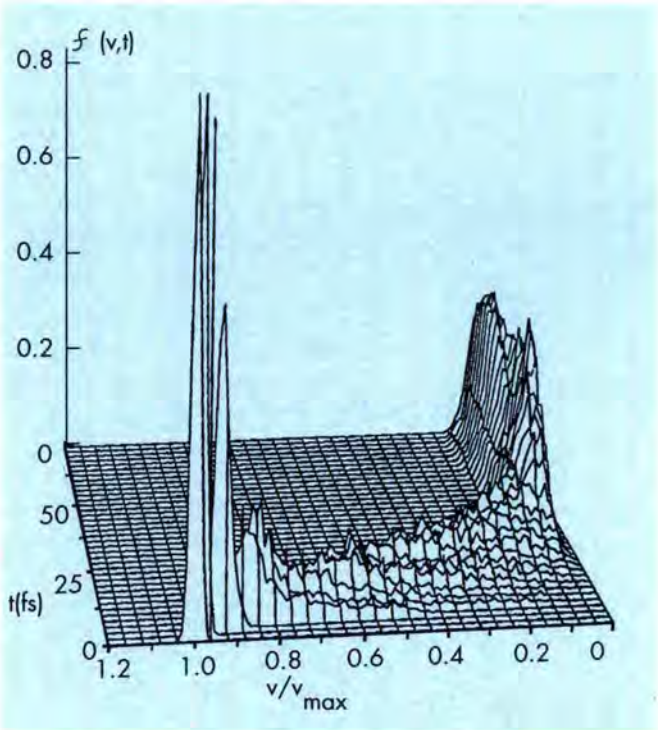


Fig. 6: Velocity distribution f(v,t) of ^{59}Ni atoms recoiling in crystalline nickel. The initial recoil velocity V_{max} was 3.3x10^4 m/s.

was not high enough to exclude the 17 keV hypothesis with sufficient high confidence [8]. An important point seemed to be that the positive findings only occurred with solid state spectrometers, while none of the magnetic spectrometer experiments could confirm them. Countering the negative results it was argued that the sensitivity to small admixtures of a heavy neutrino is limited by systematic uncertainties with instrumental shape corrections. On the other hand, since the response of a solid state detection system to monoenergetic electrons yield a strongly asymmetric pulse height distribution, a kink in these solid state detector experiments is only visible after the spectrum is deconvoluted with this response function. Very recently Hime explored the question of whether electron scattering effects could feign a heavy neutrino emission in the experiments using silicon detectors. For the reanalysis of the Oxford ^{35}S and ^{63}Ni data he used a simulated electron response function. No shape distortion was visible any more. With this reanalysis the strongest argument 'pro the 17 keV neutrino' disappeared. For a final resolution of the 17 keV problem an important step will be the lutetium experiment now running at the modified BILL spectrometer.

A first experiment in the new position has already been carried out using an external neutron activated ^{176}Lu Target. It aims at an improved search for an hypothetical 17 keV neutrino. The advantage of using an external Lutetium source is the reduction of the background compared to the inpile target position of the first Lutetium experiment. The high energy of the investigated electrons

(the kink should appear at about 480 keV in the β-spectrum of ^{177}Lu) makes energy dependent instrumental efficiency corrections negligible. The energy resolution of the BILL spectrometer is about 300 eV at 500 keV. This has to be compared with 1000 eV at 150 keV of Si(Li) detectors used in the experiment of Hime. Consequently a 17 keV neutrino with an admixture of $\sin^2\Theta \cong 0.008$ to the electron neutrino should already emerge in the raw data of the Lutetium BILL experiment.

The removal and modifications of the BILL spectrometer were sucessful. Two ^{176}Lu targets were neutron activated at the SILOE (CENG) and have been measured so far detecting about 10^6 counts/keV in the energy range around 480 keV. To demonstrate the spectrometer's sensitivity to small shape distortions, we scanned the energy range around the beginning of the second β-branch, which ends 113 keV below the endpoint of the main branch (Fig. 7). Even though the second β-branch has a different shape in comparison to a branch originated by a heavy neutrino, the magnitude of deviation is comparable to a heavy neutrino branch with an admixture of 1 %.

In Fig. 8 the spectra is shown from 390 keV upto the endpoint in the Kurie representation. No curvature of the slope is visible, so no shape corrections have to be applied. In the data analysis which is now under progress neutrino masses up to 100 keV with an admixture of a few per mill will be tested and a final elucidation of '17 keV Conundrum' seems to be feasible.

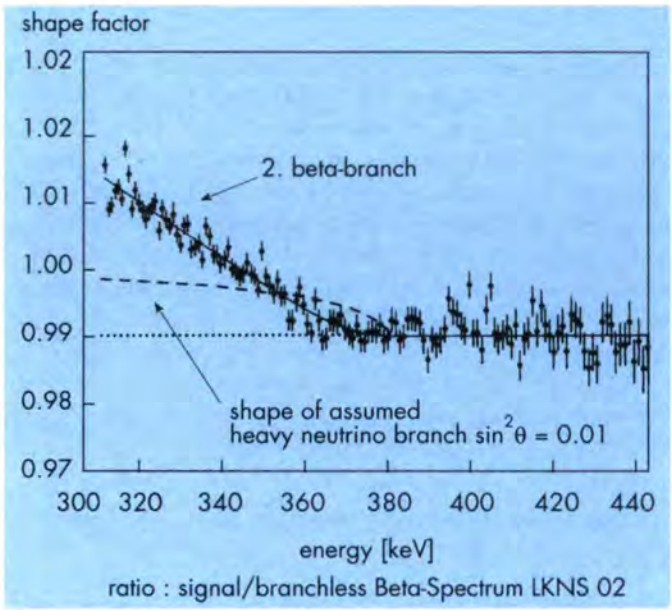


Fig. 7: Kurie plot of a single spectrum of ^{177}Lu(e$^-$)^{177}Hf. To demonstrate the sensitivity of the instrument, the energy range around the second β-branch is shown. The ratio of the data to a branchless theoretical β-spectrum, normalized above 385 keV is plotted. The solid line describes the spectrum with a second β-branch. The shape of an assumed heavy neutrino branch is inserted.

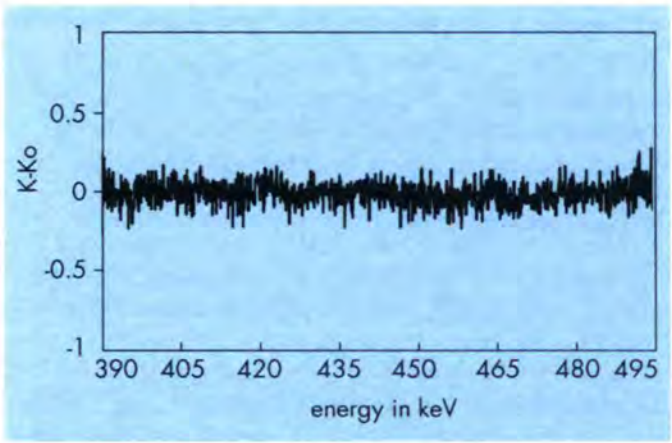


Fig. 8: Kurie representation of one spectrum. K0 is the theory Kurie function. No curvature of the slope is visible, so no efficiency corrections have to be applied.

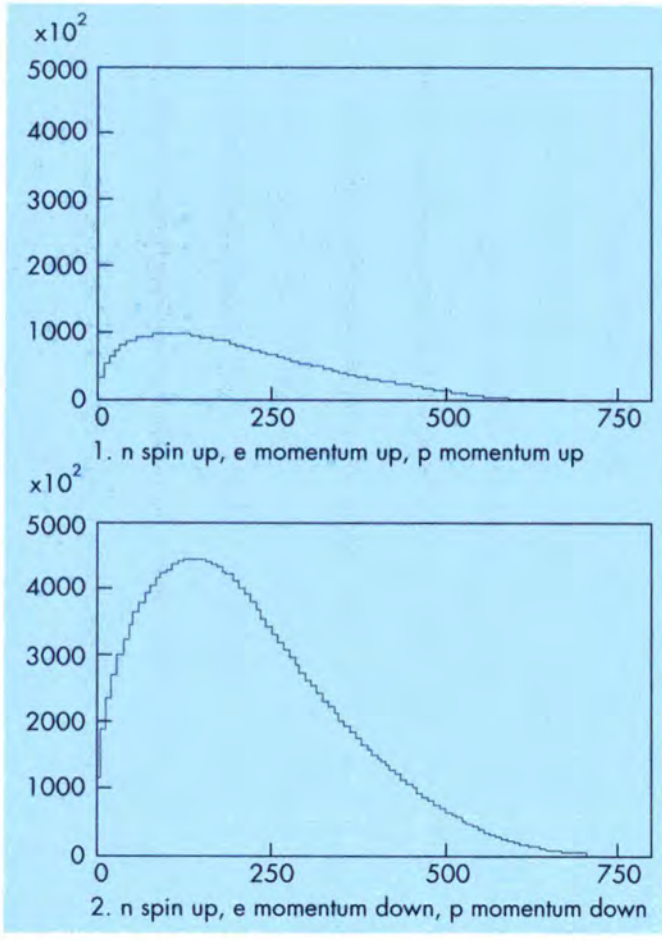
Neutron Decay Experiments at PF1

Within the framework of the Standard Model (SM) in its "allowed low energy approximation" the dynamics of the neutron weak interaction is completely determined by the two "weak" coupling constants g_A and g_V. The neutron lifetime and angular correlation coefficients are functions of these constants. Recent experimental results give a hint that this simple picture might not be quite correct. Although the evidence for a deviation from the Standard Model is not very firm there is a number of possible extensions to it which would improve the situation. One hypothesis is that there are small contributions from right-handed currents. A simple version of such an extension, the "manifest left-right symmetric model", has already been ruled out and more sophisticated theoretical approaches are clumsy and destroy the natural beauty of the SM.

There is a need for new high precision measurements of the neutron lifetime and the major angular correlation coefficients. In preparation for the future neutron beta decay experiments with the PERKEO II spectrometer at PF1, extensive Monte-Carlo simulations of the decay events were performed. The goal was to calculate energy spectra and angular distributions of the daughter particles under various coincidence conditions and values of g_A and g_V. As an example, Fig. 9 shows the energy spectra of the decay electrons for various combinations of emission directions of the proton and the electron in relation to the neutron spin.

These energy spectra can be combined to form an asymmetry function like the one shown in Fig. 10. The PERKEO II program will include attempts to measure many different asymmetry functions and to extract the decay parameters from them.

At the end of 1992 a spin rotation experiment on ^{207}Pb, originally planned to be performed earlier this year at the ILL, was set up at the HMI Berlin. It is a continuation of a pioneering experiment carried out in 1982 at the ILL by Heckel et al., who studied natural lead. The new experiment is trying to determine the origin of this particular case of parity violating spin rotation effect by measuring the contributions from different isotopes.



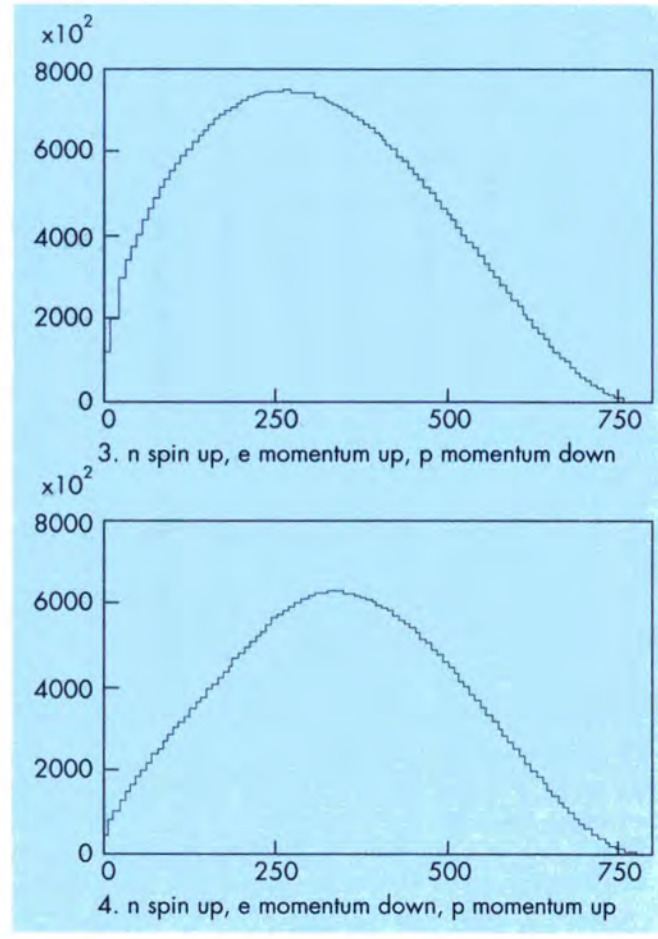


Fig. 9: Decay electron spectra for various combinations of electron and proton direction with respect to the neutron spin. The neutron spin is always pointing up.

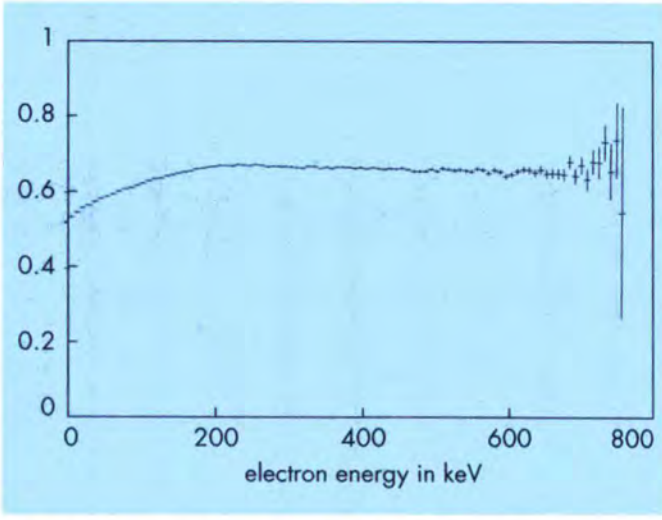


Fig. 10: Asymmetry function from a combination of spectra 1) and 2) from Fig. 9 according to (spectrum2-spectrum1)/ (spectrum2+spectrum1).

$n - \bar{n}$

The neutron-antineutron oscillation experiment is now terminated and has been dismantled. During the last year the background has been thoroughly analysed. No background event resembling the signature of an antineutron annihilation has been observed. The result for the oscillation period is likely to be in excess of 9×10^7 s (with a 90 % confidence limit). Although this value represents an increase of two orders of magnitude of the previous values, it is still consistent with the theory of Mohapatra.

At the Ultra-cold Neutron Facility PF2

UCN source

The UCN facillity PF2 on level D will profit from the refurbishment of the reactor. The vertical cold source and the vertical neutron guide which links the cold source to the UCN turbine on level D have been removed. This provides an opportunity to inspect the guide and to make such repairs as seem necessary. The automatic UCN beam changer for PF2 will be equipped with new electronics which conform to ILL standards.

EDM

A new magnetometer using mercury atoms being developed at ILL (Sussex-RAL-ILL-Washington-Harvard collaboration) which is needed for the next generation ILL measurement of the neutron electric dipole moment, has now reached the necessary statistical precision of $2x10^{-9}$ gauss rms on 2 minute measurements of the volume average magnetic field in a 22 litre cell (See the Special Instrument Group Section).

MAMBO II

The experiment MAMBO II (T.U.Munich - ILL collaboration) is in the final state of mounting and adjusting the apparatus. The aim of this experiment is to measure the neutron lifetime with a precision of one second using the method of storing ultra-cold neutrons in a liquid coated glass trap with variable volume. This successful technique was developed at the ILL [9,10] and the experience gained with the previous version provides the basis for this new design.

S51-INAA: Geology

This year the Geology Group has, thanks to the intermittent operation of SILOE at the CENG, been able to continue its work using neutron activation analysis of rock samples. We had to adjust to the different irradiation conditions, not only in terms of sample spectra, but also because SILOE has a much more complex neutron flux spectrum than the HFR.

Studies were continued on rocks from the Andean chain of South America, notably

on a series of modern volcanics from Southern Peru. Closer to home rare earth and trace elements have been measured on a series of volcanic and plutonic rocks from the Briançonnais area on the Franco-Italian border. Results have shown that during Permo-Triassic times (280-225 Million years B.P.) this part of France was in fact a mountain chain, lying above a subducting plate just as the Andes are today.

Secretary: U. Mayerhofer

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ILL Workshop on High Resolution Gamma Ray Spectroscopy

From the 5th to the 7th of October, 1992 a workshop on "Applications of High Resolution Gamma Ray Spectroscopy to Atomic Collisions and Nuclear Lifetimes" was held at the ILL. The topics of the workshop were centred around the applications of GAMMA RAY INDUCED DOPPLER BROADENING. Targets placed in the High Flux Reactor serve as sources of gamma rays following neutron capture reactions. For their analysis the instrument GAMS4 at ILL, a double flat crystal spectrometer run as a collaboration between the American N.I.S.T., Gaithersburg and the ILL, is currently the worlds highest resolution gamma ray spectrometer over an energy range 0.5 to 5 MeV. The best resolution obtained to date is close to 3 ppm. Based on this outstanding energy resolution the so-called GRID-technique (Gamma Ray Induced Doppler Broadening) was developed: after capture of a thermal neutron and the subsequent emission of a primary gamma ray the nucleus has an initial recoil velocity v where $v/c = 10^{-5} - 10^{-4}$. The kinetic energy of between 1 and 500 eV is dissipated by interatomic collisions (or, at very low energies (eV) by lattice vibrations) in the solid target within 10^{-12} s. If the level populated by the primary transition has a short lifetime of $10^{-17} - 10^{-12}$ s then the subsequent secondary gamma ray exhibits a Doppler broadened line profile which after measurement at high resolution yields information on the lifetime of the level and the slowing down process (see also ILL Annual Report 1988, "blue box contribution").

The aims of the workshop were manifold: design and performance of the GAMS4 spectrometer and its planned improvements (R.W. Deslattes and E.G. Kessler, Gaithersburg) were presented. It was demonstrated (R.W. Deslattes) that there might still be the possibility for an even greater improvement in resolution. A summary of the lifetime results which have been obtained with the GRID-method and/or their impact on nuclear physics (H.G. Börner, Grenoble, J. Jolie, Fribourg, and R.F. Casten, Brookhaven) were given. In this context it was pointed out that even for medium-heavy and heavy nuclei with complicated gamma ray cascades, important questions of nuclear structure can be answered (A. Jungclaus, Grenoble/Göttingen, R.F. Casten, Brookhaven). On the other hand it might be possible to test certain aspects of statistical model approaches (F. Becvar, Prague). An exhaustive overview of other methods for measuring nuclear lifetimes was given (J. Sharpey-Schafer, Liverpool) and finally the GRID method was directly compared to some of the more classical lifetime methods (J. Keinonen, Helsinki, T. Belgya, Lexington, C. Wesselborg, Giessen, H.H. Pitz, Stuttgart, V.T. Kupryashkin, Kiev, A.I. Fioktistov, Kiev and S. Raman, Oak Ridge).

Of special interest were the results obtained from Molecular Dynamics simulations of GRID slowing down data (A. Kuronen, J. Keinonen, Helsinki; K.H. Heinig, Dresden) which broaden the field of applications of the GRID-technique.

With the 1994 restart of the ILL reactor in view, it was also important to think about as yet undeveloped applications of the GRID-method. These might lie in "in situ" studies of anisotropic single crystal targets (K.H. Heinig, Dresden), multilayers (W. Bolse, Göttingen, A. Traverse, Orsay) and of targets with a controlled defect structure (T. von Veen, Delft).

Some areas of work which are closely related to the interests of the workshop were presented: The computation of accurate interatomic potentials (R.M. Nieminen, Helsinki), material studies using the nuclear resonance fluorescence (R. Moreh, Beersheva), molecular break-up in collisions at ~100 keV energies (W. Neuwirth, Köln), channelling experiments with cooled relativistic heavy ions (H. Geissel, Darmstadt), and neutron facilities which will be available at the refurbished neutron beam reactor in Budapest (G. Molnar, Budapest), were discussed.

A final summary (P. Lieb, Göttingen) gave some pointers to where the GRID-method might go next: its unique and increasing capabilities could lead to further highly interesting results in the future. In the past the interdisciplinary character of the GRID-method has already made GAMS4 one of the most sought-after instruments at the ILL.

H. Börner

The Neutron Electric Dipole Moment

M. Pendlebury

The size of the neutron electric dipole moment (EDM) is a significant constraint on new developments in particle physics theory. The EDM first came into prominence with the measurement made by Smith, Purcell and Ramsey in 1951, which gave the result $d_n = (0.1 \pm 2.4) \times 10^{-20}$e cm. At that time the experiment was seen as a search for a particular handedness in the neutron. However, theorists soon pointed out that, for an EDM to exist, the internal forces of the neutron have also to be asymmetric under the reversal of the sense of time, a property which at that date was thought to be even more unlikely than having a particular handedness. There were some who thought the experiment was so speculative as to be a waste of time, but Ramsey argued that such symmetry questions should be answered by experiments not by prejudice. Six years later, with the discovery of parity violation, neutrons in nuclei were indeed found to have left-handed properties, and thirteen years later, K° mesons were found to be influenced by a force which was almost certainly asymmetric with respect to time reversal. Since then, much effort, in several places, has gone into improving the measurement of the EDM. Particularly in the last ten years, the results have played a significant role in the development of particle physics theory. The most precise EDM measurement at the ILL with a neutron beam was completed in 1977. The most precise EDM measurement using ultra-cold neutrons, was carried out at ILL using the PF2 source on level D and was published in 1990 [1] as $d_n = (-3 \pm 5) \times 10^{-26}$e cm. The number of citations has already exceeded 100. By 1992, a result with similar precision $(+3 \pm 5) \times 10^{-26}$e cm had been published by the Russian group using the UCN source at PNPI, Gatchina, near St Petersburg. A new project at the ILL aims to reduce the uncertainty of the measurement by another factor of five.

If the neutron had a maximal dipolar shape distortion, the EDM would be about 3×10^{-14}e cm. From the latest measurements, it is already clear that the dipolar shape distortion is only one part in 3×10^{11} or less. This is equivalent to adding a layer, less thick than a human hair, to one hemisphere of the Earth. How does it come about that such a small effect can stimulate so much interest? The short answer is that it has an important connection with the basic forces of nature. The neutron is believed to contain three quarks bound together by the 'strong force' generated by the exchange of gluons. The quarks carry electric charges and are also acted upon by the electromagnetic forces which modify the structure by about 0.1%, and with the spin motion, create the magnetic moment. These, the most important forces, are symmetric with respect to left-handedness and right-handedness and do not act differently when time is run backwards. For these reasons they could not cause the neutron to have an EDM.

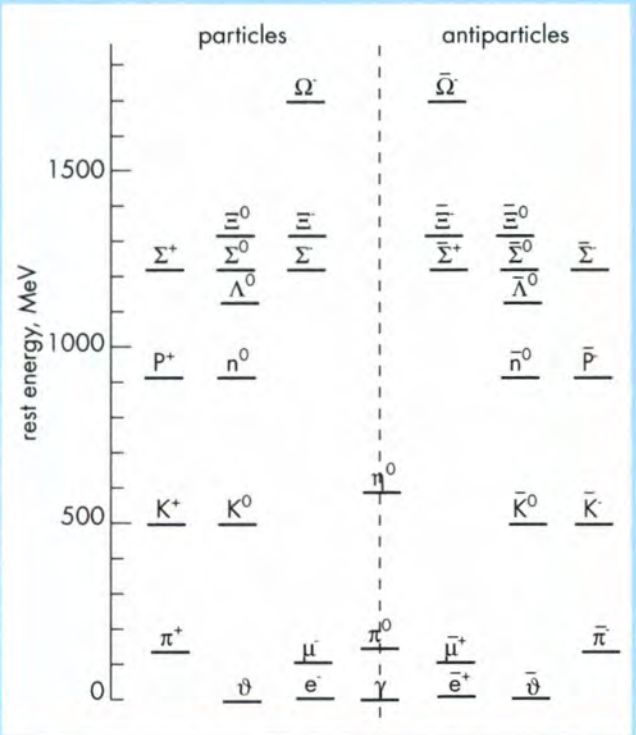

Fig. 1: The lighter particles. All those less heavy than the proton soon decay, to leave some combination of positrons, electrons, neutrinos and photons. All those which are heavier than the neutron soon decay to leave a proton or a neutron and some combination of the leptons and photons just mentioned.

The 'weak force' which is 10^7 times weaker than the strong force also produces a tiny distortion of the structure. Its most striking effect, however, is to cause the neutron to decay into a proton and electron and an antineutrino. On the time scale of internal particle motions, the decay is very slow because the force is so weak. The average lifetime of a free neutron is 888 s. The disposition of the product particles relative to the neutron spin axis, shows the weak force is left handed, but that it is unchanged by reversing the direction of time and could not cause the neutron to have an EDM.

There is evidence from just one elementary particle, the K° meson, which shows that there is also a 'very weak force' which is about 3×10^{12} times weaker than the strong force. It has some very distinguishing features. It is asymmetric under what is called the CP operator and, therefore, with most reasonable assumptions, under the reversal of time. It also has a handedness and is

parity violating like the weak force. Thus it has the two essential ingredients to cause the neutron (and other particles) to have an EDM. From its strength it could, in some types of theory, give the neutron a dipolar shape distortion of about one part in 3×10^{12} and an EDM of 10^{-26}e cm. This is just the expected resolving power of the next ILL experiment.

There is no doubt that this very-weak or 'CP violating' force exists although it has not yet been identified in any other system. (C replaces particles by antiparticles and P is the parity operator which will change a left-handed helix into a right-handed helix). The CP violating signature found in 1964 by Christensen et al. [2] is very clear cut; the K_L° meson decays mostly into three pions, but, crucially, with a branching ratio $\varepsilon_K = 2.26 \times 10^{-3}$, it decays into two pions for which the final CP eigenvalue is opposite in sign to that for the three pion case. (L means the longer lived of two species of K°). Even the main branch of this decay is a weak process, so the small branch corresponds to a very weak 'CP violating force' of relative strength more than 5×10^9 times weaker than the strong force. But that is not the end of the matter; it turns out that the weak branch comes mainly from a small CP impurity, of amplitude ε_K, in the original K_L° state where the basic CP violating force has produced an enhanced effect; so the underlying force is even weaker still. To know the true strength, one has to calculate the enhancement factor, and this requires a knowledge of the quark structure of the K° meson which is only just now becoming well enough defined for the purpose. (Analagous enhancements are seen in some states of nuclei where admixtures of the 'wrong' parity can be as much as 10^4 times larger than expected from the basic strength of the weak force). As an alternative approach, there has been a series of experiments at CERN and at Fermi Laboratory, on a different feature of K° decay, aimed at measuring the amplitude of the CP violating force directly without enhancement. The difficulty is that they are then trying to measure the amplitude, called ε' which is smaller than the already small ε_K by the enhancement factor. For the K° meson, both the theorists, and the experimenters, now agree that the enhancement must be at least 500 in place of the first estimates of 100. The change, in the theory case, follows mainly from the upward revision of the mass of the top quark which can now be estimated to within about 20%. In turn, the CP violating force strength is now seen to be about 3×10^{12} times weaker than the strong force (and 5 times weaker than estimated ten years ago). This makes the task of the K° meson experimenters harder than they expected. At the last round of e' measurements in 1991 the combined result from the two groups was $\varepsilon' = (3.3 \pm 1.1) \times 10^{-6}$ (relative to the weak force) and was in agreement with the theoretical predictions. It will probably take one more round of K° meson experiments to obtain a result which is resolved without doubt. The feature which has to be measured is a small difference between the rates of production in K_L° decay of $\pi^+ + \pi^-$ and of $\pi^\circ + \pi^\circ$. In each case the CP change involved can occur by two different paths (i) in the original state and not in the decay, (ii) not in the original state, but in the decay. The amplitudes for the two paths are proportional to ε_K and ε' respectively. The two amplitudes interfere in the final state, constructively for the charged pions and destructively for the uncharged pions. The net effect is a small fractional difference of $6\varepsilon'/\varepsilon_K$ in the production rates.

Correspondingly, over the last ten years, those predicted neutron EDM values which depended on the strength of the CP violation force seen in the K° meson, have also been reduced by a factor of five; to this extent, the goal posts for the experiments have been moved!

What about the sensitivity of other kinds of experiment to look for CP violation? It looks now as though the CP violating force is 3×10^5 times weaker than the weak force. Most experiments looking for small T (or CP) violating features in weak processes, such as neutron decay, have difficulty in resolving effects which are less than 1 part in 3×10^4; so they may not see anything unless there is some enhancement or unless they come upon some new mechanism of CP violation not revealed in K° meson decay. As mentioned below, other mechanisms are not unlikely.

One might now reasonably ask why is a force, which is as small as the CP violating force, so interesting? Mainly because of its special symmetry properties which means that it probably has something important to tell us about fundamental particles. Certainly, earlier studies of the weak force, discovered in 1957, led to the very successful theory called the Standard Model and the prediction of the existence of the heavy W^+, W^- and Z° bosons.

Perhaps the CP violating force can also explain a vital feature of the Cosmos. Soon after the force was discovered, Sakharov, in 1967, realized that its time reversal asymmetry property, could provide an explanation of the particle-antiparticle asymmetry problem [3]. In principle, it could cause a small difference between forwards and backwards reaction rates between particles and antiparticles in the fire-ball of the 'big bang' which was the birth of the Universe. This could then lead to a difference in the numbers of particles and antiparticles existing at the final non-equilibrium stage of the fire-ball. Later, the fireball cooled further and particles annihilated with antiparticles making finally only heat radiation. But, because their numbers were not exactly equal, differing by about one

part in 10^9, this tiny fraction of particles was left over to form the material from which we are made. The original numbers of neutrons and protons, before annihilation, can be calculated from the 3 Kelvin cosmic background radiation which is all that is left from them. Of course, one may ask whether the tiny particle excess was caused, not by some asymmetry in the fundamental laws, but just by statistical chance. On spinning a coin which is quite symmetric, many times, one generally obtains a different number of heads from tails. However, the mathematics of this situation is well understood, and the observed particle-antiparticle asymmetry seems to be many orders of magnitude too big to have occurred through statistical fluctuations.

A further point is that the CP violating effects which are important for this genesis of matter are those which occur in the neutron and the proton. The K° meson is unstable and soon decays giving finally massless photons and neutrinos. It is now believed there may be as many as three different CP violating force mechanisms. This complicates the question of relating the CP violation in the K° meson to that in the neutron. One mechanism might be dominant for one while a different one dominates in the other. This reinforces the notion that the neutron EDM is much more relevant to the Sakharov theory than is K° meson decay. Indeed, it has been shown that, to produce the observed amount of matter, the neutron EDM must be at least 3 x 10^{-28} ecm [4].

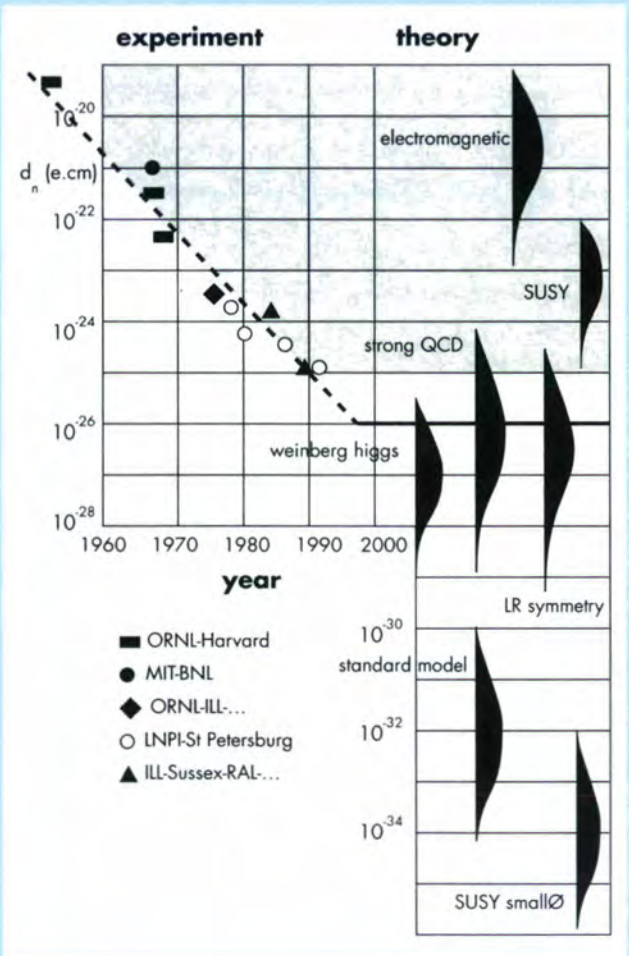

Fig. 2: The progress, over the last few decades, of the experimental results for the size of the neutron EDM in relation to various groups of theoretical predictions.

The Sakharov theory also requires the existence of reaction processes which, in high energy collisions, allow antiparticles to convert into particles and vice versa. Such processes appear naturally in 'grand unified' theories which build on the already successful electroweak unification by adding to the W^+, W^- and Z° bosons some much heavier X bosons. Evidence for such mechanisms has been sought with proton decay experiments and, at the ILL, with the N-$\tilde{N}$ experiment. The results are not positive, but they do not rule such processes. The choices in grand unification theory have simply been reduced, which is useful progress. Recent high precision scattering experiments at CERN have, in fact, lent new support to the idea of grand unification.

The Standard Model of strong and electroweak interactions (excluding grand unification) with its scheme of twelve spin half fundamental fermions plus their corresponding antiparticles and the spin one force agents, the gluons, the photon and the W^+, W^- and Z° bosons, is remarkably successful in accounting for a large domain of experimental results. Nevertheless, it has very little to say on some matters such as particle masses and gravity so it seems very unlikely to be complete. It is successful in accommodating a weak CP violating force for K° meson decay and the enhancement factor $\varepsilon_K/\varepsilon'$ referred to above. The most uncertain part of the model concerns the strong force and the way it arises from the gluons as described by the theory of Quantum Chromodynamics (QCD) which leads to very difficult calculations. Those who like to be more conservative often refer to the Standard Model of electroweak interactions only. The latter predicts a neutron dipole shape distorsion of only two parts in 10^{18} because only second order terms can be found to contribute an EDM. These involve one weak and one CP violating interaction and the EDM produced is 10^{-33}e cm. In this case CP violating in the neutron is much too small for the Sakharov argument to be successful. Almost any attempt to enlarge this minimum Standard Model, as by adding particles which could, at high energies, restore symmetry between left and right handedness (left-right symmetric models) and/or between fermions and bosons (supersymmetric models) leads to a situation in which the EDM can be created in first order, with the size of

about 10^{-26}e cm mentioned earlier. Thus, the question of whether the EDM is, big enough to be resolved experimentally, or much too small to be resolved, has seemed to be a very good test for the existence of some kind of extension, or, as it has often been said, a good test of 'new physics'.

As these more elaborate models have been studied in more detail in the last few years, including some useful inputs from string theories, it has become more evident that it is not at all easy to create models which can be reconciled with all the existing data from high energy physics. The one class of models which claims to escape naturally from most of the traps is that of supersymmetry (SUSY) within which there are two distinct mechanisms for CP violation. One involves a 'weak' mechanism to do with quark flavours (types) and one involves a 'strong' QCD mechanism concerned with coloured gluons. For quite some years theorists concentrated on the 'weak' term because K° meson decay seemed to concern the weak interaction, also this theory was better understood and easier to handle. The predicted neutron EDM was 10^{-22} ϕ e cm where ϕ seemed as though it should be about unity. However, by 1989 the EDM results were embarrassing this theory by forcing the value ϕ down to 10^{-3}. It also began to emerge that concentrating on the weak term was probably a mistake and that the larger CP violation effects might come from the QCD term [5]. An important 1989 theory paper was able to show that for an attractive range of the models the QCD term had to give an EDM at least 10^4 times larger than the weak force term [6]. In this situation the experiments constrain the QCD term to be less than 10^{-25}e cm which means that the weak term has to be less that 10^{-29}e cm. Thus ϕ has to be very small ($< 10^{-7}$) indeed so small that there has to be a particular reason. A similar situation existed earlier; the QCD term is calculated to give an EDM of 3×10^{-16} θ e cm, where the earlier models would expect θ to be about unity, but the EDM from experiment forces θ to be less than 10^{-9}. In the absence of a good reason to make θ so small, arguments had been made to suggest that $\theta = 0$, ruling out the QCD term altogether. Now, with the new arguments, it seems that the experimental result for the EDM forces both of the parameters ϕ and θ to be very small. But these parameters cannot all be zero or there would be no CP violation! Again, under strong influence from string theory, there is now an attractive group of supersymmetry models emerging which are known as N = 1 supergravity theories. Within these there is a rationale, based on the long standing and attractive idea of spontaneous symmetry breaking, which makes the values of both θ and ϕ to be about 10^{-11}. Then the contributions to the neutron EDM are 3×10^{-27}e cm and 10^{-33}e cm for the strong and weak mechanisms respectively. The dominant one is just the size needed for the Sakharov argument to give the right amount of matter [4]. Perhaps there is something in this. This size of EDM should be resolvable, but perhaps not in the next experiment, unless there is some enhancement of the EDM to help. Unfortunately, calculations of the QCD contributions to ε' have still proved too difficult to obtain a meaningful result, although this must surely change as more effort is applied to the problem in the near future.

Finally, what about the EDMs of other particles? The EDM of the electron has now been measured with about an order of magnitude more precision than that of the neutron. However, the electron is a lepton for which these mechanisms concerning quarks and gluons can only appear in higher order leading to EDM contributions which are at least 10^7 times smaller than those of the neutron. In the case of the proton EDM, the measurement precision lags about three orders of magnitude behind that of the neutron, so the neutron continues to be the particle which the theorists have to watch.

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Structural and Magnetic Excitations

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General summary

The scientific life of College 4 went on through 1992 despite the full impact of the reactor shutdown. It was marked by numerous departures: W. Petry became professor of physics at TU Munich; the inavailability of neutrons made many others leave the ILL: M. Alba, J. Bossy, B. Fåk, J. L. Martinez and L. Needham. Those who stayed had to accept the role of external reactor users and look for neutron beam-time elsewhere. This task was greatly facilitated by the solidarity of colleagues at other reactor centres, we have found friendly assistance at numerous places ranging from LLB Saclay (France) to JAERI Tokai (Japan). The experimental activities themselves became dominated by the interest of the ILL scientists rather than those of external users. Inevitably, the range of topics exhibits much more continuity compared to the past than in previous years.

Two meetings during the last year, related directly to College 4 and its members, should be mentioned. In November 1991 the still quite complete three-axis group met for a 3.5 day seminar organized by J. Bossy and B. Dorner at Luberon (Provence). Each of the 15 participants presented a talk on one of the topics covering neutron scattering from fundamentals of theory to advanced instrumentation. In order to maintain a generally comprehensible level of presentations and to encourage discussions the talks were prepared by non-specialists under the guidance of a participant working actively in the given field. Indeed, lively discussions continued during the afternoon hikes into the beautifully coloured hills of Luberon.

More recently, on May 12-14, a meeting of the French neutron scattering community was organized by R. Currat, in collaboration with E. Fries (LLB). The 2 1/2-day meeting was held at La Colle-sur-Loup near Nice and was attended by about a hundred scientists. The programme included 12 review talks on instrumentation and scientific topics and 93 poster presentations. Two evening sessions were devoted to scientific policy discussions with presentations by J. Charvolin (proposals for the ILL refurbishment), J. Rossat-Mignod (proposal for extension of Orphée reactor), J. Chappert, J. Schweizer and J. Winter. The meeting, the first of its kind, was felt to be successful and a large majority of participants expressed their support for having similar meetings on a regular basis.

Scientific trends and highlights in 1992

As in previous years the activities were dominated by three major directions: high-temperature studies of phonons in bcc metals, investigations of excitations in quasi-1D materials and crystal field spectroscopy of high-T_c superconductors and heavy fermion systems.

Symmetry breaking inelastic scattering intensity in β-Zr

The lattice dynamics of the high temperature bcc phase of the group 3 and 4 metals provides insight into the mechanisms of the displacive bcc-hcp and bcc-w phase transition. These studies have been made possible by the use of a special crystal growth furnace developed at ILL. It allows us to grow the single crystals in-situ on the spectrometer and perform the neutron scattering experiment without intermediate cooling of the sample. The measured phonon dispersion relations show a strong resemblance to each other with particularly low frequency and strongly damped branches in [ξξ0] and [ξξ 2ξ] propagation directions [1]. Recent measurements of the dispersion surface in the {110} plane showed another interesting feature which is

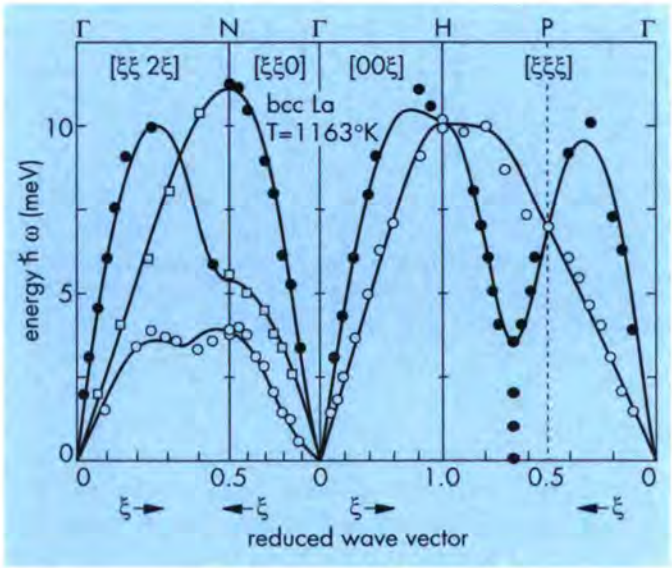

Fig. 2: Phonon dispersion of γ-La. The solid lines represent a Born-von Kármán fit including force constants up to the fifth nearest neighbour shell.

related to the pronounced anharmonicity of selected phonon branches. These experiments have been carried out at LLB in Saclay. Fig. 1 (page 102) depicts a section of the dispersion surface at an energy transfer of 1 THz in the {110} plane of β-Zr at 1333 K. The symmetry of the bcc lattice implies that the phonon dispersion can be measured at different but equivalent positions in reciprocal space. Following the one-phonon scattering law, the observable intensities scale with the square of the product of momentum transfer times the phonon polarisation and the Debye-Waller factor (DWF). In the (222) Brillouin zone there are two equivalent directions where the $T_1[\xi\xi\ 2\xi]$ phonon branch can be measured, the $[\bar{2}11]$ and the $[2\bar{1}\bar{1}]$. Along these directions the DWFs are identical for any given ξ and the products $|\mathbf{Q}\cdot\mathbf{s}|^2$ differ by only about 6% at ξ=1/3 and by a factor of 2.8 at the Brillouin-zone boundary. However, the ratio of the observed scattering intensities is about 5 at ξ=1/3 whereas at the BZ boundary it corresponds to the prediction of the one-phonon scattering law. This strong violation of the symmetry is clearly visible in Fig. 1 at ξ=1/3; a point corresponding to the dip in the longitudinal phonon branch at ξ=2/3 in the [ξξξ] direction.

Phonon dispersion of γ-La

Within the group 3 and 4 metals γ-La is the only element that transforms from a high temperature bcc phase to a fcc phase and at lower temperatures to a dhcp structure. Despite the extremely small stability range of only 53 K below the melting point, we have been able to measure the complete phonon dispersion at 1163 K [2]. Again we used our in-situ single crystal growth technique to access the high temperature bcc phase. These experiments have been performed at the IN8 spectrometer at the ILL and been continued after the shutdown at the LLB at Saclay. Fig. 2 shows the measured phonon dispersion analysed by a Born-von Kármán model with interactions up to the fifth nearest-neighbour shell. The phonon dispersion is dominated by the extraordinarily low frequency phonon modes propagating in the [ξξ0] and [ξξ 2ξ] directions. These phonons are strongly damped and close to the Brillouin zone boundary they have lifetimes of only a few vibrational periods. The polarization vectors of these phonons point into the directions of displacements towards the close-packed low temperature structures. Analysing the phonon dispersions in the fcc and bcc phase we obtain a contribution of 84% of the vibrational entropy to the total excess entropy at the phase transition. This result leads to the same conclusions as for the other group 3 [3] and 4 [1] metals, namely that the open bcc structure is mainly stabilized by high vibrational entropy caused by the low frequency phonon branches.

Elementary excitations in superfluid ^{4}He beyond the roton minimum

Inelastic neutron scattering experiments in superfluid ^{4}He beyond the roton minimum have been performed recently at LLB, Saclay. ILL has provided financial and technical support for this collaboration between ILL and CENG physicists. These experiments in superfluid and normal ^{4}He are motivated by the novel interpretation by Glyde and Griffin (GG) [4] of the nature of the elementary excitations according to which there are density excitations of zero-sound type at low wave vectors Q and single quasiparticles at larger Q's. The quasiparticles are coupled to the density fluctuations via the condensate, leading to a continuous phonon-roton dispersion curve. The GG interpretation is the first theory to describe the line shape of the neutron scattering function S(Q,E) and its dependence on temperature. High-resolution measurements were made on the thermal triple-axis spectrometer 1T1 at LLB for wave vectors between 2.3 $Å^{-1}$ and 2.7 $Å^{-1}$ at temperatures betweeen 0.6 K and 3 K, using the ILL ^{3}He cryostat. For Q=2.3 $Å^{-1}$ we observed a sharp "one-phonon" resolution-limited peak at low energy and a broad contribution at higher energy (Fig. 3a). The sharp peak disappears progressively as the temperature is raised [5], in qualitative

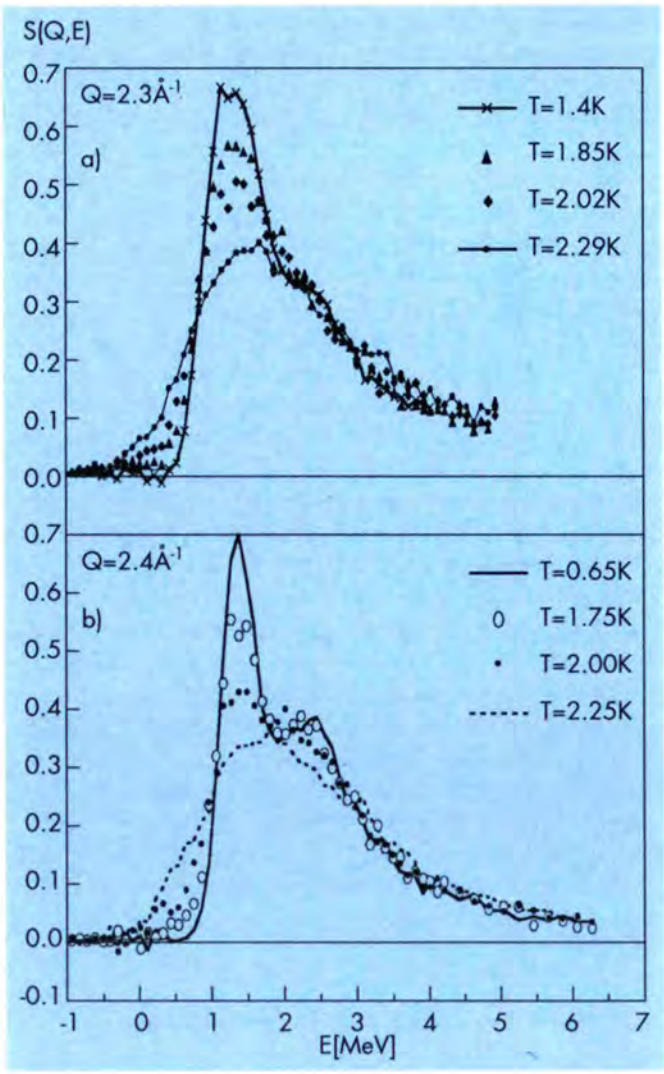

Fig. 3: Temperature dependence of the neutron scattering function S(Q,E) for liquid ^{4}He at saturated vapour pressure measured at Q=2.3 $Å^{-1}$ (a) and at Q=2.4 $Å^{-1}$ (b).

agreement with the GG theory. At larger wave vectors (Q=2.4 Å^{-1}), the sharp low-energy peak is still present, but the high-energy peak now becomes temperature dependent (Fig. 3b). The temperature dependence of the broad contribution commonly known as the scattering by the multiphonons beyond a wave vector (around 2.3 Å^{-1}) is something new. This suggests that the excitations change character, probably due to a hybridization with the multiphonons. Since the coupling of the quasiparticles to the multiphonons is not included in the GG model, further theoretical work is needed to explain the temperature dependence of the excitations in ^{4}He beyond the roton minimum.

Peierls transition in $(TaSe_4)_2I$

Transition metal tetrachalcogenides have a marked 1D metallic character due to the directional nature of the electronic orbitals (d_z^2) involved in the formation of the conduction band. The crystal structure of these compounds, of general formula $(MSe_4)_nI$, with M=Nb,Ta and n=2,3,10/3, consists in an arrangement of strongly bonded $(MSe)_\infty$ chains, parallel to the tetragonal c-axis, separated by strands of iodine ions. The anisotropy of the ionic interactions in $(TaSe_4)_2I$ is apparent in the phonon dispersion curves shown in Fig. 4, based on 3-axis measurements with cold neutrons at ILL (IN12, IN14) and LLB-Saclay (4F1, 4F2). One notices the upward curvature of the doubly-degenerate transverse acoustic mode propagating along **c***, indicating a large chain-bending stiffness. The limiting sound velocity, $v_{44}=(C_{44}/r)^{1/2}$, is controlled by interchain interactions and is found to be as low as 450 ms^{-1}, about a factor 10 lower than the longitudinal sound velocity v_{33}. The same v_{44} sound velocity is associated with (c-polarised) transverse sound propagating in the basal plane. This leads to a low-lying dispersion sheet with a zone-boundary frequency in the 0.1-0.2 THz range, as shown in Fig. 4 for propagation directions along **a*** (right hand symmetry) and **a*+b*** (left hand symmetry). The above phonon spectrum in $(TaSe_4)_2I$ is found to be largely unaffected by cooling through the Peierls instability at T_P=250±10 K. The onset of the low-temperature charge-density-wave groundstate is characterized by the appearance of diffraction satellites at $\mathbf{q_S}$=(±0.045, ±0.045, ±0.085). Detailed inelastic measurements near $\mathbf{q_S}$ show no evidence for a phason-amplitudon decoupling below T_P. As a consequence of the neutron work [6], low-temperature specific heat anomalies and optical resonances, originally ascribed to CDW-excitations have been reinterpreted in terms of the specific aspects of the compound's phonon spectrum.

Neutron scattering from $CsFeCl_3$ and $CsFeBr_3$ in an external magnetic field

The singlet groundstate systems of the type $AFeX_3$ (A = Cs, Rb, X = Cl, Br) are known to be prototype systems for 1D-behaviour because their structure is built from chains

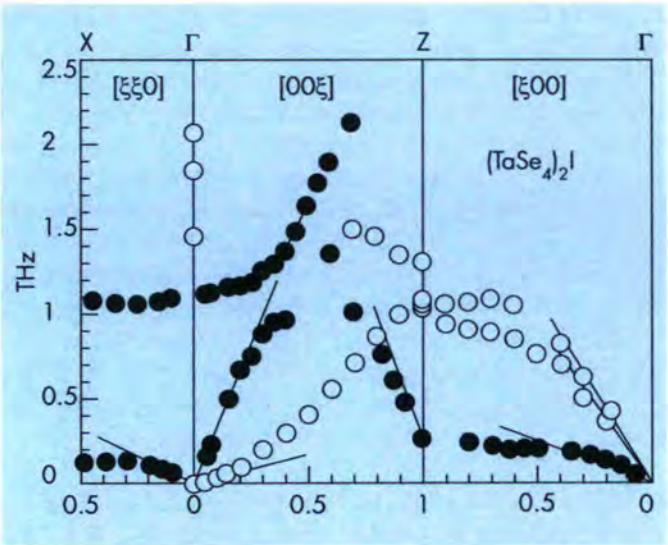

Fig. 4: Phonon dispersion curves along high symmetry directions in $(TaSe_4)_2I$ at room temperature. Modes polarised normal and parallel to the chains are represented by open and closed circles, respectively.

of face-sharing FeX_6 octahedra separated by the A-ions. The Fe^{2+}-ion with the effective spin S=1 has a singlet groundstate (m = 0) while the first excited state is a doublet (m = ± 1). This doublet undergoes a Zeeman splitting in an external magnetic field H^z_{ex} applied along the z-axis. A soft mode appears at [1/3 1/3 0] and equivalently at [2/3 2/3 0] in reciprocal space. In $CsFeCl_3$ long range order appears first as an incommensurate phase and, at higher fields, locks in into a commensurate phase with Bragg peaks at [1/3 1/3 0] and [2/3 2/3 0]. The dispersion curve of the magnetic excitations exhibits at zero field a minimum displaced by the dipolar interactions away from the [1/3 1/3 0] and [2/3 2/3 0] positions. With increasing field along the z-axis this minimum moves to the commensurate positions. We also applied a magnetic field perpendicular to the c-axis. Following the predictions of the theory [7] an increase of the excitation energies and a splitting of the excitations detected at higher magnetic fields H ≥ 3T. This behaviour of $CsFeCl_3$ with ferromagnetic exchange interaction along the chains is different from $CsFeBr_3$ with antiferromagnetic exchange interactions along the chains. In the latter case the variation of excitation frequencies in an external magnetic field perpendicular to the c-axis was extremely small [8].

Percolative superconductivity in $ErBa_2Cu_3O_x$ ($6 \le x \le 7$)?

In perovskite-type compounds $RBa_2Cu_3O_x$ (R=rare earth or yttrium, 6<x<7) the rare-earth ions are situated close to the CuO_2 planes, where it is widely believed that the superconducting carriers are located. Thus the crystalline electric field (CEF) interaction at the R site constitutes an ideal probe of the local symmetry and the charge distribution of the superconducting CuO_2 planes and thereby monitors directly changes of the carrier concentration induced, e.g. by

oxygen nonstoichiometry, pressure, doping and disordering effects. In order to understand the origin of the well-known two-plateau structure of T_c as a function of x, the CEF level structure of $ErBa_2Cu_3O_x$ has been studied in detail for a series of oxygen contents x covering the semiconducting and the metallic states. From the experimentally determined CEF potentials quantitative information on the charge transfer from the chains to the planes upon oxygen reduction has been derived. Our results exhibit a linear dependence of the charge transferred as a function of x, in contrast to Cava et al. [9] who deduced a close relation between the two-plateau structure and the charge transfer with a pronounced discontinuity at $x \approx 6.4$. Furthermore, investigating the low-energy CEF excitations of $ErBa_2Cu_3O_x$ in more detail under improved resolution conditions, the lowest-lying energy transition A is found to result from a superposition of three different components (Fig. 5), providing evidence for the formation of three different types of clusters (A_1, A_2 of metallic character and A_3 of semiconducting character) in the superconducting CuO_2 planes [10]. The fractional proportions of the three cluster types turn out to be extremely dependent upon the oxygen concentration x. These results are in agreement with the recent observation of a coexistence of two phases in the vicinity of $x \approx 6.4$ in $ErBa_2Cu_3O_x$. Based on these observations superconductivity can be shown to result from the formation of a two-dimensional percolative network. The continuous increase in the metallic states A_1 and A_2 can explain the increase of the superconducting volume fraction as observed by magnetic susceptibility measurements when the oxygen content is rising from x=6 to x=7. A two-dimensional bond percolative model predicts the critical content x associated with the transitions to the $T_c \approx 90$ K-superconducting state and to the $T_c \approx 60$ K-superconducting state to be $x_1 = 6.86$ and $x_2 = 6.42$, respectively, which is in good agreement with the two-plateau structure of T_c.

Kondo-lattice and valence fluctuation systems

$CeIn_3$ is a typical Kondo-lattice (heavy Fermion) system, while $CeSn_3$ is classified as a valence fluctuation system. The two compounds are isostructural (fcc), so the mixed pseudo-binary systems $CeIn_{3-x}Sn_x$ provide an ideal object to study the evolution from the Kondo-latttice to the valence fluctuation regime with increasing x. Evolution of the paramagnetic spectral response in $CeIn_{3-x}Sn_x$ ($0<x<3$) has been investigated on the IN4 TOF spectrometer. Fig. 6 displays the magnetic spectral response of the Kondo-lattice/heavy Fermion system $CeIn_3$ at 20 K in the paramagnetic phase as measured with neutrons of incident energies 50 meV (a) and 12.5 meV (b). The smooth curves through both of the data sets represent a common two component Lorentzian fit consisting of a crystal field excitation and a quasi-elastic (centred on zero energy) distribution. Fig. 6c shows the Fermi-liquid spectral response typical of a valence fluctuation system, in the present case $CeIn_{1.5}Sn_{1.5}$, measured at 5 K. The continuous

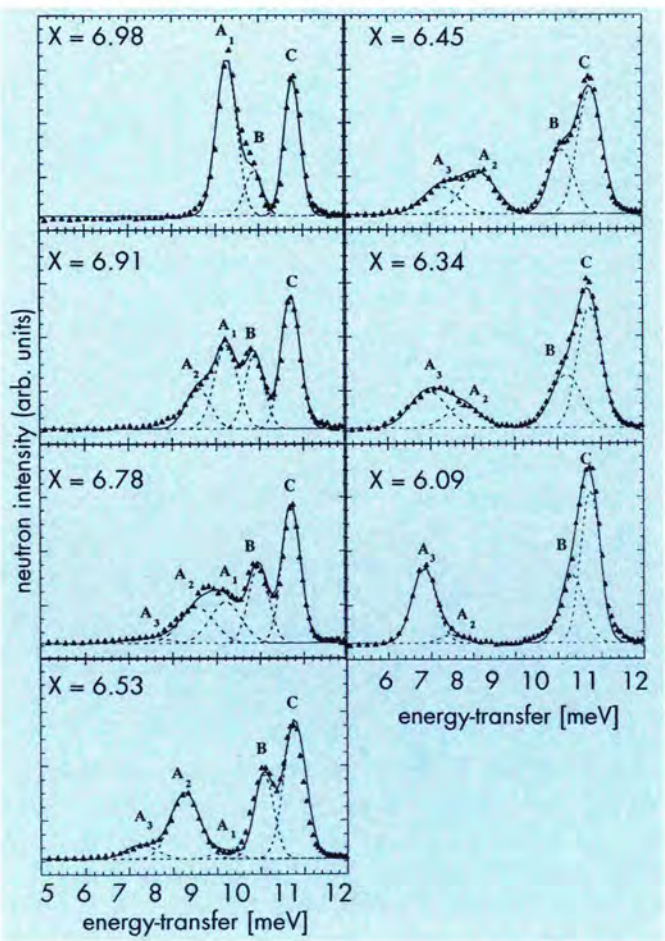

Fig. 5: Energy spectra of neutrons scattered from $ErBa_2Cu_3O_x$ at T=10 K measured on IN4.

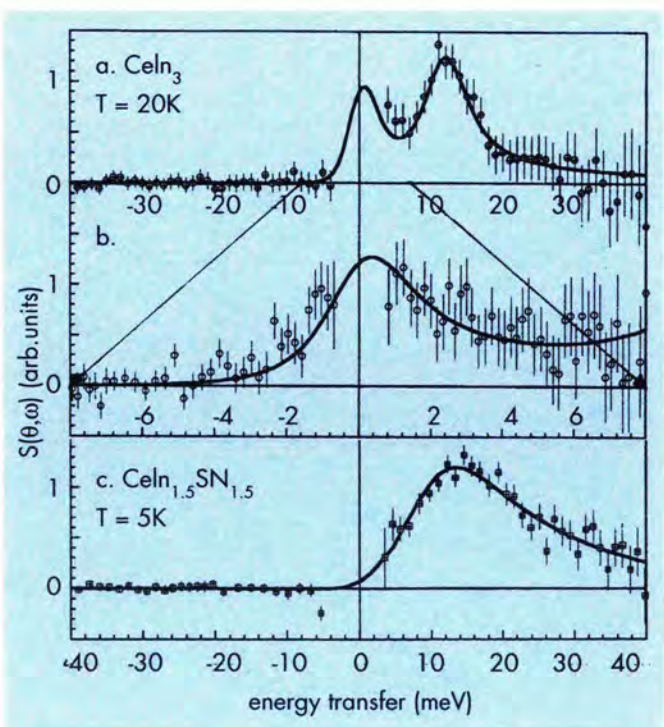

Fig. 6: Paramagnetic scattering from $CeIn_3$ at 20 K (a,b) and from $CeIn_{1.5}Sn_{1.5}$ at 5 K (c) measured on the IN4 TOF spectrometer.

curve represents the best fit to the Kuramoto-Müller-Hartmann function, which describes the Fermi-liquid response for the fully degenerate (N=6) ground state $^2F_{5/2}$. The results demonstrate the evolution with increasing k-f hybridisation from $CeIn_3$ towards $CeSn_3$. With increasing characteristic (Kondo) energy the crystal field splitting is quenched, the ground spin-orbit state ($^2F_{5/2}$) recovers its full degeneracy and the spectral function assumes the Fermi-liquid form [11].

Intermediate critical exponents in 2D-XY magnets

The 2D-XY model of collective magnetism is particularly important in solid state physics, providing a description of phase transitions in such diverse systems as superconducting and liquid crystal films, as well as being directly relevant to magnetic films and layered magnets. The model cannot sustain long range order at finite temperature, but nevertheless exhibits a "Kosterlitz-Thouless'' phase transition, which is mediated by defects in the local spin structure called "spin vortices''. At low temperature these bind together in pairs, but at a high enough temperature they become independent, driving the phase transition. Magnetic order, as measured by the sublattice magnetisation magnitude M, is directly accessible by neutron scattering, being proportional to the square root of the intensity of a magnetic Bragg reflection. Near to the critical temperature T_C, the order parameter normally shows power law behaviour $M=|T_C - T|^\beta$, with β, the critical magnetisation exponent, adopting universal values according to the dimensionality and spin symmetry of the system. For the 2D-XY model there is in theory, no magnetisation, and hence no exponent β. In layered magnets, considered to be experimental realizations of the 2D-XY model, long range order is stabilised by very weak interlayer coupling. Neutron scattering measurements on many different systems have shown that near to the phase transition there is a narrow three-dimensional critical region, with a 3D exponent $\beta \approx 1/3$. However, at lower temperature there is a crossover to a second regime with a characteristic exponent $\beta \approx 0.23$. Fig. 7 shows data measured on the D10 spectrometer, which exhibit a typical example of such a crossover. This second regime can be thought of as a region of finite size 2D behaviour, where the correlation length is too small to make the weak interplanar coupling relevant. However, the exact relation of the experimental $\beta \approx 0.23$ to the 2D-XY model has long remained a mystery. Recent theoretical work at the ILL and the ENS, Lyon [12], appears to have found the solution. Although the 2D-XY model has no long range order, the magnetic correlations decay so slowly with distance that a magnetisation occurs in any realisable finite system. A calculation of the magnetisation using renormalisation group equations, modified for finite size, shows that two dimensional fluctuations cause effective power law behaviour over a restricted temperature range, with $\beta = 3p^2/128 = 0.231$. This result is valid for a 2D-XY system of any large but finite size. Monte Carlo simulations have confirmed that it is accurate for the effective finite size of a typical layered magnet, and further confirmation comes from the observation of the same b in XY-like magnetic monolayers, where finite-size effects are directly relevant. It may be concluded that b=0.23 is a universal signature of finite 2D-XY behaviour. This result strongly suggests that vortex unbinding occurs in real magnets.

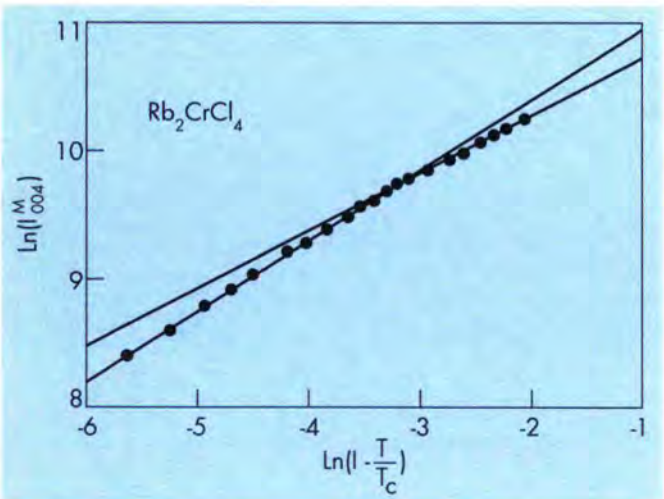

Fig. 7: Intensity of a magnetic Bragg reflection of the 2D-XY like ferromagnet Rb_2CrCl_4, plotted as a function of reduced temperature (T_C-T) where T_C=52.2 K. A crossover between the 3D behaviour with slope b^a1/3 and a 2D-XY behaviour with b^a0.23 is clearly seen.

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Displacive transitions in bcc metals: diffusion and phonons

W. Petry*

A considerable fraction of the metallic elements solidifies in the open bcc structure and transforms by lowering the temperature, or under pressure to a close-packed structure. In general, these transitions are displacive, reconstructive, of first order and are often called martensitic. How is this weakness of the bcc structure related to such apparently different properties, as the lattice vibrations or the transport of matter in these metals?

Access to the phonons of these high temperature phases is strongly hindered by the displacive transitions, which unavoidably destroy the high temperature bcc single crystal. We have overcome this problem by the in-situ growth of the single crystal on the neutron spectrometer and measured, for the first time, the complete phonon dispersion of the bcc phase of the transition metals Sc [1], La [2], Ti [3], Zr [4] and Hf [5]. Part of the results is shown in Fig. [1], which compares the longitudinal (L) [ξξξ] and the transversal (T_1) [ξξ0] phonon branch for selected bcc elements. In spite of their highly symmetric and mono-atomic structure, the vibrational behaviour of these metals is a very complex one:

- The dispersion of the longitudinal [ξξξ] phonon branch shows a pronounced dip at ξ = 2/3.
- The whole T_1 [ξξ0] with [1$\bar{1}$0] polarization is of low energy.
- All these low energy excitations are strongly damped or of a short lifetime and intensity of inelastic origin reaches down to zero-energy transfer.

The L 2/3 [111] phonon plays a particular role within the bcc structure as it displaces two out of three (111) planes towards each other (see Fig. 2). A complete collapse of the two (111) planes yields the hexagonal ω-structure, which is observed under pressure in the Group 4 metals. The other low energy mode, namely T_1 [ξξ0] with ξ = 1/2, shifts two adjacent (110) planes from a bcc stacking sequence to that of an hcp structure.

These modes can be seen as **dynamical** precursors of the approaching transition. Their eigenvectors correspond to the displacements needed to transform the bcc to the close-packed structure and because they are of low energy, they probe a low potential barrier for the displacive transition. Furthermore, the energies of these phonons are strongly temperature dependent. The mode which shifts the bcc lattice towards an hcp stacking sequence is of lowest energy at the transition and stiffens considerably with rising temperature. These low energy

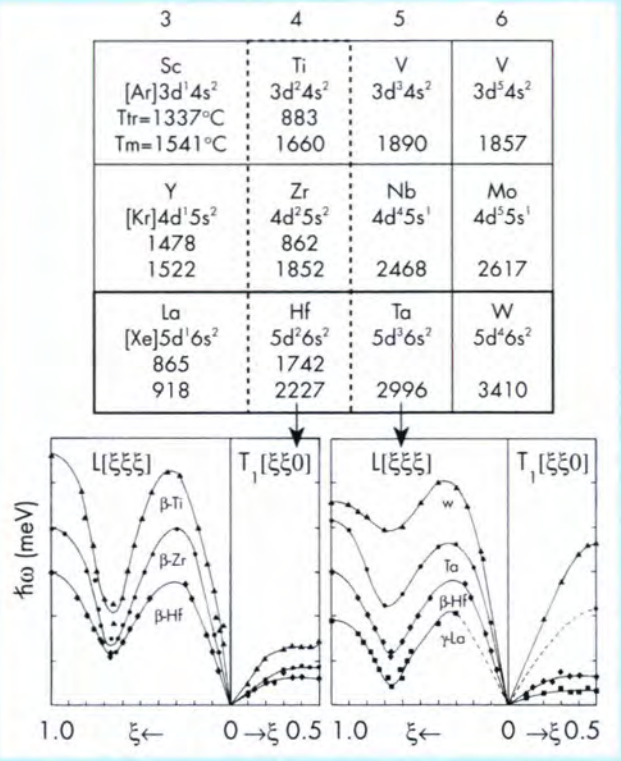

Fig. 1: Anomalous phonon branches in selected bcc metals. Within one chemical group low energy phonons are of similar frequency, whereas the frequency considerably increases with increasing d-electron density.

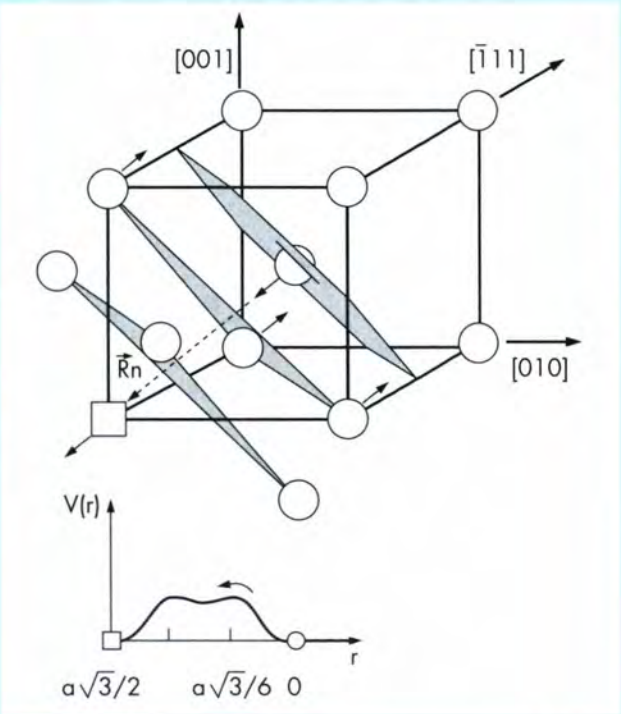

Fig. 2: Displacements of the L 2/3 [111] phonon and its relation to a nearest-neighbour jump.

modes also supply the dominant contribution to the high lattice entropy

$$S_{vib} = -3K_B \int d\omega Z(\omega)[n(\omega)\ln n(\omega) - (1+n(\omega))\ln(1+n(\omega))] \quad (1)$$

thereby lowering considerably the free energy F = U - TS of the crystal. ($Z(\omega)$ represents phonon density of states and $n(\omega)$ the Bose occupation factor). That is the reason why the low energy modes play a two-fold role: They are a sign of the weakness of the bcc lattice to undergo transformations and at the same time they stabilize the bcc structure, due to their contribution to the lattice entropy [2,4] (see Fig. 3) which then minimizes the free energy.

The broad energy distributions which are characteristic for these low energy phonons are remarkably well reproduced by a damped oscillator description. In the extreme case, their widths correspond to lifetimes in the order of one vibrational period. This makes it difficult to speak of propagating modes. More appropriate is a description in terms of dynamical **fluctuations** towards the product phase and a description by anharmonic theory which includes interference between multiple phonon excitations [6] (see also the contribution dealing with the symmetry breaking inelastic scattering in b-Zr).

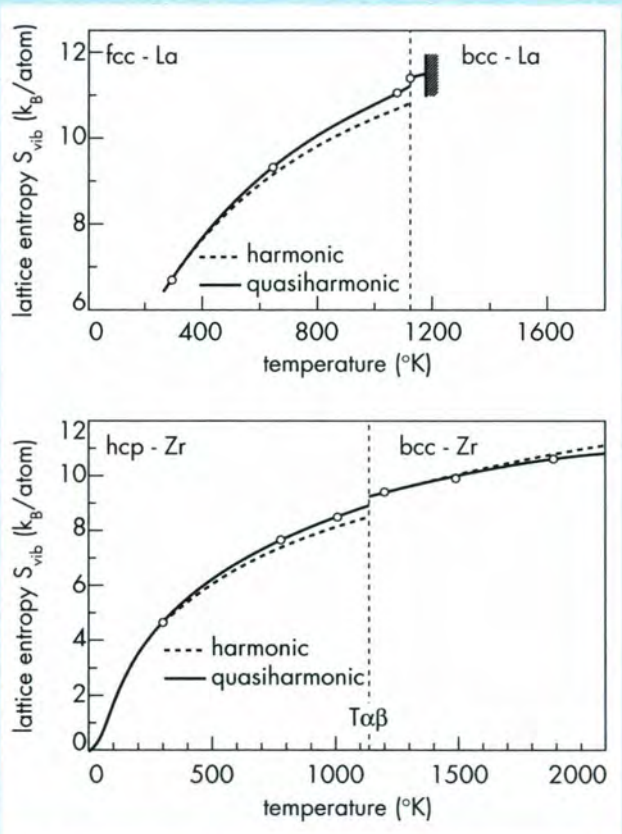

Fig. 3: Temperature dependence of the lattice vibrational entropy calculated by means of the temperature dependent phonon spectrum. The jump of S_{vib} at the transition temperature is the dominating term in minimizing the free energy of the high temperature phase. Contributions from the electronic entropy are considerably smaller [2,4].

The bcc metals are known for their unusual diffusion properties (Fig. 4). In these metals self-diffusivities D(T) differ by up to eight orders of magnitude at half of the melting temperature T_m and the faster diffusing metals exhibit a pronounced curvature in the Arrhenius presentation of D(T). The importance of these effects is seen in comparison to the diffusivities of fcc metals whose behaviour is quite "normal" as all D(T) fall on one master curve. The key information in relating this unusual self-diffusion to the vibrational behaviour in bcc elements has been obtained by an incoherent quasi-elastic neutron scattering experiment on bcc-single crystals of Ti [7]. It was shown that the elementary diffusion step is a jump into nearest-neighbour (nn) vacancies. From Fig. 2 it is evident that the displacements of the L 2/3 [111] phonon push the atoms into the direction of nn vacancies, i.e. the low energy phonon probes a low migration barrier for the diffusion jump. Similar considerations hold for the low energy phonons along T_1 [ξξ0] [8,9].

By means of the lattice Green's function, a theory has been developed which yields a quantitative relation between migration enthalpy H^m and the properties of low energy phonons [10].

$$H^m = \alpha \left(\int \frac{Z(\omega)}{\omega^2} d\omega \right)^{-1} \cdot a^2 \quad (2)$$

Whereas a is a structure specific constant (established by computer simulation), the -2nd moment of the density of states $Z(\omega)$ takes into account the element specific lattice vibrations. Fig. 5 displays the results of calculations of H^m for the bcc phase of Group 1 to Group 6 metals. For the very few cases where experimental values of H^m are available, compatibility is achieved. But the important point in Fig. 5 is that for the first time, reliable predictions were made for all bcc metals where phonon dispersions are known.

Due to the fact that the energy of the phonon modes which are related to the phase transition increases with increasing temperature, the migration enthalpy H^m shows the same behaviour. This is demonstrated for the case of bcc-Zr in Fig. 5 while Cr exhibits the opposite temperature behavior. Phonons in Cr shift to lower

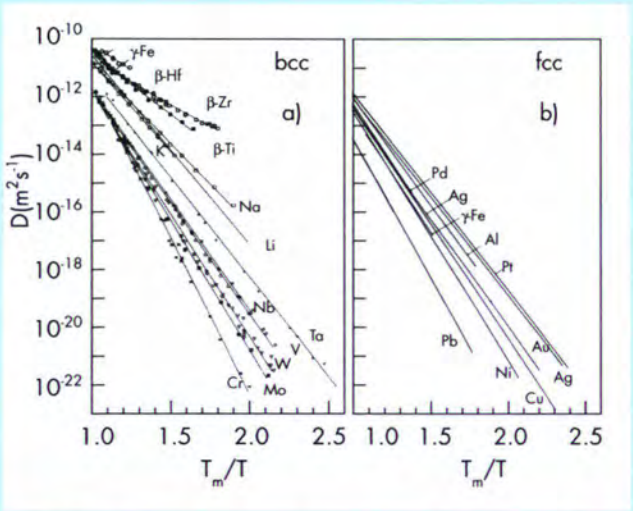

Fig. 4: Self-diffusivity D(T) as a function of a normalized temperature for bcc and fcc metals.

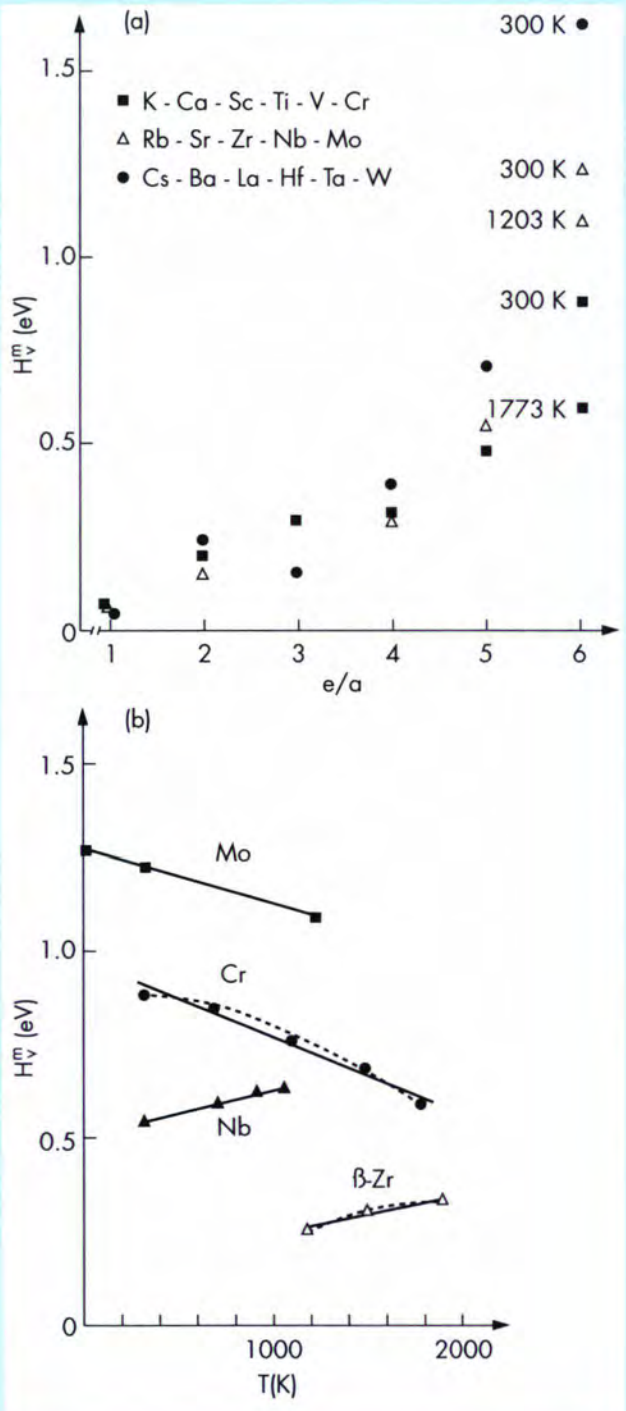

Fig. 5: Calculated migration barrier H^m for self-diffusion of the Group 1 to Group 6 elements as a function of the number of free electrons per atom (a) and its temperature dependence for selected cases (b).

energy with increasing temperature. H^m therefore decreases with increasing temperature. In this context, the evaluation of H^m as a temperature dependent quantity is of particular importance. A non-linear temperature dependence then explains the curvature often observed in the Arrhenius presentation of the self-diffusivity.

In Fig. 5 H^m is plotted as a function of the successive filling of the s- and d-band. This reveals pronounced chemical trends. In the alkali metals migration barriers are lowest. Filling the s- and d-band, H^m gradually increases. Again, this is directly related to the characteristics of the vibrations. As shown in Fig. 1, the low energy phonons are nearly of the same energy within one chemical group whereas the high energy phonons scale with their masses and lattice parameters. However, filling the d-band phonon energies gradually increase.

In summarizing, we state that inelastic neutron spectroscopy of the high temperature bcc-phases revealed the common origin a) of their tendency to transform into close-packed structures, b) of their anharmonic vibrational behaviour, and c) of their large scatter in the self-diffusivity. Filling of the s- and d-band is **the** control parameter for the potential heights experienced by jumps to vacant nn sites. The latter is the dominant self-diffusion mechanism in all pure bcc elements.

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Atomic structure and dynamical properties of the Al-Pd-Mn icosahedral phase

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Atomic structure

Quasi-periodic structures can be viewed as irrational 3-dimensional cuts of objects which are periodically distributed in an n-dimensional space (n > 3). Quasicrystals (QC) can be described by symmetry (space group), metrics (lattice parameters) and the distribution of "atomic objects" (AO) in an n-dimensional unit cell, just as for regular structures. As a consequence, the derivation of a quasicrystal structure from diffraction data follows essentially the same procedure as would be applied for a classical 3-dimensional structure. The best candidates for structure determination from diffraction data are the recently discovered, phason-less, "perfect" quasicrystals Al-Cu-T (T = Fe, Ru, Os) [1] and Al-Pd-T (T = Mn, Re) [2]. Both quasicrystals form via slow cooling procedures and large single grains can be grown [3]. Single grains of the $Al_{70.5}Pd_{21}Mn_{8.5}$ icosahedral phase were studied using four-circle single crystal diffractometry with X-rays and neutrons [4]. Indexing of the diffraction peaks for both the X-ray and the neutron experiments fully confirms the previously suggested by powder neutron diffraction data [5]. The lattice parameter, a, of the equivalent 6-dimensional cubic primitive cell was found to be 6.451 Å. The weak face-centered (F) aspect of the structure, corresponding to the weak I-character of the reciprocal Bravais lattice, comes from an uneven density distribution on sites with different parity. These features can be seen in the Patterson density maps obtained by inverse Fourier transform of the corrected integrated intensities of the indexed Bragg reflections (fig. 1). Density profiles along a perpendicular axis ($[-\tau,1,0]_\perp$ in fig. 1) are plotted in fig. 2. The Patterson maps of fig. 1 show unambiguously that AO are distributed at the lattice nodes (origin sites) and on body-centered sites. Neutron contrast variation studies measurements using isomorphous substitution [5] have given detailed information about the manganese AO, whereas the X-ray single crystal data is dominated by the Pd atom contribution. This accounts for the very large differences observed between the neutron and X-ray density profiles (fig. 2). The uneven density distribution on sites with different parity appears to be very large for the X-ray data, which is indicative of the strong chemical order induced by the palladium.

First approximations for the A0 in the 6-dimensional primitive cubic structure can be obtained by considering spheres in the perpendicular space. Modeling of the sizes of AO to the composition, density and low Q_{perp} data already gives a very restricted set of solutions. This has allowed a first model to be deduced which may be summarized as follows:

(i) At even lattice nodes, one has a core of Mn (radius 0.833a) surrounded by an intermediate shell of Pd (extending up to 1.258a) and an outer shell of Al (up to 1.547a).

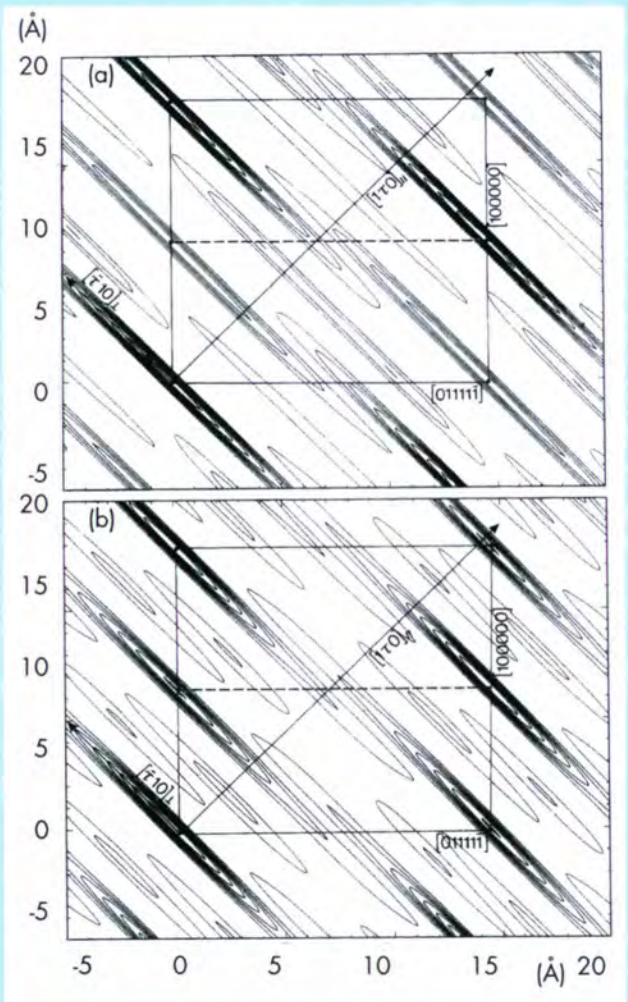

Fig. 1: The Patterson function for the 6-dimensional periodic structure as obtained with single grains and X-ray (a) or neutron (b) diffraction. The figure shows slices of the 6-dimensional space containing five-fold axes in both the physical (par) and the complementary (perp) subspaces. The density features on even and odd sites are obviously different.

(ii) At odd lattice nodes, a core of Mn (radius 0.520*a*) with a shell of Al (up to 1.639*a*),

(iii) At odd body centers, a core of Pd (radius 0.710 *a*)

(iv) At even body centers, a small core of Al or empty volume.

The resulting 3-dimensional structure contains mainly two kinds of clusters, corresponding to the external shell of the Mackay icosahedron with different decoration arising from the 6-dimensional superstructure.

Dynamical properties

Inelastic measurements were performed at the Orphée reactor (Laboratoire Léon Brillouin), using the 1T triple axis spectrometer with a PG[002] monochromator (vertically focusing) and analyser (horizontally focusing) [6]. Constant k_f scans (2.662 Å^{-1}) were used to measure excitations with an energy resolution of 0.35 THz. The sample, a single grain of approximate size 1 x 0.5 x 0.5 cm^3 [3], was oriented to provide measurements in a 2-fold scattering plane which contains all the strong Bragg reflections (fig. 3). The experimental results were analyzed by fitting the excitations with a damped harmonic oscillator function convoluted with the instrumental resolution. Typical results, corresponding to a transverse geometry associated with point C (fig. 3), are shown in fig. 4. Results of the fits are given in fig. 5. Three distinct regions may be identified:

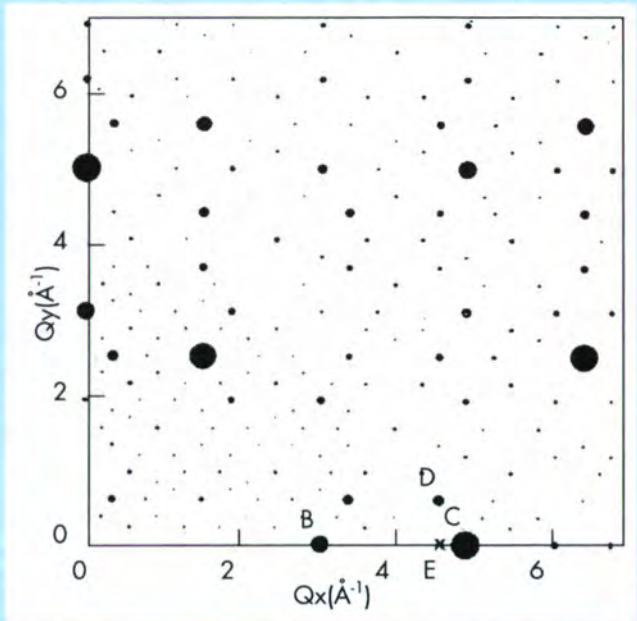

Fig. 3: Representation of the experimental scattering plane. The area of the spots is proportional to the intensity of Bragg reflections.

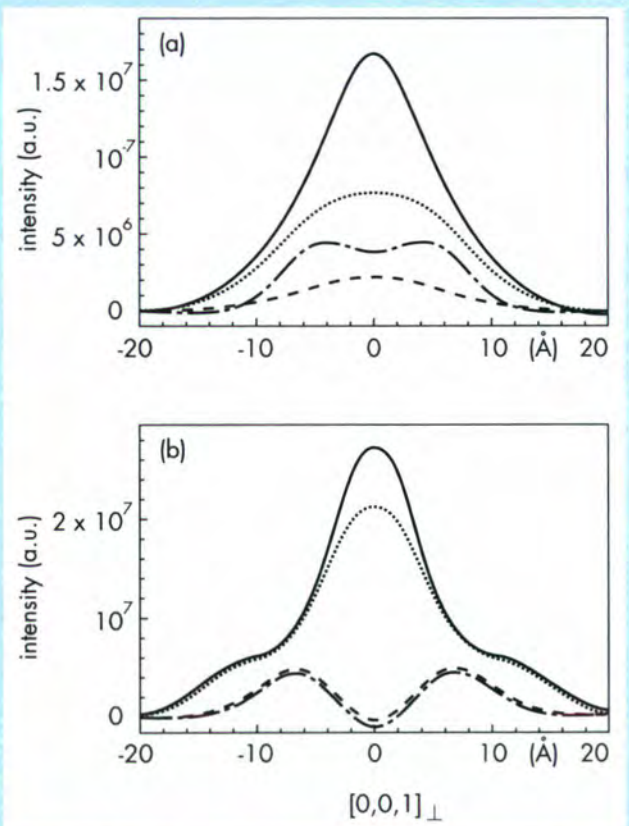

Fig. 2: Profiles of the various Patterson density features on the even (__) or odd (····) lattice nodes, and on the even (——) or odd (_ · _ · _) body centers for X-ray (a) and neutron (b) data.

- At low Q (Q <0.35 Å^{-1}), the width of the excitation is limited by the instrumental resolution.
In this region a linear behavior is observed.

- At high Q (Q >0.8 Å^{-1}), several excitations are present and there is no more evidence of a dispersion curve.

- In between (0.35 < Q(Å^{-1}) < 0.8), the width of the excitation increases (this may also indicate the presence of several excitations). There is still evidence of a pseudo-dispersion curve with non-linear behavior.
The pseudo-dispersion curve bends over around 3 THz.

In the linear regime, the isotropy of transverse modes propagating along different symmetry axes has been verified. Sound velocities were determined as 3.5 x 10^3 ms^{-1} and 6.3 x 10^3 ms^{-1} for transverse and longitudinal modes respectively, which is similar to that in AlLiCu and AlCuFe samples [7-8].

When branches cross, one would expect that a gap opens giving rise to an optic-like upper branch. These features can be measured between points C and D (see fig. 3). No such gap was actually detected.

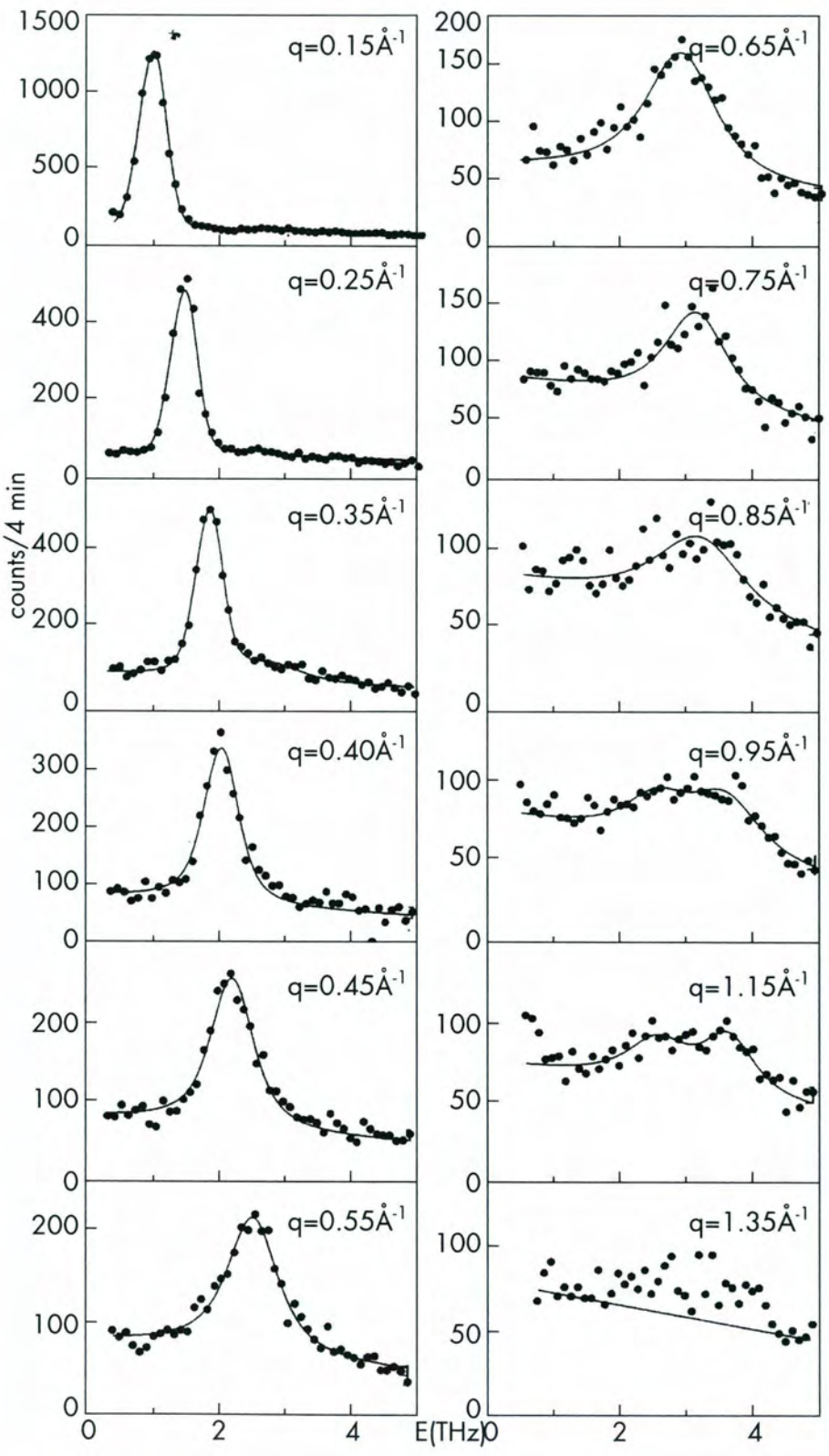

Fig. 4: Constant Q energy scans measured along a two-fold direction from point C (transverse geometry). The solid line is the result of the fit.

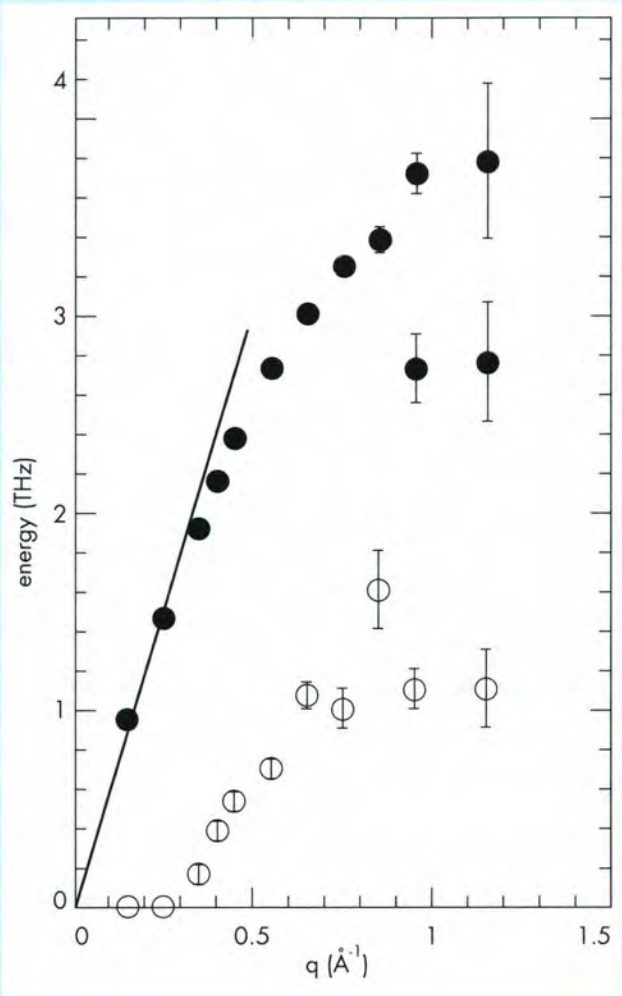

Fig. 5: The phonon dispersion relation corresponding to fig 4.

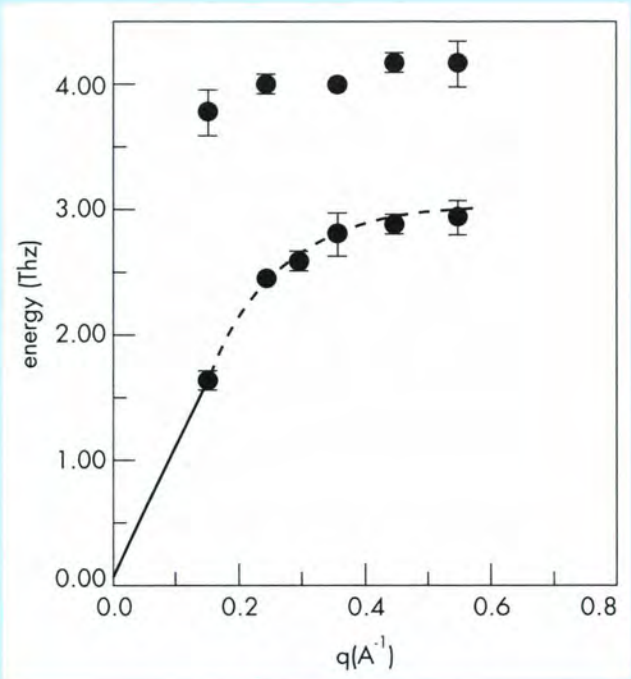

Fig. 6: The dispersion relation measured between points C and B (pure longitudinal geometry). The longitudinal branch saturates around 3 THz. An excitation(s) is observed at 4 THz.

For longitudinal excitations (see fig. 6), the pseudo dispersion curve clearly bends over around 3 THz. A non-dispersive excitation(s) lying around 4 THz can also be identified. This pseudo dispersion curve may be compared to the case of the I-AlLiCu phase [7]. There also, the longitudinal modes were seen to become dispersionless (at a lower energy, i.e., around 2.5 THz), which suggests a difference from the crystalline R-phase. This has been interpreted as an indication of spatial localization for these excitations.

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Crystal and Magnetic Structures

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Introduction

In 1991 experimental activities at ILL had already suffered from the reactor shutdown. To compensate this the collaborative scientific and experimental work of ILL scientists was further expanded at many European and overseas neutron centres. The D1A instrument was taken to the LLB in Saclay and has been available for scheduled use since October 1992. Software and hardware from the instrument D1B were taken to the Siloe reactor (CENG Grenoble) and this has enhanced the working conditions on the powder diffractometer DN5.

A number of scientists and technicians were detached from ILL for periods up to two years. The last remaining ILL thesis students are completing their theses in rather difficult conditions, again often travelling to several neutron centres to obtain beam time. Such collaborations have however usually been very productive.

College members have been involved in the joint project with the ESRF and EMBL which aims at clarifying the problems of controlling ILL and ESRF instruments under the UNIX operating system. The college has begun to study conversion of scientific and instrument programs in preparation for a substantial investment in UNIX work stations. The Cambridge crystallographic subroutine system developed by P.J. Brown and J.C. Mathewman is already running under UNIX; and for example the UNIX version of XTAL is now running at ILL.

A Silicon Graphics UNIX workstation with accelerated 3D display was purchased in 1992, together with CERIUS crystallographic software from a Cambridge company. A similar system was purchased at the same time by the ESRF, allowing favourable conditions to be negotiated, and opening the way for close practical collaboration between the diffraction groups of the ILL and ESRF.

Altogether 1992 has been a scientifically productive year and the variety of scientific contributions for the annual report is greater than ever.

Scientific Highlights in 1992

Crystallography

Modulated phases in $TlGaSe_2$

$TlGaSe_2$ belongs to the family of ternary semiconducting chalcogenides with the chemical formula ABX_2 where A and B are metal atoms and X is a chalcogen atom. At room temperature paraelectric $TlGaSe_2$ crystallizes in a monoclinic structure (C2/c) which is built up of adamantane-like Ga_4Se_{10} tetrahedra, linked through corners to two-dimensionally infinite $^{2}_{\infty}[Ga_4Se_{10}]$ layers and $TlSe_6$ prisms. The layers are stacked along [001] and linked through one-dimensionally infinite $^{1}_{\infty}[TlSe_6]$ chains. On cooling, two successive phase transitions take place: first at $T_i = 120$ K to an incommensurate phase which finally locks into a commensurate ferroelectric phase at $T_L = 110$ K. The low temperature commensurate phase has the non-centrosymmetric space group C2. It is the loss of the inversion symmetry at low temperature which leads to the appearance of ferroelectricity. It is presumably caused by the small positional shift of Tl atoms in the a-b plane accompanied by the discontinuity in the axial ratio. The appearance of ferroelectricity has been interpreted as being due to the stereochemically active electron lone pair configuration of the Tl^+ ion. To confirm this the crystal structures of the low temperature phases of $TlGaSe_2$ were investigated on the four-circle diffractometer D19, which is equipped with a 4° x 64° multidetector. Fig. 1 shows the ω-scans along the reciprocal lattice row [-9 -5 1] at 126 K, 114 K and 104 K corresponding to the paraelectric, incommensurate and ferroelectric phases, respectively. Fig. 1 illustrates the usefulness of a multidetector to record the diffraction peaks of the principal and satellite reflections simultaneously in such modulated structures. In the incommensurate phase the pairs of satellites are displaced from the superlattice positions corresponding to the wave

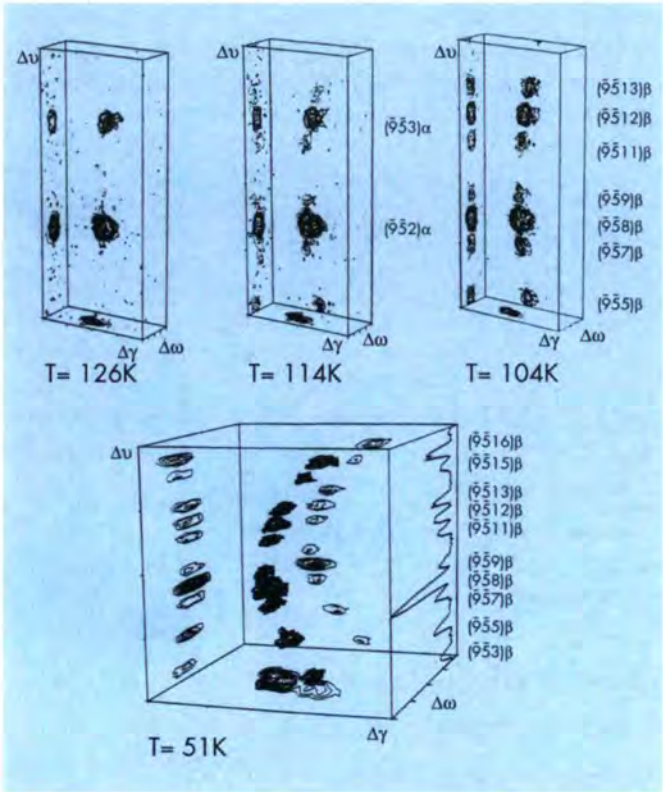

Fig. 1: Reflections of the reciprocal lattice row [-9 -5 1] of $TlGaSe_2$ at 126 K, 114 K and 104 K corresponding to the paraelectric, intermediate incommensurate and ferroelectric commensurate modulated phases, respectively. Also shown is a larger section of the reciprocal lattice row measured at 51 K in the ferroelectric phase. The position sensitive detector allows a three dimensional representation of the reflections. γ and ν correspond to the horizontal and vertical directions in the plane of the multidetector whereas ω is the rotation angle of the crystal.

vector **k** = (0, 0, 1/4) by small amounts whereas in the commensurate modulated phase they appear exactly on the superlattice positions. About 9000 principal and satellite reflections were measured in the ferroelectric phase. The structure determination of the low temperature ferroelectric phase using these intensity data showed that systematic displacements of the Tl atoms from the positions of the paraelectric phase parallel to [0 0 1] take place in the modulated phase. The $^{2}_{\infty}[Ga_4Se_{10}]$ layers remain practically unmodified. The prism changes its coordination number from CN6 to CN7. The reason for the shifts of the Tl atoms is the induced stereochemical activity of the lone pair of Tl^+ at the ferroelectric phase transition. All Tl atoms from two neighbouring $^{1}_{\infty}[TlSe_6]$ units along [0 0 1] are shifted in the same direction by the same amount. The prism units form a block. The unit cell is built of eight such blocks stacked along [0 0 1]. The shifts of two consecutive blocks are alternatively parallel to [-1 -1 0] and [1 -1 0]. The present structure model explains the quadrupling of the c axis and shows that it is the stereochemical activity of the Tl^+ ion and not the chalcogenide ion which is responsible for the appearance of ferroelectricity. This work is a collaboration with the MPI in Stuttgart.

An in-situ temperature-dependent study of texture effects

The texture of polycrystalline bulk material has important consequences for its technological applications. Depending on the intended use the existence of texture may be desirable or not.

Diffraction studies using an Eulerian cradle allow the recording of complete pole figures of a sample from which it is possible to calculate the three dimensional orientation distribution function. Referring to a single direction it is usual to describe the degree of preferred orientation relative to a random distribution in units of "multiples of random distribution" = mrd. Several studies on the influence of the manufacturing process and subsequent working processes on the resulting texture have been made by neutron diffraction techniques. D1B with its multidetector has often been used for this kind of study: in a collaboration with the GKSS in Geesthacht the first in-situ temperature-dependent texture study has now been performed by mounting a small oven inside the Eulerian cradle. Fig. 2 shows how the strong double fibre texture of cold extruded copper is influenced by recrystallisation processes at elevated temperatures. Measuring in steps of 50 °C pole figures were recorded within 20 minutes. Starting from about 250 °C the degree of orientation decreases significantly for the strong <111> component. Amounting to 17 mrd at 200 °C it drops to only 3 mrd at 600 °C the highest measurable temperature. The effect of adding 10 % Al was shown to consist in advancing the onset of recrystallisation by about 50 °C. This should be connected to the existence of inhomogeneously deformed material in the vicinity of phase boundaries in the mixed phase where for example dislocations facilitate the nucleation.

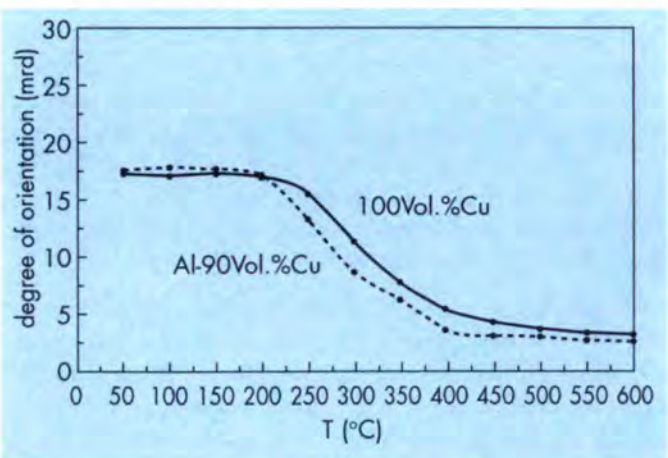

Fig. 2: Degree of orientation of the copper <1 1 1>-component as a function of annealing temperature for cold extruded pure copper and Al 90 Vol.%Cu.

Interrupting the annealing process at 300 °C has drastic consequences for the final degree of orientation: e.g. for the 10 % Al substituted sample the time-dependent recrystallisation quickly fades away. Even after 7 hours the degree of orientation stays at about 7 mrd, well above the final value of 3 mrd previously found for the 600 °C annealed sample.

In situ study of nitrogenation processes

The possibility of inserting light elements such as H, C, N, within the metal sublattice of the R_2Fe_{17} compounds (R = rare earth) has recently renewed interest in these magnetic alloys since both the Curie temperature and the magnetization are tremendously increased. In particular $Sm_2Fe_{17}N_3$ is the most promising material for permanent magnet applications.

Early studies performed on D2B have established that nitrogen atoms only occupy one interstitial site (9e), a distorted octahedron formed by two R atoms and four surrounding Fe. Nevertheless, it remains unclear whether nitrogen completely fills this site as soon as the reaction starts, or whether it leads to intermediate nitrides $R_2Fe_{17}N_x$, where x increases during the reaction.

Real time " in-situ" neutron diffraction using the diffractometer D1B, made it possible to investigate the nitrogenation process itself.

$$2\,R_2Fe_{17} + 3\,N_2 \Rightarrow 2\,R_2Fe_{17}N_x \quad \text{with } x \approx 3$$

A fine powder of Nd_2Fe_{17} was put into a silica tube. The sample was then heated under constant N_2 gas flow (10^5 Pa) from room temperature to about 730 K over a period of 1 hr and maintained at 730 K for 14 hours. During this process the diffraction patterns were recorded every three minutes using the one-dimensional position-sensitive detector.

The diffraction patterns show that only the pure Nd_2Fe_{17} phase is present at the beginning of the reaction. However an increase in the temperature results in the appearance of a new phase with slightly larger lattice parameters. From Rietveld refinement of the diffraction pattern this new phase was identified as $Nd_2Fe_{17}N_{2.7\pm0.1}$.

The percentage of each phase (Nd_2Fe_{17} and $Nd_2Fe_{17}N_{2.7}$) has been refined and is reported as a function of the time of reaction in Fig. 3. It should be noted that nothing happens upon raising the temperature from 350 K to 730 K (first hour of experiment). This is clear in Fig. 3 where the amount of nitride at first remains close to 0, then, when a high enough temperature is reached, the reaction starts.

This work has demonstrated that the nitrogenation process does not lead to intermediate nitride formation, since the 9e site is fully occupied in the nitride product. During the reaction, two phases are in equilibrium, the pure Nd_2Fe_{17} alloy and the $Nd_2Fe_{17}N_{\approx3}$ nitride. Only the relative percentages of the phases vary with reaction time.

Thermal dyotropic rearrangements in isodrin derivatives

Extensive kinetic studies have been made by NMR techniques of a thermal dyotropic rearrangement in a series of isodrin derivatives. This reaction, where isomer A rearranges to form isomer B by a 2H intramolecular transfer, is shown in Fig. 4.

These studies have revealed a wide range of reaction rates as the substituents R are varied; the unimolecular rate constant k_1 is reduced by a factor of 10^7 when substituents R = H are replaced by Cl.

In some cases it has been impossible to isolate isomer A as the reaction proceeds too rapidly to isomer B. However, as a result of the retarding effect of deuteration at sites 4 and 9, single crystals of isomer A, where R = Cl, have been obtained for the first time in deuterated form.

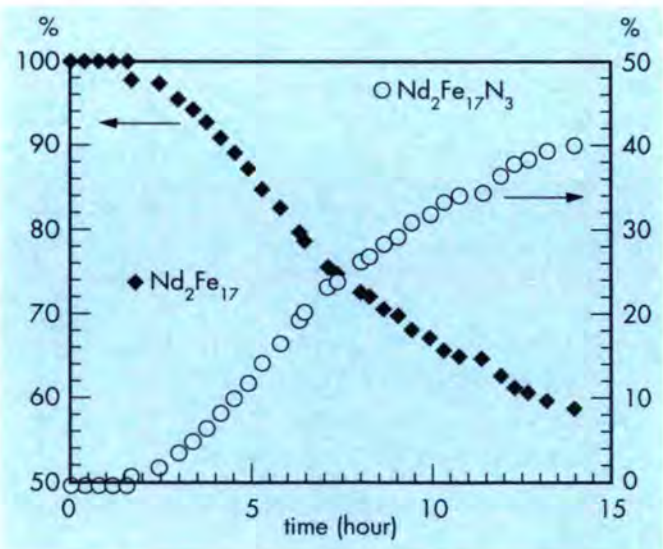

Fig. 3: Evolution of the percentage of Nd_2Fe_{17} and $Nd_2Fe_{17}N_{2.7}$ phases versus the time of reaction.

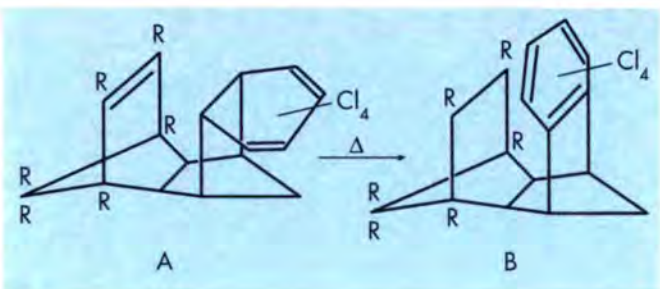

Fig. 4: Thermal dyotropic rearrangement (2H intramolecular transfer) of isodrin derivative A to B.

To determine the accurate molecular structure of this compound in which the H positions are a crucial factor, a single-crystal neutron diffraction study of isomer A has been made using data measured at the HFBR, Brookhaven on the four-circle diffractometer on port H6M (λ = 1.046 Å, T = 15 K). Isomer A, shown in Fig. 5, crystallized in the space group $P2_12_12_1$ with a = 8.664 Å, b = 14.052 Å, and c = 16.187 Å. 4472 unique reflections were measured to a $\sin\theta/\lambda$ of 0.78 $Å^{-1}$.

We now have accurate positional parameters for all atoms including the key deuterium atoms. This information, especially for the pairs of isomers A and B, is vital for understanding the relationship between the relatively small changes in the molecular structure and the rate of the rearrangement. It is also necessary for any comparison with theoretical calculations.

As part of this study we have also been able to investigate the degree of deuteration at the substituted sites, which are indicated in Fig. 5. Our results are in close agreement with those from the NMR studies, since both methods show greater than 90 % substitution.

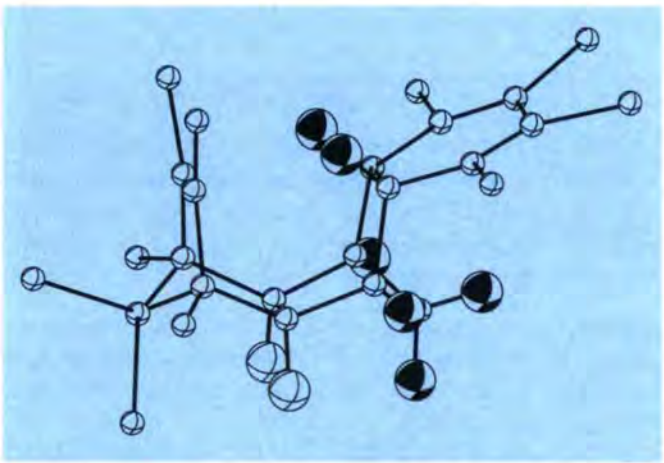

Fig. 5: Structure of isomer A (R = Cl). Thermal ellipsoids drawn at 90% probability level for all atoms at 15K (ORTEP). Deuterated sites are shown as partially shaded.

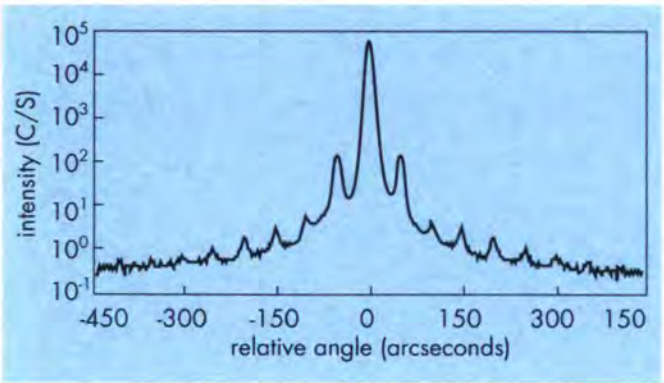

Fig. 6: Transverse angular scan around the (004) Bragg peak of a GaAs-surface grating.

Collaboration with the Universities of Durham and Bristol and with Brookhaven National Laboratory.

Characterization of quantum well wires and surface gratings by X-ray diffraction reciprocal space mapping

One tendency in present-day materials research is the increasing ability to construct solids in one, two or three dimensions. Using semiconductor systems, quantum well wires (QWW) and quantum well dots (QWD) hold a great potential for understanding the basic physics of semiconductors as well as for the improvement of integrated optical devices. One approach consists of post-growth patterning of quantum well materials, a second one of its fabrication on patterned non-planar substrates (PS).

The aim of our studies was to develop the method of X-ray diffraction as a powerful nondestructive technique for the structural characterization of periodic patterned substrates and QWW. The QWW and PS represent artificial superlattices. The PS have a one-dimensional lateral superstructure forming a surface grating with periods between 0.2 and 1 nm. The QWW are epitaxial multilayered surface gratings and show a two-dimensional superperiodicity. Thus longitudinal (Qz) truncation rods (TR) were measured near the Bragg positions of the modulated crystal lattice. The transversal (Qx) positions of the TR's fulfil the grating equation.

We combined the methods of Specular and Non-Specular Reflection (XR), conventional Triple Crystal Diffraction (TCD) and Grazing Incidence Diffraction (GID) to investigate the reciprocal space structure arround the reciprocal lattice points of the substrate ((000) by XR, (00l) and (hkl) by TCD, (hk0) by GID, with hkl being the Miller indices). A typical diffraction pattern of a transverse scan is shown in Fig. 6, obtained from a GaAs-surface grating. Transverse satellites occur around the substrate Bragg peak (here 004). The spacing between satellites is inversely proportional to the grating period. Cross patterns are formed by the longitudinal truncation rods of these satellites, centred on the substrate reciprocal lattice points (Fig. 7 for a InP-grating). This cannot be explained by normal kinematical diffraction theory. It results from Umweganregung between the grating and the dynamically diffracting substrate, since the grating acts simultaneously as a reflection and a transmission grating. For the quantitative interpretation a semidynamical treatment was developed based on a Distorted Wave Approximation. In QWW's the Qz truncation rods obtain additional longitudinal satellites, representing the superperiodicity in the growth direction.

Crystallography and Magnetism

A polarized neutron study of the magnetic form factors in $CeFe_2$

The magnetization distribution in the ferromagnetic phase of $CeFe_2$ at 10 K has been determined from a

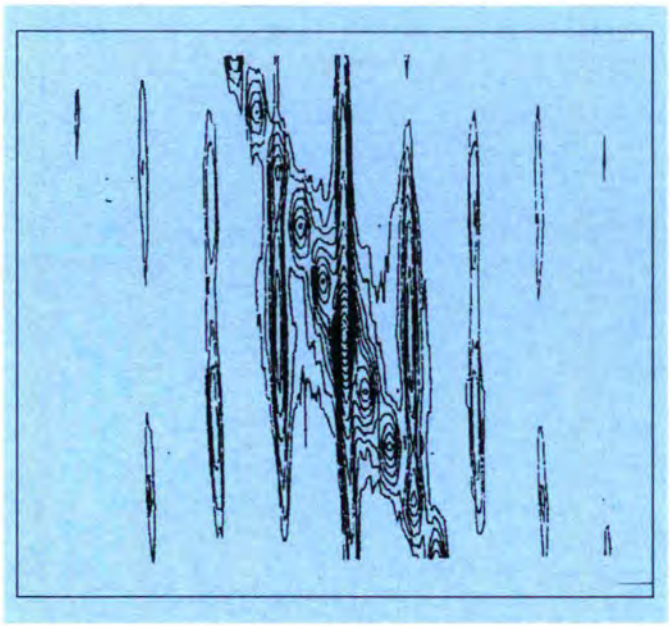

Fig. 7: Counter plot of the reciprocal space mapping of a InP surface grating in the vicinity of (002) InP.

combination of polarized and unpolarized neutron diffraction measurements on a single crystal. The neutron results confirm the theoretical prediction that the Ce atom in $CeFe_2$ carries a magnetic moment, which is opposite to the Fe one. The magnetic moment of the Fe atoms is 1.175(10) μ_B, rather smaller than the value 1.49 μ_B given by spin polarized band structure calculations. The value of the Ce moment cannot be uniquely determined without making some assumption about the ratio of the numbers of 5d and 4f electrons contributing to its magnetization. The assumption that this ratio is 0.75, as given by the band structure calculations, leads to a total Ce moment of -0.14(3) μ_B of which -0.10(2) μ_B is due to 4f spin, 0.03 μ_B to 4f orbital moment and -0.07(2) μ_B to 5d spin. The ratio of the 4f orbital to spin contributions agrees well with the band structure calculations although the magnitudes of the measured moments are almost an order of magnitude smaller than those calculated. It seems that, as is the case for Laves phases of actinide compounds, the relativistic spin polarized band structure calculations correctly predict the ratios of spin to orbital moments of Ce or an actinide, but systematically overestimate their absolute magnitudes. The magnetization distribution around the Fe atoms deviates significantly from spherical symmetry. The form of the asymmetry shows that the eigenstates of the magnetic electrons are combinations of E_g and T_{2g}-like functions which give a density with maxima in directions lying between the near neighbour bonds as illustrated schematically in Fig. 8.

Direct imaging of milli-Bohr magnetons densities in the "60 K" superconducting compound $YBa_2Cu_3O_{6.52}$

In contrast with the rather flat character in the $YBa_2Cu_3O_{6.9}$ "90 K phase", the magnetic bulk susceptibility measured at intermediate oxygen concentrations e.g. in $YBa_2Cu_3O_{6.5}$ shows an interesting thermal feature. Going down in temperature, the positive susceptibility diminishes slowly, then bends upward and reaches a positive maximum before entering the Meissner superconducting state with its large negative values.

The question then arises of the exact origin for this thermal bulk magnetic feature. The magnetic moments involved being very small, polarized neutron diffraction and its unique capability to produce an image in direct space of such a periodic density is the technique to use.

In fact, an extensive programme for measuring such magnetization density was started at the ILL on D3B a few years ago, using the 10 Tesla magnet and a YBaCuO single-crystal sample grown by the MDN/CENG laboratory. When the ILL reactor shutdown occurred, it was very fortunate for this programme that the DN2 polarized neutron diffractometer was just being commissioned at Siloe, the

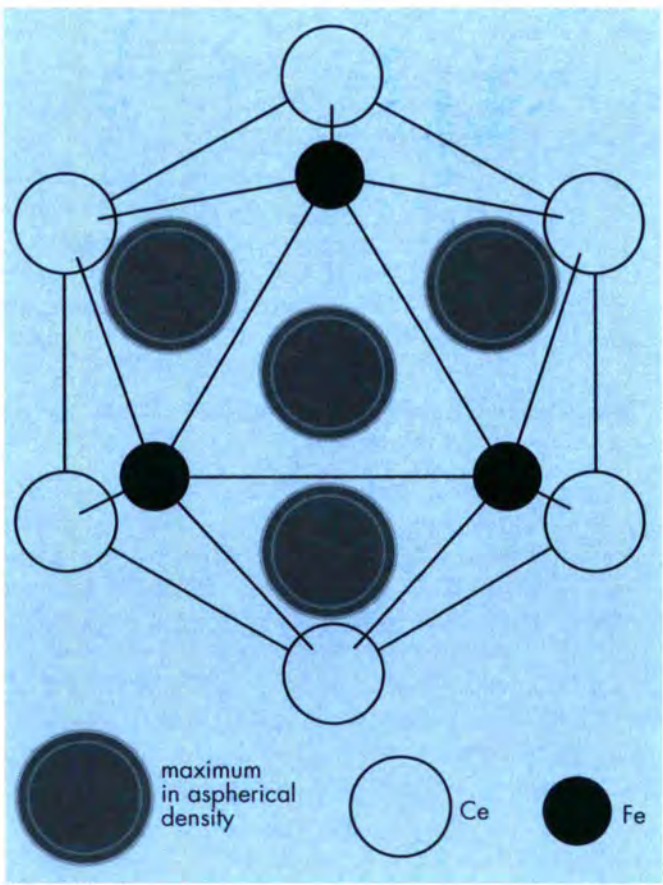

Fig. 8: Schematic representation of the icosahedron coordinating the iron atoms in $CeFe_2$. The directions in which the maxima in the spherical part of the magnetization density occur are indicated by the shaded areas.

other thermal neutron reactor in Grenoble. Therefore, by taking some of the ILL equipment to Siloe, it has been possible to continue this interesting work.

The neutron flux is reduced by the power ratio of the two reactors, but this is somewhat compensated by using longer measuring time and the progress made with the data reduction techniques. In particular, the Maximum Entropy Method turns out to be very useful for an optimal Fourier transformation of our inherently limited data.

By measuring 14 Bragg reflections of the (h h l) reciprocal space section at 3 different temperatures we were able to compute directly the "most probable" magnetization maps in projection (Fig. 9). They exhibit striking differences. In Fig. 10 we show more results of localized magnetic moments on Copper sites (Note that the scale is 10^{-3} Bohr magnetons and the precision 10^{-4} Bohr magnetons !).

Our present conclusions for these "60 K" superconducting compounds are the following:

1) As in the "90 K" compound, there is evidence on the Cu2 site for complete quenching of the spin susceptibility at the transition temperature, the residual moment being attributed to orbital contribution.

2) Unlike in "90 K" compounds the quenching seems to begin well above T_C.

3) The moment measured at Cu1 (chain sites) has a mixed Curie-Pauli paramagnetic behaviour which is not affected by the superconductivity.

4) A small magnetic moment shows up at low temperature on the apex oxygen. This may be a sign that this oxygen participates in the magnetic coupling in between the two kinds of copper atoms. At the same time the magnetic moment on Cu1 blows up and the superconducting quenching on Cu2 spins becomes less.

Chemical bonding and covalency in $NiSO_4.6H_2O$ by measurement of charge and spin densities

The experimental determination by X-ray diffraction of *d*-electron distributions around first-row transition metals has proven quite successful in recent years despite the experimental difficulties associated with the heavy atoms. It is also of interest to see if bonding features around light elements or molecules can still be observed in the presence of the much stronger scattering of metal atoms. If these include hydrogen, whose electron distribution is severely distorted by chemical bonding, the position and thermal displacement of its core must be obtained by (non polarized)

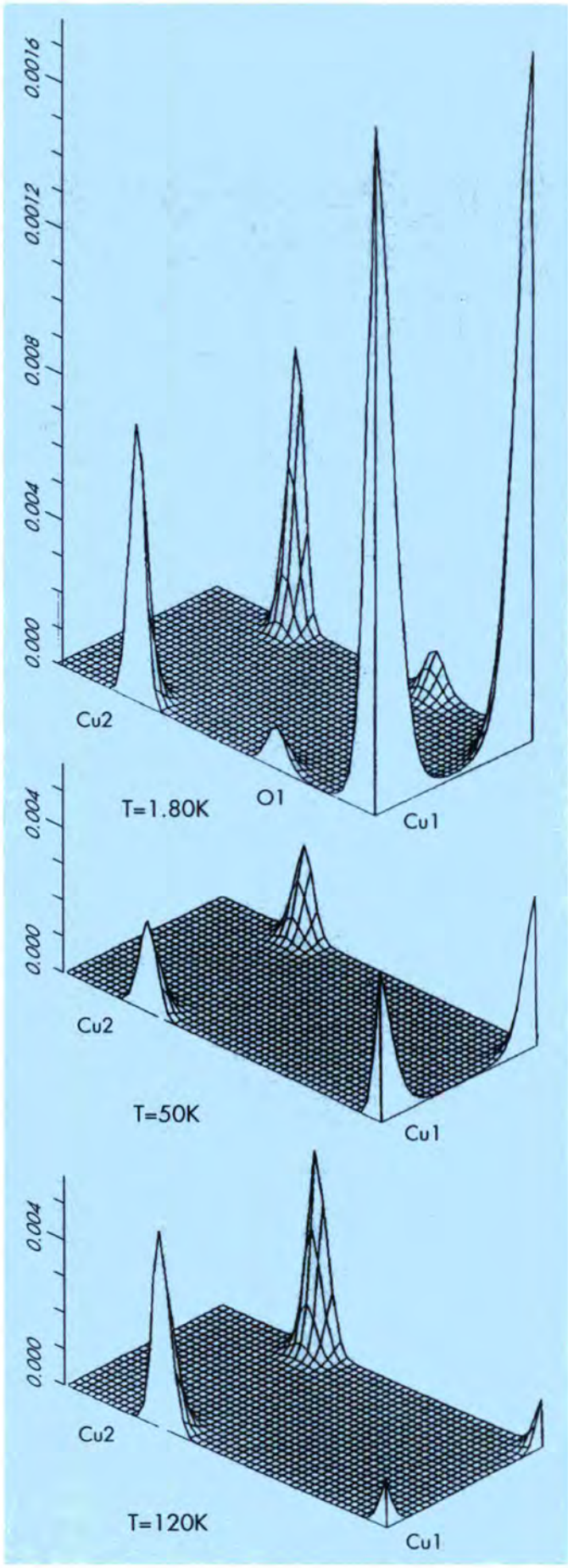

Fig. 9: $YBa_2Cu_3O_{6.52}$-[1 -1 0] Projection of the induced magnetic density at three different temperatures. The applied field is 8.2 Tesla.

neutron diffraction. Complementary information regarding the distribution of the unpaired electrons of the metal atom and the covalent transfer to the ligands can be obtained from the spin density measured by polarized neutron diffraction. Only a few joint studies of charge and spin density have been made so far. One such study is for tetragonal $NiSO_4.6H_2O$ where the X-ray data were collected at the University of Uppsala, the non-polarized neutron data at Studsvik and the ILL, and the polarized neutron data at the LLB and the ILL.

The interpretation of electron deformation densities can be confused by partial overlap of the densities associated with neighbouring atoms and molecules. It was demonstrated that the effects of superposition may be removed by considering the individual densities derived from a fitted multipole model. Analysis of the charge density for $NiSO_4.6H_2O$ at 25 K and 295 K made in this manner showed that there is clear polarization of the water oxygen lone-pair densities according to the local coordination which ranges from trigonal to tetrahedral (Fig. 11). The internal consistency amongst the deformation densities of the water molecules is quite remarkable considering the dominant contribution by nickel to the observed X-ray intensities, and is due in part to the determination by neutron diffraction of accurate structural parameters for the hydrogen atomic cores.

At both temperatures the Ni^{2+} deformations were consistent with a $t_{2g}^6e_g^2$ electron configuration with the d_{xy}, d_{xz} and d_{yz} orbitals fully occupied and the $d_{x^2-y^2}$ and d_{z^2} orbitals partially occupied, as expected from simple crystal-field theory for a weak octahedral ligand field. However there were differences observed between the deformations at the two temperatures (Fig. 12a and b), which are postulated to be due to a real change in the relative occupations of the partially-filled electronic levels; indeed, an estimation from these observations of the change in occupations agrees with magnetization measurements of the splitting of the two uppermost energy levels. If correct, this is the first time such an effect has been observed by diffraction methods.

The spin density was determined at 1.5 K using data from both $NiSO_4.6H_2O$ and $NiSO_4.6D_2O$ to maximize the number of independent data. Joint analysis of the charge and spin densities to extract orbital populations is in progress, but already a preliminary analysis of the spin density has shown good qualitative agreement with the charge density study, with the unpaired electrons of Ni^{2+} being mainly in the $d_{x^2-y^2}$ and d_{z^2} orbitals (Fig. 12c). In addition some covalent transfer to the water oxygen atoms is suggested.

Similar experiments on other compounds in the series $M^{II}SO_4.6H_2O$ are currently underway to study the bonding deformations of the different 3d electron configurations.

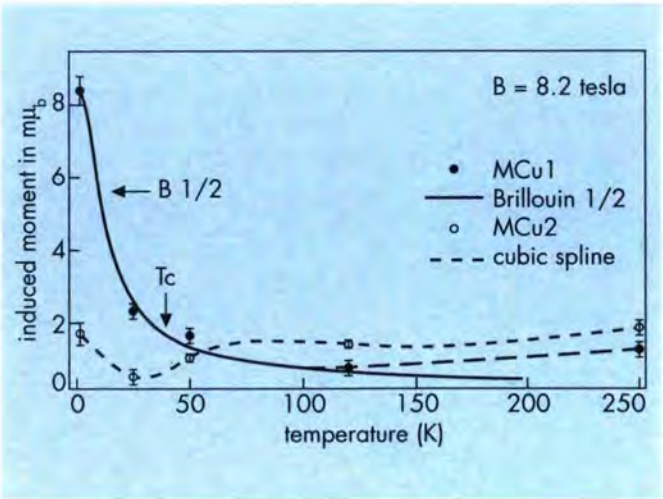

Fig. 10: $YBa_2Cu_3O_{6.52}$- A thermal plot of the induced magnetic moments on the two different copper sites: Cu1(chains) and Cu2(planes).

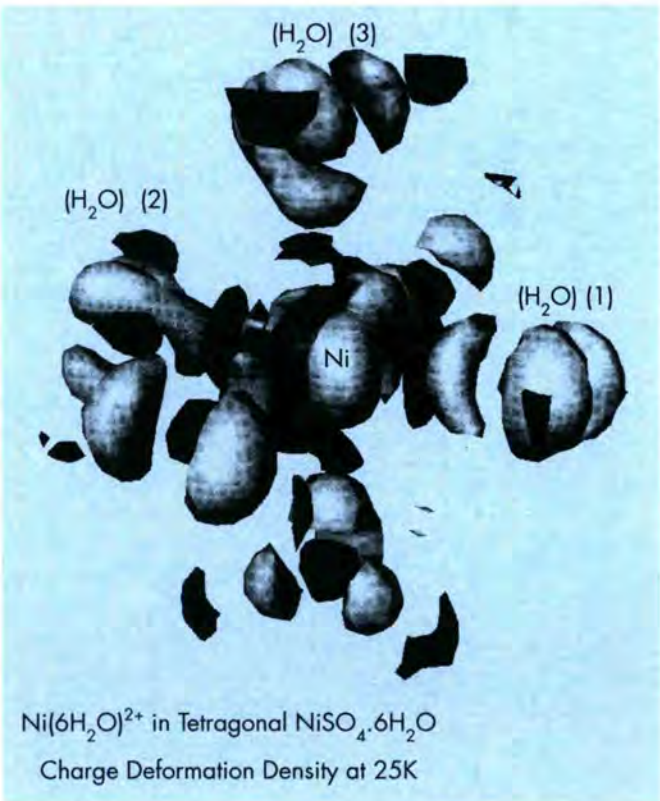

Fig. 11: The charge deformation density of the $Ni(6H_2O)^{2+}$ ion of tetragonal $NiSO_4.6H_2O$ at 25 K. This is the difference between the model that includes multipolar functions centred on each atom and the model based on purely spherical atoms.
The lighter contours envelope regions of electron excess compared to the spherical model, the darker contours regions of electron deficiency. Differences in the lone-pair distributions of the O atoms according to their coordination are clearly visible, as is the $t_{2g}^6e_g^2$ electron configuration of the Ni atom.

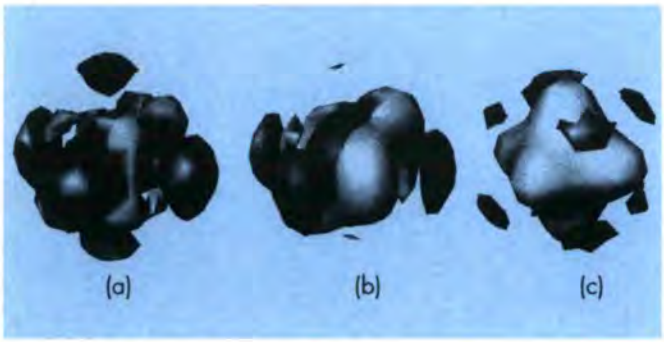

Fig. 12: Charge and spin deformation densities around the Ni atom in tetragonal $NiSO_4.6H_2O$: a) charge density at 295K; b) charge density at 25K; c) spin density at 1.5K. The differences between the charge densities at 295 K and 25 K are attributed to changes in the occupation of the uppermost 3d electronic levels.

Phases of magnetic structure factors of non-centrosymmetric magnetized crystals

Determination of the spin density from the flipping ratios of the polarized neutron diffraction experiment on tetragonal $NiSO_4.6H_2O$ was complicated by the lack of a centre of symmetry. This was circumvented by fitting a multipole model for the spin density, similar to that used for the analysis of the charge density, to the observed flipping ratios. In this compound there was little doubt as to the initial model. It was realized however that the two components of the complex magnetic structure factor could be derived directly from the observed flipping ratios by modifying the experimental technique to give two or more independent observations for each magnetic structure factor.

In its simplest form the flipping ratio for a non-centrosymmetric structure is

$$R = \frac{A_N^2 + B_N^2 + 2\,(A_N A_M + B_N B_M) + A_M^2 + B_M^2}{A_N^2 + B_N^2 - 2\,(A_N A_M + B_N B_M) + A_M^2 + B_M^2}$$

where A_M and B_M are the real and imaginary components of the unknown magnetic structure factor F_M, A_N and B_N the real and imaginary components of the known nuclear structure factor. Isotope exchange of one or more elements in the compound will change the nuclear structure factor but usually not the magnetic structure factor (to within a scale factor in the magnetization). Measurement of the flipping ratio for the same reflection from samples with different isotope content will thus give independent observations which can be solved for A_M and B_M.

The expression for R corresponds to a circle in the complex plane, and gives a graphical construction (Fig. 13) which is very similar to that used in the multiple isomorphous replacement method of macromolecular crystallography. Isotopic replacement is the most precise method, but even simple reorientation of the crystal or measurement of equivalent reflections to change some geometrical cofactors omitted from the above expression for R can give A_M and B_M independently. Variation of the nuclear polarization of selected elements could also be exploited for some compounds, which has the advantage that only one sample is used.

The validity of some of these methods was demonstrated using the experimental flipping ratio data for $NiSO_4.6H_2O$ and $NiSO_4.6D_2O$. In this case experimental determination of A_M and B_M independently was unnecessary for the study of the spin distribution, but the technique could find application in the determination of the complex magnetic structure factors of other non-centrosymmetric structures.

Magnetic phases of erbium in a c-axis field

The discovery in the mid-eighties of long-period commensurate magnetic structures in holmium and erbium rekindled intense interest in the magnetic structures and excitations of these and other heavy rare earth metals. The existence of these long-period phases is due to competition between the exchange interaction which favours simple incommensurate ordering and the crystal field interaction which favours formation of commensurable structures. Application of a magnetic field alters the balance between these interactions producing modifications of the zero-field structures, and even completely new types of magnetic order, such as the helifan observed in holmium when the field is applied along the easy b-axis.

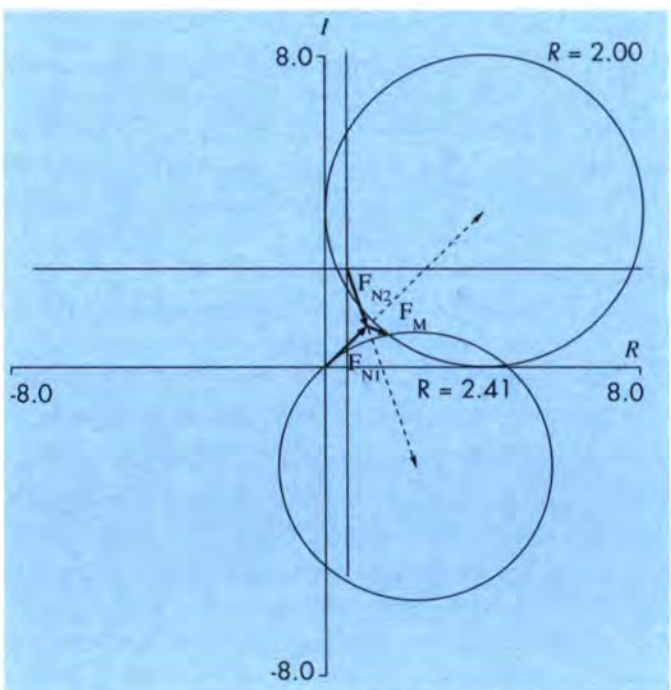

Fig. 13: The graphical solution for the complex magnetic structure from the observed flipping ratios for the same reflection from crystals with different isotopic composition. Here $A_{N1} = B_{N1} = 1$, $R_1 = 2.0$; $A_{N2} = 0.5$, $B_{N2} = -1.5$, $R_2 = 2.41$. The more likely solution for F_M is indicated. R and I are the real and imaginary axes respectively of the complex structure factor plane. The two sets of axes are offset so that the heads of F_{N1} and F_{N2} coincide.

In the case of erbium even the zero-field structures were not clearly understood until a recent comprehensive study by Cowley and Jensen showed that the cycloidal phase purported to exist between 54 K and 18 K possesses an oscillatory component perpendicular to the plane of the cycloid, and that its existence requires a magnetic interaction which distinguishes between the two lattice sites in the chemical unit cell. Their model has now pointed to detailed solutions to the structures of erbium in a c-axis field, from measurements performed comparatively recently on D10. These have allowed further detail to be added to the phase diagram (Fig. 14).

New results were firstly that in addition to the longitudinal modulation along c, the high temperature phase of erbium in a c-axis field has a small basal plane moment, probably helically ordered, with a different modulation vector to the longitudinal component. Secondly the most noticeable effect of applying a field is that the temperature intervals over which the wavevector of the cycloidal phase is commensurate are enhanced at the expense of those over which it is incommensurate. The oscillatory component perpendicular to the a-c cycloidal plane is still present but application of a field does reduce its moment, as well as the basal-plane component of the cycloid, relative to their values in zero field. Finally applying a field enhances the stability of the commensurate and incommensurate cone phases at the expense of the longitudinal and cycloidal phases, although details of the phase diagram at high field and low temperature are still uncertain.

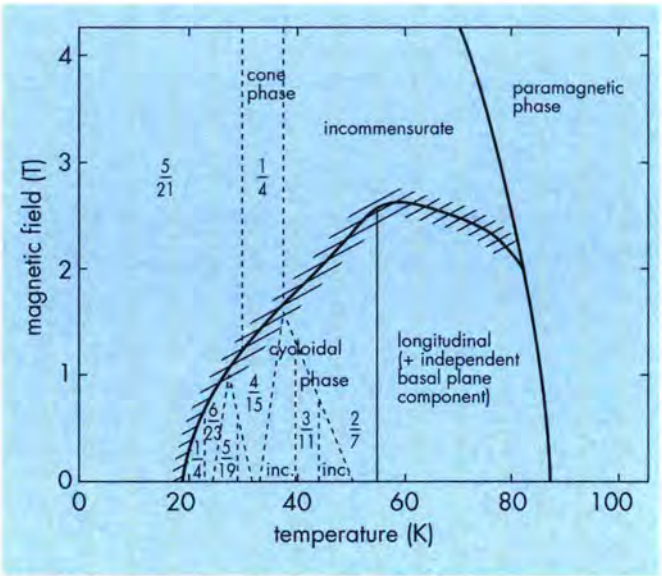

Fig. 14: Magnetic phase diagram of erbium in a c-axis field. Solid lines separate the main phases; dashed lines separate similar commensurate and incommensurate phases.

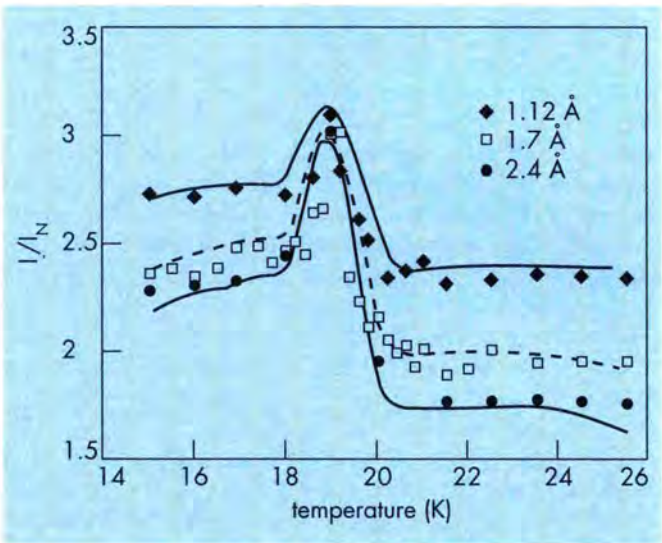

Fig. 15: The temperature variation of the ratio of the integrated intensities of the satellite 002 - τ to the reflection 002 as function of temperature and neutron wavelength; the lines represent a joint fit by the RED extinction model.

Extinction in holmium around the 19 K magnetic transition

Holmium undergoes around 19 K a first order magnetic transition from an incommensurate phase (high temperature) to the 1/6 conical (low temperature) phase. Neutron diffraction experiments on high purity single crystals reveal presence of strong extinction in the purely nuclear 002 reflection as well as in both of the magnetic 002±τ satellites. Results of detailed investigations performed on S20 imply that reduction in reflectivity is more severe for the satellites than for the nuclear reflection. Furthermore there is an appreciable reduction of the satellite intensities in the high-temperature phase as compared to the low-temperature one (Fig. 15) while they have nearly the same structure factor. It is concluded that the magnetic ordering is considerably more perfect than the underlying nuclear lattice. The itinerancy of the polarized conduction electrons is thought to be responsible for this phenomenon as a result of their weak interaction with the nuclear lattice. In particular the spin slip structure of the incommensurate phase may easily accommodate local defects in the magnetic order (keep constant the average turn angle) by introducing or removing spin slips. On the other hand the confines of a fixed wave vector in the 1/6 state will force the local propagation vector to follow more closely the crystal lattice. The fact that no change in intensity of the purely nuclear 002 reflection can be observed around the magnetic transition provides another argument for the autonomy of the magnetic system. In the immediate vicinity of the transition temperature (19 K) a considerable increase in satellite intensity is observed that can be attributed to local disorder or phase coexistence as the overall topology of the chirality domains does not change. Standard extinction models were tried to describe this behaviour. Only the Random Elastic Deformation (RED) model provides a consistent interpretation over the complete temperature range (Fig. 15) in terms of a varying mean strain gradient which in the present case refers to the spin turn angle rather than to the atomic displacement. Its

increase (5 x) in the transition region permits us to draw a picture of phase coexistence with propagation vectors fluctuating continuously both in space and time between the values corresponding to the two neighbouring phases.

The low temperature antiferromagnetic structure of Mn_5Si_3 revised in the light of neutron polarimetry

The magnetic structures which were previously proposed for the low-temperature antiferromagnetic phase of the intermetallic compound Mn_5Si_3 have been revised to take into account the results of neutron polarimetry in addition to unpolarized neutron single-crystal integrated intensity measurements. At 4.2 K the commensurate magnetic unit cell is orthorhombic with a = 6.889 Å, b = 11.901 Å and c = 4.805 Å and is related to the hexagonal cell of the paramagnetic phase by a = a, b = $a\sqrt{3}$, c = c. The hexagonal cell contains 4 Mn1, 6 Mn2 and 6 Si atoms. The total absence of magnetic scattering in the ortho-hexagonal h01 reflections shows that the moments of two of the six sublattices of Mn2 atoms must have zero ordered moment. The polarimetric results impose additional constraints on possible models for the magnetic structure. (a) There are components of moment in all three principal directions. (b) The magnetic symmetry is monoclinic and non-centrosymmetric. (c) The moments on the two Mn2 sublattices which carry moment are approximately perpendicular to one another. These constraints allowed a complete model of the magnetic structure to be refined which gave excellent agreement with both the polarimetric and integrated intensity measurements. In this final structure, which is illustrated in Fig. 16, the Mn1 atoms have moments of 1.20(5) μ_B inclined parallel and antiparallel to the direction given in spherical polar coordinates by $\theta = 116(1)°$, $\phi = 105(1)°$. (θ is measured from [0 0 1] and ϕ from [0 1 0]). One third of the Mn2 atoms carry no moment, one third have moments of 2.30(9) μ_B at $\pm$ [$\theta = 70(1)°$, $\phi = 93(1)°$] and the remainder have 1.85(9) μ_B at $\pm$ [$\theta = 21(1)°$, $\phi = 11(7)°$]. The structure is, perhaps surprisingly, rather complex and contains a variety of different Mn moments arranged in a highly non-collinear manner. The non collinearity of the Mn2 moments and the absence of moment on one third of them may be interpreted as the response to frustration in the puckered ring of six Mn2 atoms. The low moment found for Mn1 is probably due to the close proximity of its two Mn1 neighbours (2.4 Å), since such small distances between Mn atoms are known to lead to instability of the moment. The difference between the moments on the crystallographically equivalent Mn2 sites must be due to the fact that their magnetic moments have different orientations with respect to the crystal field of the coordinating Si atoms. Thus, though complex, this new structure can be understood in terms of the physics already used to describe other antiferromagnetic intermetallic compounds containing manganese.

Magnetic ordering of $TiFe_2$

The compound $TiFe_2$ crystallizes in the C14 hexagonal Laves phase $MgZn_2$-type structure ($P6_3/mmc$) in which the

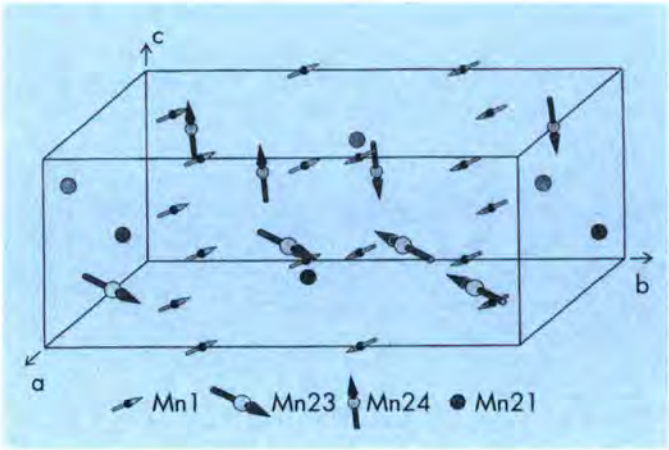

Fig. 16: The low temperature antiferromagnetic structure of Mn_5Si_3.

Ti atoms occupy a single crystallographic site (4f), whereas there are two non-equivalent sites type (2a) and (6h) for the Fe atoms which are labelled Fe1 and Fe2 respectively. $TiFe_2$ exhibits an antiferromagnetic transition below T_N = 280 K. Neutron diffraction experiments on a single crystal were made using the D15 diffractometer and the D3 diffractometer for polarized neutrons.

The positions of the magnetic peaks observed in both the powder and single-crystal diffraction measurements put severe constrain on the possible magnetic structures. Firstly the magnetic cell is the same as the crystallographic one hence the magnetic propagation vector **k** = (0, 0, 0). Next the presence of the 111 reflection indicates that the glide plane perpendicular to [1 1 0] reverses the spin direction. Finally the absence of the 001 and 003 reflections suggests that the spin direction is along the c-axis. The only structure which retains hexagonal symmetry and which is consistent with these observations is that in which the moments of Fe2 atoms in the same layer (z = 1/4) are ferromagnetically aligned while the magnetic coupling between adjacent layers is antiferromagnetic (Fig. 17). The resultant molecular field at the Fe1 atoms is zero as it lies midway between two antiferromagnetically coupled planes on a centre of symmetry which is associated with time reversal. Under these circumstances the Fe1 atoms can have no ordered moment.

On the other hand, the magnetic scattering by the magnetization induced by the applied field in the polarized neutron diffraction experiment was compared with that calculated for a simple model consisting of superposition of spherical magnetization distributions as calculated for the Fe^{2+} free ion centred at the iron sites. The magnitudes of the moments associated with Fe1 and Fe2 sites in this model were obtained from least-squares fits of the calculated structure factors to the observations. For the two orientations

i.e. the applied field parallel and perpendicular to the c-axis, the susceptibilities of the two sites were found to be approximately equal, but the absolute value of the moment induced, by the applied field of 4.6 T for the c-axis orientation (0.008(2) μ_B/atom) was ten times smaller than that with the c-axis perpendicular to the field (0.095(5) μ_B/atom).

The lack of an ordered moment on the Fe1 atoms, as in some RMn_2 Laves phases compounds, is a common feature in frustrated magnetic structures in which there are sites at which the magnetic symmetry imposes zero molecular field. In $TiFe_2$ the fact that a site with no ordered moment persists down to low temperature suggests that the Fe moment also is near to instability in this compound. The Fe1 atom would then be non-magnetic rather than magnetically disordered. Such an assumption leads to a consistent interpretation of the induced moments obtained from the polarized neutron measurements.

Antiferromagnetic ordering in $PrCo_2P_2$ and $NdCo_2P_2$

Because of the great variety of possible elements in the $ThCr_2Si_2$-type structure more than 500 different compounds of this type are known already. Some of these exhibit unusual physical properties such as superconductivity, valence fluctuations, local and itinerant magnetism. Systematic investigations of the magnetic properties of the ternary phosphides were started much later.

In the series $LnNi_2P_2$ and $LnFe_2P_2$ (Ln = lanthanoides) the transition metal atoms carry no ordered magnetic moments, whereas ferromagnetic or antiferromagnetic order was observed for the compounds $LnCo_2P_2$. Magnetic susceptibility measurements indicated antiferromagnetic order of the cobalt moments at T_N = 304 K and T_N = 309 K for the praseodymium and the neodymium compounds,

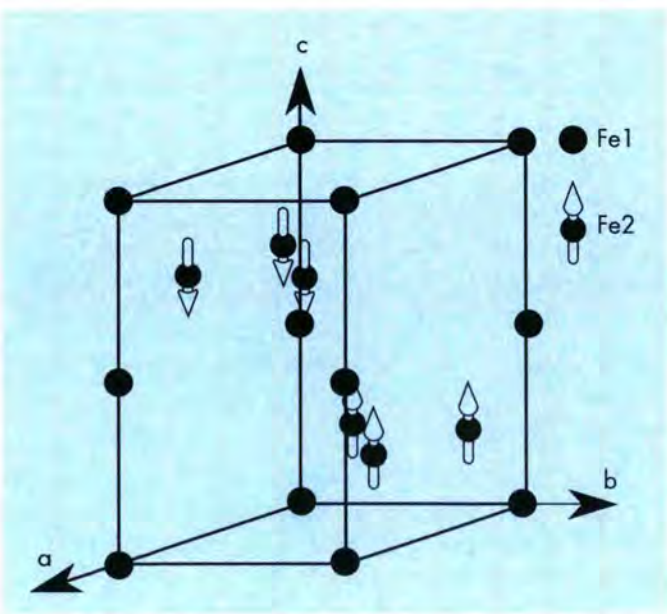

Fig. 17: Magnetic structure of $TiFe_2$. Only Fe atoms are shown.

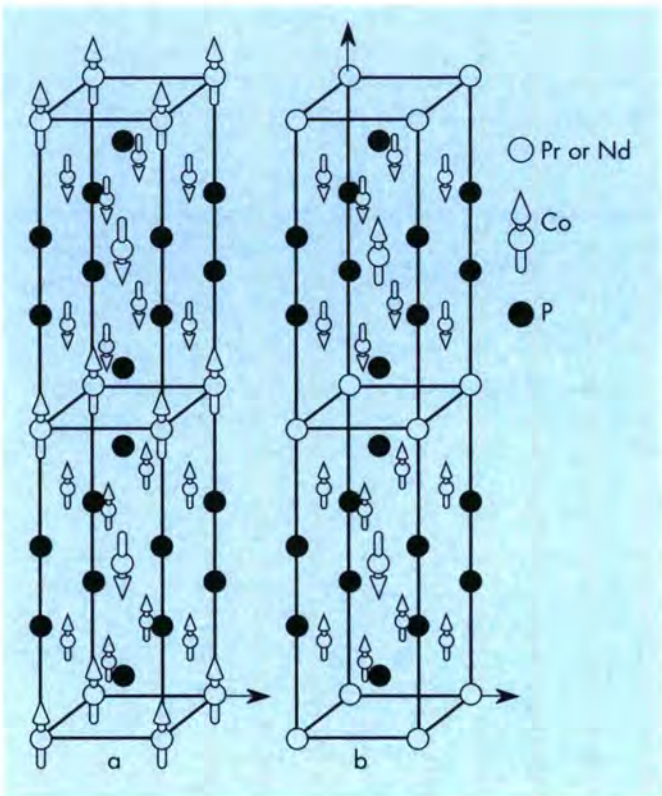

Fig. 18: Magnetic structures of $PrCo_2P_2$ (a) and $NdCo_2P_2$ (b).

respectively. A second Néel temperature T_N = 19 K was found for $PrCo_2P_2$, which was ascribed to the magnetic order of the praseodymium moments. For $NdCo_2P_2$ the magnetic susceptibility was found to behave anomalously at low temperatures.

The magnetic stuctures of the compounds $PrCo_2P_2$ and $NdCo_2P_2$ were investigated at different temperatures by neutron powder diffractometry on the instruments D1A, D2B and D20. In agreement with the magnetic susceptibility data the magnetic moments of both the praseodymium and the cobalt atoms of $PrCo_2P_2$ were found to order antiferromagnetically with different well defined Néel temperatures. The praseodymium sublattice propagates with $\mathbf{k}$ = (0, 0, 1) and the cobalt one with $\mathbf{k}$ = (0, 0, 1/2) (Fig. 18). In contrast, for $NdCo_2P_2$ only one propagation vector $\mathbf{k}$ = (0, 0, 1/2) was found for the Nd and Co sublattices, indicating that the Nd moment is induced gradually at lower temperatures. In this case the magnetic order of the Nd moment has no well defined Néel temperature, as was shown by measuring the temperature dependence of the intensity of the magnetic reflection 1 0 1/2. For $PrCo_2P_2$ the intensity of the magnetic reflection 1 0 0 vanished completely above 20 K.

The magnetic moments of the cobalt atoms of both compounds were ordered ferromagnetically within the basal plane of the tetragonal structure and parallel to the c-axis with the stacking sequence + + - - along this axis direction (Fig. 18). For the moments of the Pr atoms the order is again

ferromagnetic within the basal planes but with the stacking sequence + - + -. In the magnetic stucture of the Nd sublattice no magnetic order (0) was found for every second basal plane; the stacking sequence is of the type 0 - 0 +. At low temperatures the magnetic moment of the cobalt atoms was found to be about $\mu_{exp} = 0.9\ \mu_B$ in both compounds. The experimental moments of the Ln atoms were $\mu_{exp} = 3.08(2)\ \mu_B$ for the praseodymium atoms and $\mu_{exp} = 2.78(6)\ \mu_B$ for the neodymium atoms, somewhat smaller than the theoretical values of the free Ln^{3+} ion $\mu_S = 3.20\ \mu_B$ and $\mu_S = 3.27\ \mu_B$, respectively.

Using a dilution refrigerator with the instrument D20 a neutron diffraction pattern of $NdCo_2P_2$ was measured at 0.134 K. A change of the antiferromagnetic order to a ferromagnetic one, which was expected from our susceptibility measurements, was not found. Nevertheless such a transition may occur at finite applied magnetic fields as indicated by the field dependence of the magnetic susceptibility observed below 15 K. For $PrCo_2P_2$ a field dependence of the magnetic susceptibility was observed below the Néel temperature $T_N = 19$ K.

Magnetic structure of Ho_2BaNiO_5

Powder neutron diffraction measurements were performed on the compound Ho_2BaNiO_5 using the D1B diffractometer. Ho_2BaNiO_5 has an orthorhombic structure (Space group Immm, a = 3.764 Å, b = 5.761 Å, c = 11.336 Å), in which flattened NiO_6 octahedra form vertex-sharing chains along the a-axis.

Three Dimensional Antiferromagnetic Ordering (3D-AF) is observed for both Ho and Ni sublattices at relatively high ordering temperature ($T_N = 53$ K). Rare earth magnetic moments in oxides usually order at much lower temperatures. The magnetic peaks have been indexed within a commensurate lattice with a propagation vector $\mathbf{k} = (1/2, 0, 1/2)$. The best magnetic model has been found when the relationship between the two Ho magnetic moments of the primitive cell is $S_{2x} = S_{1x}$, $S_{2y} = S_{1y} = 0$, and $S_{2z} = S_{1z}$. The Ni magnetic moment lies also in the a-c plane. In this case the two basis vectors are directly the S_x and S_z components of the magnetic moment because the primitive cell has only one Ni atom.

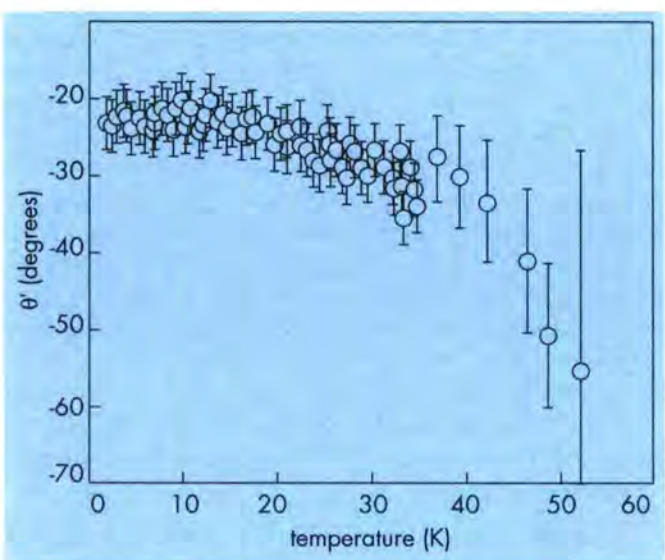

Fig. 19: Temperature dependence of the angle θ' (θ' is defined as the angle between the Ni magnetic moment and the [0 0 -1] direction).

At 1.5 K the value of the Ho moment is 9.0 μ_B close to the free ion value (10 μ_B), and is almost fully aligned parallel to the c–axis. This indicates that the single-ion anisotropy of Ho^{3+} in these compounds is clearly directed along the c–axis. The direction of the Ho moments remains nearly aligned along the c-axis i.e. perpendicular to the chains. However the direction of the Ni moments forms an angle $\theta = 154°$ with the c-axis. Fig. 19 shows the temperature dependence of $\theta' = \theta - 180°$. We observe that close to T_N the Ni sublattice starts to be ordered with the magnetic moments pointing mainly along the NiO_6 (a-axis). At lower temperature, the Ni moments start to rotate toward the c–axis, forced by the combination of the increasing ordered moment on the Ho site, the exchange $J_{Ni\text{-}Ho}$ and the anisotropy of the Ho^{3+} due to the crystal field. Around 33 K, the Ni moment is almost aligned along the c–axis with a small component parallel to the a–axis (Fig. 20)

In the case of Er_2BaNiO_5 the directions of the Er and Ni moments are almost parallel to the chains (a–axis). This reflects the effects of the magnetic anisotropy of the two rare earth ions.

The magnetic structure of $PrBa_2Cu_3O_{6+\delta}$

When Pr is substituted into the high-T_c superconductor $YBa_2Cu_3O_7$ the transition temperature T_c is found to decrease with increasing dopant concentration, and the superconductivity is entirely suppressed at 50 % substitution. This behaviour is not observed with any other rare earth dopants. It is important for the understanding of the origin of high-T_c superconductivity to know why Pr destroys the superconductivity. Evidence from crystal field excitations and magnetization measurements supports a possible explanation of this behaviour due to a magnetic interaction between the magnetic moment on the Pr atom and the electrons at the Fermi surface on the Cu-O planes.

In order to help correlate the mechanism of the magnetic exchange with high-T_c superconductivity an experiment was performed on a single crystal of $PrBa_2Cu_3O_{6+\delta}$ on TAS3 at Risφ, Denmark.

Initial measurements on the crystal, with a low oxygen concentration, revealed magnetic reflections of a h/2 h/2 l type with an initial ordering above room temperature. This can be attributed to the antiferromagnetic ordering of the Cu spins within the plane whilst the Cu spins in the chains remain disordered.

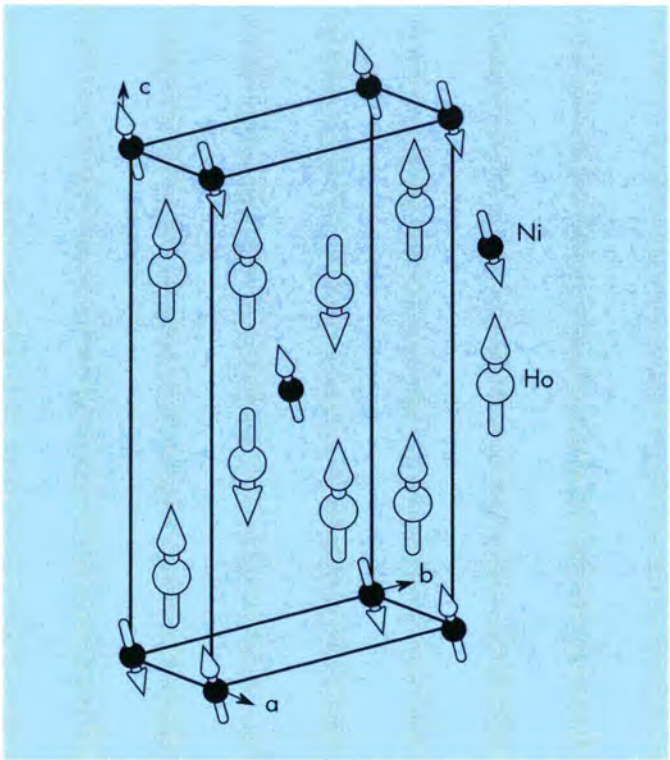

Fig. 20: Magnetic structure of Ho_2BaNiO_5.

A second ordering occurs at 40 K, with the appearance of h/2 h/2 l/2 type reflections and a decrease of the h/2 h/2 l type reflections. A simple model, with the additional ordering of the Cu spins on the chain sites coupled antiferromagnetically with the Cu plane spins, fails to describe the relative intensities of the peaks. In addition the presence of a 1/2 1/2 0 reflection, not allowed in the simple model, seems to indicate a more complex ordering involving the Pr spins.

Further measurements on the crystal, with a higher oxygen concentration, showed a lowering of the second ordering transition to 13 K. Future measurements on the fully oxygenated crystal will help achieve a full understanding of the magnetic ordering and the effect of oxygen concentration.

Magnetic behaviour of Pr_2NiO_4

Neutron diffraction measurements on a single crystal of Pr_2NiO_4 show a similar structural behaviour to La_2NiO_4 and Nd_2NiO_4. Going from high to low temperature, these compounds undergo two structural phase transitions, at high temperature the structure changes from tetragonal I4/mmm (HTT) to orthorhombic Bmab (LTO). At low temperature a second phase transition to tetragonal $P4_2/ncm$ (LTT) occurs.

The magnetic behaviour of praseodymium nickelate is also similar to that of La_2NiO_4 and Nd_2NiO_4 in the temperature range from 325 K to the LTO-LTT transition at 117 K. Nevertheless, for lower temperatures the observed magnetic behaviour of Pr_2NiO_4 turns out to be different and more complicated. The temperature dependence of the integrated intensity of the main magnetic Bragg reflections is shown in Fig. 21.

As shown from neutron powder diffraction data, the nickel moments order antiferromagnetically (AF) at $T_{N1} \approx 325$ K in a g_x-mode. Since the orthorhombic structure is derived from a high-temperature tetragonal I4/mmm phase, two crystallographic twins exist. The small intensity

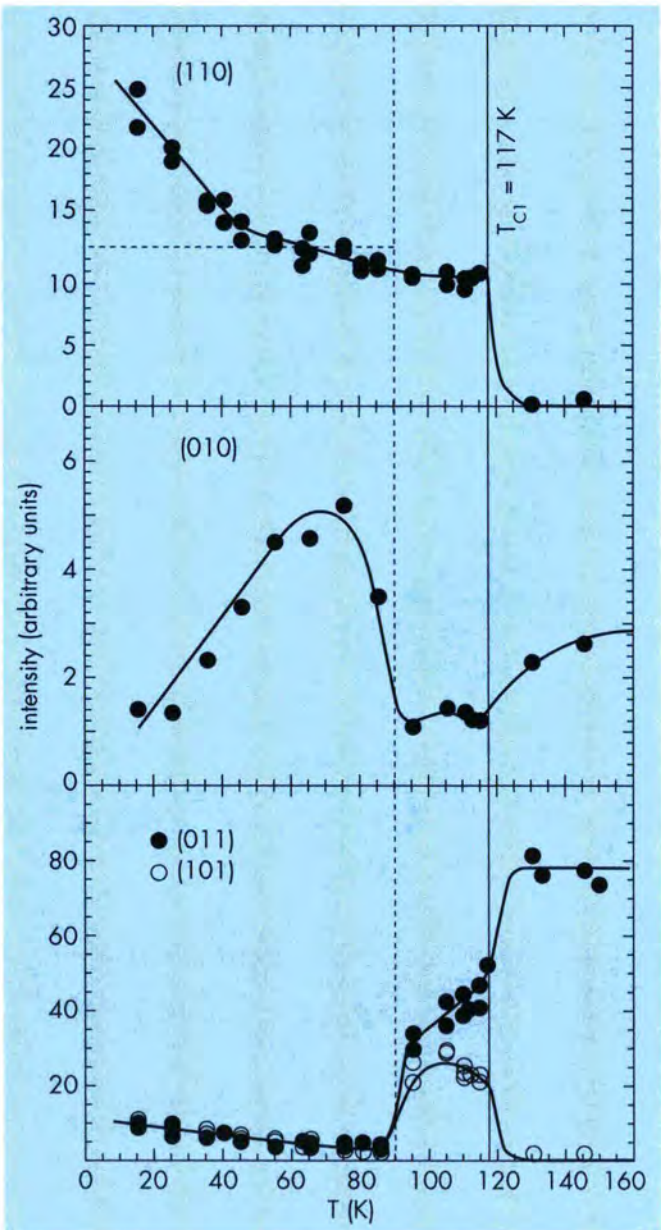

Fig. 21: Temperature dependence of the 1 1 0, 0 1 0, 0 1 1 and 1 0 1 magnetic reflections for Pr_2NiO_4 showing the structural phase transition at T_{C1} = 117 K (vertical solid line) and the magnetic phase transformation at T_{N2} = 90 K (vertical dashed line). The lines are guides to the eye.

observed for the 1 0 1 reflection, forbidden in a g_x-mode, originates from the second twin of the 0 1 1 magnetic reflection.

Due to the structural phase transformation at T_{C1} = 117 K, the magnetic modes g_x and c_yf_z are mixed. As a consequence of the average tetragonal crystal structure, it is difficult to determine the magnetic symmetry of the Ni sublattice, even using single-crystal diffraction. Either tetragonal $P4_2/nc'm'$ ($g_x+c_yf_z$), which implies that the in-plane component of the spin is along [1 1 0] for z = 0 and along [1 -1 0] for z = 1/2, or multidomain orthorhombic $Pc'c'n$ ($g_xc_yf_z$) with magnetic moments mainly along the x-direction. In the temperature range between T_{C1} = 117 K and T_{N2} = 90 K there is a spin reorientation process from g_x to g_xc_y (or g_x+c_y).

At T_{N2} = 90 K a magnetic phase transition takes place from the $g_xc_yf_z$ magnetic structure to $c_xg_ya_z$. The phase transition is specially apparent from the sudden decrease in the intensity of the 0 1 1 and 1 0 1 reflections and a sudden upward jump in the intensity of the 0 1 0 and 1 0 0 reflections. The low temperature magnetic structure has an AF out-of-plane component (a_z), similar to that observed in La_2CuO_4. This is seen from the intensity of the 1 1 0 Bragg reflection. For $T > T_{C1}$ this reflection is forbidden, while it has nuclear and magnetic contributions below T_{C1}. The nuclear contribution is represented by the horizontal dashed line in Fig. 21. Only below 90 K does the 1 1 0 intensity increase.

At low temperature the Pr sublattice is ordered within the same irreducible representation as the Ni sublattice. This means that the coupling between both sublattices is responsible for the global magnetic moment configuration. The data obtained suggest that there is an ordered magnetic moment in Pr sites below T_{C1} = 117 K. However, its amplitude is very small and difficult to estimate. The ordered moment becomes significant below 40 K, where a change in the slope of the 1 1 0 reflection is observed, associated with the growing of the AF out-of-plane component in the Pr sublattice. The magnetic moment of Pr at 15 K is much smaller than that expected for a free Pr^{3+} ion. All these observations indicate that the Pr ordered magnetic moments are induced by the local exchange field coming from the Ni sublattice.

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The structural chemistry of non-rigid molecules

T. Vogt

Introduction

Non-rigid molecules have been a challenge to the structural chemist due to the structural disorder they reveal as a consequence of their fluctuational behaviour. Probed with standard diffraction techniques this leads in general to a structure with high symmetry in the high-temperature phase as a result of the time-averaging of various competing structural arrangements with rather low energy barriers between them. This can be the result of a "floppy architecture" with a lot of rotational and orientational degrees of freedom among the structural sub-units (e.g. methyl or amino groups) or because the coordinational topology can manifest itself in two or more coordination polyhedra with rather low energy barriers between them.

An example of the first case is the diamminehydrogen ion $N_2D_7^+$, where two ammonia molecules are connected via a proton. The freezing-out of the orientational disorder of the ion, the rotation of the ammonia molecules and the appearance of a hydrogen bond network when cooling this ion in the N_2D_7I salt are responsible for the different solid state phases observed.

The second case is represented by the only two stable binary hepta-coordinated molecules IF_7 and ReF_7. The structural arrangement of these compounds in the solid state has been a longstanding problem in solid state chemistry. Predictions of the molecular geometry on the basis of the Valence Shell Electron Pair Repulsion-theory [1] are known to be rigorously correct up to hexa-coordination and independent of the force law. This no longer holds for heptacoordination, where assuming a simple variable force law of r^{-n} shows that for soft repulsions (n = 1) the pentagonal bipyramid (symmetry D_{5h}), for stronger repulsions amongst the ligands ($2 < n < 5.6$) a C_2 geometry and for very hard repulsions the mono-capped octahedron (symmetry C_{3v}) are the most stable molecular geometries respectively. Thus an increase of the repulsive interactions amongst the ligands ("hardening") leads to the puckering of the pentagonal ring of the pentagonal bipyramid which then leads to an axial bending. However, the energy difference between these different coordination polyhedra are roughly the amount it takes to deform an octahedron by one degree. These predictions have been made on the basis of some rather crude assumptions e.g. ignoring attractive forces and placing the ligands on a sphere implying equivalent bond distances. It is therefore of considerable interest to understand how nature deals with the problem of heptacoordination. It was only recently that neutron powder diffraction could shed some light onto these questions.

The diamminehydrogen ion $N_2D_7^+$

Proton transfer along hydrogen bonds is an important process in biological and chemical systems. There has been considerable theoretical interest in model systems of the type: H_3O^+-H_2O, NH_4^+- H_2O, NH_4^+-NH_3 and others. The diaquahydrogen ion $O_2H_5^+$ is known to exist in the crystalline state and has been characterized structurally. The isoelectronic $N_2H_7^+$ ion was known to exist in the gas phase revealing a $[NH_3—H\cdots\cdots NH_3]^+$ topology.

High-resolution neutron powder diffraction using D2B could not only show that this cation exists in the solid state but also reveal the "freezing-out" of various internal motions when cooling, and its subsequent distortion [2, 3]. Besides that, by comparing the deuterated and hydrogenated compound an interesting difference in the phase behaviour was found.

Both compounds N_2H_7I and N_2D_7I crystallize at room temperature in a cubic phase. This cubic phase is the consequence of an orientational disorder of the cation: its centre of gravity is located in the middle of a cube of iodine atoms. The N-N axis is statistically equally orientated along the three cubic axes and the terminal hydrogen (deuterium) atoms are disordered around each N-N axis (Fig. 1a).

The molecule now undergoes different transitions when cooling down depending on whether the hydrogenated or deuterated cation is present. In the hydrogenated case a tetragonal phase is observed at 220 K followed by an orthorhombic phase at 202 K, wheras the deuterated compound already undergoes a transition to an orthorhombic phase when cooling to 260 K. Both compounds transform into a monoclinic low-temperature form at around 155 K. The structure of the orthorhombic phase was determined from high-resolution neutron powder diffraction data.

On cooling down the three-dimensional disorder of the N-N axis along the three cubic axes is reduced to a two-dimensional disorder leading to the contraction of the axis along which the molecule is no longer

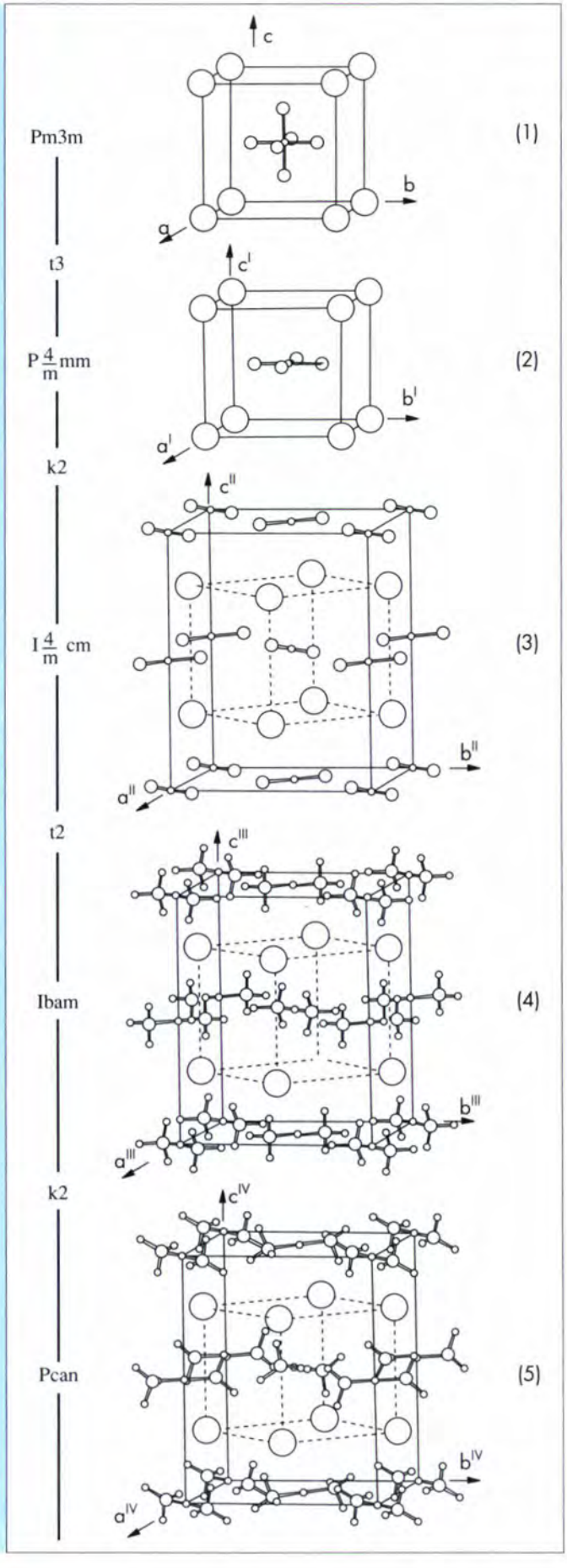

Fig. 1a. Group-subgroup relations of the phases N_2H_7I/N_2D_7I.

(1) N--N axis disordered in three dimensions. H atoms disordered.
(2) $a' = b' \approx a$ cubic, $c' \approx a$ cubic, N--N axis disordered in two dimensions. H atoms disordered.
(3) $a'' = b'' = \sqrt{2}a'$, $c'' = 2c'$. N--N axis ordered. H atoms still disordered, origin shifted to 0 1/2 0.
(4) $a''' \approx a''$, $b''' \approx b''(a''' \neq b''')$, $c''' \approx c''$. Terminal H atoms ordered, bridging H atoms disordered, cation on 2/m.
(5) $a^{IV} \approx a'''$, $b^{IV} \approx b'''$, $c^{IV} \approx c'''$. Terminal H atoms ordered, bridging H atom disordered, cation on $\bar{1}$.

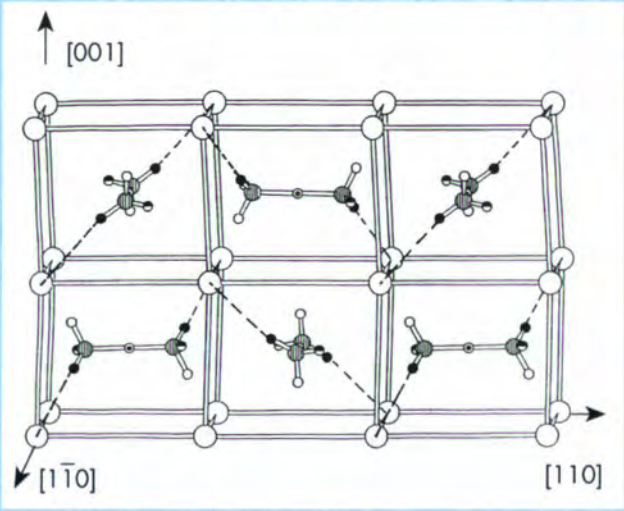

Fig. 1b. Orientation of the $N_2D_7I^+$-cations in the iodine "cubes" of the orthorhombic phase. One D atom of each terminal ND_3 group forms a strong linear hydrogen bond to an iodine atom, the other two D atoms point approximately to the middle of the edges of the cubes (bifurcated hydrogen bond).

disordered. The reduction of orientational disorder leads to larger N-N distance (2.81(1) Å) than observed in the disordered cubic phase (2.52(4) Å).

The temperature dependent powder diffraction patterns show that on transforming into the orthorhombic phase the diffuse scattering due to the rotational disorder of the terminal deuterium atoms spinning around the N-N axis vanishes. The "freezing-out" of this rotational disorder leads to the appearance of hydrogen bonds between these terminal hydrogens and the surrounding iodine atoms. A close examination of the structure revealed that one D-I distance (2.78(2) Å) was significantly shorter than the other two (3.03(3) Å and 3.17(4) Å). This is the result of an almost linear hydrogen bond of the type N-D·····I. The other N-D bonds point between two iodines qualifying them as bifurcated hydrogen bonds (Fig. 1b). The cell distortion when going from the cubic to the orthorhombic cell shows that the cell constant b along which the strong linear hydrogen bonds are orientated is shorter than a. The formation of one stronger and two weaker hydrogen bonds explains this distortion. In the tetragonal hydrogenated phase the terminal hydrogen atoms are still spinning around the N-N axis as in the cubic phase, hence no hydrogen bond network is formed which can induce an orthorhombic distortion. Fig. 1a shows the group-subgroup relations of the N_2D_7I/N_2H_7I phases. The tetragonal structure is only found in N_2H_7I, the Pm3m and Pcan structures are found for both N_2D_7I and N_2H_7I.

The hepta-coordinated molecules ReF_7 and IF_7

The only two stable binary hepta-coordinated molecular compounds are the two heptafluorides ReF_7 and IF_7. Both crystallize in a high-temperature cubic phase in which the molecules have a high degree of dynamical disorder. This shows in their ^{19}F-NMR spectra with only one line and the fact that they undergo phase transitions at much lower temperatures than the corresponding hexafluorides (e.g. ReF_6 at 277 K, ReF_7 at 151 K). Gas-phase electron diffraction data were interpreted on the basis of a pseudorotational mechanism [4] where the molecules transform between different configurations leading to a dynamical exchange of the ligands making them indistinguishable. This led to the expression "jelly-fish molecule" for ReF_7 and IF_7. On cooling one expects that this dynamical disorder diminishes by freezing-out various motions and thus one or many phase transitions may occur.

One of the first questions to be asked was: how many solid state phases exist? In the case of IF_7 it was known from earlier work [5] that at least two phases exist: a body-centred cubic phase (space group Im3m) between the melting point at 278 K and 153 K where a transition to an A-centred orthorhombic phase occurs. Weulersse et al. [6] claimed to have found evidence for two further solid to solid transitions using ^{19}F- and ^{127}I- NMR and NQR: a cubic to cubic transition at 180 K and a transition to an unknown phase at 96 K. We investigated the solid state phases of IF_7 down to 1.5 K using the high-intensity low-resolution diffractometer D1B.

At a first glance (Fig. 2a) it seems to agree with the observations of Weulersse et al. [6]. One observes the body-centred cubic phase, then at 180 K additional peaks appear where Weulersse et al. [6] observed a small discontinuity in the fluorine longitudinal relaxation time, below 150 K the known A-centred orthorhombic phase exists which transforms below 100 K into an unknown phase. However, it was impossible to index the phase below 180 K and one can see that the reflections of this phase persist down to 1.5 K. It became clear very soon that what was postulated to be a second cubic phase was actually SiF_4, which has a melting point of 183 K and stems from the catalytic reactions of IF_7 with tiny amounts of water present in the silica-glass tubes used.

Thus IF_7 has three solid state phases down to 1.5 K: a body-centred cubic phase, an A-centred orthorhombic phase and a primitive orthorhombic phase [7]. In the high temperature phase the molecules are disordered along the axes of a cubic cell, even though the molecule itself has a lower symmetry than the cubic symmetry O_h.

The A-centred orthorhombic phase still reveals orientational disorder: the equatorial fluorines form a toroidal distribution and the atomic displacement

parameters indicate large-amplitude librations (Fig. 2b). The large molecular motions still present in this phase do not allow us to claim a deviation from the D_{5h} symmetry. An orientational ordering might be the cause for the symmetry decrease and anisotropic contraction of the unit cell in the primitive orthorhombic unit cell. A definitive answer to this problem can still not be given.

The investigations of the solid state phases of ReF_7 cooling down to 1.5 K showed what we first thought to be three phases: a high-temperature cubic phase isostructural to the one observed with IF_7, a first phase transition at 139 K (162 K on heating) and a second at 129 K (154 on heating). The low-temperature phase at 1.5 K has a triclinic unit cell and the molecular geometry shows the features of a "frozen-out" pseudorotation: the puckering of the ring and the axial bending distort the pentagonal bipyramid. As one approaches the transition towards the orientationally disordered cubic phase more and more large scale molecular librations and pseudorotations are present, leading to polyhedral isomerization since the energy difference between the possible polyhedra becomes smaller and smaller. A structural refinement at 151 K, in the region thought to be a separate phase still gave the best results when using a triclinic unit-cell and a molecular geometry without symmetry, even though the deviations from a monoclinic cell are very small. The large dynamic disorder leads to large atomic displacement parameters which do not allow "clear-cut" solutions regarding molecular symmetry from time-averaged diffraction data.

Neutron powder diffraction, however, provided crucial structural insight and information concerning heptacoordination which is the basis for any further experimental and theoretical work probing the dynamics of these "floppy" molecules.

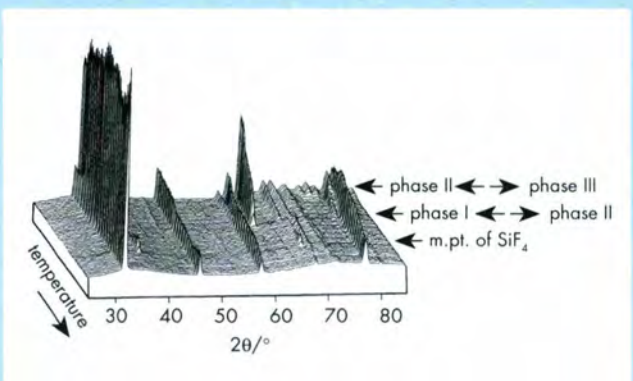

Fig. 2a. Temperature dependent diffraction pattern of IF_7 revealing SiF_4 peaks which have been attributed to a "second cubic phase".

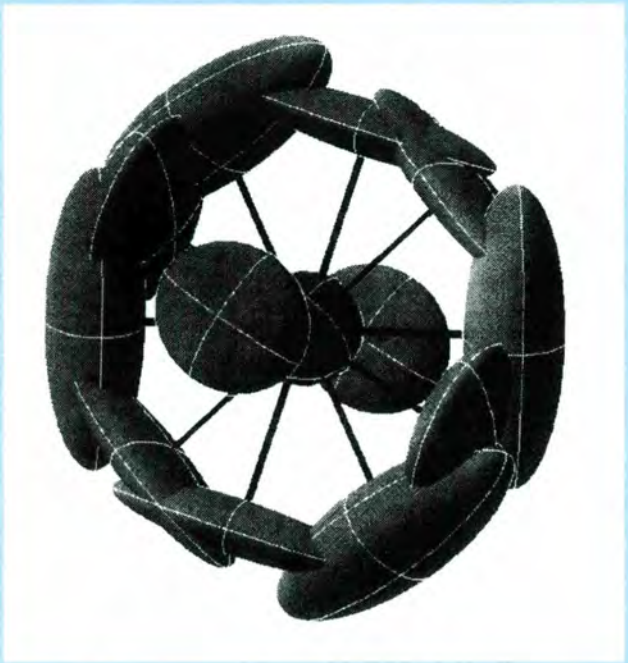

Fig. 2b. Thermal ellipsoids of 50 % probability show the disorder of the IF_7 molecule in the A-centred orthorhombic phase. The equatorial fluorine atoms form a torodial distribution of the scattering density perpendicular to the plane containing the two axial fluorine atoms.

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Liquids, Disordered Materials and Metal Physics

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Introduction

The ILL has entered a period that falls between two peaks of scientific activity. On the one hand, one sees results issuing from the last series of experiments performed at the HFBR and on the other, first results from experiments performed at other neutron scattering institutes. In the following, one finds a mixture of contributions from ILL scientists and external users of the institute that fall into both categories. Although the topics covered span a variety of interests within the college, a key area of study continues to be concerned with relaxation processes and molecular motions in glass-forming systems. Amongst the most recent scientific activity of the college, one finds a new, curious and technologically interesting class of materials: the so-called quasi-crystals. Some examples of the structure and dynamics of these novel materials are described by M. Boudard and co-workers in the Box 2 College 4. In 1992, one could say that the significant handicap caused by the loss of the HFBR has not immediately thwarted scientific life in the college. In the near future, however, we shall probably follow college activity as much through external reports as through our own.

Scientific Trends and Highlights in 1992

Physics of glass-forming systems

It is widely recognized that the α relaxation of most glasses cannot be described by a Debye behavior in time, (that is, an exponential decay). Instead, the intermediate scattering function (ISF) is more commonly described by a Kohlrausch Williams Watts (KWW) "stretched exponential" behavior on the microscopie time scale, i.e.,

$$I(Q,t) \propto \exp-(t/\tau_{WW})^{\beta}$$

where $\beta<1$. This function leads to scattering laws, $S(Q,\omega)$, which cannot be described analytically. The analysis of the scattering law is often tackled by expressing $S(Q,\omega)$ in terms of the imaginary part of the Havriliak-Negami (HN) relaxation function and relating empirically the HN parameters α, γ and τ_{HN} with the KWW parameters β and τ_{WW} (Alvarez, Alegria and Colmenero). This leads to an expression of the form

$$S(Q,\omega) \propto (1/\omega)\ \mathrm{Im}\{(1+[i\omega\tau_{HN}(Q,T)]^{\alpha})^{-\gamma}\}$$

where α and γ ($0<\alpha, \gamma<1$) are "shape parameters," τ_{HN} is the characteristic relaxation time and T is the temperature.

Recent quasi-elastic neutron scattering measurements on IN10 and IN13 from three **glass forming polymers — poly(vinyl methyl ether) (PVME), poly(vinyl chloride) (PVC) and poly(bisphenol A, 2-hydroxypropylether) (PH)** (Colmenero, Alegria, Arbe and Frick) confirm that the dynamics of the α relaxation in these glasses exhibits a stretched exponential behavior on a microscopie time scale. Furthermore the Q-dependent part of the characteristic relaxation time can be described by a power law (fig. 1), i.e.,

$$\tau(Q) \propto Q^{-n}$$

where the value of n depends on the sample. Therefore the ISF may be rewritten

$$I(Q,t)=\exp(-Ct^{\beta}Q^{n\beta})$$

where C is determined only by the temperature. It turns out that the product nβ is always close to 2 over what is a large range in the power exponent n (Table 1). These observations therefore indicate that the time and spatial behaviors of the α relaxation are directly correlated.

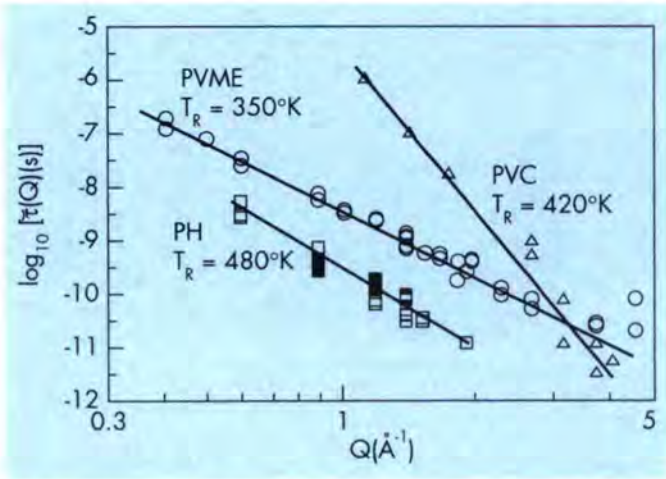

Fig. 1: τ(Q) master plot for the three systems investigated. The solid lines are linear regression fits showing the power law Q-dependence of the relaxation times.

Incoherent inelastic neutron scattering measurements on the **polymer glass, polyisobutylene** (repeat group $-CH_2-C(CH_3)_2-$) using IN6 and IN10 (Frick and Richter), show that, with increasing temperature near the glass transition, a low frequency feature appears below an energy transfer of about 2 meV (fig. 2). Although this observation is not new (see previous annual reports), it appears that, for the first time, this dynamical component is inelastic. Polyisobutylene differs from most of the previously studied glasses in that it is the least fragile polymer glass known to date, i.e., it does not show the same extreme Vogel-Fulcher behavior of the shear viscosity as fragile glasses do. The inelastic character of the additional fast dynamical process appearing near T_g practically excludes an explanation within the mode coupling theory, i.e., as a β-relaxation, but rather suggests a change of the vibrational properties around T_g. It is still an open question as to whether this observation can be generalized for glasses which tend to be less fragile. However, it is known that 'strong' or network glasses (like amorphous silica) show inelastic relaxation features even at temperatures well below T_g (Buchenau et al.). The low temperature inelastic excitation and its shift to lower frequencies just below T_g has been tentatively associated with backbone torsional oscillations which are restricted in the glass between loci of strong sterical hindrance. The shift to lower frequencies occurs due the increasing separation of these loci as the temperature increases above T_g.

Polymer	α	γ	β	β*	n	nβ
PVME	0.68	0.65	0.44±0.02	0.44	3.8±0.4	1.7±0.3
PH	0.76	0.42	0.40±0.02	0.44	4.6±0.4	1.8±0.3
PVC	0.47	0.38	0.23±0.03	0.21-0.27	9.5±1.0	2.2±0.5

Table 1: Parameters characterizing the non-Debye behavior (α and γ or β) and the Q behavior (n) of the α relaxation obtained from neutron scattering measurements. β refers to β values obtained from relaxation techniques.*

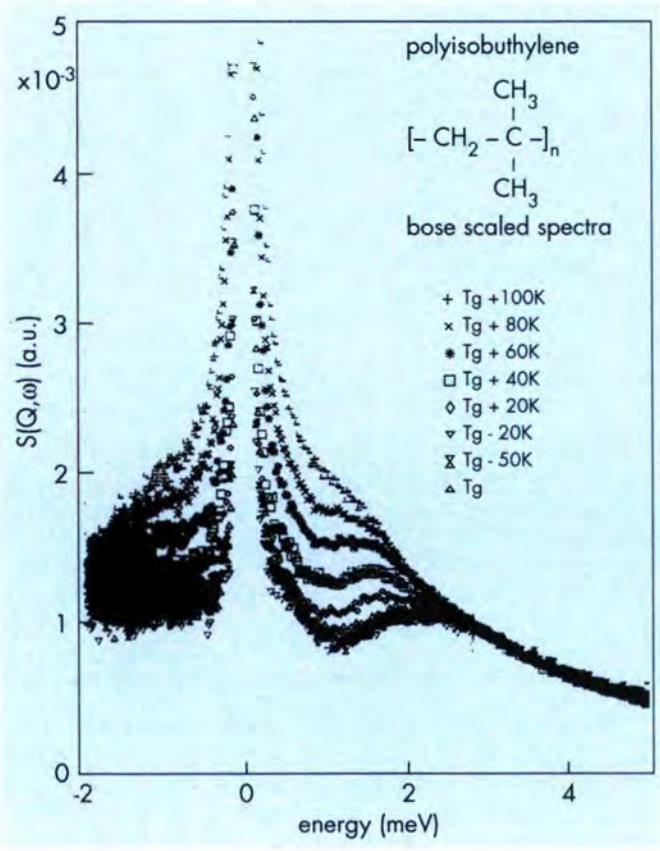

Fig. 2: The temperature dependence of the 2 meV feature in polyisobutylene near the glass transition temperature.

The low-frequency dynamics of **glassy methanol** has been investigated by inelastic neutron scattering (IN6) as well as by computer molecular dynamics (MD) simulation (Bermejo, Alonso, Criado, Mompean, Martinez, Garcia-Hernandez and Chahid). The mode assignments have been carried out using neutron data from the polycrystal as well as by analysis of the density of states (DOS), obtained from a lattice dynamics (LD) calculation. A well-resolved peak, not present in the polycrystalline reference state, is observed for the glassy phase at an energy transfer of about 2 meV. A comparison of the measured densities of states with those calculated from the MD simulations has highlighted the collective translational nature of the excitations leading to such well-defined features in the spectra of the glass. It was also found that the presence of such a peak is a direct consequence of the existence of 'excess' modes in the DOS of the glass (fig. 3). This becomes clear by comparison of the experimental and calculated spectra for the glass and polycrystal phases. From the temperature dependence of the inelastic intensities, the harmonic character of these 'excess' modes has been substantiated. Furthermore, by comparing the results from MD and experiment, this excess DOS in the glassy phase is found to be responsible for the noticeable bump in the C_vT^{-3} curves which seems to be a universal signature of the glassy state.

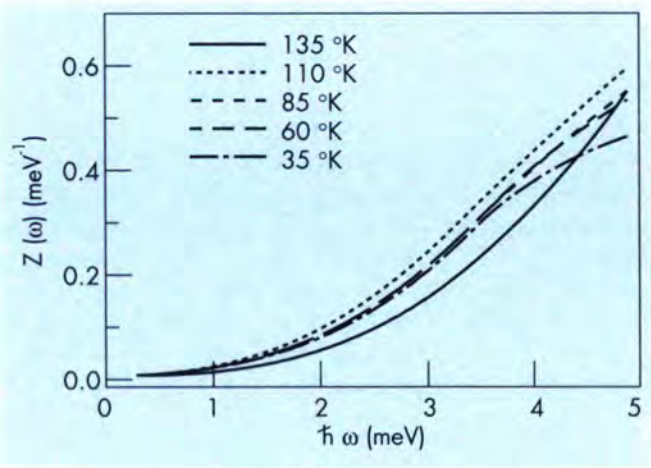

Fig. 3: A comparison of the low frequency tails of the vibrational densities of states for glassy (T= 35, 60, 85 and 110 K) and polycrystalline (T=135K) methanol. The enhancement in the DOS of the glassy samples is clearly demonstrated.

In **very concentrated aqueous electrolyte solutions**, the competition between dipolar and ionic forces (and most of the system properties) are finely monitored by the concentration. For **$LiCl.RH_2O$** (R being the number of water molecules per mole of salt), two domains of concentration exist even around hydration numbers R=6 and R=4 which can be reversibly undercooled from the liquid to the glassy state. At other concentrations, for R<12, metastability is achieved only in a restricted temperature range. For example for R=5, when warming up a sample initially quenched in liquid N_2, the pentahydrate is formed at a temperature above 171 K and it decomposes above the peritectic temperature T_p~205 K. A detailed characterization of the metastable state such as that of $LiCl.6H_20$ down to the glass transition is thus important. Inelastic neutron scattering results have been obtained on both the collective and individual atomic motions (Prevel, Jal, Dupuy, Chieux, Dianoux and Legrand). Neutron spin echo measurements (IN11) of the structural relaxation have revealed that the temperature dependence of the response follows a scaling relation and that a transition occurs near the peritectic temperature of the pentahydrate (as confirmed by viscosity measurements). Measurements of the vibrational dynamics using IN6 have shown that bending and stretching motions exist in the supercooled metastable state up to the liquid phase with a clear increase in the multiplicity of the microscopic configurations at T_p. The self and collective motions of the solvent water molecules were studied using IN5 by incoherent and coherent quasi-elastic scattering respectively (D_2O being the solvent in the latter case). A combined analysis of the coherent and incoherent scattering revealed a hydrodynamic coupling in the diffusion resulting in a departure from Fick's law behavior.

Incoherent neutron scattering measurements have been performed on the **model glass system ortho-terphenyl (OTP)**, both in its supercooled liquid (viscous) state and in its glassy state. In the viscous regime, the intermediate scattering function (ISF) has been obtained over three decades in time by combining results from IN6, IN5 and IN13 (Wuttke, Kiebel, Bartsch, Fujara, Petry and Sillescu) (fig. 4). A cross-over from α to β relaxation processes in the supercooled liquid is predicted by mode coupling theory (MCT) at a critical temperature, T_c, which lies above the glass transition temperature, T_g. The solid lines in fig. 4 represent fits of the scaling law predicted within the framework of MCT for temperatures above T_c. These fits describe well the ISF in the time range $1 < t(ps) < 100$ and the fit parameters reproduce closely the previously established value of T_c. Deep in the glassy state (typically below 245 K), all relaxations are frozen leaving only the harmonic phonons. With increasing temperature, the structural relaxations start to contribute in increasing measure to the low frequency part of the density of states. This is clearly demonstrated in fig. 5 by the increasingly non-Debye low frequency spectrum with increasing temperature.

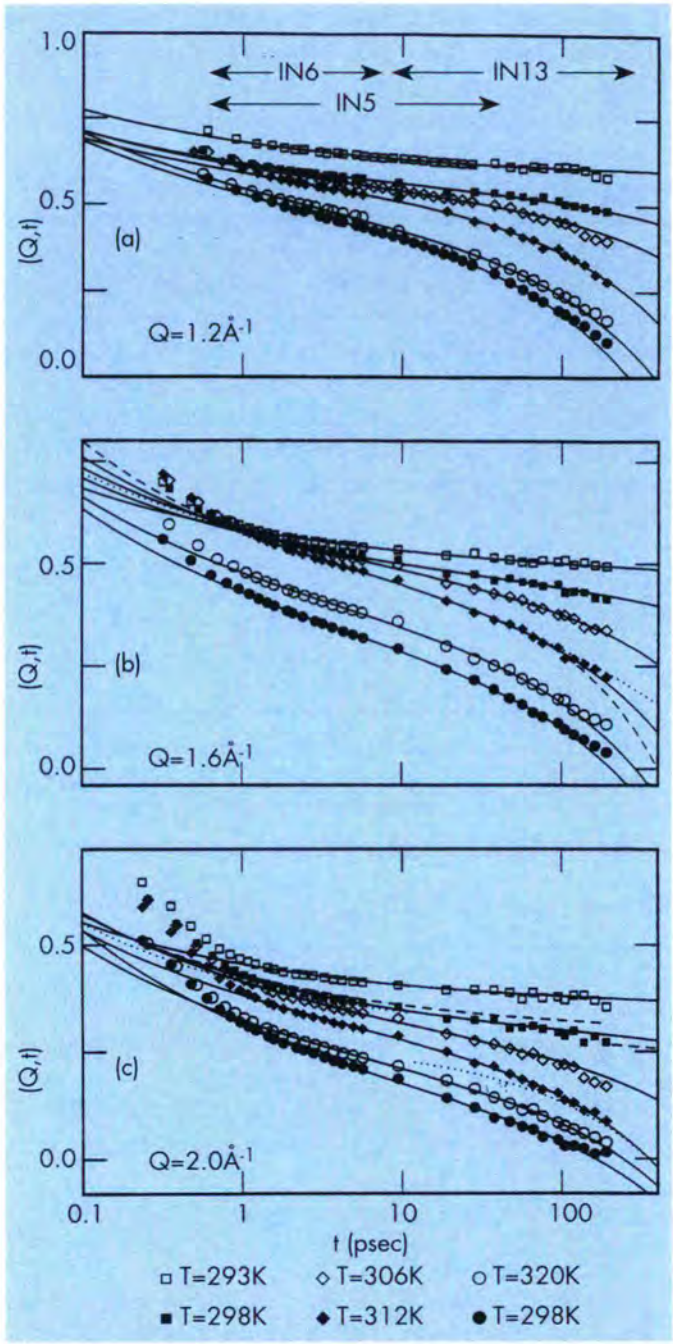

Fig. 4: The intermediate scattering law for o-terphenyl for three different values of Q as a function of temperature. The solid lines are fits of the scaling function predicted by mode coupling theory for temperatures above T_c. The measuring ranges of the three instruments used are indicated in the top figure.

Magnetic dynamics of disordered phases of oxygen

Liquid and plastic crystal phases of oxygen have been studied by high-resolution inelastic neutron scattering using IN6 (Chahid, Bermejo, Enciso, Garcia-Hernandez and Martinez). Fig. 6 shows a representative set of experimental spectra for the low temperature liquid. The broad quasi-elastic components can be considered to be a clear signature of a magnetic effect. Otherwise, the magnitude of the

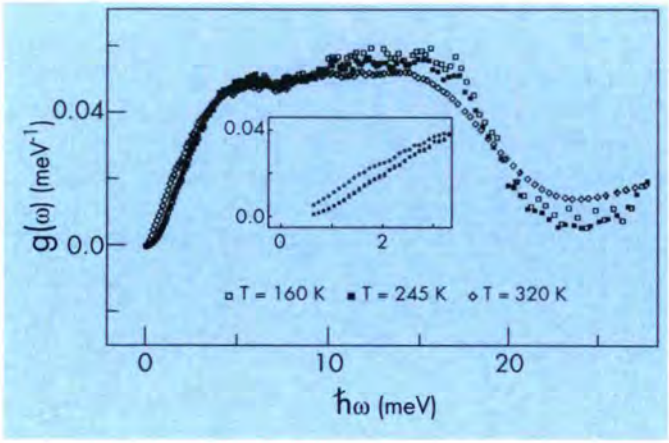

Fig. 5: The temperature dependence of the density of states in o-terphenyl, corrected for multiple scattering.

relevant transport coefficients derived from such a broadening would have to be set at least one order of magnitude larger than the value obtained by other techniques. The separation of the magnetic response from the total cross-sections was achieved by means of a computer molecular dynamics simulation enabling an estimation of the magnetic spectral weight functions. This separation has proven to be consistent with the findings of polarized neutron diffraction and the large differences (more than one order of magnitude) between the transport coefficients of structural origin (self-diffusion and rotation) and those related to the spins have enabled a safe discrimination of both components. The magnetic contribution was assumed to have a lineshape characteristic of a mono-dimensional Heisenberg paramagnet and the second and fourth moments were extracted from the analysis. For both plastic and liquid phases, it was found that the second moments in the low Q region follow a behavior which seems to be closer to a $DQ^{3/2}$ law (which characterizes an antiferromagnetic coupling mechanism) than to a DQ^2 law, relevant for simple diffusion. As far as the atomic dynamics are concerned, a remarkable similarity has been found between both disordered phases giving further support to the hypothesis of parallel arrangements also taking place in the liquid on short time scales.

A milestone in structure factor measurements

In the last few years, accurate measurements of the density dependence of the structure factor S(Q) of **gaseous ^{36}Ar** have given a direct access to the pair potential and three-body effects (Fredrikze, Van Tricht, Van Well, Magli, Chieux and Barocchi). An effective two-body potential for liquid Gallium has also been obtained using the Reatto inversion scheme (Bellissent-Funel, Chieux, Levesque and Weis). Recent neutron diffraction measurements of S(Q) for **liquid Kr** on D4B have shown that the experimental precision is now sufficiently high to test different models of atomic interactions in a classical dense fluid (Barocchi, Chieux, Magli, Reatto and Tau). Fig. 7 compares S(Q) at

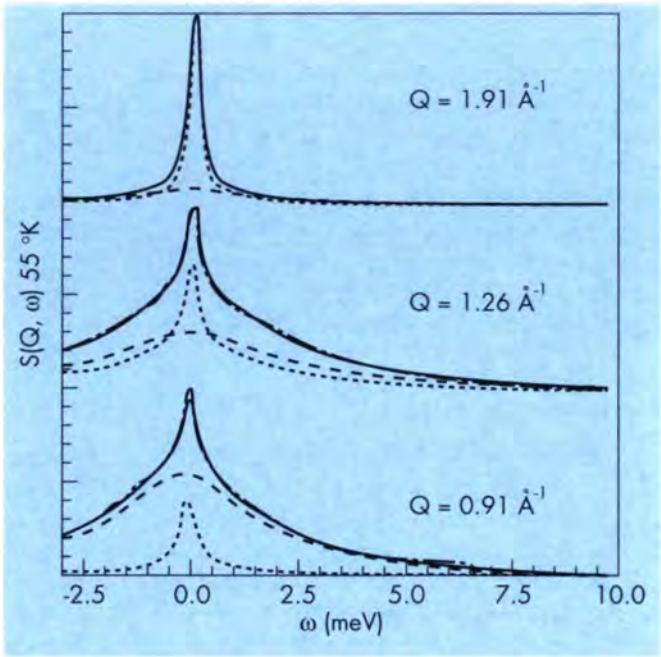

Fig. 6: Neutron spectra obtained from low-temperature liquid oxygen at 55 K, illustrating the structural contributions (dotted lines) and the magnetic contributions (dashed lines) to the total inelastic intensities (dot-dashed lines). The solid lines represent the fitted model.

T=169 K and atomic density n=14.57 nm^{-3} with the theoretical results obtained using the hypernetted chain equation (MHNC) extended to include three-body forces. On the scale of the figure, the measured S(Q) is barely distinguishable from the calculated one which refers to the Aziz model of the pair potential u_2 and the Axilrod-Teller-Muto tripole-dipole interaction u_3. The agreement $\Delta S(Q)=S_{exp}(Q)-S_{MHNC}(Q)$ is below 0.03 for all Q and for Q>80 nm^{-1} it is within experimental noise. An equivalent agreement is obtained for g(r) (see fig. 8(a)) whereas the plot of $\Delta g(r)=g_{exp}(r)-g_{MHNC}(r)$ (fig. 8(b)) indicates small additional forces of many-body character which are repulsive at small range and attractive otherwise. It is clear from fig. 8(b) that the Lenard-Jones interaction does not give an accurate representation of correlations in dense Kr. These studies provide a good illustration of the level of accuracy of both MHNC and of that achieved nowadays by experiment.

Fast ion conductors

Structural disorder in the **superionic conductors AgBr, AgI and CuBr** has been studied on D20 by making total scattering measurements (that is both Bragg and diffuse scattering) from powder samples (Nield, Keen, Hayes and McGreevy). Such experiments are considerably simpler than conventional single crystal studies of diffuse scattering and yet reverse Monte Carlo (RMC) modeling of the accurate structure factors obtained can give remarkably detailed information on mechanisms of structural disordering and fast ion conduction. In the case of AgBr measurements have been made to within 0.5 K of the melting point and it has

been found that the enhanced ionic conductivity at such temperatures is not indicative of 'pre-melting' behavior, but rather of a diffuse transition to a fast ion conducting phase which is 'interrupted' by the melting transition. In α-AgI, no evidence has been found to support the order-disorder transition that has been proposed on the basis of Raman and Brillouin scattering results. In CuBr, the γ, β and α phases have been studied (fig. 9). The Cu density distribution can be used to determine, under certain assumptions, the energy barrier to cationic conduction and this correlates well with recent conductivity and diffusion measurements.

Self diffusion in metals

Self-diffusion in **BCC metals** exhibits a strongly non-uniform behavior. For example, at one half of the melting point, the diffusivities of the different elements vary by up to 8 orders of magnitude and the Arrhenius representation of the diffusion coefficient D(T) is remarkably curved for the fastest diffusing elements. **Niobium** self diffuses at a rate which is intermediate between the fast diffusing group IV metals and slow diffusing group VI metals (see contribution by W. Petry, college IV section). Furthermore, the Arrhenius plot shows a slight but distinct upward curvature. In order to understand these properties, the phonon dispersion of Nb was measured at various temperatures up to 2223 K using the IN3 spectrometer at the ILL, HB1 at the HFR in Petten, Netherlands and DN1 at the Siloë reactor (CENG, France) (Güthoff, Trampenau and Petry). The evaluation of the complete phonon dispersion allows the migration enthalpy to be calculated at the measured temperatures (Schober, Petry and Trampenau). These calculations showed that the

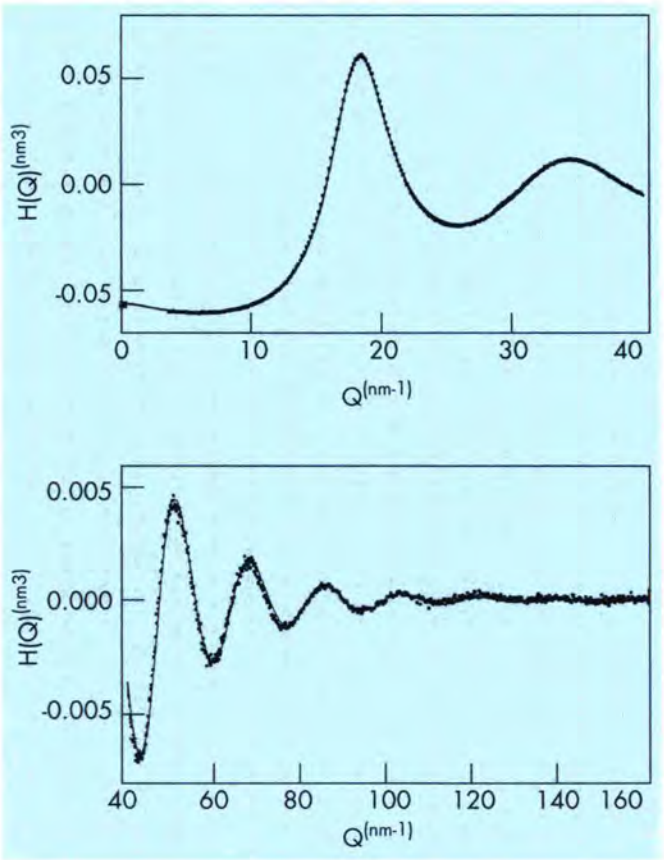

Fig 7: Detail of H(Q) = [S(Q)-1]/n at T=169 K and n= 14.57 nm^3 in the small and large Q range. The full curve is the result of the triplet MHNC equation with the Aziz pair interaction plus the three-body ATM term. The value at Q=0 was obtained from compressibility data.

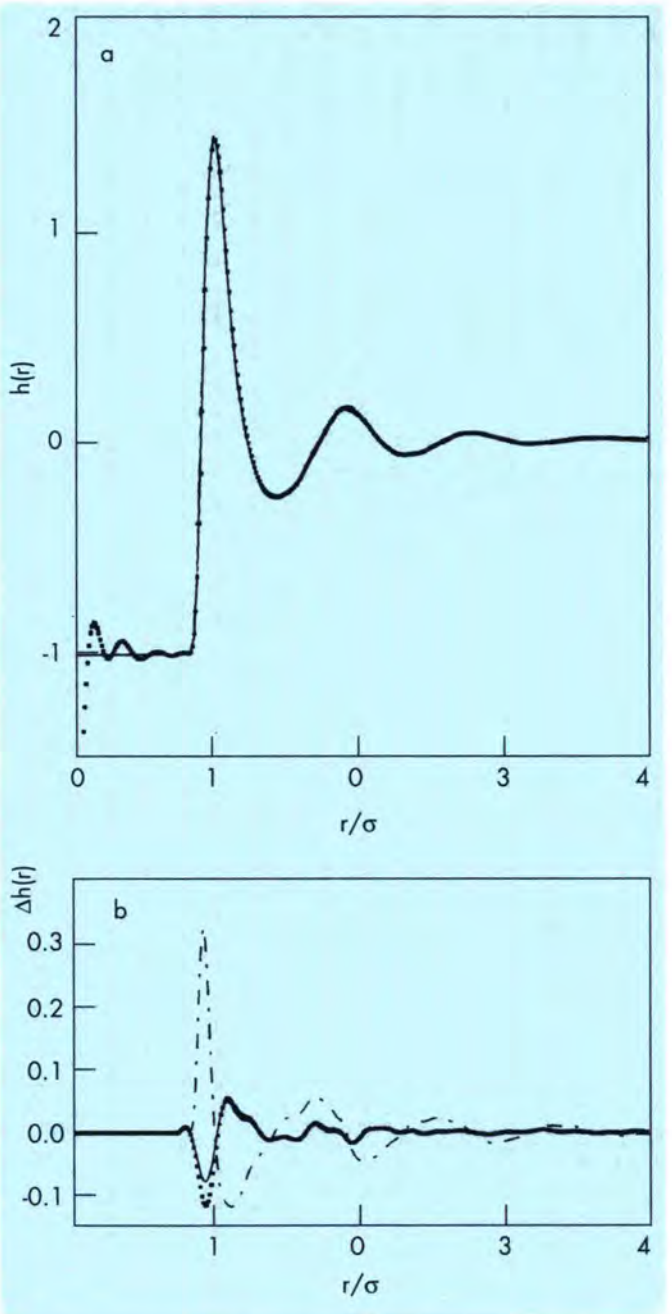

*Fig 8: **(a)** Theoretical (full curve) and experimental (dotted curve) of h(r) = g(r)-1 plotted versus r/σ where σ=0.4008 is the position of the minimum of the Aziz pair interaction.*
***(b)** Difference $\Delta h(r)=h_{exp}(r)-h_{MHNC}(r)$ for the Aziz pair interaction with (full curve) and without (dotted curve) the ATM three-body interaction and for the Lenard-Jones interaction (dot-dashed curve).*

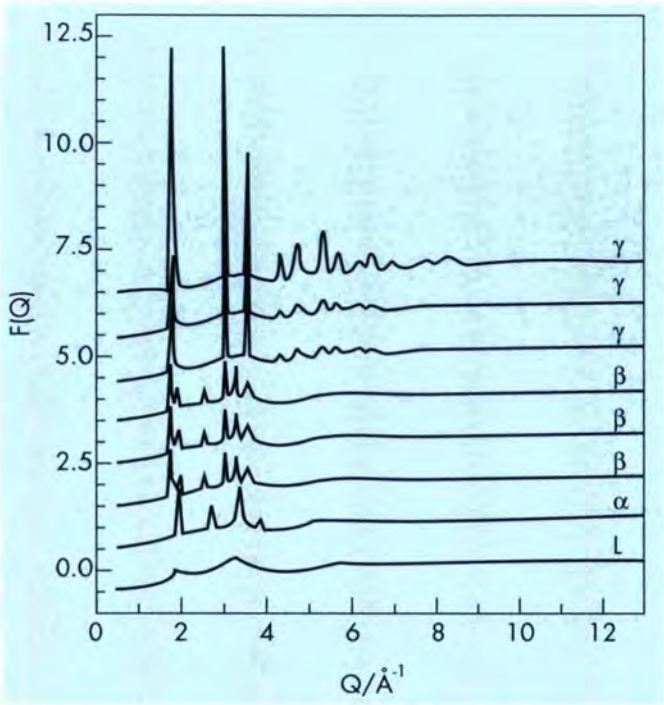

Fig. 9: Corrected and normalized structure factors for CuBr at 780, 750, 730,700, 670, 630, 610 and 293 K. Successive temperatures are displaced by 1.0 on the F(Q) scale.

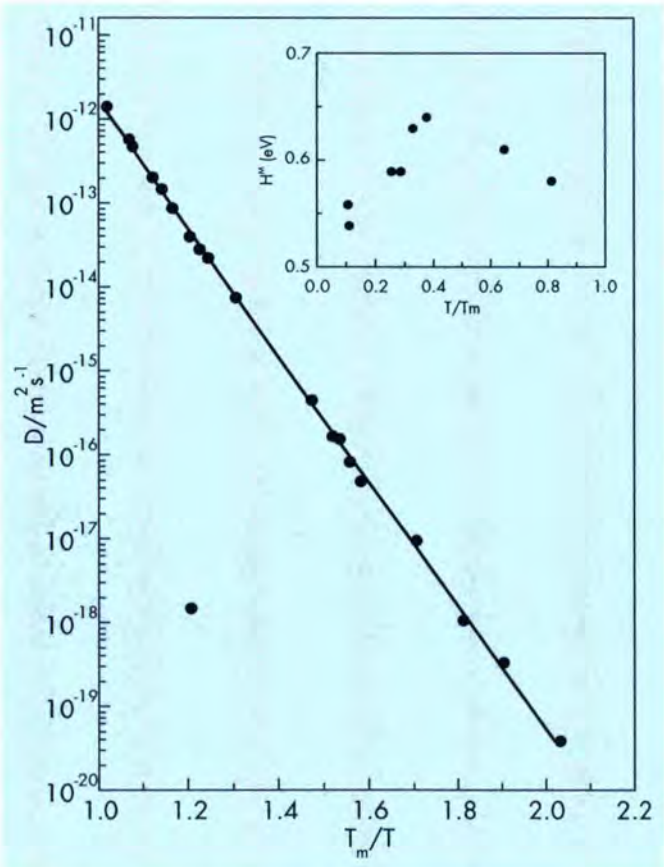

Fig. 10: A fit of the Arrhenius law to self-diffusion data for Nb. The migration enthalpies, calculated from the phonon dispersion measurements, is shown inset.

migration enthalpy increases with increasing temperature up to a maximum value around 1500 K and then decreases again at higher temperatures (see inset fig. 10). It is found that this strong non-linear temperature behavior reproduces well the observed curvature in the Arrhenius plot (fig. 10). These measurements complete a program of high temperature experiments on transition metals which aim to clarify the reasons behind their anomalous diffusion behavior.

Certain **intermetallic phases with DO_3 structure** exhibit an anomalous fast self-diffusion. A series of quasi-elastic neutron scattering measurements were performed using IN10 in order to study the diffusion mechanism in **Ni_3Sb**. Astonishingly, these measurements have shown that the quasi-elastic line broadening is approximately Q-independent. An effort was made to interpret these results in terms of several plausible jump diffusion models, however these proved unsuccessful in producing a conclusive picture of the actual diffusion process. As a first step in obtaining a more fundamental understanding of the fast diffusion (i.e., to study not only the jump mechanism but to gain some insight into the reasons behind the high mobility), the lattice dynamics of Ni_3Sb have also to be considered. Therefore a series of phonon dispersion measurements were performed on 3-axis spectrometers at Saphir (PSI,Switzerland), at Siloë (CENG, France) and at Orphée (LLB, France). The resulting phonon dispersion curve is depicted in fig. 11. The most striking features are the two low-frequency acoustic branches in the [ξξ0] and [ξξξ] directions. Besides their low frequency, they exhibit a strongly damped behavior. The longitudinal phonon [ξξξ] opens the migration barrier for nearest-neighbor jumps whereas the transverse T_1 1/2[110] phonon partly opens the "window" for the next nearest-neighbor jumps. From these results, it has been possible to deduce the particular directions in which the potential barriers are low. The situation resembles very much that of the pure BCC metals (see above).

Secretary: J. C. Cook.

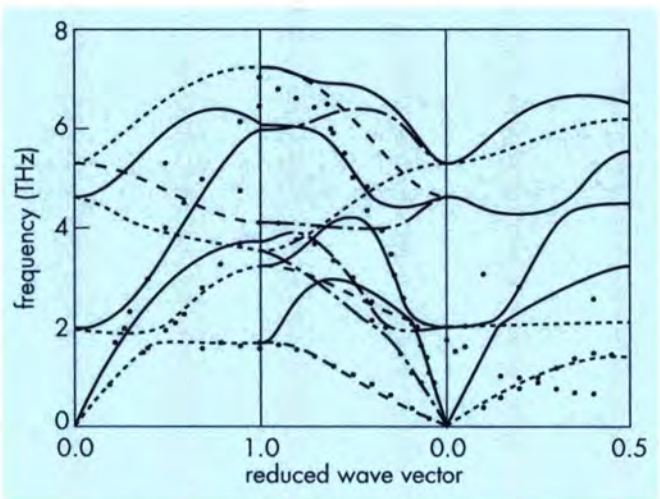

Fig. 11: The phonon dispersion curve for Ni_3Sb at 873 K.

"Neutron Scattering from Liquids"

held September 15-18, 1992 in Giardini Naxos (Italy)

This workshop was the 7th Topical Meeting of the Liquids Section from the Condensed Matter Division of the European Physical Society. The Directors were J. Teixeira (Laboratoire Léon-Brillouin, Saclay, France), A.J. Dianoux (Institut Laue-Langevin, Grenoble, France) and F. Wanderlingh (University of Messina, Italy). The Organizing Committee was composed of R. Giordano (University of Messina, Italy) and J.C. Leicknam (University Paris VI, France).

The aim of the workshop was to highlight the capabilities and developments of neutron scattering techniques in the study of liquids. Both the structure and dynamics of molecular liquids fall well inside the neutron windows of observation. Complex liquids and more generally "soft matter" have been studied within the same general framework. This meeting was intended to present recent aspects of liquid research using the methods of neutron scattering in both their theoretical and experimental aspects. An important factor was to stimulate the contacts between scientists interested in molecular liquids, colloids, glasses, proteins in solution and other non-organized materials.

The workshop took place in the beautiful resort of Giardini Naxos near Messina (Sicily) at the Hotel Ramada which offered superb accommodation as regards both the rooms and the conference hall. There was a slight disappointment from the small number of participants (~ 40), half from Italy, and the other half from France, Germany, Spain, Sweden and USA. Possible reasons, besides the high travel costs, could have come from the technical character of the topics and from the fact that several meetings on liquids took place during the same month. Nevertheless it was a lively meeting, with a lot of discussions among the participants. An account of the presentations by the invited speakers is given below.

The first lecture was given by P. Chieux (ILL, Grenoble) who communicated to the audience his enthusiasm for very precise structure factor determinations. He noted that with the improvements in dedicated spectrometers at Large Facilities, more complicated systems or more precise questions have been tackled by accurate structure factor measurements. He gave the example of the instrument D4 at the ILL where the improvement in data acquisition rate has been a factor of 1000 over the past 19 years. He has plans to gain another factor of 10. He then gave some examples which illustrate the power of the neutron scattering technique in the determination of interaction potentials in simple systems, of intramolecular structure, of local order and partial structure factors. He stressed that the isotopic substitution method in neutron scattering reveals a much better contrast ($\geq$ 10 times) than the anomalous dispersion method using X-rays from a synchrotron source. Furthermore this last technique is limited to atoms with $Z \geq 30$ in order to obtain a maximum range of $Q > 8$ Å^{-1}. In this field, he sees the future more in combined structure factor measurements by X-ray and neutron scattering. Furthermore the recent progress in the simulation of disordered sets of atoms and molecules opens the field to more elaborate questions and more accurate experimental analyses.

The second lecture by G. Tarjus (Laboratoire de Physique Théorique des Liquides, Paris) was on the theory and simulation of inelastic neutron scattering from liquid water. This theory allows a disentanglement of the quantum degrees of freedom, associated with the fast internal vibrations, from the quasi-classical degrees of freedom, corresponding to the rotational-translational motions of the molecules. The new simulation results give good agreement at high frequency ($\approx$ 450 meV) with neutron scattering spectra from liquid water at a pulsed source.

P. Migliardo (Dipartimento di Fisica, Messina) presented the influence of the H-bond connectivity on the dynamical properties of hydrogen-bonded liquids. The use of several spectroscopic techniques (Neutron and light scattering, Infrared and dielectric studies) had shed light on the rôle played by H-bonds for molecules like alcohols and water. Specifically when this class of liquids is confined in a very small space (as in reversed micelles), or is allowed to diffuse near charged surfaces (as in biological macromolecules or membranes), or is diluted in an inert solvent (like alcohols in CCl_4), the limitations of the H-bond interactions change drastically its dynamical properties. A comparison with Molecular Dynamics results and a critical review of available models ended this presentation.

F. Barocchi (Dipartimento di Fisica, Firenze) gave a detailed discussion of the dynamic structure factor in monoatomic fluids. He showed how the new low-angle facility on the spectrometer IN5 at the ILL has opened up new possibilities for studying the transition from hydrodynamics to kinetic theory in compressed monoatomic gases. One can thus work in a density range where one feels the influence of the potential, contrary to the situation in the hydrodynamic regime. As an example, neutron scattering experiments and molecular dynamic simulations, performed in a wide range of densities in Argon, were compared with light scattering results and presently available theories.

F.J. Bermejo (Instituto de Estructura de la Materia - CSIC, Madrid) reported on the short wavelength density oscillations in molecular liquids and glasses. He explained that several features which do not appear in simple liquids are important here: the short range anisotropy, the long range interactions (beyond nearest neighbours) and the complex glass transition behaviour. He then gave examples of three classes of molecular liquids: a quantum liquid (D_2),

a Lennard-Jones liquid (CCl_4) and a glass-forming liquid (CD_3OD). He highlighted the rôle of molecular dynamics simulations in the interpretation of experimental data.

W. Doster (Physik-Department, München) presented the liquid aspects of protein internal motions. The rôle of structural disorder and flexibility on biological function of proteins has gained interest in recent years. This structural disorder is apparent in the strong diffuse scattering which is observed adjacent to the Bragg peaks in X-ray or neutron diffraction experiments. The structural fluctuations of myoglobin, in a wide temperature range, have been studied by neutron scattering using time-of-flight and backscattering spectroscopy. The interpretation of the data was based on temperature dependent molecular dynamics simulations and, qualitatively, by comparison with some predictions of the mode coupling theory of supercooled liquids.

U. Buchenau, (Institut für Festkörperforschung, Jülich) went deep into the understanding of the vibrational properties of undercooled liquids. He began by describing the soft potential model, an extension of the tunnelling model, which is able to explain the soft vibrational, tunnelling and relaxational modes in glasses. The implications of this model for undercooled liquids has been investigated and it is argued that the fast picosecond relaxation is due to these modes and their damping. Dr. Buchenau then made an extensive comparison of this soft potential model with current theories of undercooled liquids.

The mode coupling theory of the glass transition has was presented by F. Fujara (Institut für Physikalische Chemie, Mainz) who recalled that the main prediction of this theory is the existence of a dynamic instability of the supercooled liquid at a temperature T_c well above the glass transition temperature T_g. He then described the experiments performed at the ILL on the van der Waals liquid orthoterphenyl which support the mode coupling theory, at least qualitatively. Some recent NMR experiments on the same sample also agree with the idea of a change in the mechanism of diffusion at T_c, from liquid to solid-like dynamics.

The last invited lecture was given by S.H. Chen (MIT, Cambridge, USA) on the determination of 3-D microstructures of bicontinuous microemulsions by combined SANS experiments and simulations. These microemulsions can be characterized by two length scales, the average inter-domain distance between two water or oil domains and the disorder parameter which measures the polydispersity of the domain sizes. The new simulation scheme, which contains three length scales, generates 3-D microstructures fully consistent with scattering data. The physical meaning of these three length scales, in comparison with the previous model, has been discussed. It seems that the third length scale (~ 10 times shorter than the other two) is related to the local curvature of the film.

The invited lectures and contributed papers will be published in a special issue of the Journal of Molecular Structure.

The organizers acknowledge the generous support they have received from the Dipartimento di Fisica (Universita di Messina), the Regione Siciliana, the Universita degli Studi di Messina, the Laboratoire Léon-Brillouin (France), the Institut Laue-Langevin and CNRS (France).

A.J. Dianoux

Workshop on Methods in the Determination of Partial Structure Factors of Disordered Matter with Neutron and Anomalous X-ray Diffraction

Partial structure factors are among the most detailed pieces of information one can get on the structure of disordered matter. As they can successfully be determined only at intense neutron and continuous X-ray sources, an ILL/ESRF workshop was organized at the ILL on September 10th and 11th, 1992, in collaboration with the CNRS in Grenoble in order to discuss different methods and their limitations used in the determination of PSF on both sources.

Even though the dense programme of the two-day workshop did not allow all topics of interest to be included, the organizers tried to include the largest part of all relevant methods. The workshop was scheduled as the third satellite meeting of the International Conference on Liquid and Amorphous Metals (LAM8 Vienna) and attracted about 65 scientists from 12 different countries, among them a large number of the world specialists in this field.

After a challenging introductory talk on "PSF in the nineties" by P.A. Egelstaff, where he outlined the rather different two particle correlations one has to deal with in condensed matter, methods related to neutron scattering were discussed. J.E. Enderby, the former British director of the ILL, presented the isotopic substitution technique in liquids and glasses, and P. Gaskell discussed the application of the first and second order difference method applied to the investigation of short and medium range order in glasses. M. Maret demonstrated the success of careful isomorphous substitution in recent years, especially in the case of icosahedral and decagonal alloys, and R. Sinclair convinced the auditorium of the profitable application of anomalous neutron diffraction in the determination of PSF for quite a number of nuclei with low lying resonances at epithermal neutron sources and with the much improved instrumentation available nowadays. E.W. Fisher discussed the decisive increase of information obtained from isotopic substitution in polymers and mixtures of them in SANS experiments and H. Bertagnolli gave a comparison of results obtained by isotopic substitution in neutron diffraction and by anomalous synchrotron radiation scattering for the structure of molecular liquids.

An introduction to anomalous diffraction with synchrotron radiation, the experiments and the difficult data treatment was given by A. Bienenstock, and this discussion was continued by A. Raoux on the determination of differential structure factors and the accuracy of the data obtained with the same method. The much more detailed information gained by anomalous small angle X-ray scattering (ASAXS) experiments compared to conventional SAXS techniques was presented by O. Lyon, and Y. Babanov defended a new regularization method and the systematic selection of compatible data sets obtained by different experimental techniques such as X-ray and neutron diffraction, EXAFS etc.

The combination of different radiations in order to change the cross-sections of the atoms in the same sample was outlined by G. Palinkas in its application to organic liquids, R.L. McGreevy discussed the results obtainable and the limitations of the analysis of PSF by the Reverse Monte Carlo techniques, and J. Hafner surprised the audience with new developments in the determination of static and dynamic PSF in computer simulations of liquids and glasses.

Nearly all of these invited review talks were seconded by one or two contributions where most recent results were discussed in the light of new developments in the methods applied to the determination of PSF, and an extended poster session gave the opportunity to present and discuss work in progress.

The discussions during and after the talks, in the coffee breaks and during the poster sessions were very lively and sometimes antithetical, the most experienced scientists often also being the most critical ones. Thus the workshop profited strongly from the presence of so distinguished experts in the field.

The workshop ended with a very complete comparison of the diffractometers which will be available at the restart of the HFR for PSF determinations, given by P. Chieux, a presentation of the new Oed-detector for D20 (microstrip technique) by P. Convert, and a visit of the storage ring and the experimental hall of the ESRF guided by Å. Kvick and C. Riekel. A very optimistic workshop summary was given by P.A. Egelstaff, who also provided the audience (and the proceedings) with a "translation kit" concerning different nomenclatures for the same topic by neutron and X-ray scatterers, in order to promote the discussion between the two PSF communities, - which obviously enjoyed meeting for the first time to discuss this topic of common interest.

J.-B. Suck

Terminal Stability of Crystals: Supersaturated Solid Solutions as an Example

Jens-Boie Suck

W. Kauzmann first realized that according to the shape of the curves describing the dependence of the entropy of a supercooled liquid and of the corresponding crystalline phase on temperature, there is an isentropic point T_g^S at low temperature (Fig. 1) below which the entropy of the supercooled liquid would be smaller than that of the ordered crystal (Kauzmann paradox) [1]. He argued that this intersection of the two entropy curves represents the terminal temperature for supercooling and that therefore the liquid must freeze to a solid, most likely in a catastrophic process.

The inverse problem was recently discussed by W.L. Johnson and H.J. Fecht [2] who, on the basis of their calculations of the temperature dependence of the entropy of liquid and crystalline Al, proposed a terminal stability point for crystalline lattices at the upper isentropic temperature, T_m^S (Fig. 1), above which the entropy of the ordered crystal becomes larger than that of the disordered liquid and which therefore sets a definite limit to superheating (and supersaturation). At T_m^S the crystal has to transform to a disordered state, a liquid or an amorphous solid depending on $T_m^S > T_g$ or $T_m^S < T_g$, where T_g is the effective glass transition temperature.

Subsequently, J.L. Tallon has argued [3] that the isentropic temperatures T_g^S and T_m^S are in fact the extreme limits for the existence of a supercooled liquid and of a crystalline lattice, respectively, but that there exists a hierarchy of catastrophes for both phases for $T_g^S < T < T_m^S$ which represent a succession of stability limits at which the systems will transform before they reach the isentropic temperatures. In particular he modified the melting condition of Born [4] in such a way that the instability limit of the lattice against shear forces is reached when the mole-volume of the crystal has become equal to that of the liquid at its freezing point.

From these different possible transitions between equilibrium and non-equilibrium states, those from a **metastable** or **unstable crystal** to a **metastable amorphous solid** are of special interest at present, as this transition is intimately related to the process of (spontaneous) solid state amorphization (and of melting), which are not very well understood up to now. A decrease in the shear sound velocity during progressive disordering of a Zr_3Al film and in the sudden transition to the amorphous solid has in fact been observed by L.E. Rehn and collaborators [5] in Brillouin light scattering experiments, i.e. in the long wavelength limit.

Several neutron inelastic scattering (NIS) experiments have been performed recently on supersaturated fcc-Al_{100-x} Si_x [6] and fcc-$Al_{100-x}Ge_x$ [7] solid solutions in order to study the rôle of the lattice dynamics when approaching the disordering transition. In the following the most recent results obtained with rapidly quenched Al_{100-x} Si_x solid solutions will be presented [8].

As Si in the solid state has the strong tendency to form covalent bonds with 4 nearest neighbours (Diamond structure) with a large atomic volume V_a of 20 $Å^3$, while Al has metallic bonds with 12 nearest neighbours and V_a = 16.6 $Å^3$, amounts of Si in excess of 1 to 1.5 at. % cannot be solved in Al in the solid state. On the contrary, at very high pressure (11 GPa) or in the liquid state Si is metallic with V_a = 15.5 $Å^3$ and can therefore be solved in Al.

Consequently, the supersaturation of the solid solution can only be achieved by a rapid quench (RQ) from the melt (melt-spinning) in order to avoid segregation, or by homogenisation under high pressure at high temperature (HPTH) (where the Si atoms, which are segregated into covalently bound clusters in the AlSi prealloy, diffuse into the fcc-Al lattice and replace Al atoms there) and a subsequent quench to avoid demixing. Both methods succeed in avoiding the formation of Si clusters, as can be seen in Fig. 2 for the case of melt-

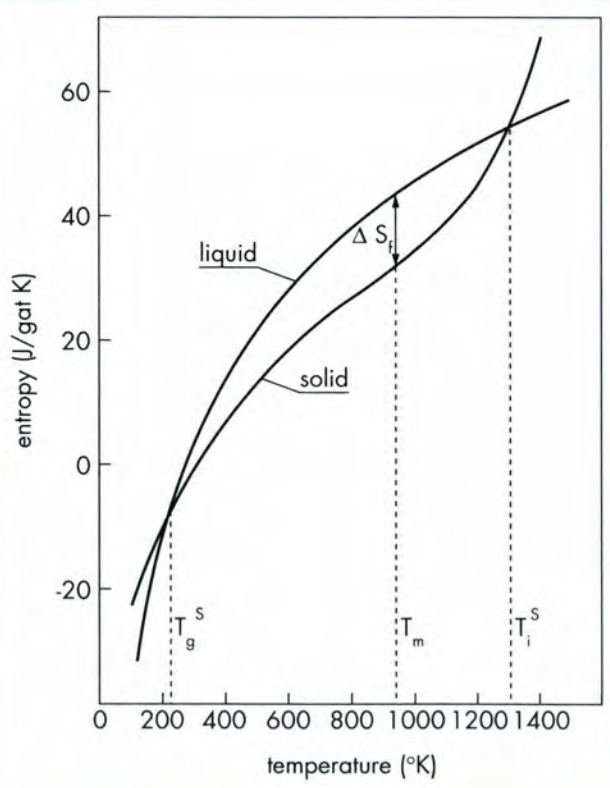

Fig. 1: Calculated temperature dependence of the entropy of liquid and crystalline Al. The lower and upper isentropic temperature limits T_g^S, T_m^S are indicated [from ref. 2].

spun $Al_{94}Si_6$, but the amount of Si atoms replacing Al atoms in the fcc lattice is different in the two cases. While HPTH apparently leads to a quantitative solution of Si in fcc Al, after RQ only part of the Si atoms seems to be stored in the lattice itself and part seems to be dispersed possibly in the grain boundaries. This conclusion can be drawn from intensive investigations of the samples using differential scanning calorimetry (DSC) at ILL. The enthalpy release on segregation increases linearly with Si concentration at least up to 10 at % Si. In the case of the samples produced by HPTH this release corresponds to the energy gained in the transition of a Si atom from metallic to covalent bonding (~ 38 kJ/mole) [9].

The enthalpy release on Si demixing in the RQ samples also rises linearly with Si concentration as can be seen in Fig. 3, but the slope is lower by nearly a factor of 2. Thus, if one ascribes the enthalpy release completely to the transition from metallically to covalently bounded Si, one has to conclude that in RQ $Al_{100-x}Si_x$ $X_{effective} \approx 0.58\ X_{nominal}$.

As the preparation methods described above produced only polycrystals up to now, all NIS experiments were done on two time-of-flight (TOF) spectrometers, IN4 and IN6. IN4 was used for a reliable sampling of the generalized phonon density of states (GPDOS) $G(\omega)$ with thermal neutrons in a large part of the reciprocal lattice. IN6 was used to investigate the total dynamic structure factor $S(Q,\omega)$ with cold incident neutrons especially in the low energy region.

In all investigations so far no change of the spectrum of longitudinal phonons has been observed, as can also be stated for RQ $Al_{94}Si_6$ (see Fig. 4). The spectrum of the transverse phonons, on the contrary, becomes slightly wider and **shifts to lower energies** This softening of the transverse phonons in the supersaturated solution increases with increasing Si concentration [9] and it seems to be slightly larger in the RQ-samples than in the HPTH-samples if the former are weighted with their

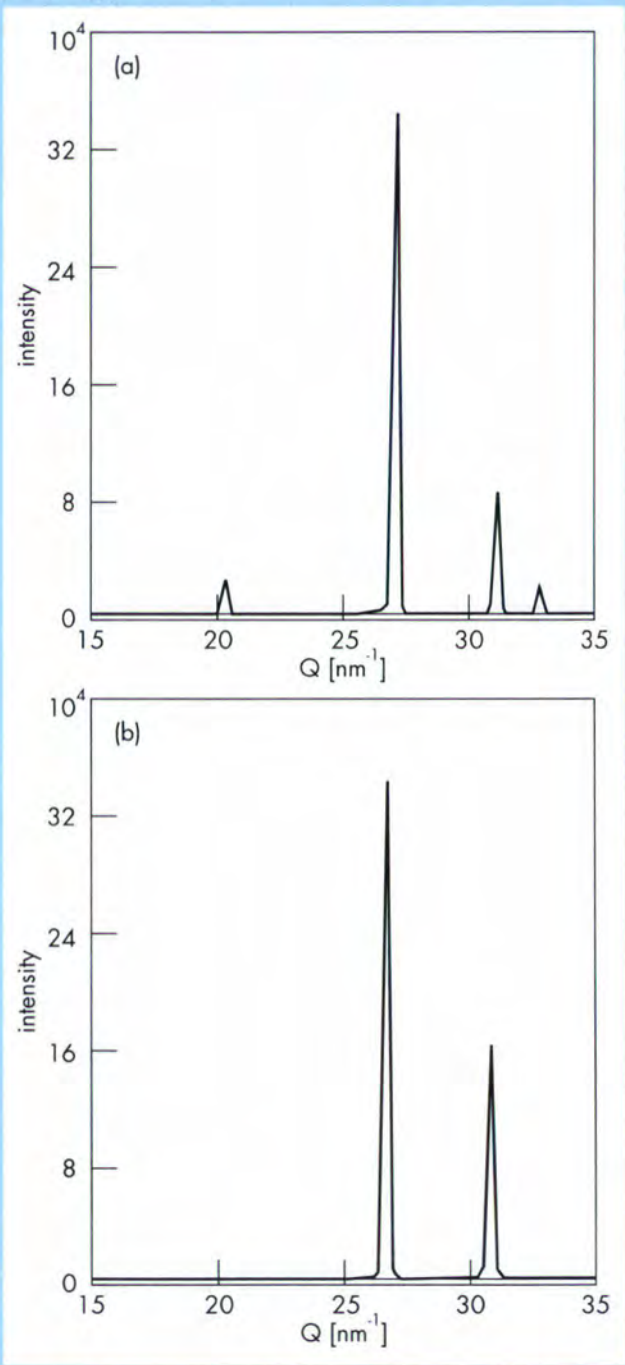

Fig. 2: Diffraction pattern (D1B) of $Al_{94}Si_6$. The Si peaks prove the demixed Si-clusters (diamond structure) in the fcc-Al matrix in the prealloy (a). After melt spinning of this prealloy the Si clusters have been dissolved in Al (b).

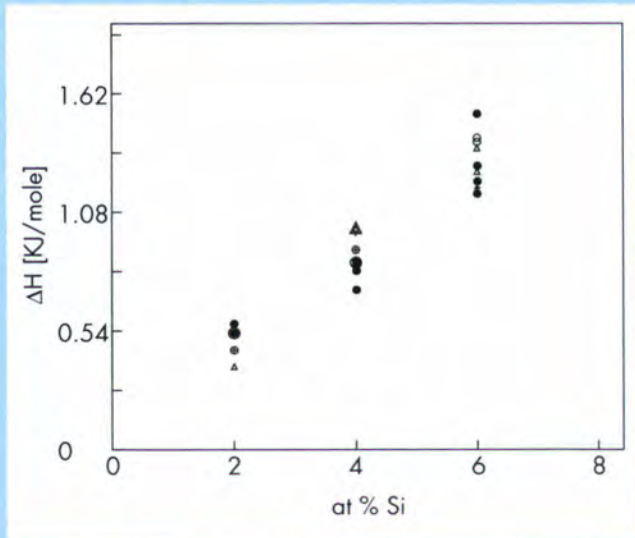

Fig. 3: Enthalpy (ΔH) release on segregation in the melt-spun solid solution of 2,4 and 6 at. % Si in fcc-Al measured in dynamical DSC scans with different heating rates (dT/dt = 5,10,20,40 K/min).

effective concentration ($X_{effective} \approx 3.5$). This latter effect is most likely due to the additional lattice defects introduced by the melt spinning process. These results demonstrate that supersaturation of the fcc-Al lattice with Si-atoms leads to a destabilization of the lattice against shear forces at short wavelength and THz frequencies.

Such destabilizations have been ascribed to the building up of internal stresses which finally force the lattice to disorder completely. Normally these stresses have been assigned to size differences of the constituent atoms. However, the atomic volumes of metallic Si (15.5 Å^3) and Al (16.6 Å^3) are nearly equal and thus we tentatively assume that **bond frustration** of the Si atoms with their tendency to develop covalent bonds in the Al-lattice is the driving force in this case.

Most recent investigations using high resolution TOF spectroscopy on IN6 show that there is not only a general shift of the spectrum of transverse modes as shown in Fig. 4 but that possibly a special low energy mode is developing a large amplitude, as can be seen in Fig. 5. The energy of this mode decreases when Q ($\hbar$Q is the momentum transfer) is approaching the (111) Debye-Scherrer peak of the fcc lattice, as has been found from the representation of the same data at constant Q. It is therefore tempting to assume that the amplitude of this **destabilization mode** increases with increasing supersaturation of the solid solution to an extent that it finally leads to the collapse of the lattice. More detailed investigations of this mode are presently under way.

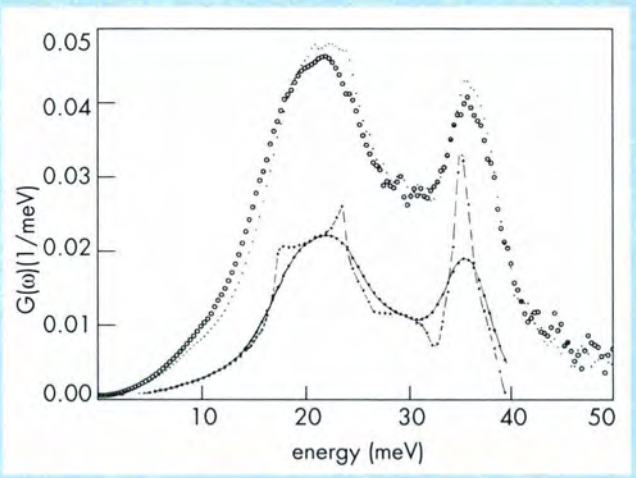

Fig. 4: Generalized phonon density of states of rapidly quenched fcc-$Al_{94}Si_6$ (o) and of fcc-Al (.) measured at 280 K in neutron energy loss on IN4 (E_o = 68.8 meV, ΔE_o = 4.7 meV). The calculated PDOS of fcc-Al before (---) and after convolution (——) with the resolution function of the TOF spectrometer is inserted below. The shift of the spectrum of the transverse phonons in the solid solution compared to that of pure Al is clearly seen.

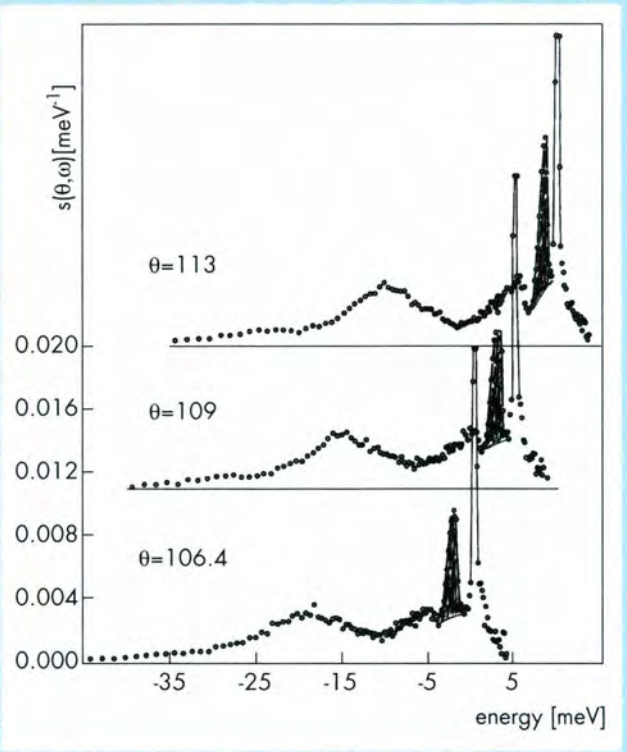

Fig. 5: Three sections through the total dynamic structure factor $S(\Theta,\omega)$ of rapidly quenched fcc-$Al_{94}Si_6$ measured at constant scattering angles Θ at 280 K on IN6 (E_o = 4.7 meV, ΔE_o = 0.125 meV). The development of a very sharp excitation (left of the elastic line) in the neutron energy gain spectra when approaching the (111)-Debye-Scherrer peak is demonstrated.

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Biological Structures and Dynamics

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Introduction

As in other colleges, the activities of the College 8 members have changed as a consequence of ILL's reactor shutdown. This is particularly true for those members of the college who belong to the ILL itself and whose work is mainly described in this report.

As expected, it turned out that ILL's facilities cannot be replaced by those of other neutron centres. Many activities had either to be stopped completely, or projects involving the use of neutrons could be pursued only partially elsewhere. It is therefore not surprising to see that many of us have started, enhanced or revitalized our interest in other domains of macromolecular biology, such as X-ray crystallography.

In 1992, quite a few of our colleagues moved to their new laboratories and offices in the newly installed Institut de Biologie Structurale (IBS) not far from the ILL. It is a sad task for me to remind you of the death of the first director of the IBS, Jean-Pierre Ebel, who died suddenly and unexpectedly on June 22nd, 1992. He played an important role in the structural investigations of biological macromolecules, especially of the translational apparatus, and in him we have lost a friend as well as a supporter of our work.

The continued collaboration with our colleagues who are now at the IBS and with those at the Grenoble outstation of the European Molecular Biology Laboratory (EMBL) is a vital element for the scientific life of our college.

Members of the college participated both in the organization, the courses and the preparation of a book for the *Hercules* course. We were represented both in the discussion of the project for the European spallation source and in the BESAC review of neutron sources and applications in the United States, which discussed the relative merits of spallation sources and steady-state reactors.

This report presents some highlights of the activities mainly of the ILL scientists, of visitors and students in College 8 in 1992.

Scientific Trends and Highlights in 1992

Protein structures

Hydrophobic protein from soy bean

The structure of a 9 kda hydrophobic protein from soybean was solved to 1.8 Å resolution by the multiple isomorphous replacement method. Mainly two heavy atom derivatives were used. The model was refined to 1.8 Å resolution by molecular dynamics using a slow cooling procedure giving a r.m.s. of 0.027 Å for the bond distances and 4.2° for the angles, and a R factor of 18 % (collaboration between ILL, UJF, CNRS and IBS). The molecular structure is shown in Fig. 1. It is a compact molecule made up of four short helical pieces connected by loops forming all together one right-handed spiral. This arrangement is one of the simplest that has ever been found, and can best be described as a distorted helix bundle.

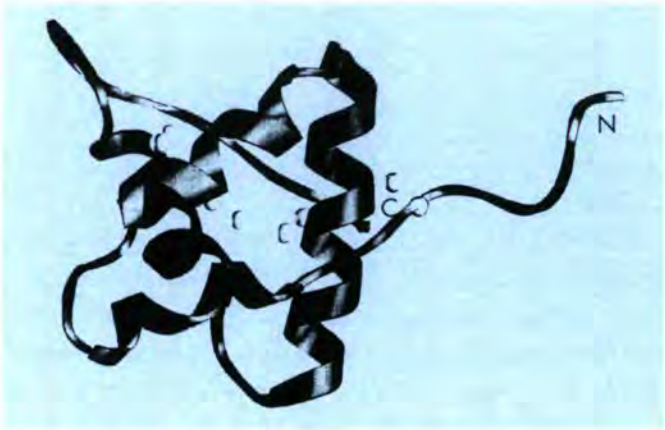

Fig. 1: Ribbon plot of the hydrophobic protein from soybean. The small spheres are sulphur atoms involved in disulphide bridges, of which there are four in all. The N and C terminals are indicated.

As implied by its name the protein is very hydrophobic. As usual for globular proteins most of the hydrophobic residues are embedded in the interior, but even then a study using a water-like probe indicates that 70 % of the surface is apolar. This is about the highest value found in proteins crystallized in a water environment and compares to for example Crambin, which has 68 % apolar surface. An interesting question is therefore how important the solvent/water interactions are in this case.

Hydrophobic moieties are expected to order the surrounding water and lead to the formation of clathrate type arrangements. Little of this is seen in the present study based on the analysis of the X-ray data. The reason is partly that hydrophobic parts of one molecule connect with similar parts from another molecule, but even where the interaction should lead to a water arrangement there is no particular indication of this. Indeed the ordering of the water is relatively low, and of the 200 water molecules available only about 30 % have been located. It is therefore planned to freeze the crystal and to see whether this will induce further order.

Work on understanding the function of the protein has also continued, both by comparison with other members of the same protein family which are known to act *in vitro* as lipid transfer protein, and by a search for homologous proteins, and in this context the protein has been found to resemble domains of larger proteins found in other plants. These proteins are known to be produced in connection with embryogenesis, from the first to the third week, and at present they are believed to be involved in stability or defense of the embryo. They consist of two parts, of which the first is proline rich and the second is homologous with the hydrophobic protein, and it is therefore possible that the protein from soy bean might have been a member of a larger complex, which was split during extraction or purification.

Phospholipid transport protein

Crystals of a phospholipid transport protein from wheat were obtained in presence of a phospholipid. Diffraction data of the native crystal were collected to 2.9 Å with a FAST detector and an image-plate device on a rotating anode diffractometer. Heavy atom derivatives studies are underway.

Lipovitellin

The location of the phospholipid in the lipid storage protein lipovitellin from lamprey eggs has been reported previously (see 1991 Annual Report). Work has continued on the fitting of the amino acid sequence to the electron density map obtained from high resolution X-ray crystallography. When completed this will allow a full description of the protein/lipid interactions which stabilise this complex (Minneapolis/ILL).

Extracellular matrix

The extracellular matrix is defined as the environment surrounding cells within tissues. This environment is made of proteins and proteoglycans. The matrix is involved in processes such as embryogenesis, wound healing and cancer. The adhesion of cells to tissues is mediated by matrix glycoproteins. Fibronectin fibres have been studied by small-angle X-ray scattering. Crystals of osteonectin as well as a fragment of fibronectin have been obtained. High-resolution isolectric focussing purification is developed to help with the isoform problems. Cryoelectron microscopy applied to matrix proteins is in development (ILL with teams in Grenoble, Lyon, London, Manchester, Edinburgh, Lausanne, Geneva and Bethesda).

Influence of glycosylation on the structure of glycoproteins

Most extracellular proteins have carbohydrate side-chains. Recent studies have started to show the role of glycosylation on the protein function but there is at present little data on the influence of glycosylation on the biophysical properties of proteins. The influence of enzymatic and chemical deglycosylation on the conformation of α-1 acid glycoprotein and ribonuclease B has been studied.

Membranes and membrane components

Porin

Porin is a protein found in the outer membrane of Gram-negative bacteria. It allows the selective passage through the membrane of polar molecules up to a cut-off value of molecular weight about 600. The X-ray structure of Porin from the purple bacterium *Rhodobacter capsulatus*, has been

solved to 1.8 Å resolution by the groups of W. Welte and G. Schultz in Freiburg, revealing a secondary structure composed mainly of ß-sheet. The crystals were produced after solubilisation of the protein in detergent which is believed to mimic the membrane lipid in its interaction with hydrophobic parts of the protein. Thus studies of the protein-detergent interaction in the crystals could throw light on the protein-lipid interactions in vivo. In the X-ray studies to date, however, no detergent structure has been observed, due probably to disorder and low contrast. A neutron diffraction study was undertaken on the crystals of Porin (Freiburg, ILL) to locate the detergent in these crystals. The results show that the detergent does indeed mimic the membrane and forms sheets within the crystal in which are embedded the protein molecules. There is no interaction between 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.

Soluble and Membrane Proteins from Halophilic Bacteria

Halophilic bacteria live in extreme saline environments such as the Dead Sea. Their cytoplasm is close to saturated in KCl, so that all their biochemical reactions take place in an environment known to inhibit function in most mesophilic proteins. For a number of years, solvent-protein interactions in halophilic proteins have been studied by neutron scattering, in order to identify the mechanisms involved in adaptation to high salt environments. These studies also contributed to the understanding of the role of protein-solvent interactions in protein folding and stabilisation in general. An integrated approach was applied to the problem. The neutron study provided a unique way to characterise the solution structure of the proteins in different solvent environments. Up-stream of the neutron study, the molecular biology and biochemistry of the proteins were developed in order to define their biological properties as carefully as possible in the same solvents. Down-stream, the data were interpreted in terms of structural models which were tested further by new molecular biology, biochemistry and biophysics experiments. In the past year two students, members of the College, presented their doctoral theses on studies of halophilic proteins including the analysis of neutron data collected before the reactor shutdown. For the first time, a halophilic protein was studied which had been successfully refolded correctly into its active structure following the expression of its gene in the intestinal bacterium *Escherichia coli*. A stabilisation model was suggested, in which the halophilic protein adapts to its environment, and is stabilised by different mechanisms in different solvents. These studies were collaborations with a CNRS unit in Grenoble, Tel Aviv University and the Weizmann Institute.

Two doctorates were awarded for studies that consisted predominantly of neutron experiments on the Purple Membrane of *Halobacterium halobium*. This membrane contains a single protein, bacteriorhodopsin (BR), organised with lipid on a highly ordered two-dimensional lattice. BR functions as a light-driven proton pump. It has been studied extensively as a model of an α-helical integral membrane protein (it is probable that many important receptors have similar structures) and in order to understand a mechanism of light to chemical energy transduction at the atomic level. One of the studies was an exploration of different structural and functional aspects of the system by using specific deuterium-labelled membrane samples. The other presented a detailed study of the dynamics of the membrane in different conditions by inelastic neutron scattering. It was the first time such a study was performed on a membrane protein and strong correlations became apparent between the type of dynamics and the ability of the protein to perform different aspects of its function. Whereas BR, when it is vibrating harmonically, can be activated by absorbing a photon and releases a proton on the outside of the cell (where the proton chemical potential is higher than in the cytoplasm), soft anharmonic motions in the protein are required for it to return to its ground state by binding a proton on the cytoplasmic side. These studies were performed in collaboration with the Institut de Biologie Physico-Chimique, CEN Saclay and a CNRS unit in Grenoble.

Detergent structure

As has been described in the case of Porin, membrane proteins can only be crystallised when solubilised in a detergent. In several cases it has been found necessary to add a second smaller amphiphilic molecule in order to induce crystallisation. Some years ago experiments were performed at D11 to investigate the effect of these small amphiphilic molecules on the structure of detergent micelles, in particular the effect of the heptane-1,2,3-triol on dodecyl amine oxide. These experiments were carried out with the high melting-point isomer of heptane triol, the only one which induced crystallisation of the photosynthetic reaction centre. It was observed that the effect of the addition of heptane-triol on the detergent micelle was to reduce its size (i.e. increase its curvature) by inserting itself into the micelle. We have now extended these experiments (Freiburg, ILL) to the low melting-point isomer which does not induce crystallisation. The experiments, performed on LOQ at ISIS, tend to confirm a qualitatively similar behaviour for the high melting point isomer but quantitative comparisons must await further interpretation of the data.

Muscle thin filaments

Just before the reactor shutdown experiments were initiated to study the interaction between actin and tropomyosin in thin filaments from skeletal muscle (UCSF/ILL). Using deuterated tropomyosin it was possible to monitor the movement of this molecule relative to the actin during regulation by Ca^{++}. In the last year these experiments have been continued in part at the H9B facility at Brookhaven National Laboratory.

Protein-nucleic acid interactions and protein synthesis

Neutrons are useful for determining biological structures for many reasons. First, they make it possible to distinguish between the main components of biological macromolecules, nucleic acids (desoxyribonucleic acid, DNA; ribonucleic acid, RNA), proteins and lipids. Secondly neutrons are sensitive to the deuterium content of these components; this can easily be varied by growing microorganisms (bacteria, yeast, etc.) in solutions containing heavy water (D_2O). Several biologically relevant molecules consist of two or more chemical classes, like ribosomes, made of proteins and RNA, or viruses, made of proteins and RNA or DNA; others form complexes containing both (like RNA polymerase, together with DNA).

In all living cells, the genetic information is contained in DNA, long chain molecules which usually form quasi-linear double-helical polymers. Before the information contained in the DNA base-sequence can be finally translated by the ribosomes into the thousands of different proteins and peptides present in a cell, base-complementary blue prints in the form of chains of messenger RNA (mRNA) are produced. This duplication process is catalyzed by the enzyme RNA polymerase, which has been studied for many years with small-angle neutron scattering.

The mRNA molecules are transferred to the ribosomes, which, by interpreting their base sequences, synthesize new proteins. Ribosomes are particles made up of two subunits of unequal size, each consisting of nucleic acid (2/3 of the mass) and a multitude of different proteins. The large ribosomal subunit (50S) *E. coli*, often used as a "guinea pig" by biochemists, consists of a short RNA chain (5S rRNA) and a very long one (23S rRNA), and more than 30 proteins (called L1 to L34, L8 being a complex of proteins, and L7 nearly identical to L12). Ribosomes and their proteins from the halophilic *Halobacterium marismortui* are much more stable than those of most organisms and therefore are more and more used for structural studies.

Low resolution neutron diffraction of 50S ribosomal crystals from *Halobacterium marismortui*.

Ab initio phasing methods developed for phasing the low neutron diffraction data from 50S ribosomal crystals (from *Halobacterium marismortui*) lead to similar density maps with different phasing methods (direct methods, maximization of entropy and likelihood). This means that the location of the ribosomal particle within the crystal seems to be in agreement between the different phasing methods. The question now is to improve the phases in order to describe with confidence the density within the particle and to distinguish between protein and RNA domains. The maps obtained are modelled in order to define two levels corresponding to proteins and RNA (in 100% D_2O the protein scattering density is about twice that of RNA). A recycling procedure is underway in order to optimize the two-level model taking into account the diffraction data obtained in 0% D_2O.

Viruses and viral components

HIV-1 Reverse Transcriptase

The genetic information of the Human Immunodeficiency Virus 1 (HIV-1), which is of the retrovirus type, is stored as viral ribonucleic acid (RNA) rather than DNA. An enzyme called reverse transcriptase contained in the virus transcribes the genetic code into DNA which then can be incorporated into the host genome to be switched on by external events. Reverse transcriptase is one of the major targets in drug design against AIDS. The solution structure of HIV-1 reverse transcriptase was first visualized by small-angle neutron scattering (MPI Martinsried, Basle, Argonne, Lyon, Cleveland, ILL; see College 8 Annual Report 1991). An ILL press release on this topic was quoted in several European newspapers and periodicals.

In the meantime, crystal structures of the enzyme have been reported by American groups. Using all the structural information available, it will be possible to study the effect of binding other molecules (tRNA, factors, inhibitors) on the solution structure of reverse transcriptase. Samples for experiments in this direction are being prepared, and it is hoped to measure them at the SANS facility of HMI, Berlin.

Disintegration of Viruses under high hydrostatic pressure

Neutron small-angle scattering studies showed that hydrostatic pressure enhances the stability of the isometric plant virus TYMV (Turnip Yellow Mosaic Virus). Contrast variation was used to observe the structural changes of the protein capsid and of the RNA core separately. The thermally induced uncoating of the RNA as well as

structural transitions of the protein capsid are shifted to higher temperature upon increasing the pressure from 5 x 10^6 Pa to 2 x 10^6 Pa. Data concerning the thermal stability in different H_2O/D_2O mixtures cannot be compared directly, even at similar pD values, because the presence of D_2O stabilizes the virions.

Another series of experiments were carried out in order to study the pressure-induced decapsidation of TYMV. The virions irreversibly released their nucleic acid; this dcapsidation led to the formation of empty protein shells that were stable under high hydrostatic pressure.

At present, the behaviour of Brome Mosaic Virus (BMV), a prototype of a virus mainly stabilized by RNA-protein interactions is being studied. Small-angle neutron scattering studies (at GKSS, Geesthacht) indicate that the diameter of BMV increases substantially upon increasing the pressure to 2 x 10^6 Pa at 20 °C, and that this swelling is at least partially reversible. In order to unravel the respective contributions of RNA-protein and protein-protein interactions, a study of the behaviour of empty shells obtained by *in vitro* reassociation of BMV protein has begun. (Osnabrück, Strasbourg, ILL, Geesthacht).

Methodological developments

Quasi-Laue diffraction and instrumentation

Development of detectors and diffractometers have continued as a collaborative effort between the EMBL and the ILL. Two lines of studies have been pursued, namely the use of position sensitive photomultipliers combined with scintillators and the application of an imaging plate with a neutron to X-ray converter.

For the photomultiplier system two detectors are now ready, allowing the possibility of testing two different read-out systems. In one case the peak location is obtained by delay-line techniques, while for the other detector the center of gravity is calculated with a PC, based on the output currents of the photomultiplier. The delay-line detector has been tested at the neighbouring Siloé reactor, and towards the end of 1992 both detectors will undergo longer tests, one at the Würenlingen reactor centre, the other at Risø National Laboratories. Both the detectors cover an area of 45 by 55 mm^2, and the expected resolution is around 1 mm, depending on the thickness of the scintillator.

Imaging plates have large detection areas, and can be either square or circular disks. These shapes are very suitable for X-ray protein crystallography where a good part of the scattering is within 45° of the forward direction. For neutron crystallography on large systems much can however be gained by using long wavelengths, and thus larger scattering angles. A good geometry would therefore be a cylinder shaped imaging plate covering all the way to near backscattering, and the construction of such a device has been started at the EMBL.

As a preparation for this detector several tests have been carried out. First, at the Orphée reactor Laue patterns were recorded using the white beam of cold neutrons at the radiology beam line. The imaging film was a standard X-ray imaging plate equipped in front with a gadolinium oxide converter spray painted onto an aluminium plate. It was read at the Molecular Dynamics reader of the small angle scattering group at CEN Saclay, and the result from an exposure of a large crystal of hen egg-white lysozyme is shown on the front cover. Further tests have since been done at the Siloé reactor, this time using thermal neutrons and a locally available reader.

These tests confirm that imaging plates are potentially useful for neutron scattering. The limitation is clearly that the measurement time for one recording is longer than the read-out time for the imaging plate, which will be several minutes. Another problem that was discovered during the measurement was that ghost images can occur from neutron absorption by ^{151}Eu, which is part of the imaging plate phosphor, and which gives rise to a longer lived isotope. The effect is small, though, and could be removed by suitable choice of isotopes or other rare-earth elements.

Synchrotron X-ray work

During the enforced stop of the reactor, members of the college have taken the opportunity to familiarize themselves with the use of synchrotron radiation, and this has lead to a collaboration between the ILL and a group at GKSS, Geesthacht for the exploitation of soft X-rays for diffraction studies. The work was done at the A1 instrument located at HASYLAB, Hamburg, and the first step was to show that it is possible to measure a large anomalous signal from sulphur atoms in a protein crystal.

The resonance for anomalous scattering of sulphur is found at 5.0 Å (2.5 keV), and the signal from f' or f'' can here attain from 8 to 10 electrons. This would typically lead to about 5 % changes in the structure factors compared to the value far from resonance, and it should thus be possible to use this effect to phase the structure amplitudes much in the same way as is done with heavier atoms.

The result would therefore as usual be an electron density map from which the organization of the peptide chain can be extracted. Due to the long wavelength the resolution of the map, expressed in minimum d-spacing, would not be more than about 2.8 Å, but this would be enough to identify the peptide chain.

Soft X-ray diffraction has a number of problems of its own, and very little work has been done till now. The reason is that these X-rays are only available at synchrotron sources, and although abundant in the storage ring they are hard to get out, mainly due to very strong absorption effects. A typical absorption coefficient for light matter is 500 cm^{-1}, so one sheet of paper would stop the beam completely. Consequently, the whole experiment has to be done in vacuum. This complicates the handling of the protein crystal, which requires a humid environment, and it was therefore necessary to hold the crystal in a cell with thin mylar walls.

Measurements were then done on tetragonal lysozyme crystals in reflection geometry, as the mean path in the crystal is only about 20 μ. This is fortunately the most favorable geometry, as it allows the use of large crystals and the unhindered observation of the 'high' resolution data, which are measured in near backscattering mode. Because of radiation damage, which is very severe at room temperature, only limited sets of data could be recorded. They showed that structure factors can be measured in a reasonable time with good statistics, and that it is possible to see the influence of the anomalous scattering on the intensities when passing through the absorption edge of sulphur.

Secretary: Roland P. May

Molecular Spectroscopy, Surfaces and Mesophases

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Introduction

1992 has not been an easy year for the Institut Laue-Langevin, however, things do now appear to be on the road to recovery. College 9A has, over the course of the last twelve months, lost a number of members. Some have left the Institute permanently, others have gone elsewhere in search of neutrons. However, the scientific life of the College continues to flourish and a number of notable projects have been completed.

Scientific Highlights in 1992

Fixed Window Spectroscopy, Structure-Property Relationships in a Series of Simple Aromatic Solids

The temperature dependence of molecular motion in the solid state is of great interest, particularly its connection to phase transitions. The melting or solid-liquid transition is surely one of the best known of all physical processes, however, the detailed microscopic understanding of the phenomenon is still elusive.

Quasi-elastic neutron scattering has been used to investigate the motion of small hydrogenated aromatic molecules in polycrystalline samples, in detail, benzene (C_6H_6), toluene (C_6H_5-CH_3) and ethylbenzene (C_6H_5-CH_2-CH_3).

The technique adopted for these experiments was that of neutron fixed window spectroscopy (FWS). Here the primary and secondary spectrometers of a high-resolution backscattering spectrometer are both set to the elastic position, we therefore define an energy bandpass, given by the energy resolution of the spectrometer. For IN13 (ILL), this window has a width, 1.9 GHz or 8 μeV.

When the molecules which constitute the samples scatter neutrons inelastically, that is, their relaxation time is shorter than a few nanoseconds, the neutrons may well be scattered out of our window of observation. As the sample temperature is increased the molecules have increasing amounts of thermal energy available to populate higher vibrational and possibly rotational levels within the solid. Then the probability of neutrons being inelastically scattered, out of the defined window, increases. One thus observes a decrease in scattered quasi elastic intensity as the molecules become increasingly thermally agitated.

We may relate the observed elastic neutron intensity to the dynamic scattering law,

$$I^{el}(Q,\omega \approx 0) \sim S(Q,\omega \approx 0) \quad (1)$$

taking into account that we observe elastic scattering only, elastic being defined as $\hbar\omega \approx 8$ μeV. The scattering law $S(Q,\omega)$ defines both the spatial and the time dependence of the motion of the scatterer. In the present study, because of its large incoherent scattering cross section our scattering particles are the hydrogen atoms present in the molecule. For incoherent scattering we may write

$$S^{inc}(Q,\omega) = DWF\ (A_o(Q)\,\delta(\omega) + \sum_{i=1}^{n} A_i(Q)\,L(\omega)) \quad (2)$$

with

$$\int_{-\infty}^{\infty} S^{inc}(Q,\omega)\,d\omega = 1 \quad (3)$$

Here DWF is the Debye-Waller factor, $\exp(-Q^2 \langle u^2\rangle/3)$, $A_0(Q)$ is the elastic incoherent structure factor, $A_i(Q)$, $i \geq 1$ is the quasi-elastic structure factor with $\sum_i^n A_i(Q) = 1$, the delta function, $\delta(\omega)$, being the strictly elastic part (present for all motions confined to a particular volume) and $L_i(\omega)$ being normalised Lorentzian functions. The width, Γ_i, of the spectral functions will increase with temperature and follow, in the most simple case, an activated temperature behaviour,

$$\Gamma_i(T) = \Gamma_{i,0} \exp(-E_{act}/kT) \quad (4)$$

The signal measured in these experiments will be a convolution of $S(Q,\omega)$ and the resolution function, $R(\omega)$. From eqn.2 we see that for small spectral linewidths only the DWF can reduce the observed elastic scattering intensity.

In the case of unbroadened spectral functions, the slope of the $\ln(I^{el})$ versus Q^2 plots defines the mean squared displacement, $\langle u^2\rangle$, with

$$\langle u^2\rangle = \langle u^2\rangle_{rotation} + \langle u^2\rangle_{vibration} + \langle u^2\rangle_{translation} \quad (5)$$

It is this property which was of interest in this study of the dynamics of different simple aromatic molecules with and without side-groups.

Plotted in Fig.1 are the relative (to 50 K) mean squared displacements, $\langle u^2 \rangle^* = \langle u^2\,(T) \rangle - \langle u^2(50\ K) \rangle$, as a function of sample temperature. Previously, the zero-point vibrational motion of benzene had been determined by inelastic neutron scattering at temperatures about ≤10 K, $\langle u^2_o \rangle = .01 \pm .005$ Å^2. For the three samples, the low temperature behaviour is seen to be linear with slopes, $d\langle u^2 \rangle^*/dT$, increasing from benzene to toluene to ethylbenzene. The rates of change of $\langle u^2 \rangle^*$ with temperature in this linear region are $(5.9 \pm .5) \times 10^{-4}$ Å^2/K $(50 < T(K) < 120)$ for benzene, $(9.3 \pm .2) \times 10^{-4}$ Å^2/K $(50 < T(K) < 170)$ for toluene and $(1.0 \pm .1) \times 10^{-3}$ Å^2/K $(50 < T(K) < 110)$ for ethylbenzene.

For benzene it is known that at temperatures less than about 140 K the main contribution to the overall measured $\langle u^2 \rangle$ comes from out-of-plane motions of the benzene ring. It was suspected, therefore, that the increase in the rate of change of $\langle u^2 \rangle$ with temperature on going from benzene to toluene and ethylbenzene, at the same sample temperatures, is accounted for by the presence of the additional methyl and ethyl side groups. These side groups would undergo

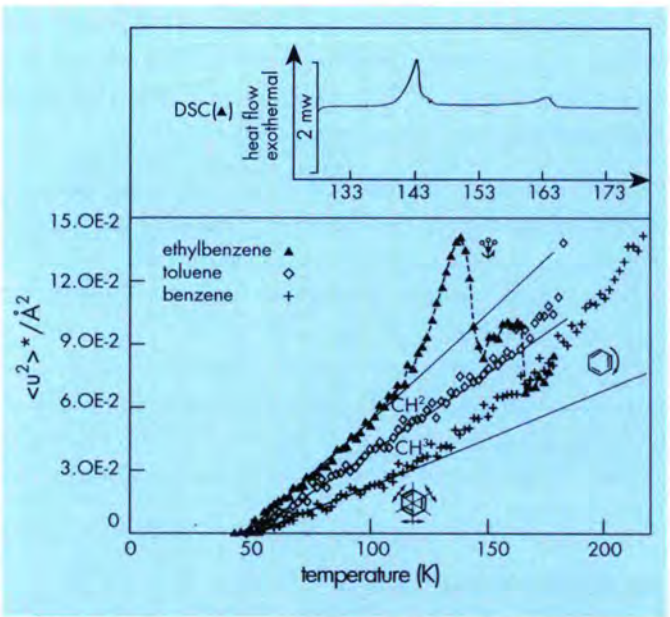


Fig. 1: Plot of normalised (to 50 K) mean squared amplitudes, $\langle u^2 \rangle$, versus sample temperature for benzene (+), toluene (◊) and ethylbenzene (▲). The out-of-plane motion of the benzene molecule is represented by the symbol under the benzene curve at about 120 K and rotations of the benzene molecule by the image under the benzene curve at higher temperatures, > 150 K. The onset of methyl rotation in ethylbenzene is represented by the image at the side of the peak in the ethylbenzene curve at T ~ 135 K. The increase in the slopes of the linear partions of the three curves is ascribed to the additional side groups in the molecules, represented by the CH_3 and CH_2 labels. The upper part of this figure, labelled DSC, contains a scanning calorimetric measurement on ethylbenzene, see text for details of the result and interpretation.

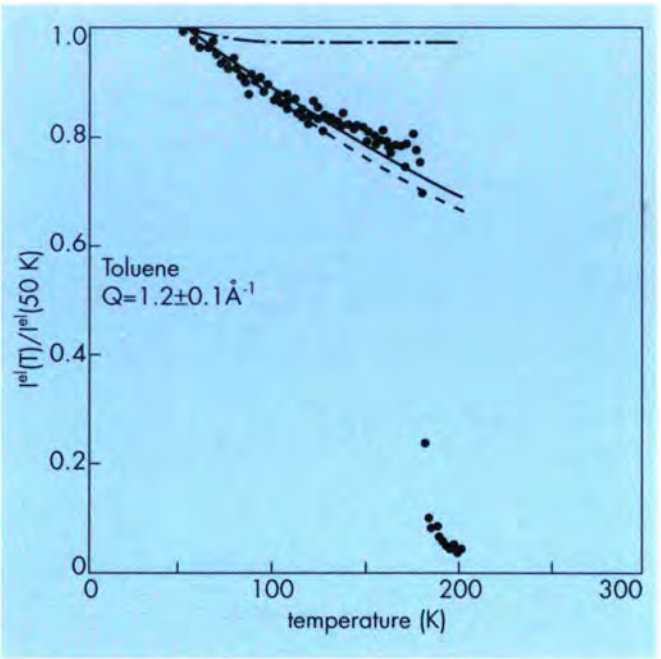


Fig. 2a: FWS for toluene, i.e. a plot of normalised, to 50 K, $S(Q,\omega \approx 0)$ versus sample temperature recorded at $Q = 1.2 \pm .1$ Å^{-1}. The dashed line represents a fit to the measured data with a DWF (obtained from Fig. 1) only. The dashed and dotted line is a fit to the data with an activated 3-fold jump for the reorientational motion of the methyl group, see text for details. The full line is the best fit with a DWF and an activated motion of the methyl group. The sample is clearly seen to melt at 178 K.

torsional oscillations leading to an increased overall amplitude of vibration. The first carbon atom of the side group is constrained by reasons of bonding to be in the plane of the aromatic ring, thereby determining the relative positions of the attached atoms. Thus, in Fig.1 it is possible to see evidence for various degrees of steric hinderance. Whereas benzene, above 120 K, starts to deviate from a linear $\langle u^2\,(T) \rangle$ behaviour, due to the onset of large amplitude librational oscillations about the C_6 axis, $\langle u^2\,(T) \rangle$ for toluene increases linearly with T up to its melting temperature (178 K).

The C_6H_5 ring torsional vibrations in the substituted benzenes are hindered by the antenna-like CH_3 and C_2H_5 groups. A deviation from linearity, due to the onset of thermally activated methyl group rotations, would be expected and a consideration of the available values for this thermal barrier implies that such a motion would already have become established below 50 K. Indeed, from the modelling, via eqn.2, of the temperature dependence of the elastic scattering, seen in Figs.2a and 2b, it was possible to reproduce the observed temperature and Q dependence with a model including three-fold jump reorientation of the methyl group protons only (the scaling factor used to weight the relative importance of the two contributions, DWF and rotational reorientation, being given by the ratio of the

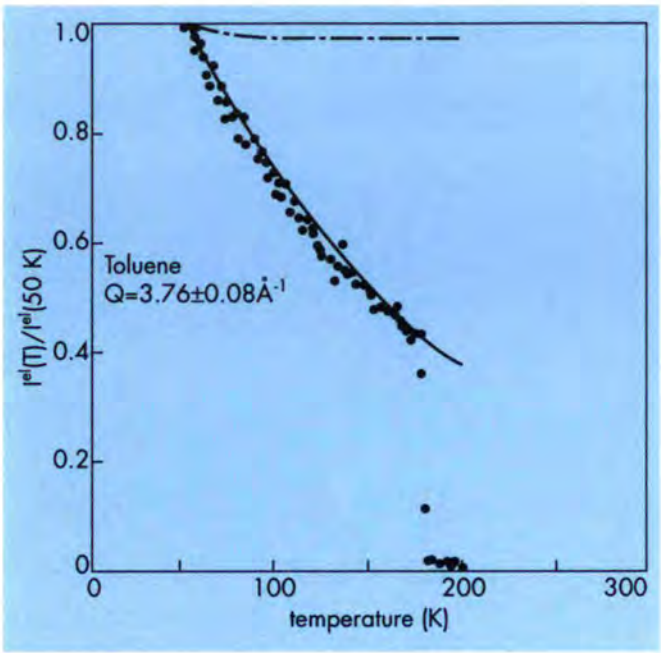


Fig. 2b: FWS for toluene at Q = 3.76 ± .08 Å^{-1}. The dashed and dotted line represents the fit to the data with a thermally activated reorientation of the methyl group only. The full line represents the fit to the data with thermally activated -CH_3 rotation and a DWF.

scattering from the methyl group protons to the total scattering per molecule). For this rotational modelling calculation, Γ_o = 5.8 meV and E_{act} = 200 K were used and we see from Fig.2a that the fit to the data is poor. However, inclusion of a DWF, determined from the temperature dependence of the measured $\langle u^2 \rangle$ in Fig.1 significantly improves the fits to the data at both high and low Q.

In ethylbenzene the methylene group is strongly sterically hindered and fixed with respect to the plane of the benzene ring. Here the linearity in $\langle u^2 \rangle$ versus temperature stops at about 110 K, thereafter it increases rapidly to 135 K and subsequently falls over 10 degrees. This sharp increase in $\langle u^2 \rangle$ was interpreted to the onset of methyl group rotation. In toluene this same motion commences at a much lower temperature, whilst here in ethylbenzene it is much more sterically hindered.

The rapid fall of the measured elastic intensity was successfully interpreted to the slowing down of the methyl group rotation. This would occur with the transference of the available rotational excitation into vibrations or librations of the whole, C_2H_5, side-arm unit. The presence of two, potentially coupled, oscillators could well be the reason for the much higher activation barrier for methyl group rotations in ethylbenzene compared to toluene. That there is a coupling between side arm and ring librations is seen in the low temperature inelastic neutron scattering studies of Cavagnat et al. (J.Physique **45** (1984) 97) on toluene.

As the temperature increases there is another rapid decrease in the observed $\langle u^2 (T) \rangle$ in ethylbenzene (lowering the value to that seen at the same temperature for pure benzene) interpreted as the coupling of the whole side arm, oscillations of the ethyl group, to the motions of the aromatic ring. Finally the available thermal energy can no longer be accomodated by molecular librations and this thermal energy is transferred to the lattice, leading to instability and melting.

It was argued that in ethylbenzene, the discontinuities in the plot of $\langle u^2(T) \rangle$ versus temperature were indicative of solid state phase transitions. This hypothesis was checked by differential scanning calorimetry measurements. In Fig.1 we include the DSC measurement for ethylbenzene. In addition to the exothermic peaks at 140 K and 166 K a very much larger endothermic melting peak at 178 K (not shown in Fig.1) was also seen. This exothermicity, at those temperatures where a slowing down of the molecular dynamics was observed, was taken as support for the above interpretation. Such exothermic behaviour would be explicable interms of crystallisation, however, additional X-ray and neutron diffraction measurements revealed no discrete Bragg lines. However, one cannot discount the possibility of a small crystalline fraction hidden below the short range order peak. This would indicate that increasing molecular dynamics triggers an ordering transition.

In conclusion, the reported elastic experiments give insight into changes of the dynamics of the different degrees of freedom of small aromatic molecules in their respective solids. It is found that these molecules show localized reorientational motions in the solid and that the coupling between the different types of these motions may even slow down the reorientation of substituent side arms. These complex changes of dynamics are observed in relatively simple systems as the temperature increases towards the melting point.

Melting of Aromatic Lattices

Above, we discussed fixed window scans (FWS), that is, the change of quasi-elastic linewidth with sample temperature as the scatterer undergoes thermally activated oscillations. This analysis has much in common with melting and lattice dynamics (instability of the solid phase). One of the earliest theories of solid state instability leading to melting was due to Lindemann who conjectured that melting should occur at a temperature, T_M , when the average displacement, $\langle u \rangle$, of the atom or molecule which constitute the solid due to thermal fluctuations reach a given fraction, r* ~ 0.1, of the intermolecular or interatomic spacing, R.

If we consider a Debye solid and neglect the frequency difference between longitudinal and transverse phonons we may write

$$\langle u^2 \rangle_{T_M} = \frac{9\, h^2\, T_m}{4\pi^2\, m\, k T_D^2}$$

where T_D is the Debye temperature and m the molecular mass. This equation suggests the existence of a liaison between relative amplitudes of molecular oscillation in the solid and the melting point of the solid. Alternatively, we may consider the amplitude of angular oscillation, $\langle \phi \rangle$. Cruickshank has given a means of relating $\langle \phi \rangle$ to the vibrational frequency, ν, of an appropriate molecular excitation, $\phi^2 = kT/4\pi^2 I \nu^2$ where I is the appropriate moment of inertia of the molecule. Bacon et al. have shown the large magnitude, 7.9°, which occur near the melting point of benzene. It has recently been proposed that melting occurs in these samples when this mean amplitude of angular oscillations reaches some fraction of the free rotation amplitude, for example, some fixed fraction of 60° for benzene. A new analogy with the Lindemann theory of melting.

Consider $\langle \phi \rangle$ in radians, if melting occurs when ϕ is some fraction of the six-fold rotation angle, 60° for benzene, hexafluorobenzene and the adduct benzene: hexafluorobenzene, we may write $\phi^2_{max} \approx (7.9°/60°)^2$. We may then rearrange the above equation for $\langle u^2 \rangle$ for the maximum value of T, i.e. T_M

$$T_M \approx \phi^2_{max} \cdot 4\pi^2 I \nu^2 / k$$

the melting point. It is well known that low frequency vibrations will dominate in any consideration of the origin of $\langle \phi \rangle$. Again it is the lowest frequency vibrations which need to be considered when looking at the melting point. This weighting in favour of low frequency and hence large mean-vibrational amplitudes reflects the coupling to the motions of the neighbouring molecules.

Consider benzene, for $\phi^2_{max} \approx (7.9°/60°)^2$, with a parallel moment of inertia of 29.6 x 10^{-46} kgm^2 and given T_M = 278.8 K we find ν = 46 cm^{-1}. Similarly for hexafluorobenzene with I_{II} = 164.2 x 10^{-46} kgm^2, T_M = 278.5 K and $\phi^2_{max} \approx (7.9°/60°)^2$ we find ν = 19.5 cm^{-1}. For C_6H_6:C_6F_6, with a reasonable estimate for the moment of inertia taken as I = (reduced mass).(3.77 Å)^2 = 130 x 10^{-46} kgm^2 , $\phi^2_{max} \approx (7.9°/60°)^2$ and T_M = 299 K we find ν = 23 cm^{-1}. A consideration of Fig.3 shows that these calculated frequencies agree rather well with the lowest frequency excitations measured in these systems by inelastic neutron scattering. This simple model has been extended to toluene and ethylbenzene. Taking the moment of inertia for the methyl rotor to be 53.45 x 10^{-48} kgm^2 and the lowest torsional excitation of the methyl rotor in solid toluene as 46.8 cm^{-1}, $\langle \phi \rangle$ is found to be 44° at 178 K, which is

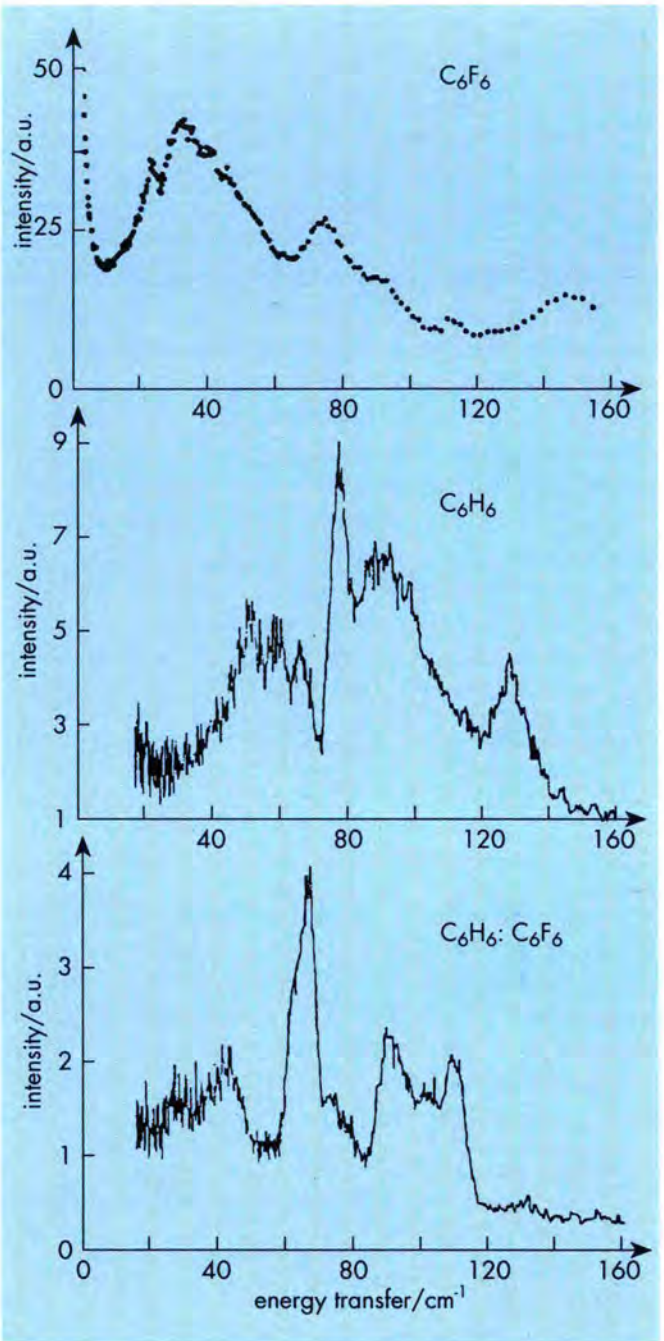


Fig. 3: Inelastic neutron spectra for C_6H_6:C_6F_6, benzene and hexafluorobenzene. The intensities are in arbitrary units. The C_6H_6:C_6F_6 and the benzene spectra were measured at the RAL, U.K. on TFXA and the C_6F_6 spectrum on IN6 at the ILL, Grenoble. The sample temperatures were, benzene 25 K, benzene: hexafluorobenzene 25 K and hexafluorobenzene 95 K.

certainly a large fraction of the free rotation angle 120°. A similar argument would apply for ethylbenzene. Cavagnat et al. (J. Physique **45** (1984) 97) point out how there is a strong coupling between methyl rotations and the phonon density of states in solid toluene at temperatures well below the solids melting point. It seem reasonable then to apply this new model and say that fusion occurs when the side group is no longer able to store the available thermal energy,

which in consequence has to be stored in other degrees of freedom which are more important in destabilizing the lattice.

In passing we note how the addition of a methyl group strongly depresses the melting point of a series of aromatic molecules. Benzene, naphthalene and anthracene melt at 278.5, 353.5 and 489 K, respectively. The addition of a CH_3-group changes the melting points to 178, 251 and 358 K, respectively. The possibility of low frequency excitations in the side group strongly effects the ability of the molecules to relax in the solid, they cannot now undergo rotational relaxation. The effect persists in the homologous series, toluene, ethyl benzene, n-propyl benzene and n-butyl benzene with melting points of 178, 178, 173.8 and 184.5 K, respectively. Whereas in benzene the molecule is able to store a great deal of thermal energy and yet remain a solid, once a side group has been introduced, strong coupling to the rotation of other molecules is produced. Then if this side group can no longer store the available thermal energy it must lead to whole molecule motion and thus to coupled lattice instabilities and finally to melting.

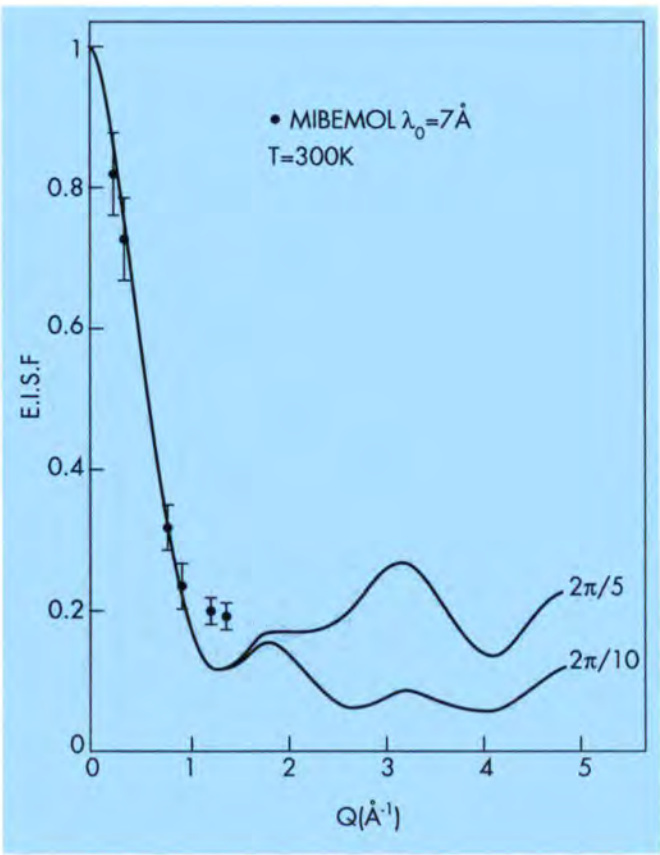


Fig. 4: The EISF for UCp_3Cl at 300 K. The model curves both correspond to motion of all three Cp rings. The jump are assumed on a circle of radius 2.23 A with (a) jumps of 2π/5 radian and (b) jumps of 2π/10 radian.

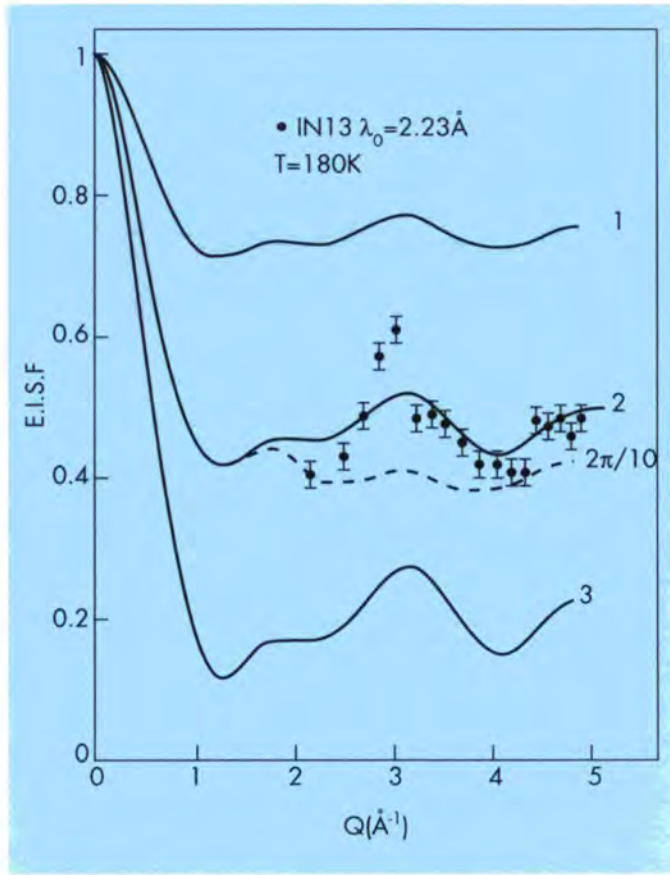


Fig. 5: The EISF for UCp_3Cl at 180 K. Model calculations are for rotations of one, two and three Cp rings and 2π/5 jump motions. For the two ring rotation model we also display the 2π/10 jump model (dashed line).

Motion of Cyclopentadienyl rings in UCp_3Cl

Organometallic systems containing actinide ions exhibit a number of interesting properties. The U—Cl chemical bond have a σ nature, whereas the metal atom interacts with the aromatic cyclopentadienyl rings via π bonds. For the solid studied here, diffraction and NMR measurements had shown that two phase transitions occur, one at 245 K and another at 78 K. The experiments undertaken at the ILL were an investigation using quasi-elastic neutron scattering of the proton motions as a function of temperature near the phase transitions.

A number of neutron spectrometers were used in this investigation, MIBEMOL (Saclay), IRIS (RAL) and IN13 (ILL). The samples were polycrystalline and placed in aluminium containers. In each case the neutron spectra consisted of a single broadened quasi-elastic response. In analyzing the corrected data two quantities were of interest. The first is the ratio of elastic scattering to total scattering, which gives the well known elastic incoherent structure factor (EISF). This ratio can be related directly to the geometry of molecular motion. The second property of

interest is the width of the inelastic response, which may be related to the residence or correlation time between two successive instantaneous jumps of the proton.

Figure 4 displays the EISF measured on MIBEMOL at 300 K, it suggests that jump motions of $2\pi/5$ or $2\pi/10$ radian are the only jump geometries that need be considered. With the known geometry of the Cp ring, it is likely that $2\pi/5$ is the appropriate angle. However, the Q-range of MIBEMOL is insufficient to allow an unambiguous determination of the motional geometry.

Below 245 K the nature of the quasi-elastic scattering changes markedly. An analysis of the IN13 data, Fig.5, at 180 K shows two developments. Now the Q-range is sufficiently large to allow us to distinguish between $2\pi/5$ and $2\pi/10$ motions. It is also observed that the motion is restricted to two of the three cyclopentadienyl rings.

Finally, measurements on the high-resolution instrument IRIS showed that below 78 K all the ring motions are blocked. However, at this temperature the first-order crystallographic transition allows two of the three rings to begin to undergo thermally activated reorientations.

The motion of only two of the three rings may be understood on the basis of "frustration" effects arising from intermolecular interactions. The phase transition at 78 K causes one of the Cp rings to approach a Cl^- anion, thereby setting up a stronger intermolecular interaction than is experienced by the other two Cp rings. Above the transition at 245 K there is sufficient energy and freedom for the three rings to undergo rotation.

Partially Oriented Samples

There continues to be interest in College 9A in scattering experiments undertaken on partially oriented samples. A great many of the samples studied with quasi-elastic and inelastic neutron scattering are powders, that is, randomly oriented collections of microscopic crystals. Large single crystals may be difficult or impossible to obtain and one has to work with averaged crystal orientations and hence an average over scattering vector.

However, much more information can be obtained from such scattering experiments if the orientation of the molecules, scatterers, in the solid sample is known. This has been demonstrated by recent inelastic experiments on polyaniline.

Conducting polymers are of interest because of their novel electronic states and for the high, metal-like, conductivities attainable upon doping. Polyaniline is one of the more versatile conjugated polymers. The polymer is

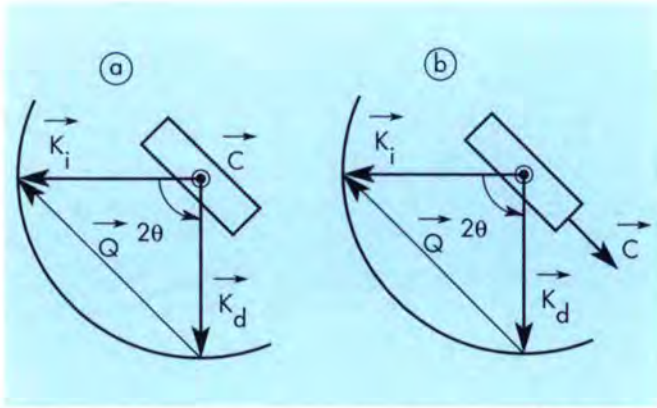


Fig.6: Experimental geometries (incident wave vector $\mathbf{K_i}$, scattered wave vector $\mathbf{K_d}$). (a) $C_\perp$ geometry, the average **c** *chain axis is normal to the figure therefore* **Q** *is perpendicular to the chain axis. (b) $C_{//}$ geometry,* **Q** *is quasinormal to the chains for small scattering angles, but it is parallel to the chains for large scattering angles.*

made up of, R—C_6H_4—NH—-C_6H_4—-NH—-R, repeat units. The basic chain structure exits in three insulator states; the fully reduced leucoemeraldine base polymer and the two oxidation states of the basic chain, the fully oxidized pernigraniline polymer and the intermediate oxidation level emeraldine base polymer. Protonation of emeraldine base, oxidation of leucoemeraldine base and reduction of pernigraniline base all result in formation of the conducting emeraldine salt polymer.

Of interest, is the role of phenyl-ring torsions in determining the nature of the ground and charge-defect states. Coupling of charge transfer between the phenyl-rings and the intermediate N atoms to the dihedral angle of the rings competes with a substantial steric repulsion between adjacent rings. It is believed that polaronic and solitonic ring-angle-alternations defect states may be relevant in determining the nature of the charged states of the polymer.

To investigate the phenyl-ring dynamics, and the more general lattice dynamics of the emeraldine-base polymer, incoherent scattering experiments have been performed on stretch-oriented films of polyaniline. The use of stretched films, that is, partially oriented samples, gives both polarization and energy information about the lattice modes, even when the mosaic distribution of chain axes is relatively large. Figure 6 defines the scattering geometry of the experiment.

These experiments have provided a new insight in the three dimensional dynamics of polyaniline. One may discriminate between modes polarized parallel and perpendicular to the chain axes. In this way one can identify

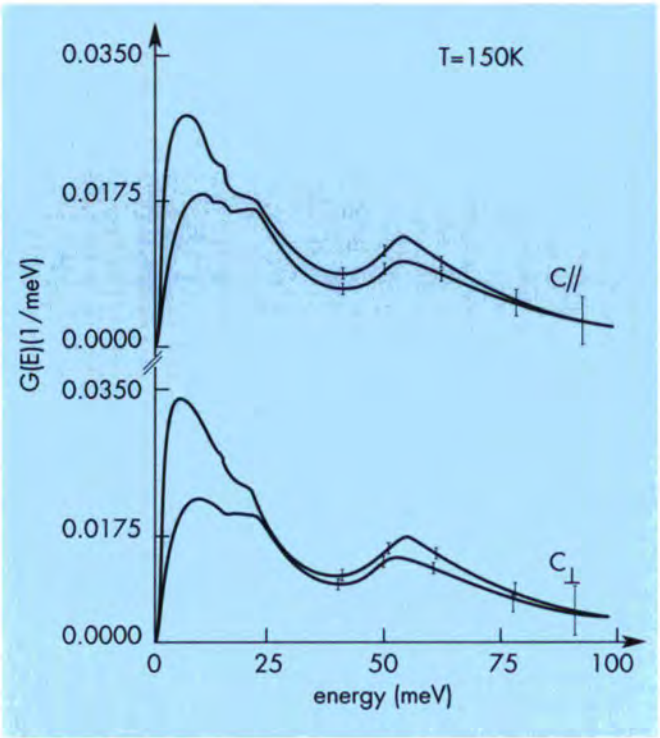


Fig. 7: Polyaniline density of states, G(E), measured at 150 K, normalized over the range 0 - 100 meV, measured for small (case a, $2\theta = 20^0$) and large (case b, $2\theta = 92^0$) scattering average angles in the $C_{//}$ and $C_\perp$ geometries. The phenyl librations occur at 7 and 10 meV. The excitation at 19 meV is believed to be a hydrogen bond stretch, RN-H - - NR_2: an inter polymer chain excitation. The higher energy excitations are vibrational deformations of the phenyl rings.

phenyl group librations, they give rise to out-of-plane (the plane containing the polymer chain) scattering. The lowest frequency peaks observed in the density of states are assigned to phenyl-group librations in a non-planar chain structure, see Fig.7. The importance of phenyl ring librations, in this and in other similar polymers, in determining dynamical properties is well known. For example, the concept of ring-torsional polarons has been proposed as an alternative to a chemical bond dimerization, or Peirerls distortion, as a means of describing the insulator-conductor transition. In this proposed model, the electron-ring angle coupling is analogous to electron-phonon coupling in polyacetylene and the ring librational dynamics play the same role as that of the C-C and C=C stretching dynamics in polyacetylene.

Secretary: Jeffrey H. Williams

Vibrational Dynamics in Solid C_6H_6: C_6F_6

Jeffrey H. Williams

The ability to predict the solid state packing of molecules and to interpret the observed molecular dynamics from a knowledge of the electrical properties of the isolated molecules is a goal much sought after but not easily realized. We have investigated structure-property relationships in solid, benzene: hexafluorobenzene. This is the simplest member of a very large class of layered organic compounds, sometimes referred to as charge-transfer complexes.

The charge distribution of the simple aromatic molecules benzene and hexafluorobenzene are of considerable interest. They have large electric quadrupole moments, Θ , of opposite phase. Simple mixing of these two liquids produces, at room temperature, a solid by virtue of the strong interaction between these two electrical moments. Solid C_6H_6:C_6F_6 melts at a temperature higher than the solids of the pure materials, and unlike the pure materials it has a structure which exhibits instabilities, there are solid state phase transitions at 205, 247 and 275 K (1).

Of interest with regard to the strength of the solid state interactions between the benzene and hexafluorobenzene molecules are the features, seen in the spectrum displayed in Fig. 1 below 120 cm^{-1} and between 420 and 540 cm^{-1}, seen in Figs. 2a and 2b in greater detail. The latter is a combination or phonon side band between the benzene ν_{20} vibrational mode, occurring at 409.6 cm^{-1}, and the vibrations of the intermolecular bonds or phonons, the latter seen in the low frequency spectra between 20 and 120 cm^{-1}. For comparison, in Figs. 2a and 2b, the intermolecular bands and the combination band have been plotted together. The ν_{20} mode of benzene is an out-of-plane vibration and is thus ideally suited to couple with the intermolecular vibrations.

The vibrational combination band or phonon side band involves a simultaneous change in the quantum number of the intermolecular bands together with a change in intramolecular mode of the benzene ring. The frequency is close to the sum of those associated with the relevant transitions considered individually, i.e. $\nu_{DIFF} = \nu_{vdw} + \nu_{20}$ where ν_{vdw} is the frequency of the phonon transitions. A comparison of the spectra in Figs. 2a and 2b shows a good match of features if we assume the ν_{20} frequency, 409.6 cm^{-1}, to be the origin of the van der Waals vibration.

The actual degree of anharmonicity may be determined from the spectra displayed in Figs. 2a and 2b by observing the difference between the sum of the

isolated vibrational frequencies and the measured combination sum frequency. The lines are red shifted in the combination sum band by an amount 1 to 3 cm^{-1}. This red shift is not constant over the whole phonon spectrum (20 - 120 cm^{-1}) but is largest, 2.5 cm^{-1}, for the line at 67 cm^{-1}.

For such a phonon side band, it is possible to construct a direct mechanism for its origin; a coupling of the two different vibrational modes (the benzene out of plane vibration and the phonon mode), through their electric moments. That is, the total moment responsible for the transition from the ground state to the manifold of two-phonon states arises by the interaction of the dipole moment, μ_D, caused by vibrational distortion of the benzene ring and the dipole moment arising by distortion of the electronic charge clouds of the chains of molecules caused by coupled vibrations, i.e. phonons, μ_T.

For the ν_{20}, out-of-plane, vibration the induced electric dipole moment has been determined from infrared measurements to be 0.61D (3). For the optic phonon induced electric dipole moment we may use the model presented elsewhere (3) which for a chain of alternating benzene and hexafluorobenzene molecule shows that for equi-spaced molecules the sum of the induced electric dipole moment, which arises by mutual polarization, is zero. However, if there is a slight difference in the distance between a benzene-hexafluorobenzene pair then a net induced electric dipole moment can arise through the polarization of one molecule by the field of the electric quadrupole moment of the other molecule.

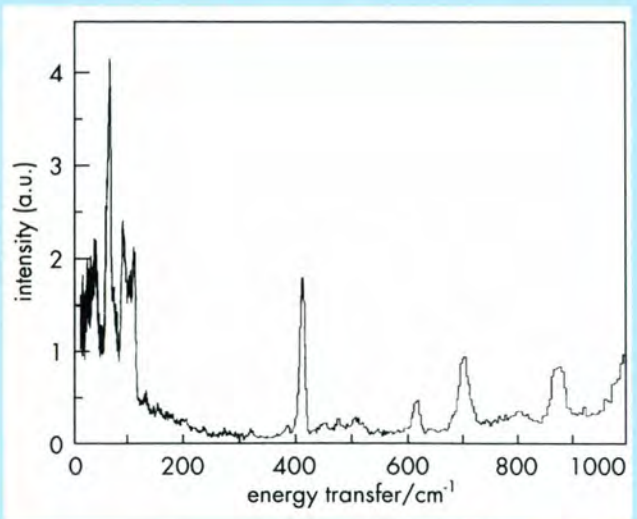


Fig. 1: High resolution inelastic neutron spectrum of C_6H_6:C_6F_6 recorded at 25K.

Consider a chain of alternating benzene and hexafluorobenzene molecules, the centres-of-mass lying on the chain axis. On the time scale of a diffraction experiment ($<10^{-14}$ sec) the benzene and hexafluorobenzene molecules appear equi-spaced along the **c** axis (2). However, on the vibrational timescale (10^{-12} - 10^{-13} sec), the chains of molecules will be unstable to vibrational motions, a Peierls distortion. If R_{ij} is the distance between a benzene molecule and a neighbouring hexafluorobenzene molecule and R_{jk} is the distance from this hexafluorobenzene molecule to the next benzene molecule, then the total induced electric dipole moment, μ^T, is given by

$$\mu^T = \frac{12\,\bar{\alpha}\bar{\Theta}}{4\pi\varepsilon_0}\left(\frac{1}{R_{ij}^4} - \frac{1}{R_{jk}^4}\right) = \frac{12\,\bar{\alpha}\bar{\Theta}}{4\pi\varepsilon_0}\left(\frac{1}{(R+x)^4} - \frac{1}{R^4}\right) \quad (1)$$

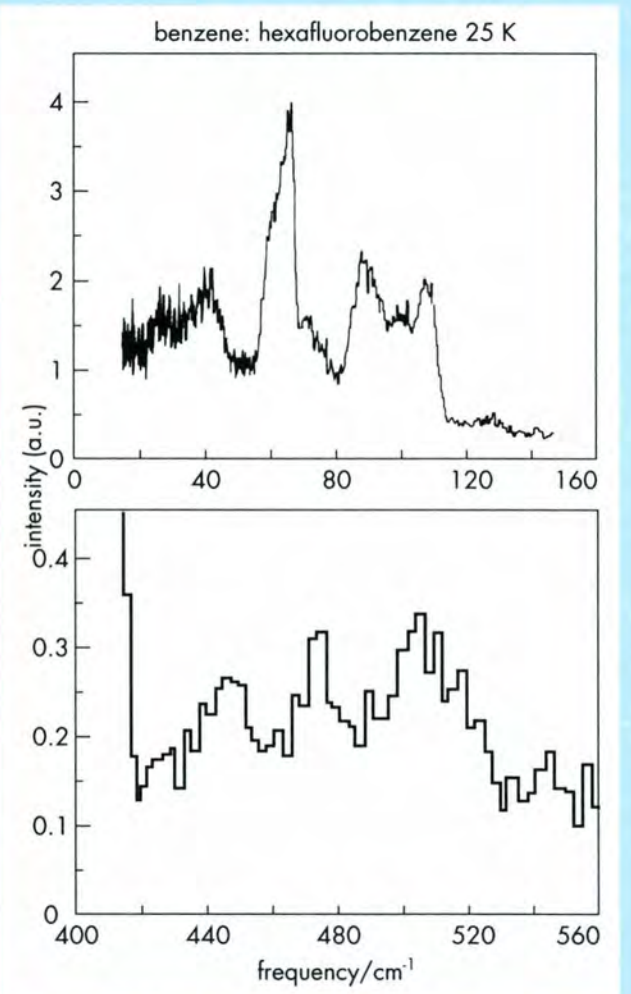


Fig. 2a: Detail of high resolution inelastic spectrum at 25K of C_6H_6:C_6F_6.
Fig. 2b: Detail of high resolution inelastic spectrum of C_6H_6:C_6F_6 at 25K showing the phonon side bands with the van der Waals or phonon vibrations (Fig. 2a).

where we represent the non-zero difference $R_{ij} - R_{jk}$, as $(R + x) - R$. Here $\bar{\alpha}$ is the mean electric polarizability in the chain direction for the pair and $\bar{\Theta}$ is the mean electric quadrupole moment.

The shift of the phonon side band lines from the unperturbed or uncoupled phonon lines arises from the coupling of the induced vibrational dipole moment of the ν_{20} vibration and the phonon induced dipole moment, $\mu_T^{C_6F_6}$, for C_6F_6. Then for a simple electrostatic interaction the interaction energy, u_{DT}, which we equate with the red shift present in the phonon side bands is given by (4).

$$u_{DT} = \frac{\mu_D \mu_T^{C_6F_6}}{(4\pi\varepsilon_o) R^3} (2 \cos\theta_1 \cos\theta_2 + \sin\theta_1 \sin\theta_2 \cos\phi) \quad (2)$$

R is the distance between the centres-of-mass, along the chain direction, of the interacting benzene and hexafluorobenzene molecules. The angles are specified in Fig. 3.

We see immediately the large difference in the interaction energy which will arise when we consider the coupling of in-plane and out-of-plane vibrationally induced dipole moments with the electronically induced dipole moment of the hexafluorobenzene molecule. For out-of-plane vibrations, such as ν_{20}, $90 \leq \theta_1 \leq 180°$ and $\theta_2 = 180$; the two induced moments lie parallel to the axis joining the molecular centres-of-mass, the crystal c-axis (2). For an in-plane vibrational deformation of the benzene ring, $\theta_1 = 180°$ and $\theta_2 = 90°$. In both cases it is reasonable to consider $\cos\phi$ to be finite. It is seen how, to first order, it is only in the case of out-of-plane benzene vibrations that there will be any coupling between the vibrational and electronic distortions within the chains of alternating benzene and hexafluorobenzene molecules.

With R, taken from the observed crystal structure, to be 3.769 Å (2) and $\mu_D = 0.61$D we find, from Eq. 2, $\mu_T^{C_6F_6} = .017$ D, assuming $u_{DT} = 2$ cm^{-1} and then from Eq. 1 we find $x \sim 0.04$ Å. This is of order the mean amplitudes of vibration measured for C_6H_6 in C_6H_6:C_6F_6 by the Q-dependence of the scattering law, $S(Q,\omega)$ at temperatures less than 20 K (5), i.e. $0.07 \leq \langle u^2(T) \rangle$ (Å^2) ≤ 0.11. We find, therefore, that it is possible with simple electrostatic models to interpret certain features of the moderately high resolution inelastic neutron scattering data from solid C_6H_6:C_6F_6.

Another observed property of the spectra which involves the nature of the solid state intermolecular potential is the strength of the mechanical coupling between the motion of the benzene ring and that of the hexafluorobenzene ring. In Fig. 1, features at 319 and at 383 cm^{-1} correspond to the ν_{14}, E_{1u} vibration and the ν_{11}, E_{1g} vibrations of the C_6F_6 ring, respectively. Their integrated intensities may be determined and compared with that of the equivalent vibration of the C_6H_6 ring. The intensity ratio of a C_6F_6 to a C_6H_6 vibrations, as seen in Fig. 1, should be of order 1: 162.

In Fig.4 we give the ratios of the integrated intensities for a series of vibrations of the aromatic rings, $I_{C_6H_6}/I_{C_6F_6}$. It will be noted that although the intensities of the C_6F_6 vibrations are lower than the corresponding vibrations in C_6H_6, they are lower only by a factor between 3 and 10, depending upon the vibration.

The hexafluorobenzene molecule has therefore considerably more vibrational amplitude than one would expect from a consideration of its mass and scattering cross section. We interpret this observation as arising from the strong coupling of the hexafluorobenzene oscillator with the benzene oscillators via the intermolecular vibrations, see Fig.3.

If there is an anomalous scattering intensity it must arise because another oscillator is scattering at the same frequency. There is thus a forced or driven oscillation of one vibrating system caused by the vibrations of the hexafluorobenzene molecule. In such a situation the frequencies of the forced oscillators, here the benzene molecules, are determined by the frequency of the driving force and not by the natural resonant frequencies of the molecule.

If F_i is a generalized force corresponding to a coordinate, η_j, then the generalized force, Q_i, for the normal coordinate, J_i, is given by the transformation

$$Q_i = \sum_j a_{ji} F_i \quad (3)$$

The equation of motion for the oscillations, expressed in normal coordinates is

$$\ddot{J}_i + \omega_i^2 J_i = Q_i \quad (4)$$

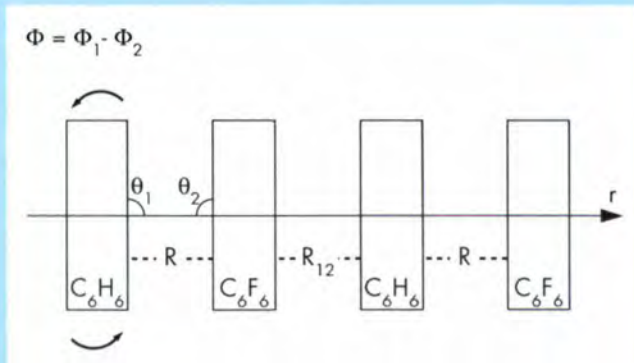


Fig. 3: Definition of the angles used to describe the electrostatic interaction between two electric dipole moments

The driving force, the vibrations of the hexafluorobenzene molecule, perturb the normal coordinates of the benzene, each atom in the hydrogenous oscillator being subject to a mechanical force whose frequency is that of a hexafluorobenzene vibrational resonance, ω.

In such systems, the driving force Q_i can be represented as

$$Q_i = Q_{oi} \cos(\omega t + \phi_i) \quad (5)$$

where ϕ_i is a phase. After standard manipulations, the complete motion of the benzene molecule may be written as

$$\eta_j = \sum_i a_{ji} J_i = \sum_i \frac{a_{ji} Q_{oi} \cos(\omega t + \phi_i)}{\omega_i^2 - \omega^2} \quad (6)$$

Thus the vibration of each particle is composed of linear combinations of normal modes, but now each normal oscillation occurs at the frequency of the driving force.

Two factors determine the extent to which each normal mode is excited. One is the amplitude of the generalized driving force, Q_{oi}. If the force on each particle has no component in the direction of vibration of some particular normal mode, then the generalized force corresponding to the mode will vanish and Q_{oi}, will be zero. An external force can excite a normal mode only if it tends to move the particles in the same direction as in the given mode. In consequence of the denominators in Eq.6 the closer ω approaches to any ω_i the stronger will that mode be excited relative to the other modes. However, because of dissipative forces and the small amplitudes of oscillation, the amplitude of the mode will remain finite at resonance.

Our measurements bear out this analysis in that we see how the intensity of the driven oscillations (in the benzene molecules) increases as one moves towards the lower frequency vibrations of the hexafluorobenzene molecules, see Fig. 4. It is seen that the ratio of the intensity of a distortion of the benzene ring to that of a hexafluorobenzene ring, of the same symmetry type, decreases as one moves towards lower frequency. Evidence for the resonance implied by Eq. 6, as it is here that one finds the hexafluorobenzene vibrations.

One has also to take into consideration the symmetry of the vibrations and the excess intensity, that is, not all the vibrations of the C_6F_6 ring couple to the driven oscillator to the same extent. The E_{2g} vibration couples most strongly, this is an in-plane extension of a pair of C-F bonds, whilst the E_{1u}, an in-plane distortion of the whole molecule (the C_6 ring moving in the opposite direction to the F atoms) couples the least strongly. The others are intermediate, however, the out-of-plane distortions all couple strongly. The crystal structure of this, the lowest temperature phase of C_6H_6:C_6F_6, is known (2) and the above observations are in line with the determined molecular orientations.

References

[1] J.H. Williams, Mol. Phys., 1991, 73, 113

[2] J.H. Williams, J.K. Cockcroft and A.N. Fitch, Angaw. Chemie Int. Ed., 1992, 31, 1655

[3] J.H. Williams, Mol. Phys., 1991, 73, 99

[4] A.D. Buckingham, Advances in Chem. Phys. 1967, 12, 127

[5] J.H. Williams and B. Frick, Chem.Physics, 1992, 166, 425.

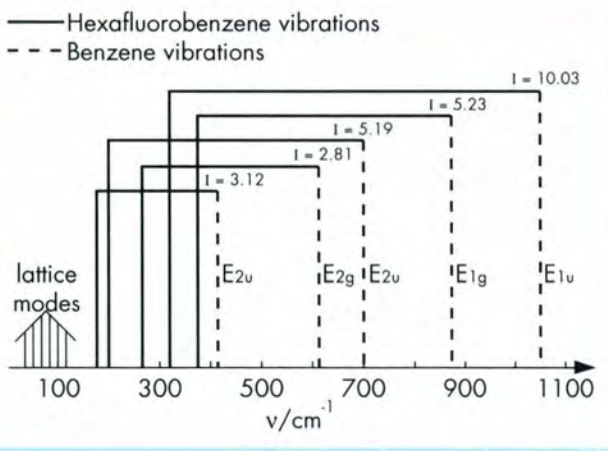


Fig. 4: Ratios of intensities of inelastic neutron scattering for various vibrations of the benzene and hexafluorobenzene molecules in solid C_6H_6:C_6F_6. The intensity ratio is defined as, ($I\,C_6H_6/I\,C_6F_6$). This ratio is seen to decrease as one compares lines, of similar type, with decreasing frequency difference. See text for details.

Large Molecules

Members of the College

E. Amalric	J.F. Legrand
P. Chieux	A. Lied
A. De Geyer	P. Lindner
B. Farago	R. Oeser
B. Frick	F. Rieutord
K. Ibel	V. Rodriguez
C. Lartigue	P. Terech

1992 was a difficult year with regard to scientific life at ILL and in particular in College 9b. Many colleagues took advantage of other facilities all around the world for performing experimental work and the scientific activities are temporarily shifted outside the ILL. This means that only a few examples can be presented at the time of writing.

Scientific Highlights in 1992

2-D crystallization of fatty alcohols at the air-water interface

The phase transitions in Langmuir films of insoluble molecules have been the subject of many investigations mainly based on macroscopic measurements, but in the past few years novel techniques using neutrons and synchrotron radiation have brought new insights in the microscopic structure of thin films made of amphiphilic monolayers.

For many Langmuir films at the air-water interface the presence of traces of impurities smears out the thermodynamical anomalies associated with the phase transitions and complicates the determination of phase diagrams. These are however systems which are less sensitive to impurities. Recently, 2D crystallization of fatty alcohols using both macroscopic techniques (ellipsometry and surface pressure measurements) and grazing incidence X-ray diffraction has been investigated at LURE.

For the series of alcohols between 1-nonanol and 1-tetradecanol, the ellipsometry results show an abrupt discontinuity of the monolayer thickness at a temperature T_c which increases with the chain length (Fig. 1). From X-ray diffraction results this is interpreted as the melting/crystallization temperature of the monolayer as the Bragg peak observed at low temperature disappears at T_c (Fig. 2). In addition, upon cooling below T_c this single narrow Bragg reflection in the powder diffractogram increases in intensity and shifts towards higher Q indicating a high disorder and a large thermal expansion coefficient of the 2D lattice ($\alpha = 10^{-3}$ K^{-1}). The complete interpretation of this unusual behaviour in terms of possible tilt of the chains, Debye Waller factor, proliferation of defects, etc. requires additional information to be obtained on the vertical structure of the monolayer. As shown by J. Penfold et al. such information can be obtained by neutron reflectometry techniques using molecules with deuterated chains while X-ray reflectometry measurements would suffer of a lack of contrast between the monolayer and the water.

(ILL Grenoble, Laboratoire Spectrométrie Physique Grenoble, Institut Curie Paris, DRF-CEN Grenoble).

Semidilute polymer solutions under shear

There is increasing interest in studying the scattering of polymer solutions under shear, both from experimental and from theoretical aspects. Previous small angle neutron scattering experiments on *dilute* solutions in a good solvent have revealed the shear induced deformation of one single chain. In this case, the chain appears elongated along the flow direction. Striking effects are to be expected when a *semidilute* polymer solution is subjected to shear flow and

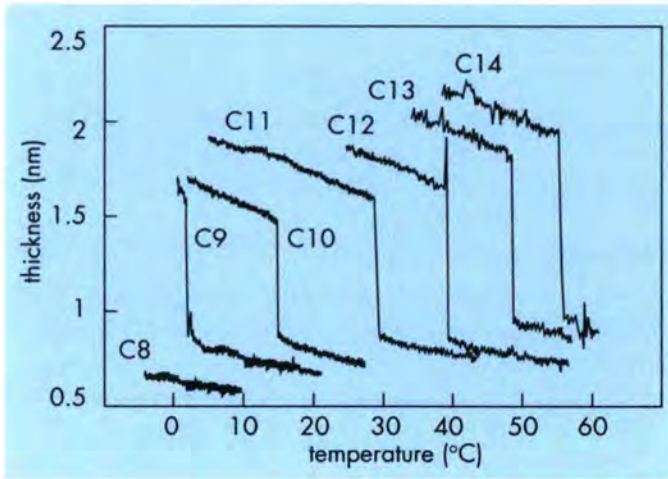


Fig. 1 : Change in the thickness of the monolayer films as deduced from ellipsometric measurements.

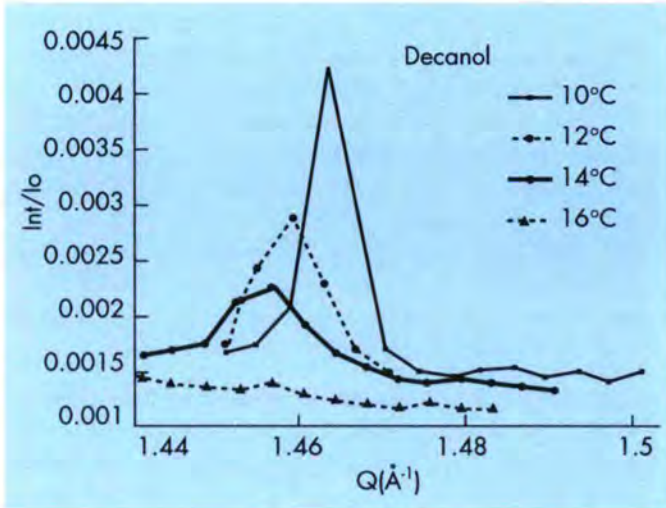


Fig. 2 : In plane X-ray diffraction of a decanol monolayer at different temperatures above and below T_c.

the environment (thermodynamics) for the entangled system is changed from good solvent- to theta-conditions. Small angle neutron scattering experiments with a semidilute polymer solution in laminar shear flow have recently been performed at the Laboratoire Léon Brillouin in Saclay.

The picture on page 102 presents an interpolated colour image of the raw scattering measured at a temperature of 30°C (near the theta point) at a shear rate of 300 s^{-1} (flow direction horizontal). In comparison to the isotropic scattering of the solution at rest (not shown) the contours are slightly anisotropic at large q, with a long axis perpendicular to the flow direction. At low q, a different behaviour is observed: a pronounced increase parallel to the flow direction leads to a double winged shape of the pattern. This resembles closely the butterfly patterns already observed with SANS in deformed gels and rubbers.

(ILL Grenoble, LLB Saclay).
Secretary: P. Lindner

Les Journées des Polymères et des Colloïdes
(14-15 April 1992)

The meeting, which was held in the past in the form of a "Journée des Polymères" was extended to two days this year, as it expanded to cover colloïdal systems. The "Journées des Polymères et des Colloïdes" were held at ILL on 14 and 15 April 1992 under the aegis of the French Polymer Group and the ILL.

This meeting of about sixty physicists, chemists and biologists from the Rhône-Alpes region on various aspects of soft matter, consisted of 35 communications, including about 20 oral presentations and about fifteen posters. The numerous subjects covered included radiation scattering, structure, rheology, the electrical and mechanical properties of polymers and their application in industry, and the structure and formation of membranes and amphiphilic systems.

E. Geissler
P. Lindner

Neutron, X-ray and light scattering in the study of 'soft matter'

For the second time a European School on "Neutron, X-ray and Light Scattering as an Investigative Tool for 'Soft' Condensed Matter" was held in Bombannes, Gironde, France, from May 31 to June 6 1992, following the first workshop of this kind in Spring 1990.

Both workshops were devoted to a simple practical approach to neutron, X-ray and light scattering experiments, involving mathematical transformation back to real space and structural model calculation of the scattering. They were aimed at colloid and polymer scientists using scattering methods in their home laboratory or at common research facilities, who already have some background in this domain and want to exchange their experience and computing programs. The primary objective was to explain the current methodology of elastic and quasi-elastic techniques (avoiding both under and over-exploitation of data) rather than a general course on colloids and polymers. Basic information on data interpretation, on the complementarity of the different types of radiation, as well as information on recent applications and developments was presented.

Experience with the 1990 workshop showed that there is a need for a basic course on scattering and that there is a demand of about 50 young scientists in two years, who wish to be trained in such a school. This European community is spread out in physical chemistry, chemistry, physics and biology laboratories, but the language in scattering is common. It had been proved to be extremely important that the workshop be held in a remote area with housing and the lecture rooms located in the same environment, providing a common leisure activity (in this case sailing) nearby. This ensures permanent contact between lecturers and students and is a guarantee that all participants stay the whole week!

The 1992 meeting gathered together 44 participants from 9 European countries, i.e. Germany, France, Spain, Portugal, Switzerland, Austria, Italy, Sweden and Czechoslovakia. The morning and late afternoon lectures (22 hours of general presentations given by 14 lecturers during the whole week) were followed by late after-dinner evening sessions. Those were devoted to obligatory short contributions (20 minutes) given by the students, where the specific project or problem of each participant was discussed.

The workshop was jointly supported by: Institut für Festkörperforschung, Jülich; Institut Laue - Langevin, Grenoble; European Synchrotron Radiation Facility, Grenoble; Laboratoire Léon Brillouin, CEA Saclay and Service de Chimie Moléculaire CEA, Saclay. Financial participation of all partners is gratefully acknowledged.

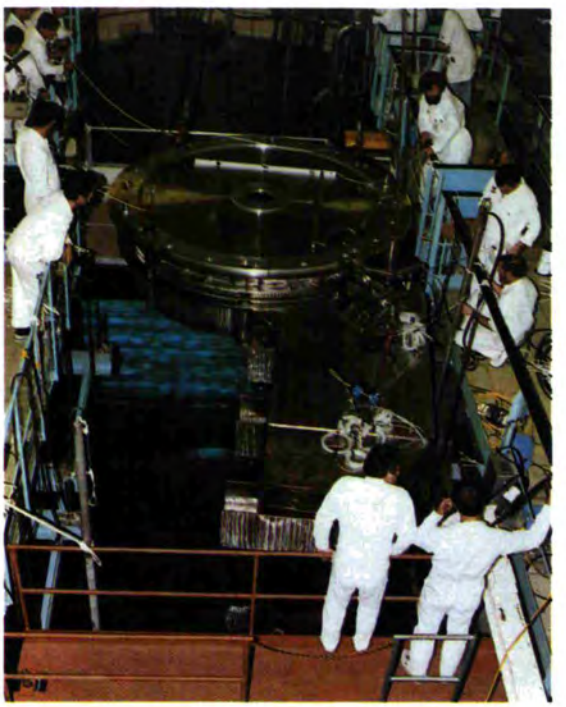
Peter Lindner

Lead coffin for the removal of the H5 liner (Horizontal Cold Source).

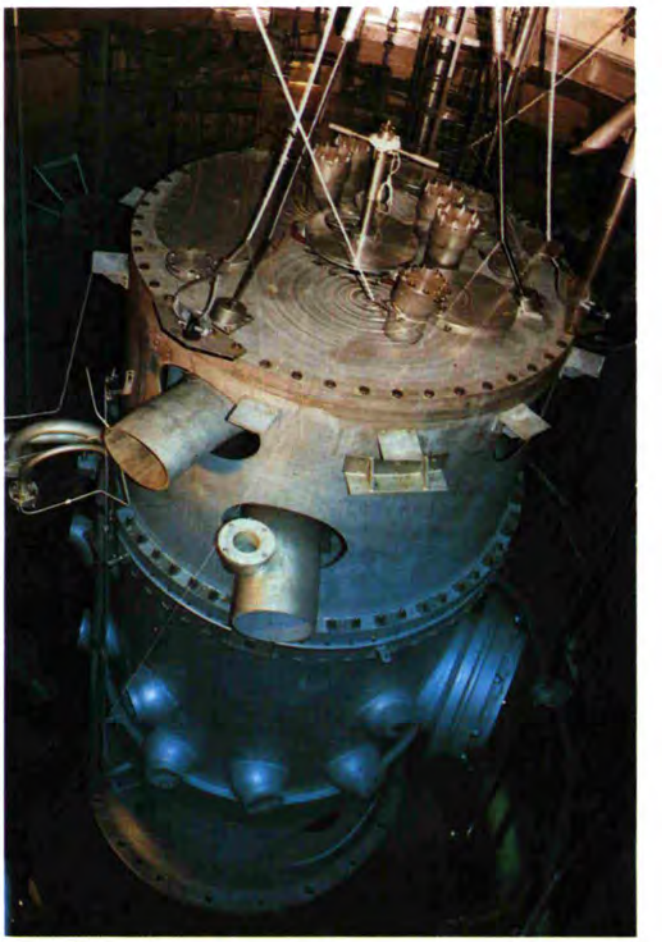
Removal and cutting of the rear part of a liner.

Removal of the H1-H2 coupling sleeve.

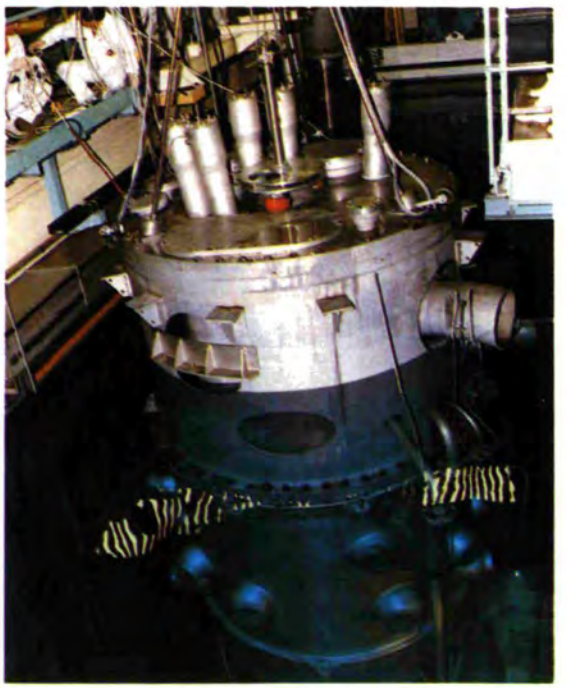
Cutting the H1-H2 beam-tube coupling sleeve in the swimming pool.



Positioning in the HFR storage pool of the turn-table for cutting the reactor vessel.



Dismantling of the reactor vessel and upper structure assembly in the swimming pool.

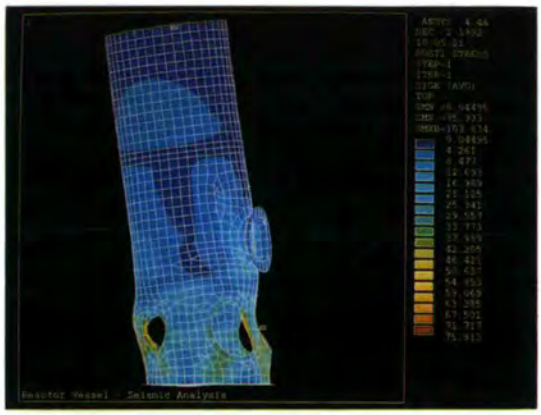


Positioning on the turn-table in the storage pool of the reactor vessel and upper structure assembly.

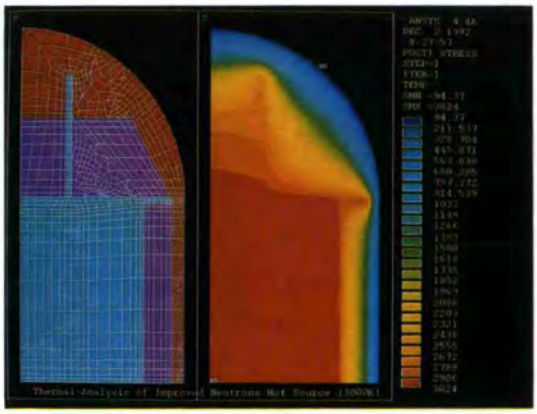
The empty swimming pool of the HFR (December 1992).

Some examples of the finite-element analysis carried out by the mechanical engineering group of the D.I.M.

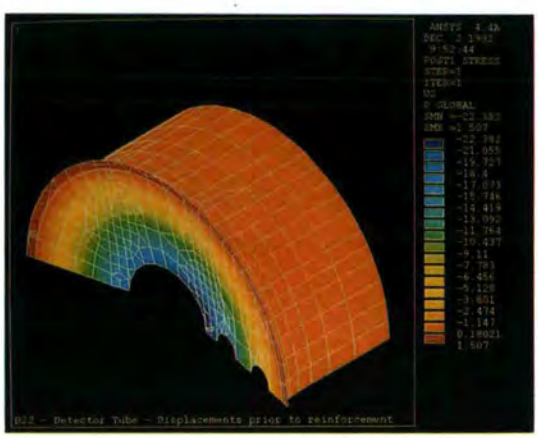
(The models shown in photos 2 to 6 represent the "asymmetric units" of the structures in question).



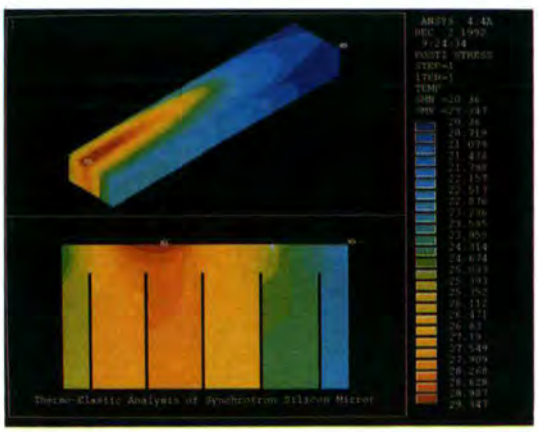
(1) Results of a static analysis of the D22 vacuum vessel - these calculated displacements were confirmed by physical measurements.



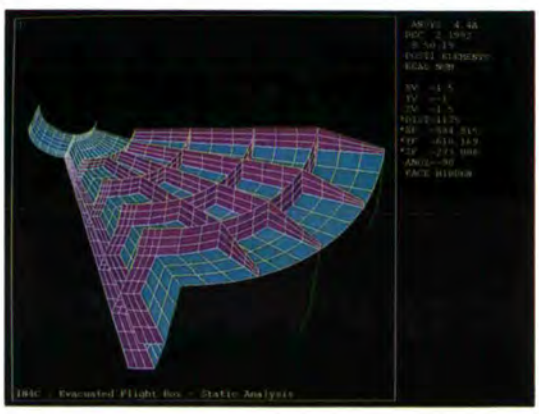
(2) F.E. model and results of a non-linear thermal analysis of a possible higher temperature hot-source.



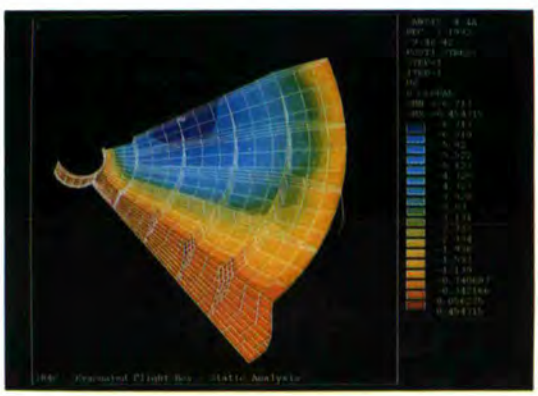
(3) Results of a seismic analysis of the reactor vessel, showing the stress distribution and the mode-shape for the first natural frequency.



(4) Results of a thermo-elastic analysis of a synchrotron mirror, showing the temperature distribution (work subcontracted for the ESRF).



(5) Finite element model of the evacuated flight box for the new TOF spectrometer IN4C (a snapshot of the work in progress on the optimisation of this component).



(6) Displacement distribution of the IN4C flight box (vertical direction) - showing that further reinforcement is necessary.

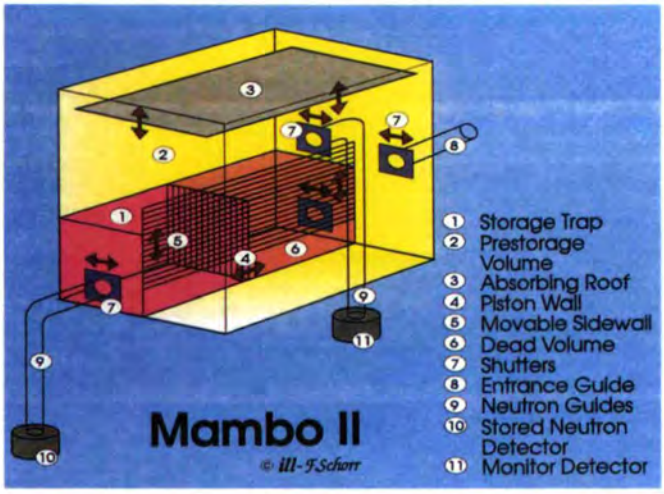
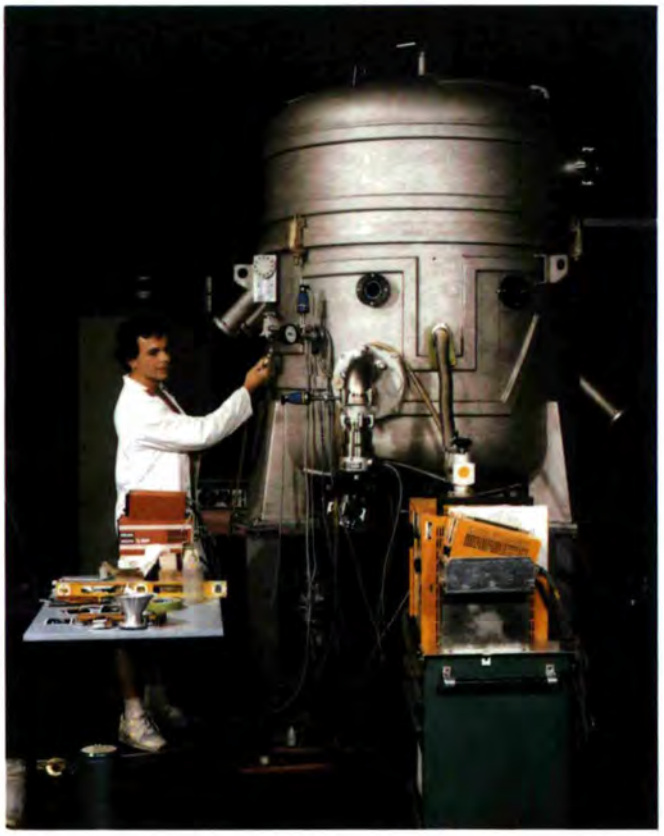
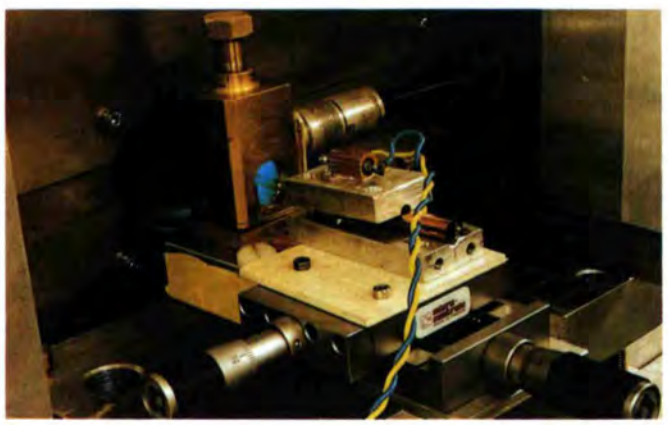


Fig. 3: The principle of the Mambo II experiment (see report page 127).

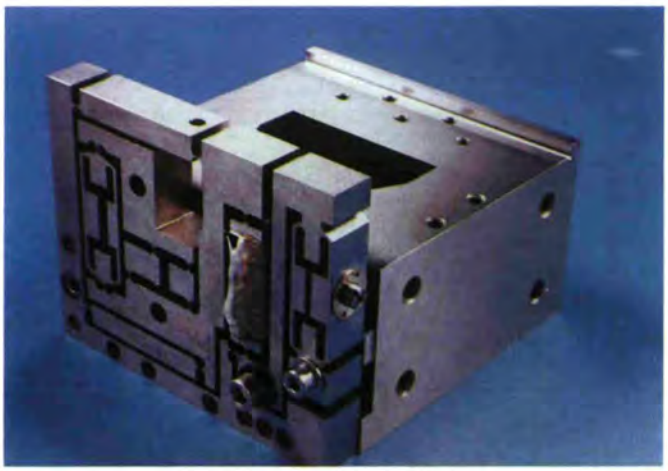


The vacuum vessel housing the Mambo II equipment (see report page 126).



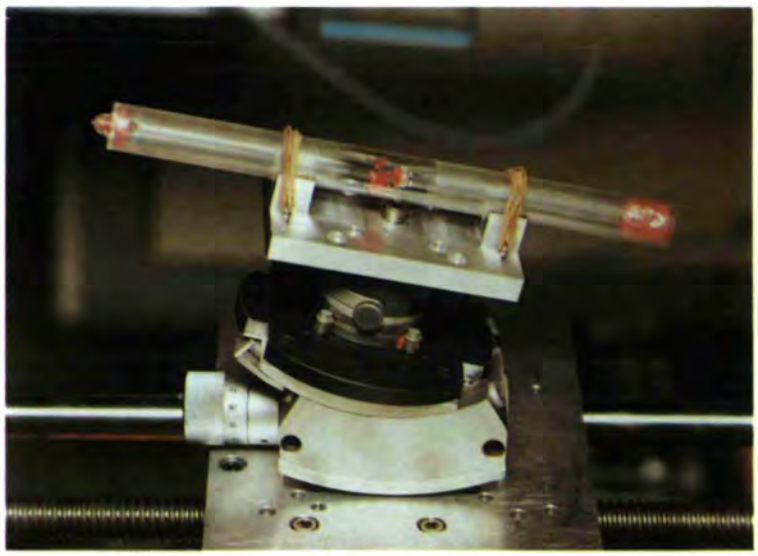
The microwave excited mercury discharge lamp, which generates the 204Hg ultra-violet resonance radiation used to monitor the orientation of 199Hg nuclei in a cell which is about 1 m away inside the magnetic shield and vacuum system of the neutron EDM experiment.

The new multidetector for the high flux diffractometer D20 (see report on page 124).

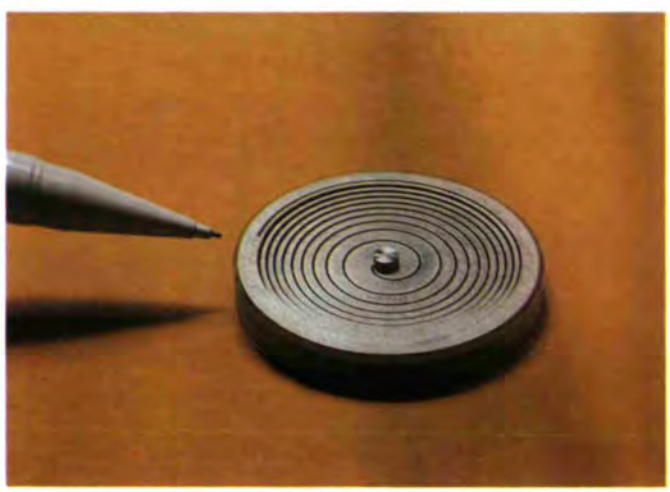


The gamma ray spectrometers GAMS1 and GAMS2/3 use germanium crystals which act as diffraction gratings to provide high resolution with respect to wavelength. To adapt efficiently to the angular divergence of the arriving gamma ray beam, each 6 cm long plate of single crystal must be bent slightly into a circular arc. Shown here is a mounting used to bend a crystal with high precision. The elaborate cutting of the end plate provides a graded system of mechanical levers used to push on one end of the crystal.

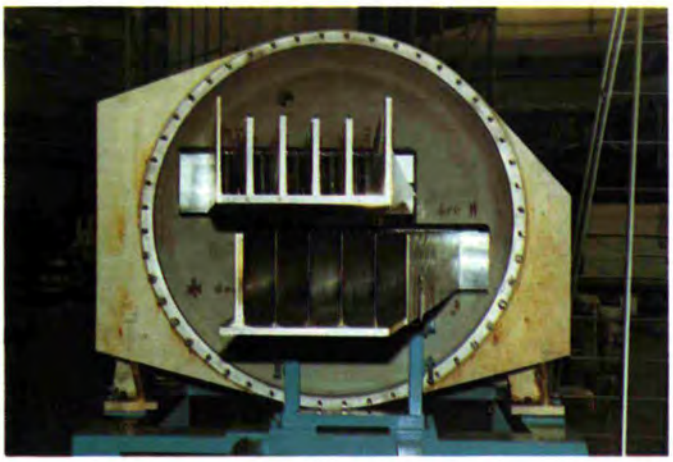
Automation of the dilution refrigerator inserts
(see report on page 104).



A HgI_2 crystal grown from the vapour phase in microgravity is mounted in the γ–diffractometer
(see report on page 136).



Double-spiral correction coil to be used on IN20 TASSE as part of the design of the new superconducting OFS precession coils (see report "Instrument Groups", 3-axis spectrometers).



In-pile part of the H1-H2 neutron guides. View of the support structures after the dismantling of the glass elements.

The detector of D22.

Extraction of the support structure for the cold guides H1 from the housing.

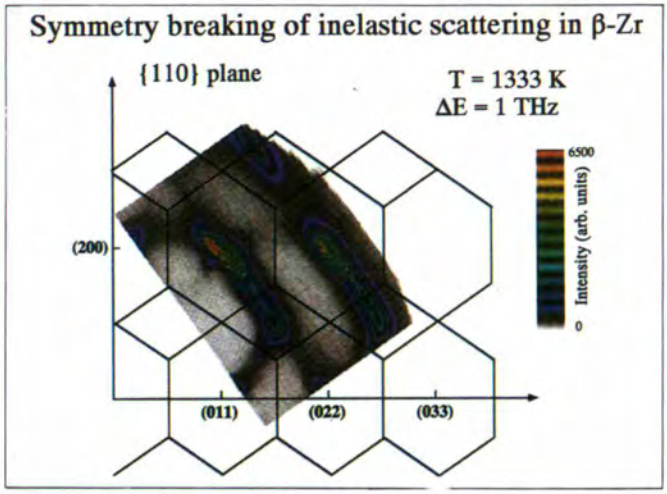


Fig. 1, Coll. 4: Isointensity plot of the dispersion surface at 1 TH_z in the (110) plane of β-Zr at 1333 K. The Brillouin zone boundaries are shown as solid lines.

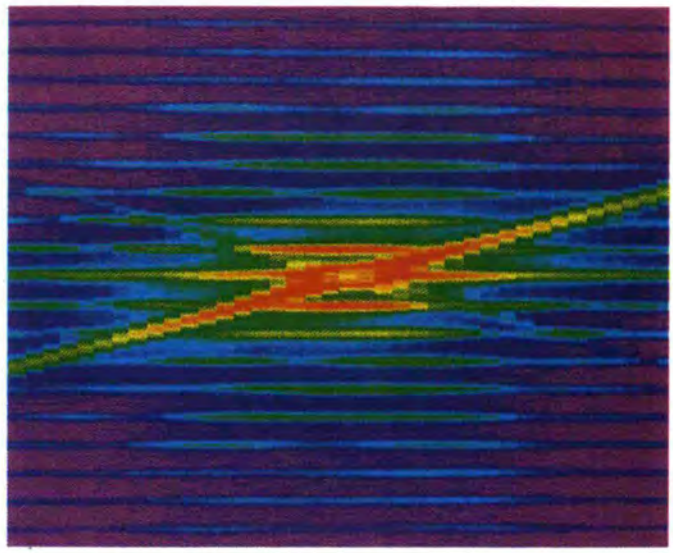


Fig. 7, Coll 5: Counter plot of the reciprocal space mapping of a InP surface grating in the vicinity of (002)InP.

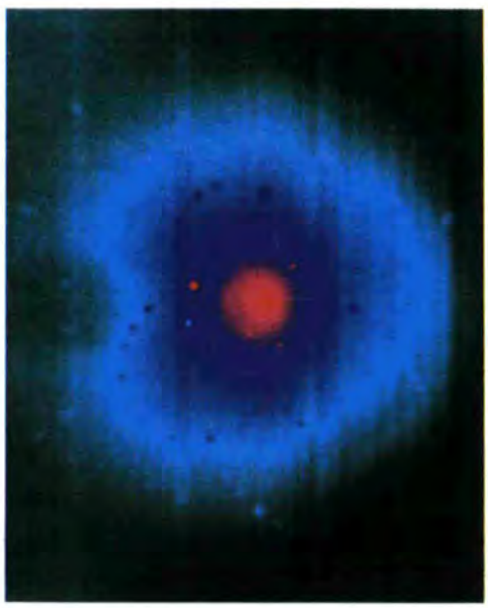


Fig. 2, Coll 8: Laue picture of a large crystal of triclinic hen egg-white lysozyme observed with cold neutrons at the radiology beam line of the Orphee reactor. Regions of higher intensity are coloured red. The recording device was an X-ray imaging plate equipped with a gadolinium oxide converter screen (collaboration involving staff from EMBL, ILL, LLB and CEN Saclay).

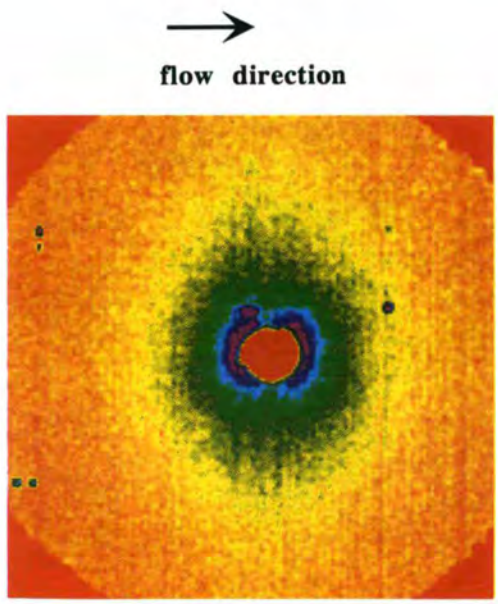


Fig. 3, Coll 9b. Interpolated colour image (raw data) of a sheared semidilute polymer solution as measured at PAXY/LLB with the ILL couette type shear apparatus.

Introduction

The dismantling of the instruments and of the experimental sites in the reactor hall which had started in October 1991, was finished at the end of February 1992 under the coordination of the Department EDEX. We have started to prepare the programme for the reinstallation of this equipment in 1994. The basic idea is to restart and test all the instruments in the two neutron guide halls by the end of 1993, in order to have all the remaining technical staff available for the immense amount of work in the reactor hall in 1994. We foresee difficulties in the execution of our programme due to the loss of experienced personnel.

During the year 1992 the total number of staff in the Department was reduced by more than 35 %. This was achieved by detachment of personnel to other sectors in the ILL and to outside companies as well as staff leaving the Institut definitively. The work of the remaining staff was concentrated on the following actions:

▲ Maintenance of site and buildings.
The staff of the Maintenance Service took on most of the maintenance work which is normally subcontracted to outside companies in order to make economies.

▲ Some development work on our instruments (small improvements).

▲ Work on the replacement of all beam shutters of the ILL instruments.

▲ Development work for external institutes in the domain of sample environment (6 furnaces, 2 transuranium sample inserts, etc.).

▲ Technical support on experiments performed at other neutron sources.

▲ Preparation of posters describing the ILL instruments.

Special Cryogenics Service

The activity of this service has been oriented in two directions:

▲ Loan of specialised equipment, including the corresponding technical assistance for experiments (LLB, ISIS, RISØ, HMI, CENG).
The main long term loans are: 3 cryomagnets, 1 dilution refrigerator, 20 temperature controllers and several 'Orange' cryostats.

▲ Developments
Previously started developments have been continued:

❍ The automation of the dilution refrigerator have been finished (see photo on page 100).

❍ The final setting-up of a gravity insensitive dilution refrigerator for use on a Eulerian cradle has been completed. Temperatures down to 65 mK have been reached.

❍ The construction of the 5 mK dilution refrigerator in collaboration with the CRTB (CNRS, Grenoble) has been continued. First tests have been done.

❍ The development of the new sample environment controller ILLSEC has been pursued energetically.
The order for the delivery of two prototypes has been placed. Tests on these are planned in 1993. A first batch of 20 new controllers will be available in 1994 for the start up of the instruments.

The following projects have been started:

❍ The study and design of a special He cryostat for neutron polarization analysis (Cryopad 2). The order for the main parts has been placed.

❍ A feasibility study of a special cryomagnet for neutron polarization via the Zeeman effect has been carried out: a horizontal magnetic field of 7 Tesla in a room temperature bore of 46 mm diameter can be obtained at relatively low cost. The order has been placed.

❍ A design study of a ^{3}He purifier has been made to allow the purification and recycling of large amounts of ^{3}He used in neutron multidetectors.

Central Service

The Central Service is responsible for the general organisation and maintenance of the experimental halls, assistance for the running of instruments and provision of sample environment between 1.2 K and 2000 K and at high pressures. The staff of this service has been temporarily reduced by about 50 %. The major work carried out in 1992 includes:

▲ Dismantling of instruments.

▲ Participation in the modernisation of all beam shutters.

▲ Preparation and surveillance of two risk experiments at the ILL without neutrons (Curium on PN1 and Lutetium on PF2).

▲ Video recording of all major technical events (instrument and reactor dismantling).

▲ Maintenance and improvements of sample environment equipment.

▲ Work for external institutes (see introduction).

▲ Test rig for pressurizing a 12 kbar clamp in situ in an 'Orange' cryostat.

▲ Technical assistance in high pressure experiments with ILL equipment at PSI (Würenlingen).

Building Maintenance and Modifications Service

The essential activities of the Service are maintenance, repairs, improvements and construction, renovation, modifications and equipment of site buildings, technical installations (except the reactor), instruments (shielding) and zones around instruments.

The major difficulties encountered by the Service result from the budget and staff reductions, which no longer allow necessary repairs, and requests for work, to be carried out as quickly as previously.

In 1992 the Service was mainly involved in:

▲ Completion of the dismantling of the experimental sites in the reactor hall.

▲ The installation of the new site entrance guard house and the ILL/ESRF Joint Medical Service building.

▲ Completion of installation work in the second guide hall ILL22.

Outlook

The new management structure of the ILL will be implemented in the middle of 1993. The EDEX Department will be divided into three different sections. Before this happens I would like to take the opportunity to thank all the members of my department for their excellent work and for the collaborative spirit which was always present. It was a pleasure for me to work with this cooperative team and I am convinced that the EDEX members will be at least as efficient in the new organisation as they were in the old one.

Nuclear and fundamental physics

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

PN3 Two curved crystal spectrometers GAMS1, 2/3 and one flat crystal spectrometer GAMS4 on the through beam tube H6-H7 (S. Ulbig, H. Boerner, A. Williams, R. Oliver)

PN4 Ge (Li) pair spectrometer on beam tube H7 (A. Williams, U. Mayerhofer)

PF1 Former PN7 - cold polarized beam at the end position of guide H142 (J. Last, U. Mayerhofer, H. Just)

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

PN1 Fission product separator

The project to provide energy focussing in the ion optics of the LOHENGRIN mass separator has reached its most active phase. When completed it will increase significantly the ion collection efficiency and reduce the background. The principal new element is a reverse energy dispersion (RED) magnet which weighs 6 tons and which was delivered at the end of 1991. Modification of the focal plane region of LOHENGRIN is nearly complete. Changes have been made to the roof and to the walls of the casemate and $5m^2$ of marble floor have been laid so that the magnet position can be adjusted using air pads. A new magnet vacuum chamber was designed and completed in June and the support frame for the magnet is expected at the end of 1992.

Following the installation of the power supply unit, including its connection to a PC-compatible computer for remote operation, the RED-magnet has been tested on PN1 using α-particles from a ^{241}Am radioactive source, assumed to be monochromatic with an energy of 5.479 MeV. To simulate the energy dispersion found along the LOHENGRIN parabola, the α-particles were injected at three different positions along the magnet face, and different values of the magnetic field strength were set according to the position. The positions corresponded to the highest, the average, and the lowest energy points of the parabola. The α-particles were detected using a 5 x 1 cm^2 position sensitive silicon detector. For each of the three injection positions, measurements were made with the detector at several different distances from the exit face of the magnet covering a range of 6 cm around the calculated focus. The experiments were repeated with several alternative collimators for the α-particle source giving angular half-widths ranging from 0.37 to 0.91 degrees. The results obtained for an input beam collimation of 0.81 degrees are displayed in Fig.1 where the error bars correspond to the half-widths of the beams. The focal distance and the total lateral width are both in agreement with calculations. In order to check the influence on mass resolution which involves the direction perpendicular to the plane of Fig.1, the detector was rotated through 90 degrees. In this case only the beam collimation of 0.36 degrees was used, and the results shown in Fig.2 confirm the prediction of a constant image width over more than 10 centimetres.

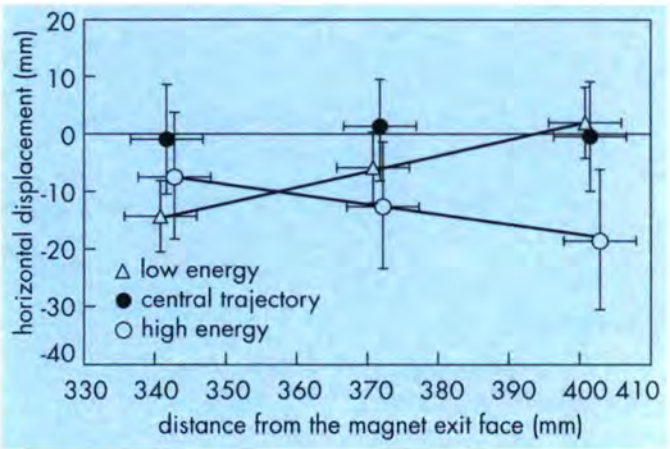


Fig. 1: Measured trajectories at the focus of the LOHENGRIN mass separator when using the new magnet for energy focussing. These results were obtained in a simulation with an alpha particle source collimated to 0.81 degrees. Without the energy focussing, these trajectories would have been spread over a width of 40 cm. In addition the new system will reduce the flux of background particles arriving at the focus.

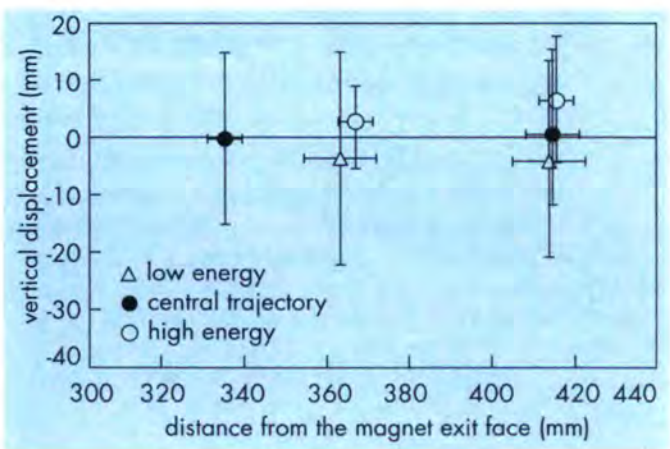


Fig. 2: Trajectory displacements in the vertical, mass resolving direction for LOHENGRIN with the new energy focussing in operation. The measurements were made in a simulation using an alpha particle source collimated to 0.36 degrees. These results confirm the prediction of a constant image width over a distance of more than 10 cm in the vicinity of the focus.

The new ionisation chamber

To exploit the energy focussing capability, it has also been necessary to develop a new detection system. According to Liouville's theorem the phase space occupied by a beam of particles will be conserved when they are passing at constant energy through a well behaved ion optical system. Thus, the reduction in area of the focal image will be accompanied by an increase in the divergence, with the angles of the trajectories at the focus now reaching as much as +17 or -11 degrees. This divergence spoils the charge resolving power of the detector unless the angles can be allowed for.

An ionisation chamber has been developed (see Fig. 3) which possesses both ΔE and E_R sections to provide charge resolution for fission fragments. A new method based on the time delay ΔT for the electron signals from the two parts of the anode has proved to be suitable for the measurement of the angle of the incoming particle. The system has been tested with an α-particle source and the behaviour over a range of values of electric field strength and pressure has been investigated. In Fig. 4 the correlation is shown between the angle of the trajectory θ and the measured ΔT between the signals ΔE and E_R. The plots are labelled with the ratio of the electric field strenght to pressure,E/p. They show that there is an approximately linear relation between ΔT and the angle θ which obtains for the wide range of E/p values which may be used. With α-particles, the resolution in angle reached about ±1.5 degrees, which is largely sufficient for the requirements .

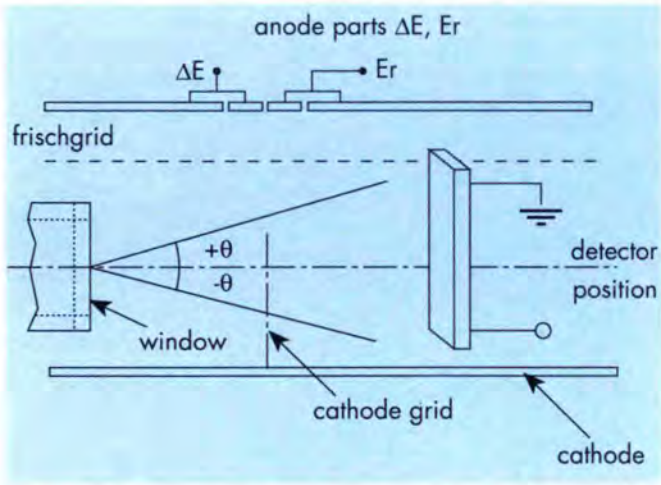


Fig. 3: The new ionisation chamber for PN1 in the test configuration used to investigate its resolution for particle trajectory angle. The angles were measured independantly using a position sensitive silicon detector and the results were correlated with the time delays ΔT between the electron signals from the ΔE and E_R parts of the anode.

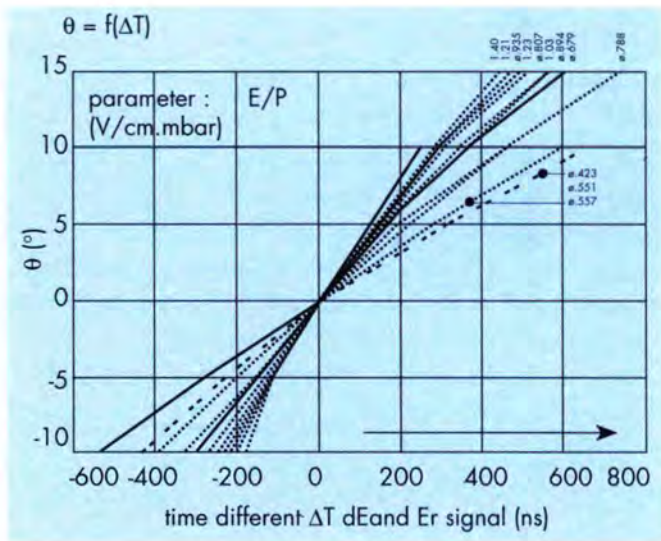


Fig. 4: Plots of the trajectory angle θ as a function of the time delays ΔT between signals from the two parts of the anode in the new ionisation chamber for PN1. The plots are labelled by the various ratios of the electric field to pressure, E/p, which were used inside the chamber.

PN3,4 Gamma ray spectrometers

The upgrade of the GAMS spectrometers has begun with the rebuilding of the interferometers of GAMS2/3 as a Munich-ILL collaboration.

For the interferometers giving control of the angle of the crystals, a design was chosen which is based on a newly developed and tested approach. Laser beams are split and reflected from two arms on opposite sides of the pivot and brought together to interfere with each other as shown in figure 5. A measure of the angle about the pivot is provided by the path difference in the two arms. Ultimately, the phase representing a tiny fraction of an interference fringe must be resolved. A two frequency laser with orthogonal planes of polarization in the two beams is used. Both arms of the interferometer are fed with light of both polarizations so that there are two sets of interference fringes, one for each polarisation. Comparison of the two intensities at a special detector allows the phase difference between the arms to be determined free of errors due to laser amplitude variations. Signals representing deviations from a chosen reference phase are fed back to control the angular position using piezoelectric crystals.

The support frame of the instrument has been modified to increase its stiffness and resistance to relative rotation of the upper and lower crystal interferometers as a whole. In order to give better vibrational damping, the entire instrument is now suspended on three chains to minimise coupling to ground vibrations. For the data aquisition and control of the spectrometer, new hardware and software is being developed with the aim of being compatible with the other GAMS spectrometers. By the end of the year it is envisaged that the assembly of the instrument will have been completed so that testing can be carried out in 1993.

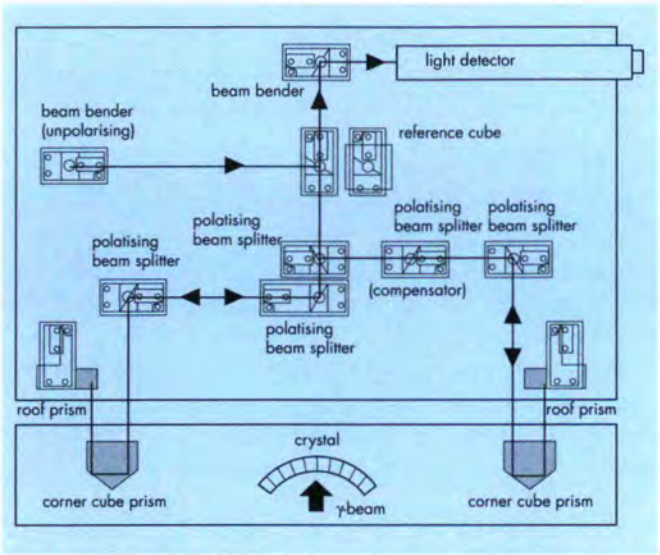


Fig. 5: The new interferometer arrangement being installed to control the angles of the crystals in the GAMS2 gamma ray spectrometer.

A test version, GAMS5T, of interferometers forseen for a new two axis bent crystal spectrometer, has now been designed in a Munich-ILL collaboration financed by the BMFT. It is based on the use of glass ceramics for key interferometer parts exploiting the very low thermal expansion coefficients of these materials. Assembly and testing is scheduled for the first half of 1993. A new generation of high precision crystal benders for the new spectrometer have been designed and built (Goettingen-ILL collaboration). These are due to be tested in 1993 at NIST, USA. The crystals to be used are currently being shaped in collaboration with the ESRF.

PF1 (PN7) cold polarized beam facility

A refurbishment of the polarizer system is being carried out in preparation for the reactor restart. Part of the old support structure for the supermirror polarizer has been replaced by a stepping motor controlled table which allows for computer controlled fine tuning of the polarizer angle around a vertical axis. An identical system has been aquired for the analyser mirror. Since a change in the angle of the polarizer leads to a change in the outgoing polarised beam direction, the analyser system will have to be mounted on a further table which allows it to be displaced horizontally.

Two new supermirror polarizers for PF1 have been built by O. Schaerpf, I. Anderson and W. Graf. These have a multilayer coating on both faces of each glass sheet which increases both the neutron transmission and the polarization. It is planned to test the polarizers in HMI shortly.

The planning and pricing of a new building to house the PF1 facility, in place of the temporary shelter in which it has existed for some years, has been finalised in 1992. The support of the EDEX team who did this work is much appreciated.

A significant effort has been devoted to a theoretical study of a neutron focussing device which could be used with the new guide NG13 which is planned for this facility. The original idea was to use two symmetric stacks of concentrically bent glass plates whose length increases as a function of the distance from the central axis as shown in Fig. 6. Neutrons would be guided through the narrow channels between the supermirror coated plates. As shown

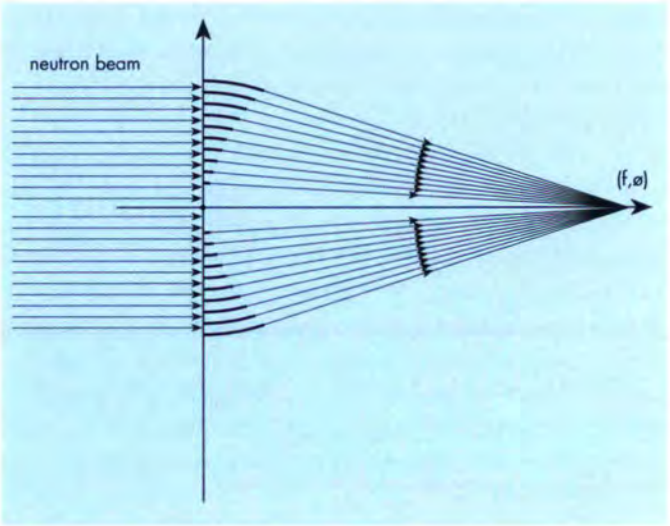


Fig. 6: A schematic view of a neutron focussing element using curved channels between two stacks of appropriately bent and cut glass plates.

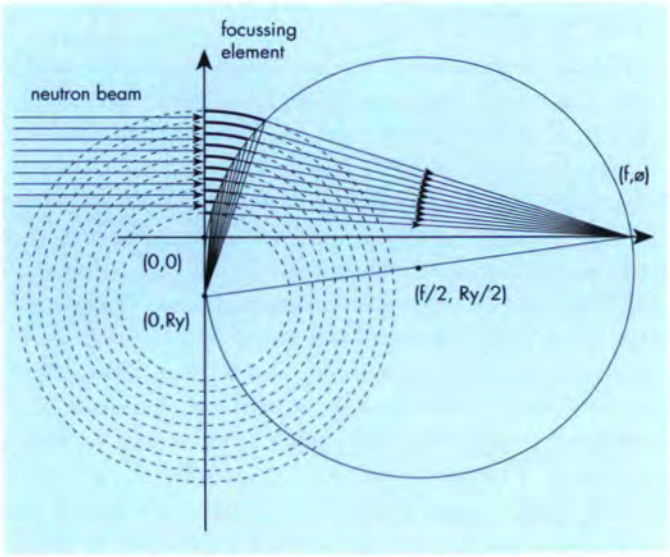


Fig. 7: The cut-off line for the glass plates of a focussing element is a Thales circle with the radius and the position of the centre depending on the focul length and bending radius.

in Fig. 7 the cut-off function of the glass stack is a Thales circle whose centre and radius are functions only of the radius of curvature for the stack R_y and the focal length f. A typical value for R_y is 30 m at a focal length of 2.5 m. Although detailed Monte-Carlo studies of such a device show that concentration factors up to one order of magnitude can be achieved (Fig. 8), the practical realisation of such a glass lens hardly seems possible because of serious mechanical problems. The latter come mainly from the requirements for the precise mounting of the more than 1 m long 0.2 mm thick glass strips and the sensitivity to surface waviness.

These problems could be overcome if, instead of glass plates, stacks of thin silicon wafers with supermirror coatings were used. In this case, the neutrons would be guided internally through the silicon bulk material. Because the channels can then be much narrower, a silicon lens could be made as short as 10 cm using a radius of curvature of the order of 2 m. A major disadvantage is the reduction in transmission due to neutron scattering in the silicon. Taking into account results from transmission measurements by Magerl et al. , calculations show that concentration factors in the range of 3 to 5 are possible. Further studies will therefore pursue the silicon version.

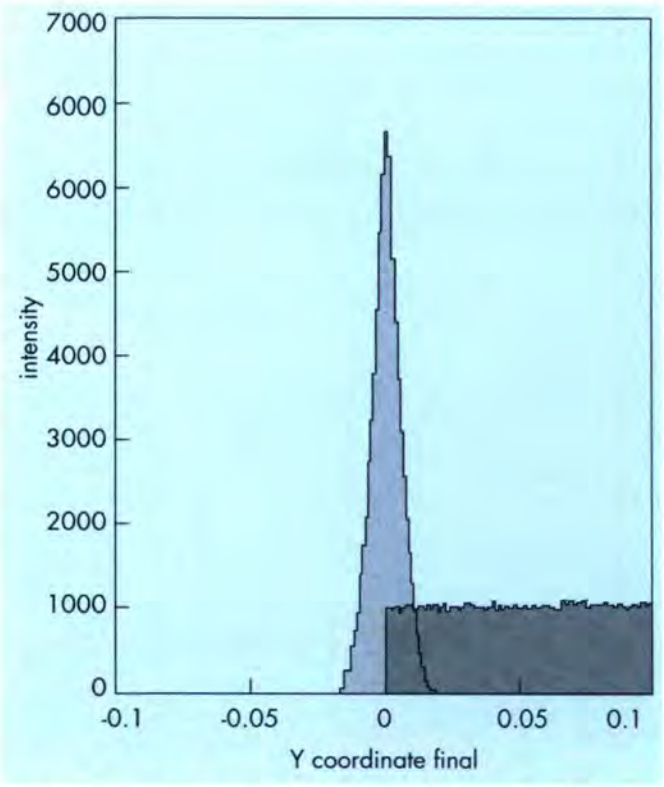


Fig. 8: Results of a Monte-carlo simulation for the upper half of a glass plates focussing element as shown in Fig. 6. The original beam is homogenious and extends from Y = 0 to Y = 0.1 m. The peaked distribution centred on Y = 0 is the neutron intensity at f = 2.5 m for the case where the radius of curvature R_y = 30 m. For a beam of large vertical extent, such as that from the projected NG 13 guide, the lower half of the focussing device would also contribute to the peak thereby doubling its intensity.

The BILL magnet at PF1

The second magnet of the BILL spectrometer was moved, from its position as part of what was the PN2 instrument on level D, to the site of the PF1 (PN7) facility. It was decided that we should use this opportunity to carry out an experiment of great topical interest, the search for a heavy (17 keV) neutrino as a component of beta decay. An experiment of this kind, carried out at PN2 two years ago, had been limited by the high background level associated with the use of an inpile target. It was estimated that a better experiment could be achieved by placing the spectrometer well away from the reactor and using a source transported to the spectrometer after being produced by neutron activation in the neighbouring reactor SILOE (CENG). At the same time, the experiment has provided some experience of using the spectrometer in a situation which is similar to that which would exist if it was used to analyse electron spectra from in-beam neutron capture sources at PF1.

To run the spectrometer in this way, a source chamber suitable for radioactive sources has been designed, built and installed as a T.U. Munich-ILL collaboration. The chamber is suitable for the 100 mCi ^{176}Lu source needed for the heavy neutrino search and the relevant procedures have been agreed with the Radioprotection Service. Spectra have now been obtained from two sources and the programme of measurements will continue into 1993. The resolution of the spectrometer, consisting now of only the second magnet, has been found to be comparable with that of the previous two magnet arrangement.

PF2 ultra-cold neutron facility on level D

The work on the reactor has resulted in the temporary displacement of the vertical cold source and of the straight vertical neutron guide and the curved neutron guide which lead neutrons from the cold source to the UCN turbine. It has been possible to profit from this situation to put in hand the refurbishment of the vertical neutron guide by ILL staff, and of the curved guide, by ILL staff in collaboration with the original fabricators T.U. Munich. On the output side of the turbine, the electronics for the UCN distribution switching which had developed serious faults, is being replaced by a system conforming to ILL standards.

Concerning experiments at PF2, the diffractometer and the long-wavelength interferometer have been taken away to be worked on in the institutions from which they came. For the neutron electric dipole experiment, the magnetometer development program has been continued on level D without interruption.

M. Pendlebury

Three-Axis Spectrometers

IN1, IN1B 3-axis and Be-filter spectrometer on the hot source beam tube H8 (H.J. Lauter, B. Dorner and P. Palleau).

IN8 3-axis spectrometer on the thermal beam-tube H10 (J.L. Martinez, J. Bossy and T. Hornsby).

IN12 3-axis spectrometer on the cold guide H142 (S. Bramwell, B. Fåk, and D. Puschner).

IN14 3-axis spectrometer on the cold guide H53 on the horizontal cold source (R. Currat and A. Brochier).

IN20 3-axis spectrometer for neutron polarization analysis and spin-echo option on the thermal beam-tube H13 (M. Alba, J. Kulda, C.M.E. Zeyen and A. Dorn).

The state of the instruments at the end of the year is as follows:

1) IN1, IN8 and IN20 have been disassembled in connection with the current operations on the reactor beam tubes. The instruments IN1 and IN20 are stored near their respective sites in the reactor hall while parts of IN8 have been transported into the new guide hall.

2) IN14 (on the horizontal cold source), IN3 and IN12 (in the guide hall) are not affected by the reactor refurbishment programme.

The reassembly work is due to begin in the spring of 1994 after the new beam tubes are installed.

A limited instrument development programme was maintained during 1992 and will be pursued into next year. So far it has involved the replacement of the shaft encoders and related electronics, on IN1 and IN8, a step motivated by maintenance difficulties on the existing electronics.

A modification of the IN14 monochromatic beam geometry is presently under study. The aim is to reduce the monochromator-to-sample distance by integrating part of the beam equipment (beam shutter and Soller collimator) in the primary protection. Also planned for next year is the installation on IN8 of a horizontally curved graphite analyser together with a vertical-axis counter.

Under the proposed ILL "Unix plan", it is planned to replace the PDP11 instrument computers by Unix workstations. The type of workstation to be installed is the subject of current consultations. The new control system will be implemented on IN1 and IN8 for the reactor start-up, and on IN14 at a later stage.

No upgrading work, other than required by operational safety, is envisaged on IN12: as a consequence of the recent decision to reduce the number of scheduled ILL instruments from 30 to 25, IN12 has been put on the list of proposed CRG instruments, which already includes the thermal guide spectrometer IN3. As a cold-neutron 3-axis spectrometer, IN12 is second only to IN14, in terms of flux (only down by 30 % at $E_0 = 2$ meV). The instrument also offers a uniquely uncontaminated monochromatic beam in the energy range $6 < E_0 < 10$ meV, when higher-order neutrons are suppressed by the cut-off of the s-curved H142 guide. The instrument is equipped with a supermirror bender and a Heusler (111) analyser and is fully operational as a polarised-beam spectrometer.

The Larmor precession magnets for the neutron spin-echo option to be implemented on IN20 (TASSE) are under development.

For thermal neutron spin echo, line integrals of the order of 1 Tesla x Meter (10^6 Amperes) are required. For reasonable magnet lengths, even OFS (Optimal Field Shape, Zeyen 1988) magnets of field lengths L of 1 to 1.5 m have relative residual radial and path length inhomogeneities of the order of 10^{-4}. Further line integral corrections are obtained by introducing suitable current distributions in the beam. The best corrections are obtained for an OFS coil with a set of two spirals (second order spirals with small quadratic contribution) placed at particular axial distances z_c from the coil middle. The optimal positions can be calculated analytically, for OFS one finds $z_c = 0.37L$ (for solenoids a slightly larger value). The figure (photo) shows a recently developed double Aluminium spiral, spark-erosion cut from a massive plate, which could also be a single crystal if SANS has to be avoided. The usable beam diameter is 35 mm and the cutting gap is 0.2 mm. Two spirals are connected electrically in the centre (screw), and slightly held apart at the circumference to assure electrical insulation of the windings, better cooling and mechanical stability in a magnetic field (the slight deformation of the spiral is taken into account in the shaping). The minimum conductor cross-section is $1mm^2$ and the maximum current is 5 Amperes. This gives a total maximum correction of 200 Amperes, or 2×10^{-4} Tesla x Meter, enough to correct the superconducting OFS coils for the IN20 TASSE option. Thicker or larger coils are feasible by the same technique. Larger corrections can also be obtained by using more coils, the neutron absorption being negligible.

Coordinator: R. Currat

Ref. Zeyen C.M.E. and al, Optimal Larmor precession Magnets, IEEE Transactions on Magnetics 24, pp 1540-1543 (1988).

Time-of-Flight, High Resolution and Diffuse Scattering

Due to the tight budget situation, it was possible to do active work only on some instruments. This is why this year presentation has been changed, and a report is given only for those instruments where a sizeable investment was realized.

IN4C Thermal TOF project with Brillouin option on the thermal tube H12 (H. Mutka)

IN10A/B Backscattering spectrometer on the cold guide H15 (J. Cook, P. Joubert (technicien))

IN11 Neutron Spin-Echo on the cold guide H41 (B. Farago, J.F. Legrand, E. Thaveron (technicien))

IN15 High resolution spin-echo spectrometer for long wavelengths on the cold guide H511 (C. Lartigue, F. Douchin, J.F. Barthelemy (technicien))

IN16 New backscattering spectrometer on the cold guide H53 (formerly IN10C) (B. Frick, R. Rebesco (technicien))

D7 Diffuse scattering instrument with polarization analysis on cold guide H15 (O. Schärpf, R. Rebesco (technician))

D11 Small-angle scattering diffractometer on the cold guide H15 (P. Lindner, P. Timmins, R. May, R. Baker (technician))

D17 Low-Q, low-resolution diffractometer on the cold guide H17 (R. May, P. Terech, M. Cruz (technician), R. Gay (technician)

D22 New low-Q diffractometer on the cold guide H512 (project) (R. May, M. Thomas, R. Gay (technician))

Group Engineer : F. Douchin

IN4C Thermal TOF project with Brillouin option on the thermal tube H12

A decisive momentum to the project has been given through the association of an Italian partner (coordinator F. Sacchetti, Perugia) whose contribution to the spectrometer will be of great importance. The firm engagement on their side has been demonstrated by the purchase of pyrolytic graphite crystals that will cover one face of the double curvature monochromator. These crystals have already been tested in Italy. Meanwhile, growth of copper single crystals is in progress at the ILL monochromator group.

The persisting progress in the design of the instrument has been assured by the efforts of the project office. The elements of the primary spectrometer, including the choppers with their mountings and the monochromator assembly, have found their positions inside the necessary shielding. The dimensions and material of protections have been defined and fabrication will be finished before end of 1993. (See fig. 1).

The detector group of the ILL has constructed and tested a prototype of a small-angle detector with three sectors of 45 degrees and six radial cells. The basic concept proved to be sound and a final design consisting of 96 elements (8 sectors, 12 radial cells) is underway. This detector will equip the small angle region of the vacuum flightpath whose detailed design is a major part to finish.

In parallel with the main design, the small-angle inelastic instrument, Brillouin spectrometer, has been laid out. The operational capacities of this instrument have been evaluated in detail (H. Mutka, J. Mol. Struct., to be published, Proceedings of the EPS conference on Neutron Scattering from Liquids), and a future accommodation will provide unique means for investigating long wavelength excitations in various systems, such as fluids and magnetic materials.

IN10A/B Backscattering spectrometer on the cold guide H15

The programme of modernization of the IN10 electronics, proposed last year, is under way. Currently, 4 motor axes have been equipped with the "Synchro" or "Moore-Reed" type coders which are compatible with the new "NIM" motor-control/coder reading units. It is envisaged that the movements which are essential for the operation of IN10B will be completed in the first half of 1993. The construction of the "high-temperature" IN10B monochromator cryofurnace prototype is virtually complete. The only task that remains is the welding of the niobium heat exchanger to the stainless steel sample well. This has been referred to a specialist company. A mechanism for fast exchange of the Doppler drive (IN10A) and the IN10B cryofurnace is currently being studied.

A new and cheaply implemented monochromator option is currently being researched. This involves the ultrasonic excitation of a monochromator via a piezoelectric transducer. Following promising initial measurements on IN10 with a $LiNbO_3$ transducer [1], it has been shown that a resonant ultrasonic wave creates a strain field in which the lattice spacing is modulated (in space and time) according to the form of the ultrasonic standing wave. It has been demonstrated that, by varying the exciting amplitude for elastic crystal deformations, the resulting energy resolution of the reflected neutron beam is a linear function of the ultrasonic strain. By using this technique, a continuously tunable energy resolution - intensity can be achieved (fig. 2). Work is currently under way to compare the performance of $LiNbO_3$ and quartz transducers. Indium foils are being investigated as a possible bonding-coupling medium between the silicon and the transducer.

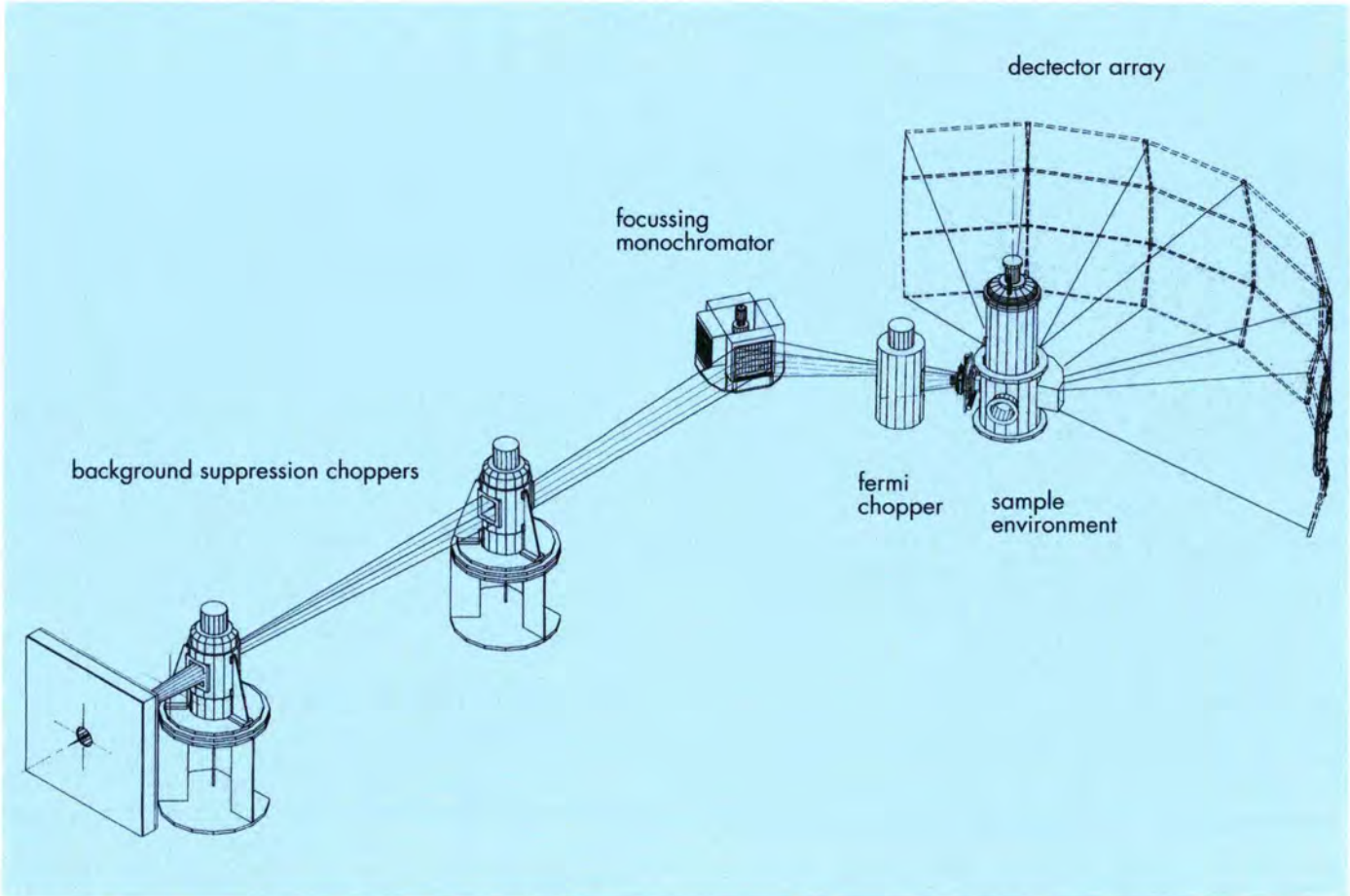


Fig. 1: The main elements of the IN4C thermal time-of-flight spectrometer along the beam path are the background choppers, the double curvable multi-face monochromator, the Fermi chopper, sample environment and the secondary flight path with the detectors.

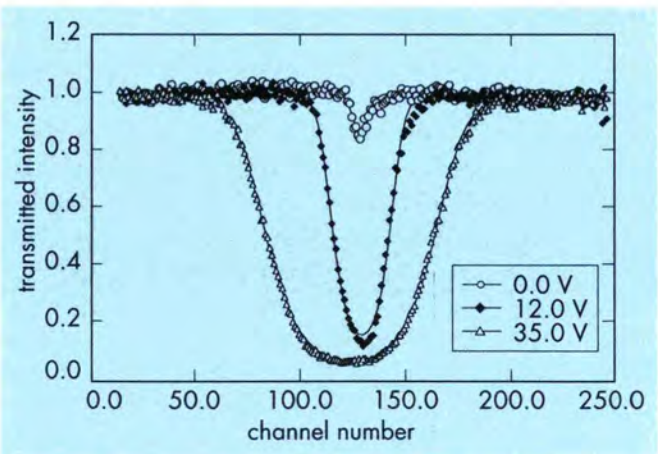


Fig. 2: The normalized transmission curves measured on a silicon crystal of thickness D = 9.933 mm vibrating at a frequency of f = 2.37 MHz fitted by the mosaic crystal profile (solid line); the curves correspond to transducer voltages of 0 V, 12.0 V and 35.0 V.

[1] Hock R., Vogt T., Kulda J., Mursic Z., Fuess H. and Magerl A., Z. für Physik B: Condensed Matter (to be published).

IN11 Neutron spin-echo on the cold guide H41

We are trying to profit from the shutdown of the reactor to bring some improvements to IN11 within the tight budget situation of the ILL.

The largest investment will be the change of the main precession coils. There will be no fundamental changes, but more carefully wound coils were ordered. From test measurements we know that the imperfections of the windings of the old coils led to limitations of the resolution. This was a relatively cheap improvement, since the existing power supplies are capable of providing twice the power used so far. In addition, after more than 15 years of service we have to fear corrosion problems in the hollow copper conductor.

In collaboration with the KFA-Jülich we are trying to develop new Fresnel correction coils with less neutron absorption for higher correction currents.

IN11C will be an optional extension of IN11 for large scattering angles ($2\theta > 15°$) (see fig. 3). It will have a detector bank covering 30° scattering angle for simultaneous measurement. The price for this intensity gain will be a reduced resolution compared to the single detector IN11.

The magnets are at hand, the main parts of the mechanics are expected before the end of the year, or will come from recuperation of existing parts. The instrument is expected to be available for tests at the restart of the HFR.

IN15 High resolution spin-echo spectrometer for long wavelengths on the cold guide H511

The VME electronics as well as the software for running the experiment from the VAX were intensively tested and debugged. A special box for housing the sample with an opening of 30°, glass windows and controlled atmosphere (inert gas as well as vacuum) for small angle scattering has been made.

In order to check the performances of the prepolarizing FeCo neutron guide, we tested two pieces at BENSC in Berlin with neutrons. The polarization and the reflectivity were measured as a function of the magnetic field. It has been shown that within the $\pm 0.5°$ divergence used on the instrument there are 16-20% intensity losses in the guide and only a small gain in polarization at wavelengths shorter than 10 Å. The transmission polarizer which follows the guide should achieve the necessary polarization at $\lambda \geq 9$Å, while intensity can only be recovered by changing the coating. The possibility of improving the guide is under study.

The prototype toroïdal mirror for the focussing option (≈10.7 m focal length, 50 cm length) coated with Cu^{65} to ensure a μ-roughness less than 3 Å pp was delivered from Zeiss in November 1991. A test experiment was installed at the LLB-Saclay in February. The source (exit of the velocity selector) and the detector were respectively set at each focus of the mirror. At 10 Å, a 1 cm diameter spot was perfectly imaged on the detector, while at 20 Å one could observe aberrations due to falling neutrons (with gravity). However, the important result concerning the background to peak ratio around the image could not be measured precisely: the surface of the mirror which was perfect before starting the experiment was suddenly damaged by a strong oxidation. The effect is clearly seen on the scattering pattern. This oxidation is still a mystery: we were unable to explain and reproduce it on natural Cu coating. A new sample coated with Cu^{65} will be delivered by the end of the year to be tested at BENSC-Berlin. Great care of all details will be taken to avoid oxidation.

For the time-of-flight option, after some modifications of the software and optimization of the parameters to drive the "big" chopper, the whole system of 4 choppers is still under tests at the ILL using the control from the MacIntosh. The first 3 choppers can be perfectly phased with an accuracy of 0.2°, while 0.5° is achieved for the "big" chopper. The zero positioning of the latter needs to be revised as well as the modification of the theoretical flipper functions. The software for the remote control (OS9 system+Vax) is being developed by both the ILL and the KFA-ZEL group at Jülich .

IN16 (formerly IN10C) New backscattering spectrometer on the cold guide H53

The new backscattering spectrometer is finished as regards all technical components. A formal procedure for taking over the instrument from the DIM department was undertaken and reviewed the status and the remaining work to be carried out. The major task is the analysis of crystal deformation on the polished "high resolution" analysers and monochromator. The construction budget for IN16, ending in 1992, was spent by the purchase of a second set of 7 m^2 unpolished Si(111) analyser single crystals (the "low resolution" set-up). These crystals will be glued under deformation onto the spherical analyser supports in order to increase $\Delta d/d$ and the reflectivity, and to obtain an energy resolution of about 1.2 μeV.

For the high resolution crystal set, an undesirable deformation had been detected by photographic and γ-ray investigations and this was studied intensively by neutrons in 1992. As no suitable backscattering instrument is currently in operation around the world, we prepared at the beginning of 1992 a miniature backscattering set-up using a Mössbauer drive (from Univ. München) for mounting a perfect Si(111) single crystal in transmission and the test analysers in reflection. The data acquisition experiment control was handled by dedicated VME electronics. We acknowledge the support by both LLB Saclay and NIST Gaithersburg, in giving beam time on regularly scheduled instruments for these test experiments.

A first measurement of 4 days was undertaken in March 1992 at the cold triple axis spectrometer of LLB, Saclay (Brocker, Frick, Liss, Neumann). Two analyser sets of IN16, a polished analyser of IN10 as a reference, several unpolished deformed crystals, Boron doped Si(111) crystals of different thickness and a SiGe prototype crystal were investigated. In spite of the short time available, and the long time required for high accuracy adjustment, the results were encouraging, but not conclusive, concerning the question of deformation. The measured spectra were resolution limited (FWHM ~ 0.7 μeV) due to beam divergency and deviation from backscattering geometry. A comparison with the IN10 polished Si(111) analyser resulted in a similar linewidth.

A second attempt at NIST, Gaithersburg, was undertaken in October 1992, using very clean collimation conditions, exact backscattering and improved background level. These conditions have drastic consequences for the available flux, as only $2cm^2$ of beam cross section can be used, in addition flux losses from the chopper and the 50% efficiency detector

add up to nearly a factor of ten. Fig. (4) shows the spectrum measured at NIST (Frick, Gehring, Neumann) testing the mobile analyser of IN16. An energy resolution of about FWHM = 0.39 ± 0.03 μeV was measured, a value still being slightly too large for perfect Si(111) single crystals but diminishing the importance of the crystal deformation. About 0.3 μeV could be expected with the configuration used. Currently laser interferometer measurements are carried out, in order to test the precision of the Mössbauer drive motion and to calibrate the energy scale. The main difficulty, however, seems to be the alignment of the crystals to perfect backscattering, a task which becomes very difficult with the low neutron intensity available (the spectrum in fig. (4) was measured for 39 hours). A further improvement in this direction is planned.

At the instrument IN16 the following work was carried out during the past year:

- the shielding of the secondary spectrometer was improved,
- at the entrance of the focussing guide into the shielding, pneumatic mobile shielding blocks and a system of security end switches were installed,
- a conical helium flightpath from the graphite-deflector-chopper to the Doppler drive was installed in order to reduce neutron losses from air scattering and absorption,
- the mechanical coupling of the analysers to the mobile platform and the height of the monochromator was checked and adjusted,
- an electric security system for the control of the water cooling, the presence of vacuum and the vibration level on the two choppers and the oil flow on the Doppler were installed,
- the electronic phasing of the choppers was tested,
- the connection of the instrument to the local network of electricity, gases and effluents was installed and the cabling to the electronics cabin was completed.

D7 Diffuse-scattering instrument with polarization analysis on cold guide H15 (See Blue box in this section)

D11 Small-angle scattering diffractometer on the cold guide H15

Despite the shutdown of the reactor, work on the improvements to D11 has continued during 1992. Indeed these otherwise unfortunate circumstances have enabled the instrument team (technician and physicists) to carry out work from design to manufacture of some components.

The projects initiated in 1991 have largely been completed. The new velocity selector has been exhaustively tested and a piece of guide tube added to compensate for the 60 cms of difference in length compared with the previous selector (Brunhilde). A new attenuator system has been designed and built. It comprises three separate attenuators (attenuation factors 300, 1000 and 3000) consisting of cadmium plates with small holes drilled in them. The attenuators are fully automated and under computer control. The 20 metre section of guide after the velocity selector is now motor driven and the movement has been integrated into the new collimation control system installed last year.

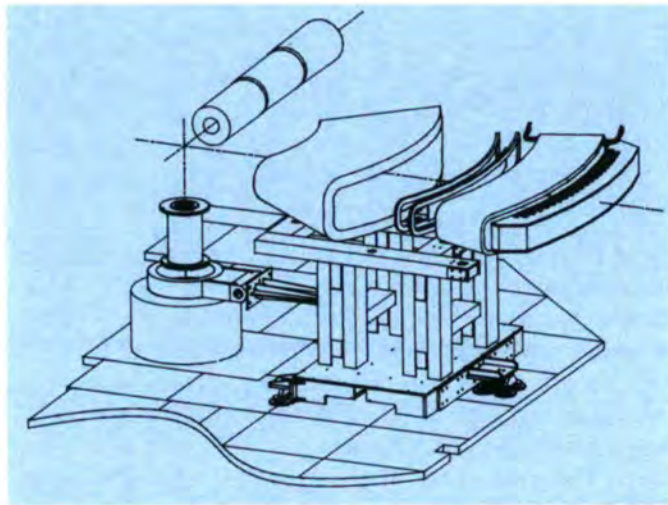


Fig. 3: Schematic view of the IN11C option. The first part of IN11 (solenoids) is kept, the second part is detached from the sample table, and the sector magnet assembly is attached as a replacement, covering 30° of the scattering angle.

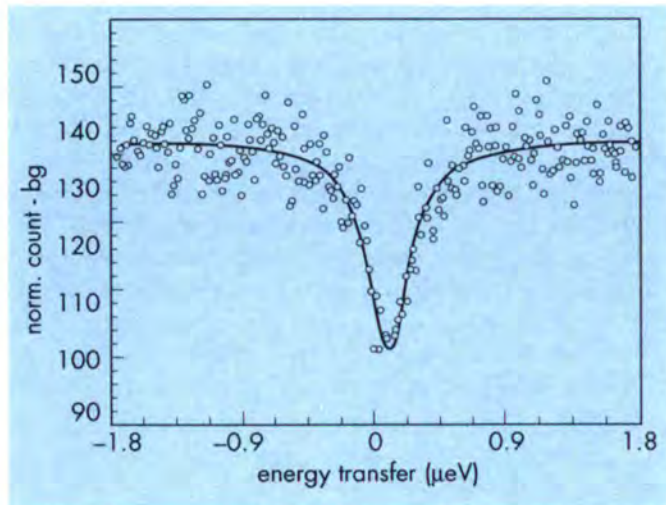


Fig. 4: Resolution measurement of the mobile IN16 analyser at NIST using a test backscattering set-up (Frick, Gehring, Neumann).

Improvements to the sample area are being continued with the design of new sample diaphragms and an improved sample table XYZ adjustment.

D17 Low-Q, low resolution diffractometer on the cold guide H17

A number of improvements were started on D17 in 1991 when it became clear that the HFR would be shut down for two years. The drives of all mechanical velocity selectors (5, 10, 30 %) are being changed from DC to AC motors. This will allow for selector speed control by the new ILL standard REFU 317 power supply which has been purchased for D17. Furthermore, connection of the REFU with the MicroVAX instrument computer will make automated wavelength changes possible in the future.

A completely new, compact attenuator and alignment system similar to D11 is under construction. A choice between three different attenuators (2 made of Cadmium sheets and one made of PMMA) will be available. The process controller of the compressed air pistons will be connected to the instrument computer via the CAMAC system. The alignment system will consist of a combination of a laser and a stroboscopic light source mounted outside the collimating guide. The light beam will be reflected from a neutron transparent silicon wafer into the path of the primary neutron beam.

For 1993 further improvements are planned in the sample area, in particular with regard to D17's reflection mode.

D22 New low-Q diffractometer on the cold guide H512

The budgeting and the construction of D22 finished at the end of 1992. The 1 x 1 m detector with 16K pixels of 0.75 x 0.75 cm from CERCA was tested at a beam-line of the Orphée reactor at Saclay. It was delivered to the ILL in the first week of December, 1992. The detector was then mounted on its carriage for tests and subsequent installation in the 2.5 m diameter and 20 m long vacuum beam tube.

The mechanical items still missing at the beginning of 1992, such as the beam-shaping device in front of the sample, the entrance cone to the detector tube, the beam-stop mechanism, and most of the sample environment, including a platform serving for ancillary equipment and as a support for the radiation protection, have been designed, manufactured and installed in the course of the year 1992. Some mounting remains to be done in 1993.

The Dornier velocity selector, turning at a maximal speed of 28300 rpm for neutrons of 4.5 Å at a resolution ($\Delta\lambda/\lambda$) of 10 % (FWHM), was successfully tested at the ILL for 100 h at full speed. After a check on of its bearings, it will be installed on a translation and rotation table in its "casemate". Devices for monitoring its vacuum, vibrations and temperature have been purchased, and its supervision will be incorporated into the industrial process control system already installed for the collimation and the instrument vacuum and temperature control. The supervision program (InTouch) running on a PC compatible under Windows has been interfaced with the instrument control computer, a Vaxstation 3200.

The data acquisition and shaft-control electronics (VME) was implemented by the ILL electronics group in the course of 1992. A preliminary version of the user interface program (compatible with that of D11 and D17) written by the ILL instrument computing group has been tested, and will be finished in early 1993.

The feasibility of an on-line direct-beam monitoring system incorporated in the beam stop mechanism was tested at the sample position of the SANS facility of the Hahn-Meitner Institut in Berlin. It will be mounted on the detector carriage and tried out with the first neutrons to arrive.

Coordinators: A.J. Dianoux
R.P. May

D7 What it can do: SRO-parameters, magnetic moments, order and disorder in polymers, elastic and quasielastic nuclear and magnetic scattering.

At the ICNS91 conference in Oxford, 7 experiments performed on D7, without and with polarization analysis [1,2,3,5,6,11,12] have been reported. These papers give a good survey of what sort of problems can be treated on this instrument. They include measurements on short range order [1,2], experiments for which the instrument was originally developed by Bauer [4] in Jülich and built by W. Just in the ILL, and which are now even easier with the switch over to measurements without analysis, using in this case 64 detectors with an angular distance of 3 degrees, and with three different wavelengths and a double focussing monochromator.

Another group of measurements, which were reported at this conference, were obtained with polarization analysis, and concern the separation of coherent and incoherent scattering. This possibility was reported with measurements on polymers [5,6,3] and ionic conductors [11]. In [3] it was demonstrated that the origin of R_i in $\sum_i b_i \frac{\sin(Q \cdot R_i)}{Q \cdot R_i}$ for amorphous samples has to be taken as the "centre of scattering", given by $\frac{\sum_i b_i R_i}{\sum_i b_i}$. This relation was used to get meaningful results in calculations [8] for measurements on polymers with polarization analysis. This report describes the method used on D7 for such materials very comprehensively, and serves for users applying this method to polymers as an introduction to the problems which can be solved on D7 [9,6,3,5] and to the methods applied.

Two other publications discussed at Oxford [5,6] showed that the instrument D7 with polarization and TOF analysis is well suited to the analysis of short range order in amorphous polymers and that the simulations of the structure used in the past, such as the "amorphous cell" method [7], need to be modified. The measurements on D7 permit an easy quantitatively absolute cross-section determination by the "internal calibration" method, relating the observed scattering to the incoherent scattering from the known hydrogen/monomer content. This incoherent scattering is separated by spin flip scattering and is then used for calibration instead of a vanadium calibration sample. This new possibility requires that any theory has also to deliver the absolute cross section and not only the qualitative behaviour. Fig.1 shows that the quantitative behaviour is not yet well described by the theory, only the qualitative behaviour, so that here too the measurements on D7 gave completely new insights.

Results on liquids were presented at the conference on Quasielastic neutron scattering at Windsor 1992 [10]. We further mention a paper about Li diffusion in the superionic conductor Li_2S measured on D7 in quasielastic mode to find whether there is a coherent contribution [11].

A third group of publications (fig.2) is related to magnetic scattering. Mezei et al. [12] show an example of a measurement on V_5O_9 with the polarization analysis of D7. This is an example of a material showing a metal-insulator phase transition. Here again the D7 results contradict all expectations, this time concerning the magnetic behaviour at metal-insulator phase transitions, and they call for new theoretical ideas for the understanding of the transition in the V_nO_{2n-1} series.

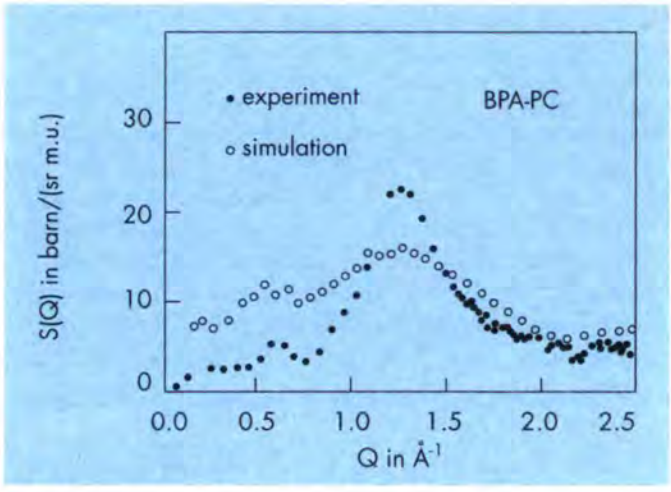


Fig. 1: Coherent structure factors for the polycarbonates measured by spin polarized neutron scattering, compared to calculated structure factors obtained from amorphous-cell results for bisphenol-A-polycarbonate. Notice especially the absolute scale on the ordinate.

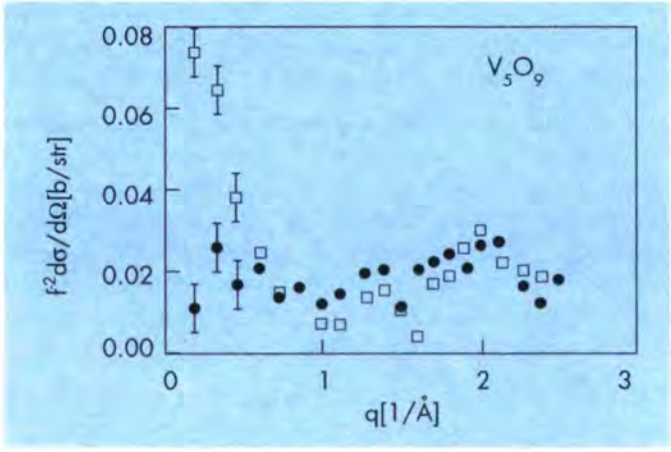


Fig. 2: Wave number dependence of the magnetic neutron scattering cross section in a V_5O_9 powder sample in the metallic phase at 70 K. The error bars indicated are representative for all the data points. Only the higher q data are given, corrected for the magnetic form factor of vanadium. This contradicts all expectations about the magnetic behaviour at metal insulator transitions and calls for new theoretical ideas.

In a forthcoming publication [13] a theory of polarization analysis from magnetic scattering into a multidetector has been derived. Here the II⊥ method of [14] is generalized to the xyz or three dimensional polarization analysis. The formulae can easily be extended to include the most general case of Blume [15] and even the case of nuclear polarization [16,17] , using the method of treatment derived there.

The way the polarization rotates in the three directions x,y or z is also investigated in detail. Fig.3 shows the guide field resulting from the permanent magnets on the banks. Fig.4 shows this field in and around the spin turner coils. Fig.5 shows the rotation of the field in stereographic projection on the way from the sample to the detector just behind the corner of the coil. From this an estimate of deviations is found which turns out to be smaller than the size of the detectors. The error resulting from this deviation is also estimated and should be not more than 0.15%.

The derivation of the cross sections for magnetic scattering with polarized neutrons in three dimensional polarization analysis shows that the investigation of helical structures should also be possible, not only with one detector but simultaneously with 32 detectors and with polarization analysis and time-of-flight energy analysis on all 32 detectors. This operating mode can very easily be switched over to the mode without polarization analysis to see whether there are contributions with higher energy, which may be lost by the analyzers. At least without polarization analysis one can find them in upscattering and then concentrate on further investigations of these.

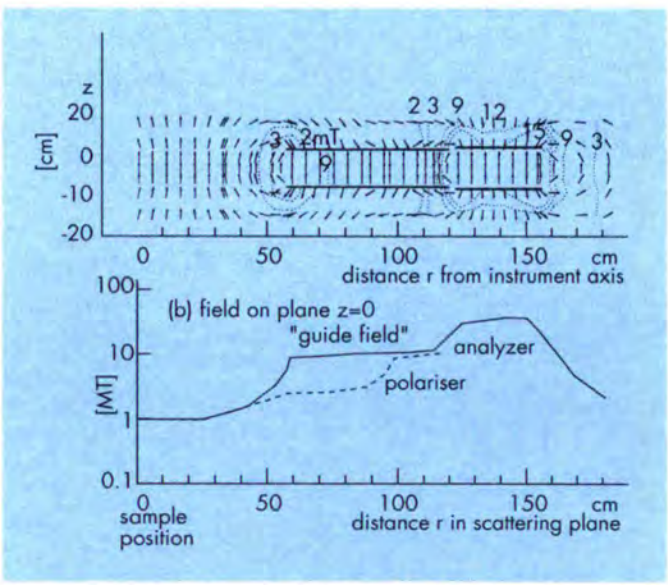


Fig. 3: (a) Field pattern of one detector bank in a vertical cut. Some lines (dotted) of constant field strength are given, near the points where the field changes strongly. The arrows show the field direction in the centre point of the arrow line. (b) Field strength in the scattering plane on the way from the sample centre to the centre of the detector without current in the spin turn coil.

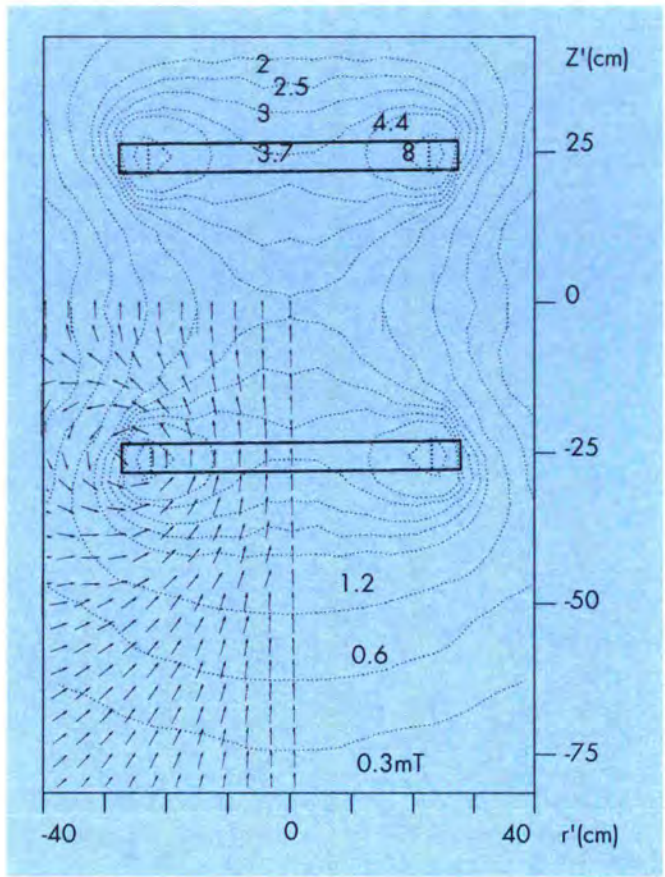


Fig. 4: The field in and around the spin turn coil of D7. The dotted lines are lines of constant field strength in mT for a current of 7.7 Ampère. The arrows in the lower left quarter show the field direction in this part of the plane at the centre of the arrows. Solid thick lines: position of two circular coils with the coil axis z' in the figure plane through the zero point of the abscissa. This makes it possible to follow exactly the direction of the field in the instrument and to verify whether the spin direction can follow this field direction and to what degree.

Another publication in the press [18] describes extensively investigations of the quantitative exactness of the magnetic cross section measurements (fig.6). With this possibility of measuring absolute cross sections one has for example a new way to look for intermediate valence, because these materials should then have another total magnetic cross section. It is also shown that the temperature dependence of the absolute magnetic cross section can in certain cases replace the measurement of the energy of a crystal field transition. In fact it is itself a quantity which can replace another parameter normally measured but not accessible in a particular case, for example because it is at a much too high energy. Another result of these investigations is that one can even find correct cross sections in the superconducting state, something which was very often in doubt. For this one has to use a procedure described in the paper cited. A criterion is also given as to whether in this case the method works correctly.

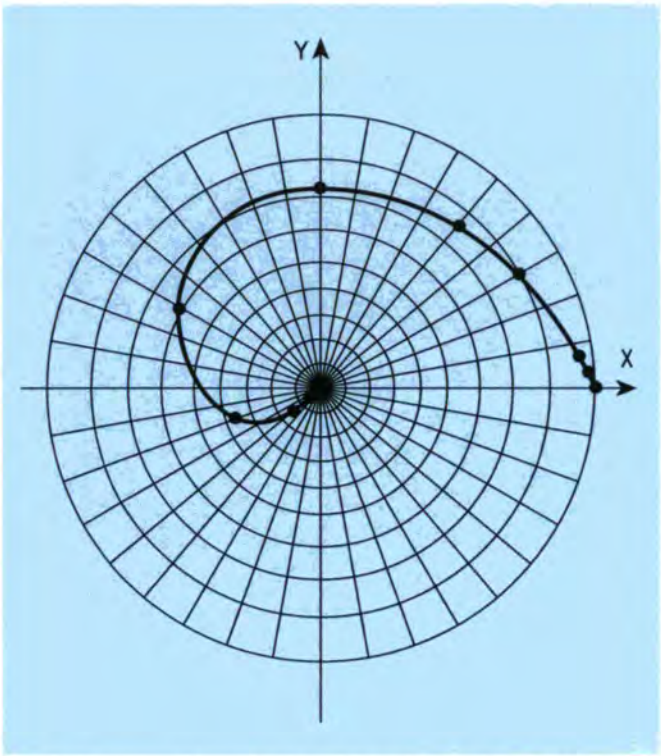


Fig. 5: Stereographic projection of the rotation of the field direction on the path from the sample to the detector. This path has an angle of 50 degrees to the forward direction and passes just behind the corner of the coil, where the field direction is changing considerably.

How important such quantitative possibilities are can be seen in publications on magnetism in high T_c superconductors. There one can get the impression that they are fully magnetic. But if the absolute size of the cross section is measured one can see that it is really very weak. In the case of G.Shirane's Koshu #1 [19], where the magnetic scattering is so strong that we could even find on D7 the whole magnetic ridge (fig.7), but broader and lower than in the pure crystal without strontium, this scattering is just 3% of the scattering expected for 1 μ_B. If you find only 3% of what you expect you ask whether it is clear that this is coming from the superconducting phase, especially if you hear that this sample is only 80% [19] Meissner effective.

With these publications on multidetector polarization analysis things routinely possible on D7 are put now on a solid foundation, enabling the users to see what they can expect from the instrument. First extensions of the theory showed that it is easy and clear to apply also to a generalized polarization analysis. To permit access to the full possibilities of such a unique instrument it should be transferred to an endposition of a cold guide. Then one could really gain at least a factor ten in intensity and with the monochromator option, which should not be abandoned, one would not lose the normal possibilities necessary for routine diffuse scattering for short range order parameters etc. When the reactor restarts it will be possible to allocate routinely submitted proposals a maximum of 1 week. In this way it

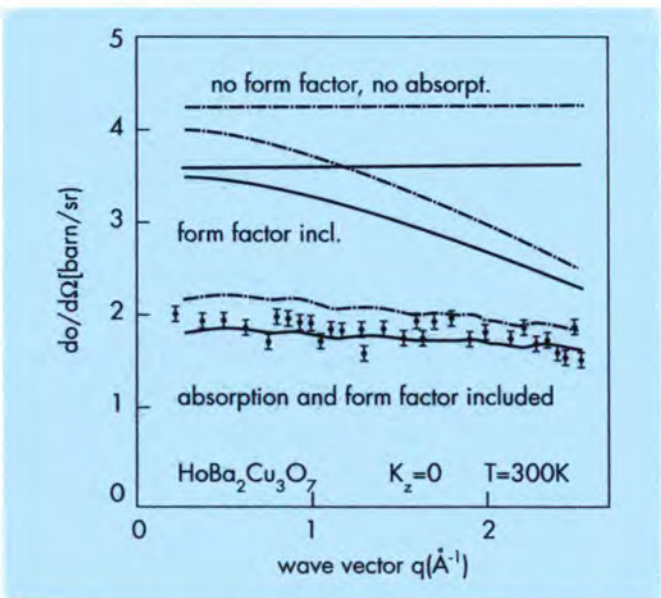


Fig. 6: Comparison of the experimental data for T=300 K with calculations of the magnetic cross sections as a function of the wave vector q (dash-dotted curves: not including analyzer transmission, solid curves include the effect of the analyzers.) The measured points show how well the theoretical behaviour is reproduced, if all corrections are included.

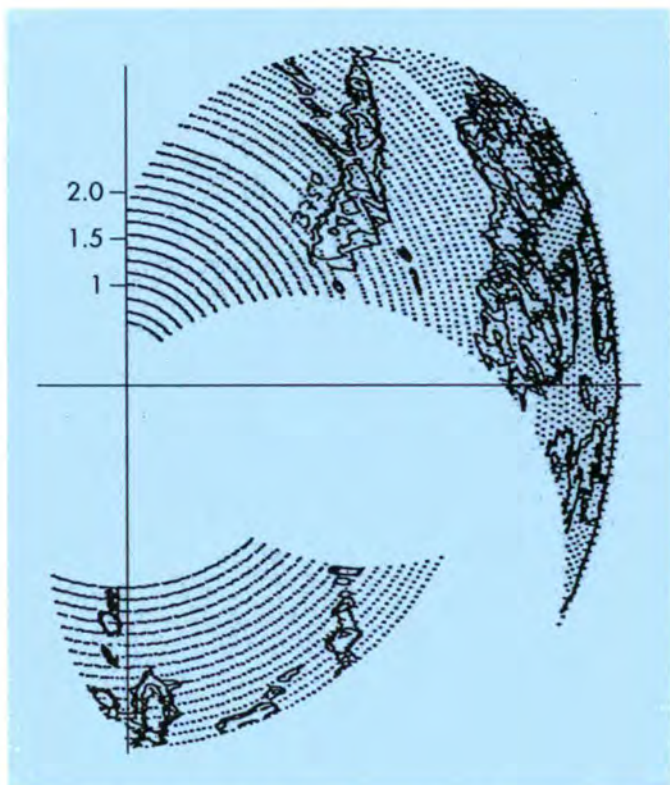


Fig. 7: Shirane ridge in a superconducting sample $La_{1.85}Sr_{0.15}CuO_4$ at room temperature measured with D7.

will be possible to have much easier access to this instrument than in the past. There it was still necessary to investigate the full reproducibility of the calibration measurements. Meanwhile these measurements were very carefully done and compared, and this showed that for most cases one can rely on calibration measurements even done long before. This allows a great saving in time.

O. Schärpf

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Diffraction Instruments

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

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

D1B: Two-axis diffractometer with multidetector a 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, P. Feder (to May 1992))

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)

D10: Four-circle triple-axis spectrometer on thermal guide H24 (G.J. McIntyre, C.M.E. Zeyen, R. Chagnon (to Sept. 1992))

T12: Neutron camera on thermal guide H23

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

D16: Four-circle MK6 diffractometer on cold guide H16 (G. Zaccai, V. Rodriguez)

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

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

DB21: Four-circle diffractometer with PSD for biological macromolecules on the cold guide H15 (C. Wilkinson (EMBL), E. Pebay-Peyroula, P. Agnès).

Important issues for the Diffraction Group

The division of diffraction work between the various sources of radiation promises to be a key question for the next decade. Most favourable in that respect is the fact that ILL will start again with a reliable, first rate neutron source. But obviously, the balance will depend not only on the source but also on the associated instruments and techniques.

Because of the tight budget expected in 1994, the ILL has to focus attention on its 25 leading instruments. It is therefore the scientific responsibility of the Group to prepare the diffraction instruments now so that they will reach their best possible performance quickly after 1994.

Data visualisation and modelling software link our specialized techniques with the outer scientific world. They often determine the users' satisfaction and the quality of the final output of the Institut and should have all our attention.

Novel ideas and techniques are essential for our future. We should not forget them. Here, the possibility of finding extra money and help from outside exists, and we shall pursue it.

Rebuilding the Instruments

To proceed with the exchange of the reactor vessel, most of the instruments in the Level C reactor hall had to be dismounted. Because the individual beam-tubes have to be extracted longitudinally out of the reactor vessel our primary spectrometer biological shields are necessarily in the way. Some can be pulled back on rails but most of them were lifted and stored in various locations. Not to be destructive for delicate, precise instrumentation which is buried deep in the shielding such major dismounting required good general coordination.

For rebuilding, it may seem enough to proceed in reverse order but there is a crucial difference: the adjustable equipment has to be carefully monitored in good time, especially where the sequence of adjustments is critical. In that respect the loss of technical expertise which we are experiencing now could one day hamper our chance of getting our instruments rebuilt properly. We must remain extremely attentive to it.

D1A: High Resolution Powder Diffractometer on thermal guide H22

D1A was moved to Saclay in 1992 for the duration of the ILL reactor shutdown. Dr Juan Rodriguez and Peter Cross were detached from the ILL to help run the machine, which will be available by application to the Saclay 'tables rondes' committees for $^2/_3$ of the beam time, and to the ILL for the remainder. All of the D1A ancillary equipment, including its He-cryostat and automatic temperature controller, were moved with the machine. However the D1A PDP-11 computer was replaced by the micro-Vax from D2B for instrument control and data reduction, since there are no DEC computers at Saclay, and it would have been difficult to connect the PDP-11 system to the local network. It was relatively easy to connect the D1A Vax to the Internet at Saclay, so that remote users, in particular from ILL, can log-on. This work was carried out by A. Barthelemy and J. Allibon of ILL.

We are also indebted to the EMBL laboratory in Grenoble, for whom John Allibon now works, for allowing him to continue to help with the D1A Vax at Saclay. And of course we are particularly grateful to Rossat-Mignod, Bourée, Pinot and others at Saclay for making this move possible.

D1A is installed on a cold guide at Saclay (the only position available), and naturally the neutron intensity is significantly lower than it was at ILL. However good quality, high resolution diffraction patterns can be obtained at 1.984Å in the acceptable counting time of 2-3 days (compared to 12-24 hours at ILL). To improve the efficiency of D1A, a new bank of 25 detectors (instead of 10) is being constructed at ILL, and this will be available before the machine returns to the ILL in 1994.

D1B

Despite the strong support it got from the user community at the Uriage meeting in late 1991 D1B will be one of the instruments not to be officially scheduled any longer at the reactor restart. It is hoped that this machine which has been used by over a hundred research groups in the last 20 years resulting in over 500 publications will find a future in terms of a CRG (Collaborative Research Group) comprising several different scientific partners. A collaboration between e.g. 4 groups with scientific interests in respectively a) magnetic structures, b) structural phase transitions, c) kinetic studies, in situ reactions and d) texture studies would be ideal to preserve and enhance the experimental possibilities of this highly versatile machine. Due to its situation in the neutron guide hall D1B has not been dismantled and is therefore one of the few diffraction instruments ready to start with the first 'new neutrons' in 1994. Research groups interested in participating in the CRG for D1B are urged to contact the instrument responsible Dr. C. Ritter, or the ILL directors.

D2B Very High Resolution Neutron Powder Diffractometer on thermal beam H11

D2B was one of the machines, together with D11, that produced the largest number of scientific publications in the 3 year period preceding the reactor shutdown. It is therefore rather sad to see the machine sitting idle in storage. Because D2B uses very high collimation, it needs a very high neutron flux to operate, so it was not feasible to move it to another European reactor, as was done for D1A. However, it is encouraging to see that machines very similar to D2B are becoming operational at reactors at NIST and BNL in the USA, and also in Japan.

Indeed, the scientist responsible for D2B, Dr. Thomas Vogt, was selected from a number of excellent applicants to construct a similar machine at Brookhaven National Laboratory. Although Dr Vogt is currently employed by BNL, it is hoped that he will return to ILL in 1994. In the meantime, he is working with BNL and ILL staff to develop

a new kind of focussing monochromator, made from thin silicon or germanium wafers obtained from the electronics industry. The present D2B monochromator, although it is highly efficient, produces a non-regular peak shape that detracts from the performance of the machine at the highest resolutions. It is expected that the new monochromator will be available when the ILL reactor restarts, improving the performance of D2B still further.

D2B is also scheduled as one of the first instruments to receive a new control computer, since its current computer is used on D1A at Saclay. Because D2B can collect data very quickly as well as at high resolution, it is necessary to compare results at many different temperatures or sample stoichiometries. It is hoped that the Cerius software, puchased in 1992 for the new Silicon Graphics workstation, will greatly aid with the data analysis on machines such as D2B.

D3B: Two-axis polarised neutron diffractometer and CRYOPAD

Polarisation:

During the last two decades, optimised sources of short wavelength neutron (HFR Grenoble Hot Source, ANR, ISIS, LANSCE spallation sources) became available. New experimental techniques were developed for polarised neutrons and the traditional ones were refined. Exciting new fields of Solid State Physics (Heavy Fermions, Paramagnetic excitations, Low dimensional systems, High energy magnetic fluctuations, High Tc Superconductors) emphasised that polarisation techniques can help in several unique respects. At the same time, severe limitations in the experimental possibilities came to light, which appear inherent in the use of single crystal polarisers. This led to strong interest in a novel polariser: the optically pumped ^{3}He spin filters. When combined with the best monochromators they promise more flux and flexibility at thermal and short wavelengths.

D3B- A Polarised Neutron Diffractometer for High Magnetic Field

D3B is a Normal-beam single-crystal diffractometer with a polarised incident neutron beam. In practice, the instrument is set at a Bragg peak of an already known crystalline structure. Then by simply reversing the beam polarisation, D3B can make a highly sensitive measurement of the spin-dependent nuclear-magnetic interference amplitude term which is present in the Bragg scattering of polarised neutrons from a single-crystal specimen magnetised in a field.

This technique is not restricted to ferromagnetic samples but it is sensitive enough to deal with milliBohr-magneton magnetic moments which can be induced in many paramagnetic samples at low temperature under a strong magnetic field. An interesting example is the study of YBaCuO high-Tc superconductors shown in the College V section of this report.

For paramagnetic studies it is often necessary to work at low temperature in heavy cryomagnets with the kind of precision required in single crystal studies. The normal beam geometry with lifting detector is invaluable in permitting a simple geometry with the cryostat vertical so as to collect partial 3d data out of the horizontal plane. D3B uses a Harwell MkVI diffractometer which is not equipped with the coaxial two-shaft design which was judged too costly at the time. We have now bought such a used base from the recent Harwell Equipment Sales and it is planned to have it in place for the reactor start-up. The base has been checked, it is good and will provide the best geometrical precision for studies using the heaviest cryomagnets.

The D3B instrument has the overall capability to collect high precision flipping ratios in a reproducible way. Automatic wavelength change helps for extinction corrections and the system reaches the highest standard in such measurements.

An interesting further option is being discussed which would incorporate a small multidetector of the D15 kind. Because different "Stern-Gerlach" deviations in large field gradients will break the symmetry in the two spin states when combined with a position sensitive detector, this detector might not reach the required standard. Nethertheless it should certainly be made available in case D15 is stopped because many magnetic studies of a more general kind (phase transitions, incommensurate structures etc.) require such a facility.

CRYOPAD-The Zero-field Neutron Polarimeter

In Spherical Neutron Polarimetry (SNP) all three components of the neutron polarization are under control in the incident beam as well as in the scattered beam giving the best possible neutron insight into the vector nature of the scattering process.

To accomplish this difficult magnetic task in a compact and precise way, CRYOPAD takes advantage of the magnetic Meissner shielding effect provided by superconducting thin niobium cylinders which surround the sample chamber. These cylinders are transparent to thermal neutrons.

Because the prototype cryostat was designed to study periodic magnetic structures involving relatively large scattering cross-sections in discrete Bragg peaks and satellites, the variable temperature chamber was 2cm in diameter and the precessing coil arrangement could only deal with relatively small samples (a few mm^3) and a single scattering angle at a time.

Recent proposals for work on inelastic cross sections and diffuse scattering require much larger samples and/or more general scattering conditions. At first, we have investigated

Meissner shielding effects in an open-ended cylinder using computer simulation. We are now building the corresponding annular cryostat; it comprises a large room-temperature bore, 19 cm in diameter, with free top and bottom access. This is a volume large enough to think of many different sample environment devices. We are also working on a new design for the precession coils aiming at a wide neutron scattering angular window.

By measuring the full rotation of the neutron polarisation in zero field CRYOPAD was shown to be a powerful tool for the investigation of complicated antiferromagnetic structures (see for example, Mn5Si3 in College V Report). For such magnetic scattering measurements, this new polarimeter CRYOPAD-II ought to be a second generation tool, more flexible and easier to use than the prototype. For example it will provide enough free space at the sample axis to host an ILL Dilution Cryostat. It could also serve as a bench for the implementation of Spherical Neutron Polarimetry in low temperature physics, quantum liquids and nuclear spin order phenomena where this technique is not exploited yet.

For the moment, at thermal wavelengths, only IN20 can host CRYOPAD at ILL, but the Heusler crystals used for neutron polarisation cause severe loss of intensity, and the available energy transfer is limited (50 meV maximum incident energy).

To enlarge successfully the range of SNP studies we need improved polarisation tools like the ^{3}He polarisation filter.

D9 Four-circle diffractometer on the hot beam H3

With the advent of very strong X-ray sources, notably the neighbouring ESRF, more and more precise data can be measured for more and more complicated systems. The good use of these data is a challenge to all researchers dealing with structural problems, and the combination of high resolution X-ray and neutron diffraction results will undoubtedly play a part in unraveling many of the problems encountered. This is due to the complementarity between the nature of the scattering processes, which favours X-rays for the determination of electron densities and neutrons whenever questions about the distribution of the nuclei arise.

In the new group of official instruments a major role for D9 is therefore to cover this important part of all structural research, but it will also be vital that studies taking specific advantage of the small position sensitive detector are continued. At present this covers 32 by 32 pixels with 2 mm spacing, but it would clearly be of interest to have detectors with more elements and higher resolution. It is therefore hoped that in not too far a future D9 would be able to benefit from the developments that gave the new detector for D20. Another possibility is to shift to a photomultiplier technology and in this case to take advantage of the test that have been done in collaboration with EMBL, and that is discussed in the report of college 8. In both cases a resolution of about 1 mm can be approached with more available elements.

Such developments of position sensitive detector applications is in line with the other diffractometers at the ILL, and with a coordinated effort it should, as mentioned below, be possible to keep up with new demands as they will arise.

When D9 was dismounted it only took two mornings. It is clear that it might take somewhat longer to assemble it, especially because the collimating systems before the monochromator housing have to be realigned. There are however no major plans for changing any of the collimators, and only for the monochromator unit is a recabling envisaged during 1993. Likewise at present there are no plans for any changes in the diffractometer and its environment control units, mainly because the D9 was already well equipped, but also partly due to complete lack of man-power. Hopefully this will change at the approach of the restart when considerable testing of the equipment must be made.

D4B Disordered materials diffractometer on the hot beam H8

Further progress in the study of disordered material structures always requires higher accuracy in data acquisition. This is true for the local order investigations around a reference atom (e.g. using the isotopic substitution method) for which a statistical accuracy of 0.03% or better would be very useful. It is also true for accurate absolute structure factor (S(Q)) determinations for which accuracy at the per mille level allows us to discriminate between existing models or potentials.

Reactor based disordered material diffractometers offer the advantage of well-defined experimental conditions (low background, appropriate sample environment, defined resolution function, constant incident neutron energy, constant flux over the Q range investigated, well established chain of data treatment). Experiments are reproducible within the claimed statistical accuracy. In the last 20 years, the present machines (e.g. D20, D4B) have already been improved by a factor of about thousand due to focussing monochromators and small position sensitive detectors, further improvements (factor 10) will come in the next 5 years from the banana detector on D20 and eventually a bank of small PSD's on D4. Gains on the monochromators by a factor 2 or 3 are also possible [Graphite Monochromators on D20, Be on D4B]. Such a gain in data acquisition will normally provoke a reassessment of the whole chain of data analysis and increase the need for accurate sample characterization.

Computer simulation (M.D., Reverse Monte Carlo, Simulation of experimental conditions and data analysis) takes an increasing role in the study of disordered matter and has allowed us to compare theories, models and potentials to the measured S(Q). For the time being however a rather clear line demarcates the computing effort and simulation necessary for the optimization of the experimental conditions and accurate data correction or analysis from the one needed for the physical interpretation of the measurements which is more specific. We have always tried

to provide the ILL users and visitors with at least one updated chain of data analysis, but there is a great need for a Common Standard and updated pool of programmes for data treatment. This probably implies some common policy if we move to UNIX System.

D10 Four-circle three-axis spectrometer on thermal guide H24

The installation of the electronics for the new five-phase stepper motors were completed and successfully tested. The staff of Département des Instruments et Méthodes and Calcul Scientifique as well as Service Electronique are thanked for their enthusiasm and effort.

But what lies ahead? In the immediate future it is vital that D10, being the only four-circle diffractometer in the guide-hall and thus perhaps the only four-circle diffractometer immediately available at the reactor startup, be kept fully and reliably operational. To ensure this, mock experiments will be run at frequent intervals until then.

One long-term goal is to improve the user-friendliness of the instrument. Nowhere is the need for a user-friendly interface to the control program as great as on D10 with its dual role as a diffractometer and spectrometer. The types of experiments go from conventional diffraction data collection, through mapping of reciprocal space at high resolution for quasi-elastic scattering and at low resolution for measurement of diffuse scattering, to inelastic phonon and magnon measurements, all in full four-circle geometry. The extra demands that fewer instruments and fewer experienced ILL scientists will impose on the instrument responsibles make improved user-friendliness a priority for the future. The current joint ILL-ESRF-EMBL project on diffractometer control by UNIX workstations might appear to have little relevance to those of us for whom the replacement of our VAX computers is many years away, but we should all be watching carefully the development of the user interface in this project.

It is hardly an overstatement to say that position-sensitive detectors have caused a minor revolution in neutron single-crystal diffractometry in recent years, especially for macromolecular crystallography. With beam-time at an even greater premium in the years ahead, position-sensitive detectors should be installed on all diffractometers, and tried on seemingly inappropriate instruments such as polarised-neutron diffractometers and triple-axis spectrometers. D10 will also be joining the revolution. When D19's new larger detector has been commissioned, the present D19 detector will be installed at D10 to improve efficiency of structural data collection and measurement of diffuse scattering, and to provide valuable test data for the new flat-cone diffuse-scattering spectrometer D5B.

D15 Two-axis diffractometer with lifting counter on the inclined thermal beam IH4.

D15's location on an inclined beam maintains reasonable resolution out of the equatorial plane, which together with the out-of-plane access allowed by the tilting counter, means that it is one of the few instruments that can give nearly complete 3D diffraction data even when bulky or heavy sample environments are used. Of particular note is the routine use of cryomagnets and pressure cells. The sitting of ancillaries, such as vacuum pumps and liquid nitrogen supply, has been steadily refined over the years to give an instrument which is mechanically very easy to use. Another feature is the recent installation of a small position-sensitive detector which offers several advantages such as significant reduction in experiment start-up time and to much easier understanding and measurement of incommensurate diffraction patterns.

Despite - or perhaps because of - its proven reputation as a steady workhorse since the early days of the ILL, D15 will not be one of the 25 normally scheduled instruments at the reactor start-up. Nevertheless we believe that its future is assured, under the full responsibility of an external collaborative research group. Without wishing to limit the possibilities, we suggest that the interests of this group might cover magnetic and nuclear structure, including incommensurate structures, particularly at low temperature, or in strong magnetic fields, or under high pressure. Any groups interested in this collaboration are invited to contact the ILL Directors, or the D15 Instrument Responsibles.

D16 Four-circle MK6 diffractometer on cold guide H16

D16 is a versatile neutron diffractometer which remains unique for whole sets of experiments requiring good Q-resolution at low Q. It has extremely flexible collimation conditions and sample environment area, 2 circle or 4 circle options, and the possibility of using crystalline, partially disordered or solution samples. With its graphite monochromator on a cold source guide providing a large beam of high neutron flux-λ between 4 and 6Å for $\Delta\lambda/\lambda \approx 1\%$ —and its narrow wire spacing (high angular resolution) two-dimensional psd on a scanning arm, it is unique in filling a gap in neutron diffraction studies between the small angle scattering cameras like D11 and crystal diffractometers.

Studies in this gap are essential for structural determinations in a number of fields and D16 has increased our understanding of biological membranes, collagen, polymer solutions, protein interactions, surface lattices and intercalated compounds, ordering in alloys, liquids, magnetic frustration, liquid crystals, micro-emulsions. Because of the low signal to noise inherent in most of these studies (the H content of many of these types of sample is relatively high and coherent diffraction is often weak on a strong incoherent background) a high flux reactor is essential.

D16 features open and accessible sample area, flexible collimation, a large beam cross-section and the possibility of using partially disordered and solution samples of variable size (from $\approx$ 1mm^2 to $\approx$ 10cm^2 in cross-section). Sample environment facilities are available for the different

types of sample and they include cryostats, furnaces, magnets, pressure cells, constant humidity chambers, automated multiposition sample changers with temperature control for solutions. The users of D16 are not professional neutron scatterers. They are interested in problems in which neutrons can make unique contributions which are then used in a complementary fashion with results from other experimental methods. In the field of biological membranes neutron diffraction makes an important contribution because of deuterium labelling, the use of long wavelengths with negligible absorption and the possibility of studies as a function of environment while maintaining the sample active (hydration, very concentrated salt solutions, temperature, pressure) which are very difficult or impossible by X-ray diffraction or electron microscopy (the complementary techniques). The need for such studies is growing especially because of increased knowledge in the biochemistry of membrane proteins and of the interest which goes beyond the determination of a protein structure and questions how a protein interacts with the water and salt ions in its environment and how it moves. Questions that can only be addressed by neutron experiments.

It is interesting to trace the development of D16 in response to the needs of a specific scientific problem (biological membrane diffraction) and how this created an instrument that became useful in many other fields. First, the beam size on the original Mark 6 diffractometer was increased to the guide maximum and a 5cm diameter single detector was installed in a new shielding. Variable angular resolution was obtained from different sets of Soller slits, including a high transmission set made with cadmium coated mylar. Secondly, the next set of improvements included the small scanning two-dimensional psd and mounting the instrument on a Tanzboden to provide easier wavelength changes. D16 is easy to use and functions very smoothly with minimum maintenance. In case a third generation instrument could be envisaged the monochromator and detector arrangements would each be improved in order to profit even more from the high neutron flux on that guide position, and to increase the potential of the instrument for studies with even weaker signal to noise than the present ones.

D19 Multidetector diffractometer for protein crystallography on the thermal beam H11

D19 is a single crystal diffractometer with position-sensitive detector. The new 20° x 64° position-sensitive detector, built by CERCA, Romans, France will be tested with neutrons at the end of 1992 and the final shielding and support table will be built during 1993. If money is available in 1993, the D19 monochromator drum will be re-built to eliminate interference with the D20 beam.

With something approaching a full-sized area detector D19 should benefit for some experiments from installation of the data reduction system MADNESS used by many protein crystallographers. How to marry this with the present MAD diffractometer control software, and with the ADVANCE area detector software pioneered for the ILL by Clive Wilkinson and John Allibon (now both at EMBL) is an open question. The co-existence of D19's VMS systems with newly-purchased Unix work-stations will certainly create extra work for scientists and programmers. Much work will be needed to help users understand and exploit the possibilities offered for all experiments by the new detector coupled with state-of-the-art software. Hopefully at least the user interface will be similar to those used in other laboratories such as ESRF.

More generally the place of D19 in the diffraction group instruments will perforce be rediscussed when the new ILL list of at least 25 official instruments is implemented. Either D19 will be used frequently for protein data collection or it will have to move toward experiments at thermal wavelengths under non-ambient conditions. Most such experiments can benefit from position-sensitive detectors, but the closeness of the detector to the sample position causes both mechanical and background problems. More challenges for all.

D20 High Flux multidetector on the thermal beam H11

The year 1992 has been devoted to the completion of essential parts of the 160° PSD detector and of its electronics. By the end of the year all 50 glass plates, each carrying 32 detecting elements (cells), will be at hand, tested and ready to be mounted and aligned inside the detector vessel. This large body weighing 1900 kg has been outgassed during three weeks at 200C and is now leakproof. Fifty-two pieces of high quality graphites (HOPG) have been ordered to build a new monochromator for long wavelengths (λ=2.4Å).

The construction of the definitive D20 will take place in the next two years in two stages:

– In 1993, completion of the detector, of its complete dedicated electronics (1600 amplifiers and logic, of its VME data acquisition system and computer control (under Unix).

– In the second part of 1994, the rebuilding of the whole instrument at its previous position on beam H11 in level C.

The PSD used on D20 up to now had a 12.6° horizontal angular aperture. Due to this limitation experiments requiring data on larger Q ranges were done in angular scan mode. This hampered the development of time resolved experiments requiring synchronous detection over a large angular range. In addition, the quality of the monochromators and filters was not optimum and the poor angular resolution at high diffraction angles limited the use of D20 in powder crystallography.

The new instrument will feature a higher flux and better resolution through the use of better monochromators and filters. The priorities are with the HOPG (λ=2.4 Å) and Cu monochromators (λ=1.3 & 0.9 Å).

The detector aims at perfection: 160° angular aperture with a high efficiency & homogeneity and a perfect stability. The Data Acquisition System & Instrument Control

(DASIC) is equipped with 1600 independent buffers. It will permit counting rates up to a few MHz over the detector and the control and live display of stroboscopic data acquisition (time slices down to 20 μs). The instrument will have dedicated standard low and high temperature environment, sample changer, sample orienter (Eulerian cradle and translations), room temperature vacuum vessel.

This very powerful new powder diffractometer will concentrate on two kinds of experiments:

1) those requiring close to Giga-counts in order to reach the high statistical accuracy ($\Delta I/I \approx 10^{-4}$)needed for the study of small features in the Q dependence (disordered systems) or subtle differences due to bulk transitions and surface effects.

2) those requiring high counting rates for taking "movies" of systems evolving continuously or periodically with time (time resolved experiments).

DB21

The normal function of DB21 has been to investigate at low resolution the structures of protein single crystals with large (normally ~ 100 Å) unit cells, using 10 Å wavelength neutrons produced by an intercalated graphite monochromator. Before the start of the reactor refurbishment, tests made on single crystals with comparatively small (~ 60 Å) unit cell edges demonstrated that it is practical to use the instrument with 4 Å neutrons to determine these structures to 5 Å resolution. From cells of this size, data was still measurable at scattering angles of 90°, and a second (stationary) two-dimensional position sensitive detector is being placed on the instrument to collect reflections at high angles. In order to have several wavelengths available on the instrument, a carousel of novel design which will allow the monochromator crystal to be changed remotely has been constructed and is shortly to be installed in the H15 guide.

Coordinator: F. Tasset

Special instruments and experiments

It became clear in 1992 that activities in this field in the future will differ greatly from what they looked like at the time of the reactor shutdown. ILL's share in these ventures has probably to be reduced to zero, but it seems to be possible for Collaborative Research Groups to get the opportunity to work on specialised applications of slow neutrons at the ILL high flux reactor.

The following groups have expressed their interest in continuing to work at the ILL after the reactor restart:

University of Vienna	-thermal neutron interferometry
CNRS Grenoble	-neutron topography
HMI Berlin	-depth profiling
CNRS Grenoble	-Laue diffractometry
PTB Braunschweig	-precision determination of ħ/m
University of Grenoble	-neutron activation analysis
University of Munich	-evanescent wave diffractometer
University of Innsbruck	-interferometry with very cold neutrons

The UCN/VCN-source on level D was used by numerous research groups in the years since its installation and became a highly appreciated research tool. It was therefore proposed to convert it into a normal scheduled instrument (PF2) on the formal basis of a long-term loan from the TU Munich to the ILL. Future experiments on this source (such as the EDM experiment or the precision measurement of the neutron lifetime MAMBO-II) will then be treated like proposals on any other scheduled instrument.

During 1992, equipment of several S-instruments has been removed from the ILL. The neutron-antineutron oscillation experiment has come to an end and S20 (neutron topography) will be moved to the ORPHEE reactor at Saclay during the shut-down period of the ILL HFR.

Major development work has been performed on the EDM experiment, the search for an Electric Dipole Moment of the neutron on the new neutron lifetime experiment MAMBO-II and the PIAFE project. This work is summarised as follows:

Development work on the Neutron EDM experiment

In the absence of neutrons work is concentrated on setting up a system using nuclear spin polarised 199Hg atoms to measure the magnetic field with high precision in the 20 litre storage cell which will ultimately contain simultaneously ultra-cold neutrons and 199Hg atoms. Mercury vapour at 2×10^{-5} torr is optically pumped by circularly polarised mercury resonance radiation of 253.7 nm wavelength. The pumping takes place in an adjacent 1 litre cell while the Hg atoms are diffusing in and

accumulating steadily. At a stage in the two minute cycle of operations which is the point when the 22 litre cell has been filled with neutrons, a valve opens and the now spin polarised mercury then takes about 2s to flow in and mingle with the neutrons. During this time the two cells reach a common mercury pressure of about 10^{-6} torr. In the process about 1% of the neutrons will be lost through the Hg entrance aperture. In the next 2s the mercury spins are turned by magnetic resonance into a direction perpendicular to the magnetic field and subsequently allowed to precess freely. The precession is observed as the sinusoidally varying intensity of a second beam of mercury resonance radiation which has passed through the 22 litre cell along a diameter perpendicular to the magnetic field. The oscillatory signal is amplified and then digitised 100 times per second with a 16 bit ADC. The data, extending over an interval of about 100s is used to determine the frequency of the free precession averaged over the interval. The oscillation is now seen with an initial signal-to-noise ratio of 2500 using a 2 Hz bandwidth.

The first half of the year was devoted to (1) improving the stability and reliability of the two mercury light sources (2) optimising the mercury flow circuit (3) investigating the pumping conditions, for example, the spin relaxation times in the prepolarising cell, with and without the pumping light for various conditions of the surface (4) installing the on-line RISKOS Archimedes microcomputer to take and analyse the data and to pass the results to the main computer (5) investigating the affects of gas discharge treatments of the deuterated polystyrene coating of the main cell in relation to the spin relaxation time of the 199 Hg. Oxygen is the only gas found to have beneficial effects. There is a strong suspicion that small numbers of single atoms of hydrogen on the surface can catalyse the spin relaxation, perhaps by the formation of loosely bound paramagnetic HgH molecules which dissociate soon after they have had time to disorient the Hg spin. Oxygen may help to remove these lone hydrogen atoms. Factors of four improvement in the spin relaxation time have been obtained with oxygen. The improved time of about 60s is just long enough for the requirements of the experiment. Fomblin oil coated glass appears to give a satisfactory relaxation time for the prepolarising cell and to remain in a good condition without recoating for at least six months.

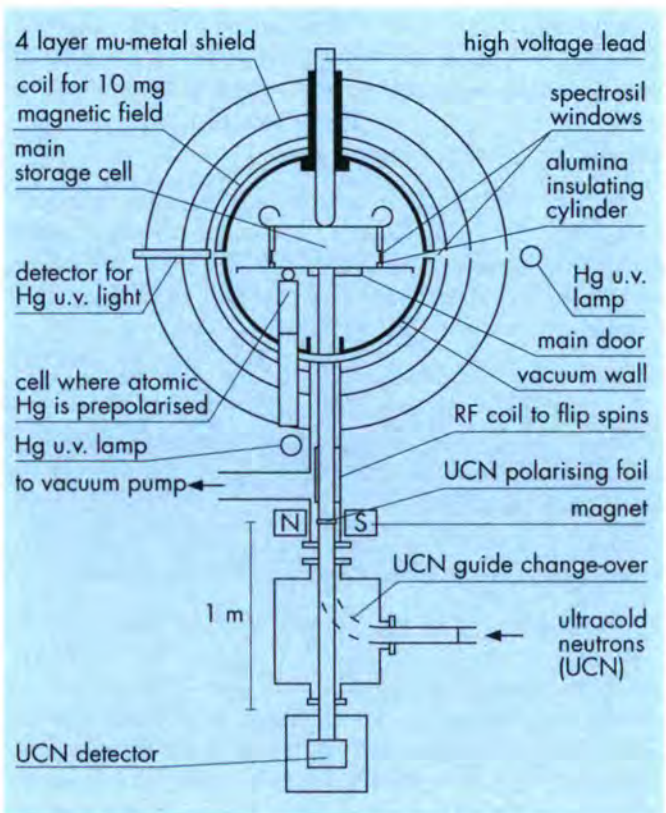


Fig. 1: The new instrument for measuring the neutron electric dipole moment.

Over the summer it has been possible to run the Hg magnetometer routinely measuring the magnetic field for several days at a time. The precision is being steadily increased and now corresponds to 2 nanogauss rms for a 60s relaxation time. The ultimate required is about 1 nanogauss rms. The latest improvements came with the installation of some very large calcite crystal polarisers. Figure 2 is a plot of 330 readings taken at 2.3 minute intervals extending over 12 hours in October. Here the relaxation time was only 25 secs and the rms noise was 5 nanogauss or about 5 parts in 10^7 of the field. The best rubidium magnetometer which runs alongside can measure with an rms noise of 2 nanogauss so it is known that the true short term magnetic field noise is $\leq$ 2 nanogauss. The long term drift seen in Fig. 2 is almost certainly a real magnetic field effect due to temperature changes. The neutrons will measure the field with similar precision and at this point it would be interesting to be able to compare Fig. 2 with a similar plot obtained using neutrons.

The 199 Hg magnetometer fulfils much better the need to measure the same volume average field as that seen by the neutrons. The 85 Rb is in a coated glass bulb 30 cm away from the centre of the neutron cell. Attempts to run rubidium or caesium in a similar way to the mercury ran into difficulties due to their greater reactivity with surfaces.

MAMBO II, the Neutron Lifetime Project

A new experiment for the determination of the neutron lifetime is currently under development. The aim is to reach a precision of one second using the method of storing ultra-cold neutrons in a liquid coated glass trap with variable volume. This successful technique was developed at the ILL by W. Mampe et al [1,2]. The experience gained with the previous version provides the basis for this new design which includes the following features:

– **Stored ultra cold neutrons:** UCN in a material trap are lost due to beta decay, absorption by the trap walls, escape through gaps and scattering by residual gas

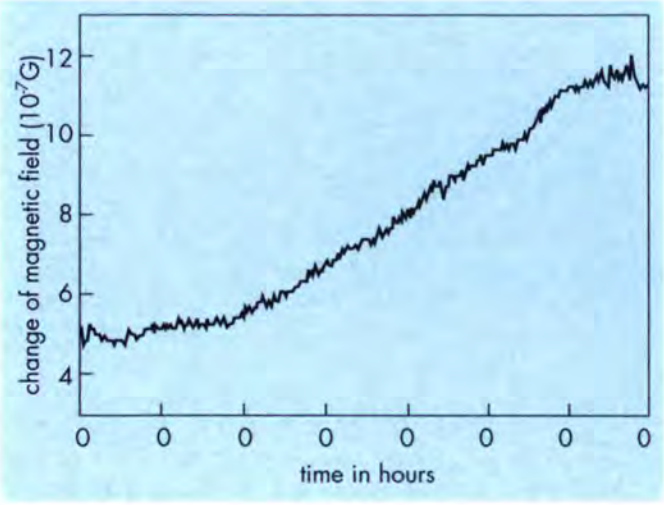


Fig. 2: The magnetic field strength, averaged over the volume of the 22 litres ultra-cold neutron storage cell, as a function of the elapsed time for the night of 20th October, 1992. Only the off-set is shown; the strength is 0.01 gauss. The data were taken with the atomic 199Hg mercury magnetometer which is under development. There are 330 measurements at intervals of just over 2 mins. The short term rms noise is about 5 nanogauss and mostly comes from the mercury and not the magnetic field. This is now close to the target of having the short term noise be less than 2 nanogauss. The longer term drift shown is probably caused by thermal expansion of the inner magnetic shield in response to the daily temperature changes.

molecules. Counting the remaining neutrons as a function of time and accounting for all other effects lets us extract the beta decay time constant.

– **Variable geometry:** The neutrons are stored in a trap with a variable volume to surface ratio. Extrapolation to an infinite volume to surface ratio yields the lifetime of the `free' neutron. Moving a side wall with a piston can change the storage volume in the range from 0-150 litres.

– **Liquid walled storage trap:** The storage trap is coated with a special oil, Fomblin, containing only C, F and O atoms, which has a relatively high Fermi potential, a very low average absorption cross-section and which wets the glass well and closes small mechanical leaks in the trap. Hydrogen atoms which much increase the wall losses in solid walls easily diffuse out of the oil and into the vacuum pumps. The expected uniformity of the liquid surface in all regions of the trap is crucial to the success of the extrapolation just mentioned.

– **Controlled maximum and minimum UCN energy**: The storage trap is filled with neutrons in a well defined energy band. This prevents the entry of neutrons with energies higher than the Fermi potential of the wall and those with less than the minimum needed to reach the highest parts of the trap. Such neutrons would greatly complicate the behaviour. The tailoring of the spectrum is achieved by pre-storing the neutrons in a large surrounding volume with an absorbing roof, within which is contained the measuring trap as shown in Fig 3 (see page 99).

– **Volume independent fill spectrum**: As another condition for the successful extrapolation, one has to ensure that the fill spectrum does not depend on the magnitude of the storage volume. The only solution is to make the entrance cross section proportional to the trap volume, by placing the trap inside the pre-storage volume and designing the whole trap sidewall to open as a neutron door.

– **Isotropic fill spectrum**: As a result of placing random scatterers in the pre-storage volume, the neutron spectrum gets isotropic in momentum space, which is also an important condition for the extrapolation. This may reduce the amount of irregularity needed inside the trap.

– **Gap free storage trap, guides, and shutters**: The trap and pre-storage volumes, the piston and all shutters are made of glass. The movable wall moves inside the trap with 0.1 mm play, which is sealed with the oil. All neutron guides are connected to the shutters without gaps and the shutter plates slide on oil films, leaving no gaps.

– **Monitored neutron flux**: The neutron number density in the pre-storage volume is continuously monitored.

– **High quality neutron guides**: All neutron guides are covered with nickel and are produced by the 'replica technique'.

– **Temperature control**: Since the wall absorption depends on temperature it is necessary to stabilise and to make uniform the temperature of the storage trap to better than 1°C. In addition, performing experiments at different temperature settings provides for important consistency checks.

Design and construction of the instrument take place in close collaboration between the ILL and H. Nagel at the Technical University of Munich, where the apparatus is currently mounted. The vacuum vessel (see photograph on page 99) the storage trap, motors and electronics have been delivered, most pieces are already machined and the final assembly will soon be finished. The experiment should be ready for operation at the ILL with the reactor start up.

[1] W. Mampe et al., Phys. Rev. Let. 63 (1989) 593-596.

[2] W. Mampe et al., Nucl. Inst. and Meth. A284 (1989) 111-115.

The PIAFE Project (Production, Ionisation, Accélération de Faisceaux Exotiques)

The PIAFE project was launched by the Institut des Sciences Nucléaires (ISN) Grenoble, about two years ago. The aim is to use a fission source of the ILL reactor to provide neutron rich isotopes which will be transported 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.

The general scheme is shown in Fig. 4. At the ILL reactor, the fission product isotopes will be generated from about 1 gram of ^{235}U in a dedicated reactor channel where the neutron flux is about 10^{14} n/cm^2 /s. The more volatile isotopes produced will diffuse into an ion source and, after ionisation preacceleration and passage through a mass selecting magnetic field, they will be transported to the SARA complex. On arrival, the isotopes will be put into much more highly ionised states in an ECR (electron cyclotron resonance) source and then accelerated with the two cyclotron arrangement there. Table 1 shows some of the estimated beam intensities for various nuclear species.

PIAFE will be a powerful tool to study the influence of neutron excess on the probability of fusion yielding very heavy nuclei. A second aim will be the study of neutron currents in binary collisions.

During 1992 there has been increasing activity on the R and D studies required for the reactor source, the transport, the coupling to the ECR source, and safety studies. The collaboration for the project already involves groups from France, Germany, Belgium, Denmark, Sweden, Poland and Russia.

W. Drexel

Nucleus	Usable beam First cyclotron	Usable beam Second cyclotron
Rb^{93}	$2.\ 10^9$	$3.\ 10^8$
Rb^{95}	$2.\ 10^8$	$3.4\ 10^7$
Rb^{97}	$4.\ 10^6$	$7.\ 10^5$
Kr^{91}	$1.\ 10^9$	$1.7\ 10^8$
Kr^{93}	$9.\ 10^7$	$1.6\ 10^7$
Kr^{94}	$2.\ 10^7$	$3.4\ 10^6$
Cs^{142}	$2.\ 10^9$	$3.4\ 10^8$
Cs^{144}	$1.7\ 10^8$	$3.\ 10^7$
Cs^{145}	$3.\ 10^7$	$5.\ 10^6$
Xe^{142}	$6.\ 10^8$	$1.\ 10^8$
Xe^{144}	$2.\ 10^7$	$3.4\ 10^6$

Table 1

Estimated usable beam intensities in pps at the output of the first and second cyclotrons.

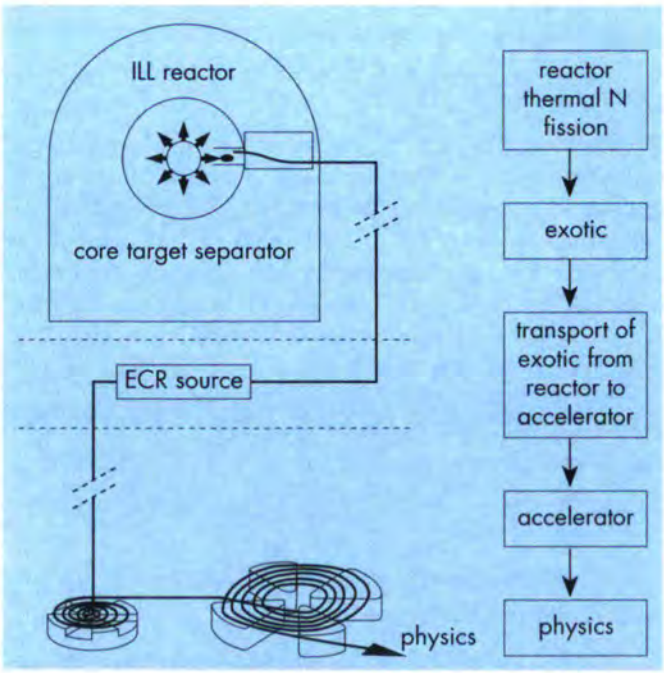


Fig. 4: The scheme for the project PIAFE to use the ILL reactor and the neighbouring accelerator complex SARA as a Production, Ionisation, and Acceleration Facility for Exotic beams. The project was proposed by staff of the Institut des Sciences Nucléaires (ISN) Grenoble.

Scientific Coordination and Public Relations

Scientific Programme

In view of the reactor shutdown during the whole year, many scientists have spent their time at host neutron centres for carrying out their experiments.

To compensate for the lack of experimental activities at the ILL, a series of workshops was organised by the ILL:

- Journée des Polymères et des Colloïdes.
  ILL (P. Lindner, E. Geissler) 14-15 April 1992
- 2nd European Workshop on neutron,
  X-ray and light scattering as an investigative tool for soft condensed matter.
  Bombannes (France) 31 May - 6 June 1992
  (P. Lindner)
- Determination of partial structure factors of disordered matter by neutron and anomalous X-ray diffraction. Joint workshop with the ESRF.
  ILL 10-11 September 1992 (J.-B. Suck)
- Applications of high resolution gamma-spectroscopy in studies of atomic collisions and nuclear lifetimes.
  ILL 5-7 October 1992 (H.G. Börner, M. Pendlebury)

In 1993 the following workshops will be organised:

- Neutrons and X-rays in the study of magnetism.
  Joint workshop with the ESRF.
  ILL (G.H. Lander (EITU Karlsruhe) ,
  W.G. Stirling (Keele), C. Vettier (ESRF)) 21-23 January 1993
- Memorial Colloquium Walter Mampe
  ILL (M. Pendlebury) 29 January 1993.
- Dynamics of Disordered Materials II.
  ILL (A.J. Dianoux, W. Petry, D. Richter (Jülich))
  22-24 March 1993
- Focussing Crystal Optics.
  ILL (A. Magerl) + PTB Braunschweig
  10-11 May 1993
- Réunion annuelle du groupe français d'étude des Quasicristaux.
  ILL (C. Janot (CNRS) 2-4 June 1993

Projects for 1993:

- Workshop on detectors.
  ILL (P. Geltenbort)
- 3rd European Workshop on neutron X-ray and light scattering as an investigative tool for soft condensed matter.
  Bombannes (P. Lindner)

Public Relations

The ILL has participated in 2 public events at Grenoble: on 12-14 June 1992, the French Ministry of Education organised get-togethers in various French cities between the population and representatives from the pertinent research institutes in each region of the country (Journées "La Science en Fête").

On 15-18 October an exhibition of high tech firms and research institutes (TEC 92) was organised by the town of Grenoble.

At both events the ILL participated with a stand showing its activities.

SCAPRO in collaboration with EDEX started to establish a permanent exhibition hall (former library) on the first floor of the ILL main building. Historical and up-to-date pieces of equipment in the neutron field will be displayed as well as many posters describing neutron instruments and neutron experiments.

Also many brochures, leaflets and workshop proceedings will be on display.

Safety, Medical and Health Physics Group

Health Physics and General Safety

Apart from the usual duties of assistance to the different departments, the Health Physics and General Safety units were occupied in 1992 with monitoring the dismantling work in the reactor.

The Health Physics Unit in particular has set up a strict system of radiological monitoring of persons working on the project. It has also carried out two essential technical functions:

- Decontamination of various slightly active reactor components,
- Disposal of active parts which cannot be reutilised.

Training of staff in health physics and general safety has continued. Instruction in the use of fire extinguishers has been added to this programme.

Medical Service

The establishment of the ESRF/EMBL/ILL Joint Works Medical Service has continued. The second nurse is now working full time. The project to install the Medical Service in another building has been finished in February 1993.

In the frame of the ILL security training program, the doctor has also organized a number of information meetings, on back problems, on the biological effects of radiation, etc. The whole staff is concerned by this training program, with the intent to improve the general work safety in ILL.

Joint ILL-ESRF Library

1992 Scientific Literature Budget: 1190 KFF, HT

ILL Share: 65% = 773 KFF, HT

Despite the budget difficulties of the ILL and the tremendous increase in the cost of journals (more than 10% per year), the library could operate in good conditions thanks to the participation of the ESRF to all library expenses:

- Staffing levels were completed since January 1992 resulting in a team of both ILL and ESRF employees reporting to the ILL Director and giving equal service to all common site users, as well as to many visitors from neighbouring institutes.

- The Joint ILL-ESRF Library moved to the Common building last June:

  20 000 bound volumes of journals,
  10 000 books,
  and about 30 000 other documents

were transferred and reinstalled within one month by the staff of EDEX Department. The existing furniture was also moved and reinstalled: Due to the increase in the library surface from 350 to 700 square meters, it had to be completed by new shelves, additional chairs, display for new journals...

- Library automation prepared since 1986 became a reality in 1992: the implementation of the LORIS-DORIS software under UNIX on a microcomputer Compacq 4856/33 by the ESRF computing services was done in March 1992. Up to now 3300 notices have been entered and are now searchable from the library. In the future, the access to the library catalogue of books will be extended to all offices on the ILL-ESRF site.

- Current Contents on Disquette with abstracts has been installed from 1992 on the Appletalk network of the ILL, giving an outstanding current bibliographic tool to ILL as well as to ESRF scientists. The number of computerized literature searches remained constant (200)

- 10 new titles of scientific journals could be subscribed to in 1992, bringing to 250 the number of current titles.

- 850 Books were processed

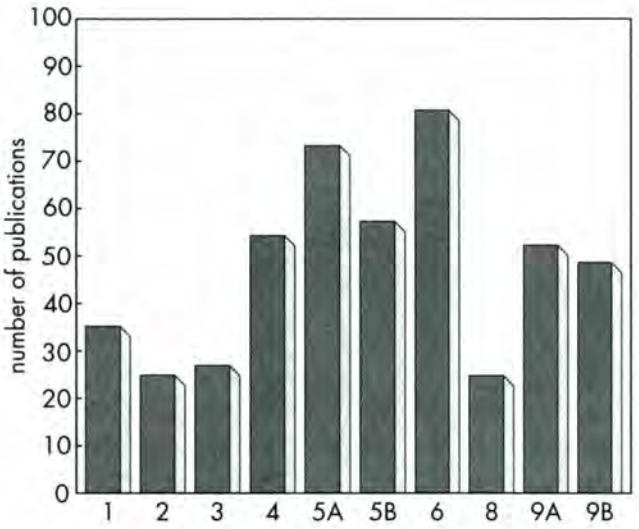
  – 500 for the Joint Library
  – 230 for ESRF Departments or Divisions
  – 120 for the ILL Divisions

- 500 volumes of journals were bound

In close relation with ILL scientific activity, the library compiled and edited the 1991 volume of Experimental Reports and Theory College Activity, the last after 20 years of regular publishing.

Publications received in 1992 by Subject:

600 Publications were received in 1992.



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

General

In 1992 the department was faced with two contradictory requirements:

on the one hand the reactor shutdown offered an exceptional opportunity for work on numerous instruments available for maintenance operations or modifications which had generally been desired for some time;

on the other hand the need for economies on ILL funds in favour of the reactor refurbishment led the DIM to offer its services to external laboratories. While giving priority to assistance to the ESRF, the department has tried to make contacts and to start collaborations which should prove fruitful in the future.

The response to these two requirements does not affect the increased contribution to the work associated with the reactor refurbishment and to the neutron distribution facilities.

Mechanical engineering

Although the ILL's scientific activity is reduced, the mechanical engineering group's workload has not diminished, in view of the amount of work in progress on the instruments, but also because of its contacts with external laboratories (collaboration with ESRF, PSI, HMI).

The mechanical engineering group is also making its contribution to the effort for the reactor refurbishment, both in practical form (dismantling, study of auxiliary assemblies, machining, reinstallation, etc.) and in theoretical form, for example by modelization of the reactor vessel and studying its dynamic behaviour in the presence of seismic excitations.

Workshop and Assembly Hall

In addition to a normal retirement, there was a considerable reduction in the staff of the assembly hall in 1992, due to one resignation and three detachments (to the reactor, ESRF and HMI). Despite this reduction in personnel the assembly hall, with the assistance of some members of the Instrument Operation Department staff, undertook the project for rebuilding the beam shutters and safety loops. The aim was to redefine and rebuild the 80 beam shutters of all the ILL instruments, while improving the safety and the qualities of design, construction, assembly and tests (Quality Assurance). Certain traditional activities of the assembly hall have been maintained, as for example balancing and endurance tests on choppers (IN15) and velocity selectors (D22 "Dornier" selector).

As before, mechanical manufacture has been directed to external firms or to the ILL workshop.

Because of the considerable reduction in the assembly hall's potential for intervention work, the workshop has had to extend its skills: for example to mechanical maintenance and metrology of modular assemblies for the instruments, precision cutting of glass sheets which support the electrodes (microstrips) of the D20 multidetector.

The workshop is assisting with the reactor refurbishment work by responding very quickly to its requirements, and by machining slightly radioactive assemblies such as the beam tubes (machining which it is very difficult to subcontract outside ILL).

Drawing Office

Two of the seven draughtsmen in the drawing office have devoted the majority of their time to special tasks; the first has worked on the assembly of several beamlines for ESRF, and the second designed auxiliary equipment necessary for the reconstruction of the reactor (e.g. storage container for beam tube H5, mechanical part for the new cold neutron guides NG12 and NG13).

The other draughtsmen have worked either on improvements for existing instruments, or on new instruments.

Improvement of existing instruments

PN1: adaptation of a new focussing magnet.

GAMS2/3: complete rebuild.

D3B: reconstruction of the polarizing monochromator area.

IN11C: new magnetic configuration after the sample.

Continuation of studies for D22: standardization of "standard" areas of the SANS D11, D17 and D22.

Continuation of the studies for the installation of the new multidetector on the existing instrument D20.

New instruments

- New very high resolution gamma spectrometer GAMS 5.
- Intensive continuation of studies for IN4C.
- Feasibility study for NESCA, a Neutron Strain Scanner.

Calculation laboratory

The most significant of the studies carried out were as follows:

dynamic behaviour of the reactor vessel subjected to seismic excitation:

– modal analysis, quasi-static analysis, study of sensitivity of vibration eigen frequencies resulting from structure modifications of the reactor vessel;

– magneto-elastic study of a superconducting coil (vertical field 2.5 Tesla);

– thermo-elastic study of mirrors and monochromators under thermal load, and minimization of induced curves (contracts with ESRF);

– study of static behaviour of the vacuum box of the future instrument IN4C;

– analysis of critical rotation velocities of the IN4C chopper;

Electronics Group

The beginning of the year was characterized by the task of dismounting the experiments in the reactor hall. Some experiments had been dismounted so that they could be reinstalled relatively easily (without cables being cut, etc.) in the future. Others had been dismounted less delicately, especially in radioactive areas, where cables had in any case been corroded by radiation. Others will undergo considerable modifications during the reactor shutdown; so they will need a new construction anyway.

Some instruments or copies of them had been moved to other centres: in particular:

- IN10: simplified copy moved to NIST (Washington) - (electronics)
- IN15: simplified copy moved to SACLAY - (electronics)
- D1A: moved as a whole instrument to SACLAY
- T13A: moved as a whole instrument to SACLAY
- IN6: moved to SILOE - (electronics)
- D13C: moved as a whole instrument to SILOE.

Progress or acceptance test of new experiments.

D20: data acquisition electronics in VME for the new D20 with the 1600 Banana has been going into series production (6 crates of VME electronics) part of which is already delivered. The three dimensional real time display has been completed and improved and is already used in addition to D20 in other VME experiments with time-of-flight analysis and/or multidetectors.

IN15: acceptance was effected with certain reservations as some items could not be tested without neutrons.

D22: the first level of "Programmable Controller" has been operated and accepted. This type of electronics is based on VME but includes reliability and programming techniques of programmable controllers.

The first level of data acquisition has been installed and tested. This type of "Histogramming" accepts data from a multidetector and increments them at an event rate of 1 million per second. This was implemented in using programmable gate array logic, which is a modern way of producing hardware which can be edited and modified via software.

A joint project was started together with ESRF to show feasibility of ILL VME electronics together with UNIX architecture influenced by ESRF. DB21 was selected as an available four-circle instrument. The existing CAMAC electronics were duplicated by VME electronics. Full functionality was demonstrated to the joint ILL/ESRF working group. A major input was given to the project by the ILL Computing Department.

A demonstration was given by using an artificial neutron source on the 128 x 128 cell multidetector, with a coloured three-dimensional real time display originally developed for D20; but now used on all area detectors or time-of-flight instruments with VME.

The Electronics Group lost 50% of its technician staff, mainly detached to ESRF; this fact proves the competence of the ILL electronics staff and the modernity of ILL electronics standard, especially in respect to the VME standard, also selected as the principal standard within ESRF.

Monochromator Group

It is vital for the work of the group to have experimental facilities at hand which allow a detailed analysis of the reflection properties of large single crystals. Of course, the most important information for the purpose of the group is obtained on a neutron diffractometer. The transfer of our test instrument T13C to the nearby SILOE reactor at the CENG proved most valuable. In spite of the reduced beam quality available (fixed wavelength position behind a 4-circle instrument, small beam size, limited space) T13C was heavily demanded for numerous tasks and it produced valuable results all year long. SILOE will be shut down at the end of the year for an extended period. To cope with this situation the second diffractometer of the group T13A including the entire electronics will be transferred to LLB at Saclay.

In further compensation for the loss of neutron beam time we have upgraded our-X ray single-crystal diffractometer. It now features higher resolution (K_{a2} radiation suppressed) and a more stable mechanical design for the tube and the monochromator part. It is used for example routinely for studies on the plastic deformation of beryllium single crystals. A further X-ray generator and associated equipment which so far has served the diffraction group has been transferred to the group's X-ray lab.

During this year we have defined a number of procedures to make improved monochromator materials and we have prepared several crystals which will be assembled during 1993. For example Ge crystals as needed for D2B and for D20 will be made by a novel wafer-based technique which results in very homogeneous reflection profiles for large areas. In addition, it provides a favourable anisotropy for the mosaicity. This development driven during the last few years by L. PASSELL from Brookhaven National Laboratories has come to maturity and it can now be used in the construction of spectrometers.

A further large effort has been devoted to the growth and the characterisation of a large number of copper crystals which are needed for IN4, D9, D19 and D20.

The status of the beryllium project has been discussed on a broad basis during two workshops in Jülich (April) and in Stuttgart (November). The Max Planck Institut in Stuttgart is making an increased effort to improve the quality of the as-grown crystals by a modified pulling technique and by subjecting the crystals to high temperature annealing cycles. The present results are very encouraging and it can be expected that an appropriate plastic deformation can be achieved more readily with the new quality standard of the crystals.

A particular experiment should be mentioned: HgI_2 crystals were grown in microgravity during a mission of the American space shuttle early this year. This experiment was provided by CNES. (Actually, there was a second experiment on the growth of HgI_2 on the same flight). The Monochromator Group has been asked to characterize structural properties of these crystals on our high energy g-diffractometer and to compare them to crystals grown by the same procedure (identical furnace) on earth. Following visual inspection these experiments were the first in a series of investigations on HgI_2 crystals grown in space. The photograph on page 100 shows a specimen in its original quartz ampoule on the instrument.

Multidetector Group

Last year was the first full year without neutrons from the reactor and without users. In this difficult period the detector group was also not spared from changes. Two technicians have already left the Institut, and within the scope of staff reduction and reorganization even more sacrifices will have to be made. Fortunately, the importance of the development of new detectors for progress in physics and other sciences has been underlined by the this year's Nobel prize in physics awarded to Georges Charpak from CERN. Incidentally, Georges Charpak was a member of ILL's instrument subcommittee from 1983 to 1986. Parallelling his work, published in 1968, on one-dimensional Multiwire Proportional Chambers (MWPC) for charged particles, a technology of two-dimensional MWPC for neutrons was developed in the framework of a LETI-ILL collaboration (patent in 1968 by J. Jacobé et al.). Such position sensitive detectors (PSD) have contributed to the success of many instruments not only in particle physics but also in neutron research. That is why the ILL group is putting a steady effort into improving existing detectors as well as developing new ones based on this wire technology. Thus the prototype small angle detector of the future IN4C instrument (cf. Annual Report 1991 and figure 1) has been completed and tested with a neutron beam at the LLB, Saclay. The tests[1] have shown that the wire structure envisaged is valid and just some minor adjustments and modifications have to be carried out in the realisation of the final detector.

This year, however, the lion's share of research and development work went into Microstrip Proportional Counters (MSPC). This new approach in gas filled detectors was initated at the ILL (patent in 1986 by A. Oed) and offers many important advantages, amongst others, by overcoming the limitations in countrate capacity and spatial resolution of classical MWPCs. As already pointed out in last year's report such an MSPC works impeccably in pure noble gases without any quenching gas. All of the five noble gases and various noble gas mixtures have been tested, leading to the following conclusions[2]: the higher the molecular weight of

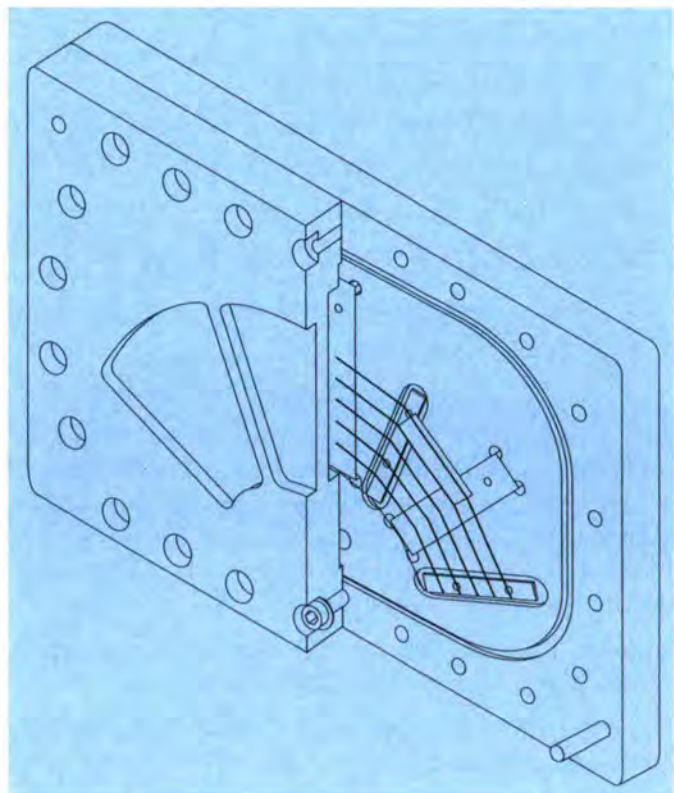


Fig. 1: Prototype of IN4C detector (3 sectors with only 6 cells each).

the noble gas the higher the limiting gas amplification, and Xenon behaves like a quenching gas when mixed with other noble gases. As a consequence of the large avalanche and absence of quenching, such an MSPC can be used as an active scintillator by making use of the light emission within the avalanche just above the MS-plate. That is why comparative measurements with the standard scintillator material NaI(Tl) have been carried out. From the spectra shown in figure 2 it can finally be deduced that the light emission in the visible region is 60 times higher with an MSPC, just used to make the avalanche in the gas, than it is with the scintillator. Furthermore, the first ever two-dimensional position sensitive detector for neutrons based on microstrips has been successfully put into operation[3]. Its design is shown in figure 3. The glass support is 0.5 mm thick and has a size of 5"x5". Through the uncovered glass surface the ion cloud around the thin anode strips induces a signal on the rear strips which are perpendicular with respect to the MS structure on the front. The signal height on the back depends on the thickness of the substrate, since the metallic strips on the front act as a screen. In this particular

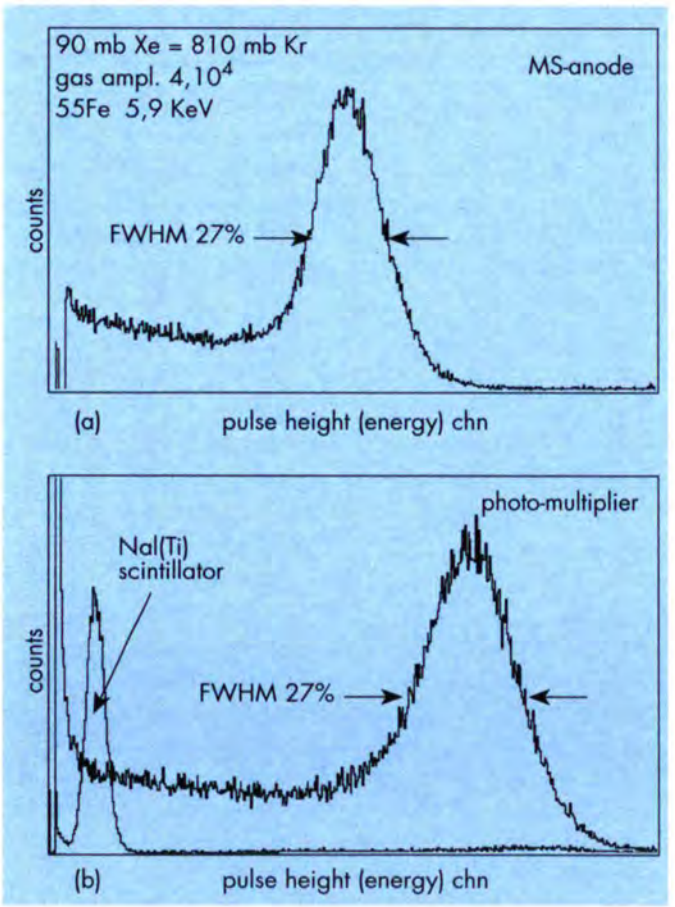


Fig. 2a: Pulse-height spectrum of the 5.9 keV X-ray measured with the charge pulses of the MS-anode.
Fig. 2b: Pulse-height spectrum measured with the PM observing the emitted light from the MS-anode during the measurement. The line on the left side serves for calibration of the multiplier by using a NaI (Tl) scintillator irradiated with the same X-rays.

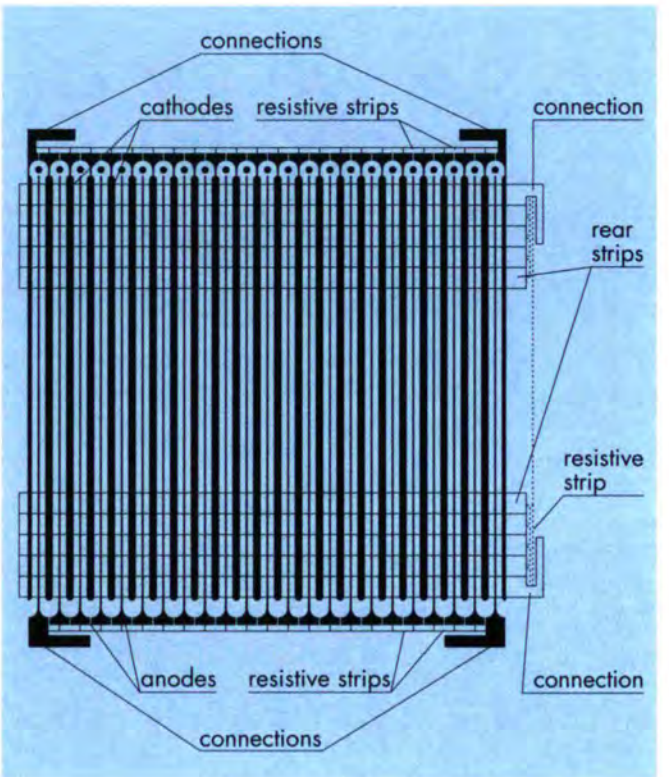


Fig. 3: Two-dimensional microstrip plate with integrated resistive line.

case, with a glass thickness comparable to the distance between the thick cathode strips the induced signal is about 1/3 of the anode signal of the front. All electrodes belonging together are linked via a resistor line which is integrated onto the plate. Thus the position coordinates can be easily determined from the charge division of the signals. To determine the spatial resolving power of the detector it was filled with 3.5 bars of ^{3}He and 1.5 bars of CF4 as the stopping gas. Neutrons from a collimated Am-Be-source were used. With a count rate of 4 n/s a measuring time of 240 h was needed to accumulate the data for figure 4. The distance between point i and "i" is about 2 mm, hence the measured position resolution is about 1 mm and corresponds to the mean variation of the centre of gravity of the ionisation tracks of charged particles of the ^{3}He(n,p)^{3}H + 770 keV reaction in the gas. It should be emphasized that an MS plate does not necessarily require an orthogonal strip structure as shown in figure 3; any structure adapted to the experiment, such as circles, or segments, etc. can be produced by the microlithographic technique. Furthermore, it is possible to bend an MS-plate in a furnace.

In the domain of transferring the MWPC technology to industry, several PSDs have been finalized by continuous support of our experts, amongst them the new D22 detector.

In these days without neutrons PSDs have already been, or are being prepared to be installed at other neutron research centres.

Fig. 4a: Letters of the ILL-logo "iLL" made from neutron absorbing B_4C. The distance between point and line of the "i" is 2 mm.

Fig. 4b: Neutron image of the above letters taken with a microstrip gas detector. Since reactor neutrons are presently not available, the detector was irradiated by a collimated Am-Be source. The exposure time was 240 hours at a rate of 4 counts per second. (see also picture on page 2).

To improve the basic installations within the ILL group a ^{3}He-gas recovery unit is under construction in collaboration with the cryogenic service of the Institut.

1) D. Feltin, Essai du détecteur prototype d'IN4C, DIM-92/198-DF

2) P. Geltenbort, A. Oed, Features of microstrip proportional counters, Conf. on Slow Neutron Imaging Detectors SPIE '92, San Diego, USA

3) J.-E. Assaf, Etude et réalisation d'un détecteur gazeux à microrubans pour l'imagerie des neutrons thermiques, Thèse 1992.

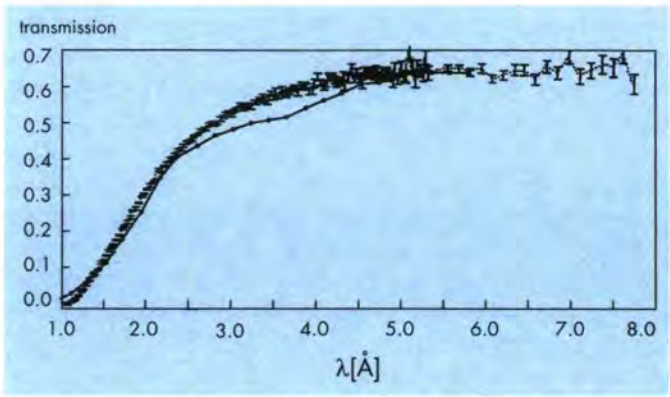


Fig. 5: Measured transmission of a supermirror bender at the Reactor of the TU München. The solid curve is a theoretical estimate using the individually determined reflectivity curves (from K. Raum, diploma thesis).

Multilayer Laboratory

Despite the lack of testing facilities due to the reactor shut-down, the multilayer group has continued the usual efficient production of neutron mirrors in response to the increasing demand for optical devices for both internal and external use.

On a commercial basis neutron guide elements have been coated with supermirrors for the Risø National Laboratory (Denmark) and polarizing supermirror elements have been supplied to the KFA Jülich. The latter are to be implemented in a wide beam analyzer for the multidetector of a small-angle instrument.

On a more collaborative basis polarizing supermirrors have also been supplied to the Technical University Delft (The Netherlands) and to LLB (France). In addition, two supermirror benders have been lent to HMI Berlin and a further bender is in use at PSI (Switzerland).

A fruitful collaboration with U. Schmidt and D. Dubbers led to the construction of a non-polarizing bender which has been installed in a beam tube of the Munich reactor. The 60 cm long, 2.3 cm wide bender effectively reduces the γ-background and maintains a useful solid angle down to 1.5 Å. The transmission of the bender, shown in Fig. 5, is well matched to the beam tube spectrum. A second focusing supermirror bender is presently under construction for the Munich reactor and a further one is planned for installation at Braunschweig (in collaboration with Stockmeyer, Jülich). In the meantime work has started on the production of polarizers for the IN11C analyzer, a project which will occupy the Electrotech evaporator for at least one year.

Besides the evidently productive side of the group's activities, a significant amount of effort has been invested in research and process development, essential to keep ILL at the forefront of neutron multilayer technology. We have profited from collaboration with A. Menelle at LLB, Saclay

to investigate multilayers (both polarizing and non-polarizing) by neutron reflection. In particular, the EROS reflectometer at Saclay was modified to operate with polarized neutrons and measurements performed on various TiCo multilayers. The experiments clearly evidenced the existence of a non-magnetic region at the surface of the Co layers. Further measurements are planned in a continued collaboration.

Another fruitful cooperation with PSI (Switzerland) has allowed a number of developments to be investigated. In particular a gradient layer monochromator has been fabricated and tested. Such a monochromator could be used to obtain a variable wavelength at constant 2θ, an interesting development for a reflectometer.

Although the evaporators have served the ILL well for a number of years, future developments will require the use of new and composite materials, thinner layers and better control of layer and interface characteristics, i.e. the deposition technology must be updated. Development towards sputtering technology is an inherent part of the group program and has been initiated with the acquisition of an rf-excited ion beam gun what will be put into operation in the near future. The controlled bombardment of a growing film by an ion beam of variable energy allows essential properties such as film stress, structure and interface roughness to be modified. The test programme will rely on continued collaboration with LLB (Saclay) for neutron reflection measurements as well as the development of in-house facilities for grazing incidence X-ray and stress measurements.

With the growing demand for optical elements in scattering experiments the development program will enable ILL to meet the needs of the future.

Publications and conference proceedings

1) O. Elsenhans, P. Boni, H. Grimmer, P. Buffat, K. Leifer and I. Anderson 11th International Conference on Vacuum Metallurgy, Antibes 1992

2) I. Anderson Proc. SPIE, San Diego 1992

3) O. Elsenhans, P. Boni, H.P. Friedli, H. Grimmer, P. Buffat, K. Leifer and I. Anderson Proc. SPIE, San Diego 1992.

Other Activities

Neutron Guides

The order for the refurbishment of the glass part of the H1-H2 guide system has been placed. The work has been continued by ILL staff with the dismantling of the glass in the housings of the swimming-pool part and in the mechanical supports of the in-pile part (see pictures on page 101). The delivery of the glass guides is planned in autumn 1993 and the mounting of the guides has to be commissioned for the reactor restart in 1994.

The design of the mechanical part for the new NG12-NG13 guides project on the vertical cold source is finished. The quotations resulting from a call for tenders are available. The decision on the project has to be taken.

The replacement of the electrical controls and the valve system for the vacuum pumps of the neutron guides has been started.

Refurbishment of the beam-shutter

The refurbishment of the beam-shutter system is scheduled to be finished for the reactor restart. The complete system consisting of the mechanical shutter, the electro-pneumatic control and the electrical control is being reviewed and rebuilt under Quality Assurance.

Computer aided design

The drawing office is working with 5 PC based Autocad Release 11 and most of the PC are connected to the local area network DECnet.

One of the two workstations, operating since 1987 for the EUCLID CAD system, was replaced by a VAX station 3100 M76 borrowed during the reactor refurbishment from the Computing Department.

Overall, the year has been dominated by the preparation of the Unix Plan, that is to say, a plan for progressively converting all the Institut's computing activities to run on Unix-based systems.

The key issue has been how to take into account the existing stock of programs which have been developed over a period of 20 years and which represent an enormous investment for ILL. Even in the absence of Unix conversion, many of them would no doubt have benefitted from being tidied up and adapted to make use of the functionality available on modern workstations, but the availability of sufficient manpower to make a comprehensive review seems in doubt, especially at this time of reductions in overall staff numbers.

Nevertheless, a proposal was made to the Spring Meeting of the Steering Committee, and subsequently revised for the Autumn Meeting, where the general outline of the Plan was accepted and an initial budget accorded to start in 1993.

The immediate aim is to have achieved the conversion of the general infrastructure (central facilities and network) before the Reactor restart, as it is feared that, from that time on, the daily obligations in respect of the experimental programme will seriously limit the rate at which conversion work can continue.

Whilst the Project will be pursued with enthusiasm, there is inevitably a feeling that, given the never ending sequence of technological developments in the computing field, long-term plans stand little chance of being adhered to for more than a few years. For example, with Digital's announcement of the arrival of the Alpha range of machines, one finally has equality between VMS and Unix in respect of performance/price ratios.

Central Facilities Service

Operations

The Group has responsibility for the following systems:

for scientific purposes-

– a cluster of 5 DEC VAX machines (8700, 8650, 3 VAXStations) running under VMS

– 2 systems running Unix (DECStation 5000-200, HP 9000-710). Together these machines (each with a license for 8 simultaneous users) provide a useful computing resource, and an environment for converting programs to Unix.

for management information services-

– a PDP11 for applications developed at ILL

– 2 microVAXes for the areas of finance, medical, benevolent fund (mutuelle)

– 2 HP systems running under Unix for new applications developed under Oracle

In the scientific area the level of activity has been:

– for the Cluster, a mean total of 800 hrs CPU/month (normalised to the VAX 8650 processor), with a peak of 1000 hrs in September and October

– for the Unix machines, 200 to 400 hrs CPU/month

Concerning these statistics, one notes that the level of use is holding up despite the Reactor shut-down, principally due to simulations and modelling calculations. The introduction into the cluster of a workstation with twice the power of the VAX 8650 has helped to speed up this type of job.

Work coming from ESRF has tended to steadily rise, reaching 100 hrs CPU/month towards the end of the year.

The Operations Group also has the responsibility of providing the first level of intervention when problems arise on the distributed terminals, printers, Macintoshes and PCs. This has enabled significant savings to be achieved on external maintenance contracts.

Systems and Networks

On the Cluster the main event has been the installation of the latest version of VMS, 5.5-1, which has introduced important changes in the verification of software licenses, management of queues and sharing of peripheral devices.

On the Unix side, the HP 9000-710 has been installed with network protocols enabling terminal access via the DECServers. A total of 3 DECStations running Ultrix is supported (2 used by DIM for structural calculations).

As part of the studies on compatibility between Unix systems, the discs on the DECStation Ultrix machine have been made accessible from the HP system (and also from the Cluster).

Concerning external networks, access to Internet has been introduced. Apart from interest in Internet as such, this has become essential because, within France, EARN is being superseded by the new regional and national research networks. The EARN link between Grenoble and Montpellier will cease to be supported in 1993, obliging users either to move to another network such as Internet, or use special links to access EARN and BITNET.

Access to the other external networks: Transpac, JANET, HEPNET, remains unaffected.

Mathematics

The environment traditionally available on VMS systems, notably NAG subroutine library and Fortran Compiler, has been installed on the Unix systems (DEC and HP).

In respect of the conversion of programs to run on Unix systems, the following preparatory work has been carried out.

The scientists have been provided with certain guidelines to aid conversion, and a range of tools has been installed on the target Unix systems.

A detailed study of Fortran 90 was made, leading to the recommendation that it seemed to offer the best solution for converting VMS Fortran programs. Currently it is a compiler supplied by NAG which is in use, but with others now coming on the market, one is looking to achieve better compatibility with libraries compiled under Fortran 77.

A study is being made of the various conversion tools which are now coming onto the market. These tend to be based on analysing the structure and quality of the program, with a view to restructuring.

The ABFFIT package (which fits data from powder diffractometers and similar), has been modified to allow the inclusion of external executable code. Additional mathematical functions now permit its application to asymmetric peaks. In this way, time-of-flight data generated at the RAL ISIS neutron source has been fitted.

A statistical analysis package, ABCDATA, offering statistical tools such as linear and non-linear regression, suitability fitting, Monte Carlo simulations, etc. has recently been completed.

To help ILL improve its image amongst the general public, the Group has played a leading role in creating on a Macintosh (together with scientists and two outside software houses) a hands-on interactive program simulating neutron scattering experiments. This product has successfully been put on display at two local science fairs, 'la Fête de la Science' and TEC92.

Graphics

The graphics environment for Unix systems has been enhanced by the addition of the NAGSPLT and NAGHPLT libraries, and the latest Bordeaux version of PHIGS/GKS.

X11 drivers have been introduced for the DISSPLA library and for client-servers between VMS and Unix.

The performance of the Tektronix colour printer has been improved by enabling it to be accessed on Ethernet under TCP/IP.

With the aim of establishing the new graphics standard, a number of studies have been carried out in close collaboration with the scientists. These include the use of MOTIF, the emulation of X11 on PCs and the future replacement of DISSPLA.

Telecommunications

The major part of the Group's activity concerns its responsibility for the complete telephone network on the joint ILL/ESRF site (designated as The Joint Telephone Service). The new exchange installed in 1991 has proved very satisfactory. Only 2 hours has been lost (on the ESRF module), this due to violent storms.

With the build up of their activities, an additional 400 lines have been installed in the ESRF sector, giving a total of 1500. The progressive transfer of ESRF staff to their permanent buildings has also generated a great deal of work.

The other area of work for this group concerns computer networks. The Group has responsibility for Appletalk (network connecting Macintoshes), many new zones of which have been installed. In ILL4 each floor now comprises a separate zone directly linked to Ethernet. Buildings ILL7, ILL17 and ILL22 also now have their own zones. The Group also provides a cabling service to the rest of the Department.

Administrative and Office Computing

Finance and Purchasing

Having decided against a major rewrite of the package, changes have been limited to some small specific improvements, including following up late deliveries, orders spread over several years, and checking the correct cost centre for charging orders. This work is done partly in-house, partly by the original supplier, DEAL. Most members of the Finance Service now have their own Macintosh for spreadsheet displays of data generated by the DEAL package.

Salaries and Personnel

The Group continues to support the HERA package for personnel management.

Office Computing

The Group supports secretaries and administrative staff, principally with the use of Microsoft's WORD (word processing) and EXCEL (spreadsheet) on Macintosh.

In-house Developments

Applications that are particular to ILL are normally developed in-house.

The ESRF's package for handling travel claims (based on Oracle) has been adapted to ILL's needs and installed on two PCs (one a data-base server, the other a workstation). It came into operation in October.

The implementation of the new system controlling access to the joint ILL/ESRF site started at the beginning of the year, and is also based on Oracle. Two HP 9000-807S computers running Unix are used, one as data base server, the other for data treatment. The watchkeepers and receptionists use PCs capable of running the applications programs. Secretaries and others authorised to input data normally use their own Macintosh, (linked by Ethernet) which, as yet lacking Oracle, provisionally operate in terminal emulation mode. This came into use in November.

Instruments Service

It might be thought that 1992 would have been a quiet year for the Service. On the contrary, the various activities associated with the introduction of Unix, including preparations for the modernisation of the network, have generated a very heavy workload for the reduced numbers of staff who have been present. In spite of the present uncertain climate, members of the Service have maintained their morale and make good progress on their projects.

The principal aims have been to

– keep the equipment in good condition, awaiting the restart of the instruments.

– complete (in so far as is possible) development on the instruments IN16, IN13, D22, IN15

– investigate possible collaboration with ESRF

– continue training on Unix

– improve the performance of the internal and external computer networks.

Maintenance

Maintenance contracts for the VAX/VMS systems have been suspended during the reactor shut-down, but breakdowns have been few and caused no problems. A VS3100/76 has been installed in the drawing office to assist the work of Mechanical Services. Considerable time has been spent helping Macintosh users; unfortunately the needs here continue to outstrip resources.

Developments on Instruments

Here one has tried to ignore the general uncertainty surrounding the future of instrument system design, in order to complete the projects in hand. The IN13 package has been completely rewritten on transferring from a PDP11 to a VAX/VMS; general tests have been carried out on IN16; the ILL part of IN15 has been installed and tested; on D22 testing proceedes as the various electronics modules become available.

Collaboration with ESRF

Since May a number of members of the Service have worked intensively on a joint ILL/ESRF/EMBL project. Within four months a typical ILL instrument package (essentially that of DB21) had been converted from VMS to Ultrix, including the interface to OS9 and VME. It was considered of particular importance to create a general-purpose standard interface between the computer and the VME crate.

Although at the present time it seems uncertain as to whether this design can also be used by ESRF, it has given ILL staff confidence that they can create Unix-based systems within tight time schedules.

The other area of collaboration is in the field of networks (internal and external). The Service maintains the Ethernet link between ILL and ESRF, and also provides access for ESRF to Internet. It has also provided some assistance to ESRF on their own sector of the network.

Unix Familiarisation

The DB21 project mentioned above gave staff very valuable experience on a real Unix project. Having developed the program on a DECStation under Ultrix, the portability of the interface to OS9 was checked by transferring it to HP-UX and VAX/VMS.

A user interface based on OSF/Motif is also being developed.

The protocol TCP/IP is becoming increasingly important on the network, and better tools for managing it have been installed.

Networks

The computer network is becoming an essential element in almost all computing activities and has to be continually improved. One is still in the process of completing coverage for all buildings, and the bridges between Ethernet and Appletalk have been extended and improved. The start-up of the site entry management project has entailed a number of additional terminal connections being made, and a fibre optic link between ILL7 and the new guardhouse was needed. The ILL/ESRF Common Building has been connected to the ILL network. With rapidly increasing growth of CAD facilities, the Mechanical Services laboratories have had to be completely recabled.

Some measurements have been made in preparation for providing a dual protocol solution on the terminal network. The product DECMcc has been installed to provide network surveillance for both DECnet and TCP/IP. Tools are being developed to measure traffic passing through the routers to the external networks.

Support for external organisations

The Service has played its part in the Institut's plan to provide help for other organisations during the shut-down. One programmer has been detached for three years to EMBL, whilst an engineer and a programmer have spent several months at HMI, Berlin.

The Service has also participated in the design of the local research network, ARAMIS.

Nuclear Physics and Special Instruments Group (NUPSI)

The Group participated in the preparation of the Unix Plan, and has subsequently started to study how the ideas should be interpreted in terms of new instrument control systems. Progress has been affected by the fact that one of the two Group members spent seven months at HMI, Berlin, as part of the plan to make staff available to other centres.

Existing Systems

A new version of the PN1 program has been installed, with a PC Vectra to interface user commands.

The experiments GAMS 2/3 and GAMS 4 have been transferred and reinstalled. Likewise, PN2 (BILL) has been moved to the Guide Hall for use with an autonomous source.

Future solutions

In examining possible future solutions, it seems that the Nuclear Physics instruments could well profit from using some of the new dedicated software, intended to run on PCs, that are now coming onto the market. Among the products which have been tested on S20A have been 'Visual Basic' of Microsoft and 'Labview' of national Instrument. A CAMAC-PC coupler has also been satisfactorally tested.

The design of the acquisition system for the new instrument GAMS5 has started, but seems to need a specialised data acquisition interface.

Data and Projects Group

The Group has been preoccupied with studies for changing over to Unix. Apart from direct involvement in preparing the formal Plan, there has been much practical work on the Ultrix systems at ILL, and also on HP-UX and SUN-OS systems, to which access was generously offered by ESRF. This enabled some real appreciation of the subtleties of these differing flavours of Unix and Posix implementations to be gained directly.

Implementing Unix system facilities to match those presently in use with VMS has required some research and experiment; inevitably this has required members of the Group acquiring competence in C language programming. Faced with providing simple-to-use tools for exploiting sophisticated libraries such as PHIGS, there has been collaboration with ESRF on basic scientific graphics. First steps in developing Motif-based X-window interfaces were helped by acquisition of the DEC-VUIT interface builder software. After some practice, the Group was able to help other members of the Department in the use of this GUI toolkit.

In gaining the background knowledge necessary to aid conversion of scientific programs using up-to-date software standards, the Group has also experimented with the Fortran 90 compiler. This augmented language would appear to offer as standard many useful DEC extensions to Fortran 77. It has also been used in tests of mixed-language programming on the different systems.

As a complement to conversion of ILL programs, easy direct access to Internet has stimulated the search for and evaluation of public domain programs for data presentation and treatment. Use of these packages would eliminate the strict license constraints on commercial packages such as PV-WAVE which preclude developing and offering portable data treatment facilities with an advanced user interface. It is likely that such research will significantly save effort in developing equivalent software in-house. Nontheless, the WAVE software is continuing to be maintained and updated since, for the present, it provides comprehensive functionality, against which other packages can be measured.

Disappointing delays in the manufacture and delivery of the Transputer-based multidetector interface restricted progress on this Project to general studies of monitoring and debugging programs distributed over a Transputer network environment.

– REACTOR DIVISION P.148

Major steps in the life of the reactor

On 28.11.91 the Steering Committee decided on the refurbishment of the reactor, initially requesting a study and costing of the various possible options. This task, carried out jointly by the ILL teams and an international Consortium including AEA Technology (UK), SIEMENS (Germany) and TECHNICATOME (France) was carried out between November 1991 and February 1992, when the final report was forwarded to the Steering Committee which, on 13 February 1992, opted for the replacement of the reactor vessel.

Following the Steering Committee's decision in May 1992 on the refurbishment of the reactor, the ILL Management delegated the responsibility for this to the Head of the Reactor Division, assisted by a 'Project Group' and an 'Industrial Architect'.

The Project Group applies the directives given by the Management, and prepares at a technical level all the operations to be carried out as a function of the desired aims. It deals with the technical follow up of the operation and the financial management. It places the contracts with suppliers of goods and services.

The Project Group also provides the liaison with the Industrial Architect, consisting of engineering companies representing the three member countries (UK, Germany, France). The Industrial Architect is responsible for the ordering of certain elements of the reactor, and in particular for the operations on the site between the clearing of the swimming-pool and the leakproofing tests of the 'second barrier' after installation of the new reactor block. It is responsible in particular for the equipment ordered being available at the appropriate time.

1. Progress of work

Until the decision in May 1992 to replace the reactor block, the work initiated was limited to dismantling which was common to the various options envisaged: this covered essentially the removal of experimental instruments and of internal elements in the reactor block which could be dismantled without constituting irreversible steps.

The work of the reactor teams in 1992 was subsequently centred on the separation of the reactor block from all the circuits connected to it; this phase ended on 24 November 1992 with the transfer of the reactor block into the storage pool, where it will be cut up before disposal.

1.1. Work in the level C experimental hall in the reactor building

The completion of the work of removing the experimental instruments gave access to the beam tubes and made it possible to withdraw them and their associated beam shutter plugs. The following beam tubes have been removed in this order: H3, H4, H8, H10, H11, H6, H7, H13, H1/H2, IH3, IH4, IH1, H5, H9.

As the removal work progressed, the most active front parts of the beam tubes were cut up in the hot cell and disposed of; beam tube H1/H2, because of its unusual dimensions, had to be cut up by a special machine working under water in the H1/H2 swimming-pool. This operation took place between early March and early June 1992. Certain non-active rear parts of beam tubes have been put in store and will be used for production of new replacement parts.

The withdrawal of the beam tubes was completed at the end of June, and was followed by the removal of the coupling sleeves and the annular shielding plugs when the level of radioactivity permitted.

The coupling sleeves were removed in the following order: IH4, IH3, IH1, IH2, H9, H11, H10, H8, H6, H3, H5, H4, H12, H7, H13. At the beginning of September, all the coupling sleeves had been removed, apart from that of beam tube H1/H2, which was taken out on 3 December 1992, after the reactor block had been transferred into the storage pool.

The following stage consisted of the removal of the annular plugs of the horizontal beam tubes kept in place until the removal of the reactor block into the storage pool, and the removal of the waterproofing sleeves, after cutting up the bellows. This operation was completed at the end of December 1992.

1.2. Work in the level D swimming-pool hall in the reactor building

The removal of the components which could be dismantled from the interior of the reactor block has continued, and at the time of the transfer only the anti-turbulence grids and the diffuser remained inside. All the assemblies in the swimming-pool whose presence causes inconvenience for the removal of the reactor block or the inspection of the lining have also been removed.

On conclusion of this dismantling work, and after obtaining the necessary authorisations from the nuclear safety authorities (DSIN), the collectors connecting the heavy water circuits to the reactor block and the tail of the tank permitting passage of the push rod of the control rod were cut up.

To permit the reactor block to be transferred into the storage channel, the extrusions on the reactor vessel were cut off (except for H1/H2 where the cut was made at the end of the coupling sleeve).

In parallel to the disconnection work on the reactor block from the associated circuits in the swimming-pool, the work necessary to receive it was carried out in compartments 1 and 2 of the transfer pools.

As it was necessary to remove the used fuel elements from the storage channel before the reactor block was transferred there, they were transported to the Pégase storage pool at Cadarache between 19 October and 16 November 1992.

1.3. Evacuation of radioactive waste

The components removed from the reactor which are not reused will be conditioned as waste and dispatched to the storage areas envisaged, in close collaboration with the CENG services.

At 1 December 1992 the quantity of radioactive waste evacuated was as follows:

3 cylinders C1, 9 cylinders C3, 2 containers of 5 m^3, 100 drums of 100 l, 10 drums of high activity waste, for a total activity of approx. 10^3 TBq.

1.4. Metrology of the reactor block

Precise measurements were made during the construction phase. After withdrawal of the beam tubes, and before the reactor block was taken out, geometrical measurements were taken to evaluate the variations from the original situation; the axis of the waterproofing sleeve of the control rod and the centre of the waterproofing sleeves of the chimney and the hot and cold sources were noted before dismantling the reactor block.

2. Studies carried out or in progress

2.1. Verification of the reactor block

The new reactor block has been checked by calculations in accordance with the ASME Code, Section III. The results show that the structures are compatible with stresses in normal operation, transition phases and in exceptional situations. The fatigue behaviour of the structures examined is compatible with the lifetimes envisaged.

2.2. Seismic studies

Since the construction of the reactor, the seismic conditions to be taken into account in the calculations have been modified. A verification of the reactor shell carried out in 1984 confirms that the present building will withstand the 'SMHV' (Maximum Historically Probable) earthquake.

The reactor block and the internal structures (swimming-pool, transfer pools and hot cell) are currently the subject of verifications by calculation.

2.2.1. Measurements of the ground modulus

The ground modulus of the ILL site has been measured by the Cross Hole method. For this purpose three 35 m deep holes were made near the reactor building. In addition, samples of the ground were taken and the characteristics of the samples were determined. The results give a better indication of the actual characteristics of the ILL site, to be taken into account in the calculations under § 2.1.

2.2.2. Vibration behaviour of the reactor block

It is difficult to determine theoretically a number of characteristics such as damping and the added mass of water, which influence the inertia of the structures. ILL has accordingly had vibration measurements carried out for the whole of the reactor block, first with the heavy water collectors connected, and then with them disconnected. The results make it possible to determine precisely the actual characteristics to be taken into account in the calculations. It should be noted that the amplitudes measured in the tests are of the order of magnitude of the amplitudes predicted for a 'SMHV' earthquake. This 'full scale test earthquake' was tolerated by the structures with no detectable damage and with no permanent deformation. The data obtained during these tests made possible part of the calculations in § 2.2.3. ('SMHV' earthquake behaviour).

2.2.3. Behaviour of the reactor block

Calculations were carried out on the basis of a three-dimensional model subjected to quasi-static stress. The conclusion was that the structure is resistant to the 'SMHV' earthquake stresses without damage. The dynamic calculation is in progress, and will be completed before the end of 1992.

2.2.4. Internal structures

The study of the behaviour of the swimming-pool, the transfer pool and the hot cell is in progress. Modelisation is complete and the first results are available.

Although it is not yet possible to give a final assessment of the behaviour of the structures, it may be noted that the initial results are very encouraging.

2.3. Design study for the new anti-turbulence grid

The design study has started for a new smaller anti-turbulence grid, to facilitate its removal if necessary: the results obtained to date are extremely encouraging; at the end of the current experimental stage, it should be possible to submit this for approval by the safety authorities early in 1993.

2.4. Study of metal seals

An analysis and a test programme have been initiated to confirm the operation of the metal seals which ensure leakproofing in the highly irradiated areas in the reactor block. The results will make it possible to optimise the type of seal and the installation conditions; the current results have already enabled us to stop definitively the sampling of flanges from deliveries.

3. Purchases

3.1. Aluminium AG3 NET

The orders for AG3 NET are not encountering any significant difficulties; deliveries are in progress and will be completed by the end of 1992 or early 1993; all the stocks necessary for production in progress have been purchased.

3.2. Manufacture of the new reactor block

The preparation work for the manufacture of the reactor block has started. The company concerned has drawn up its schedule and at the end of 1992 is carrying out welding tests, qualification of welders, various tests for making extrusions, production planning and quality assurance programme. The delivery of the reactor block on the ILL site is scheduled for not later than 31.12.93.

3.3. Tools for cutting-up the reactor block

The production of the tooling is progressing normally.

The turntable on which the reactor block was put after removal was delivered on 13 November 1992 and installed in the storage pool.

The cutting tools for the internal elements of the reactor block were delivered in November and December 1992.

4. Timetable

The various operations are progressing overall according to plan, which makes it possible to envisage the reactor restart around the middle of 1994.

Finance

Implementation of the 1992 Budget

The 1992 budget is characterized by the authorization of the Steering Committee to start work on refurbishment of the reactor. Total expenditure is expected to amount to approximately 310.7 MF, comprising a normal budget of 242.4 MF and the setting-up of a reserve for the reactor refurbishment of 65.4 MF. It is assumed that out of this reserve the Institut will use 42.6 MF in 1992, thus leaving a balance of the reserve of 22.8 MF at the end of 1992.

The following table shows the changes in expenditure and income between 1991 and 1992:

Expenditure	Expenditure 1991		Estimated Expenditure 1992		Change
	MF	%	MF	%	%
1. Staff costs	178 546	56.3	173 720	55.9	-2.7
2. Fuel elements	36 257	11.4	9 774	3.2	-73.0
Consumables	22 048	6.9	16 551	5.3	-24.9
Long term supplies and services	10 835	3.4	6 756	2.2	-37.6
Short term supplies and services	10 750	3.4	7 731	2.5	-28.1
Travel	2 808	0.9	2 596	0.8	-7.5
Miscellaneous adm. costs	4 598	1.4	3 025	1.0	-34.2
Taxes and fees	1 371	0.4	1 341	0.4	-2.2
3. Operation	**52 410**	**16.4**	**38 000**	**12.2**	**-27.5**
Buildings	7 000	2.2	2 950	0.9	-57.9
Equipment	7 483	2.4	2 239	0.7	-70.1
Instruments	13 261	4.2	11 035	3.6	-16.8
Other investments	8 822	2.8	4 682	1.5	-46.9
4. Total Investments	**36 566**	**11.6**	**20 906**	**6.7**	**-42.8**
5. Normal Budget (1-4)	**303 779**	**95.7**	**242 400**	**78.0**	**-20.2**
Reactor refurbishment:					
6. Setting-up of reserve	**(13 542)**	**4.3**	**(65 400)**	**21.1**	**NC**
7. Expenditure			**42 600**		
8. Balance of reserve at end of year	**13 542**		**22 800**		
9. Additional reserve	**-**	**0.0**	**2 943**	**0.9**	**NC**
10. Total expenditure (5 + 7 + 8 + 9)	**317 321**	**100.0**	**310 743**	**100.0**	**-2.1**

Comparison of 1991 and 1992 Budgets - Income

Income	Income 1991		Estimated Income 1992		Change
	MF	%	MF	%	%
Collaboration with ESRF	1 451	0.5	1 639	0.5	+ 13.0
ILL's own income	7 324	2.3	11 004	3.6	+ 50.2
Spanish, Swiss, Austrian contributions	13 689	4.3	10 850	3.5 *	- 20.7
Associates' contributions	281 672	88.8	287 250	92.4	+ 2.0
Carry forward 1991 on 1992	8 430	2.6	-	-	NC
Use of general reserve	4 755	1.5	-	-	NC
Total income	**317 321**	**100.0**	**310 743**	**100.0**	**- 2.1**

** Spain: 4 650 KF, Switzerland: 4 650 KF, Austria: 1 550 KF.*

The normal budget was decreased from 303.8 MF in 1991 by about 20 % to 242.4 MF in 1992 in order to enable the setting-up of the reactor reserve. This decrease affected all parts of the normal budget.

Staff costs have been reduced by 2.7 %. This decrease shows the result of the large number of departures during the year 1992: staff will decrease from 469 at the beginning of 1992 to about 421 at the end of the year (see section on Personnel and Human Resources). Also the Institut has seconded and detached staff to other scientific institutes and to industry in order to make economies.

The decrease in fuel costs is due to the fact that in 1992 the Institut has decreased its fuel element order to one element. The remaining irradiated fuel elements have been transported from the reactor to Cadarache for interim storage, thereby liberating space in the reactor swimming-pool for the refurbishment project.

Operation costs have been decreased by 27.5 % due to the effect of the reactor shutdown and the absence of scientific experiments.

The investment sector shows a particularly pronounced decrease of 43 % between 1991 and 1992. In the scientific sector the emphasis was put on the termination of the cold source instruments (IN10C, D22, IN15) as well as on improvements of existing instruments (D20, D18, refurbishment of guides). Two major infrastructure projects, jointly financed with ESRF, were finalized in 1992: the Joint ILL/ESRF Building (library, theoreticians' offices, restaurant) and a new guard post at the site entrance.

As planned, the execution of the budget 1992 permitted the setting-up of a reserve for the refurbishment of the reactor of 65.4 MF. Expenditure for the project in 1992 is estimated at 42.6 MF, thus leaving 22.8 MF at the end of the year to be carried forward.

Forward Look

Clearly the priority objective for the Institut in 1993 and 1994 remains the refurbishment of the reactor and the preparation for the restart of the reactor and of scientific experiments. Consequently the 1993 Budget, adopted by the Steering Committee on 26 November 1992 with total expenditure of 326.9 MF comprises a Normal Budget of 232.3 MF and a setting-up of a reserve for the refurbishment project of 94.6 MF.

The Institut plans to finalize the reactor refurbishment in the middle of 1994. The financing of this last part of the project is assured by the carry forward of the reactor reserve remaining from the years 1991, 1992 and 1993.

Purchasing

The Purchasing Group participated actively in all commercial aspects of the refurbishment of the reactor and carried out a number of other purchases mainly in the scientific sector.

Reactor refurbishment

During the first three months of the year Purchasing cooperated with the Project Group for the reactor refurbishment in the appraisal of the tenders received for the manufacture of the new reactor block and other major orders in this connection. After the decision to go ahead with the reactor refurbishment at the Steering Committee meeting in May 1992, and the first meeting of the Subcommittee Refurbishment in June 1992, the first major orders were placed, in particular:

– GRAVATOM (GB) for the cutting tools

– NOELL (D) for tools for cutting the upper part of the reactor block;

– NTG (D) for the supply of the waterproofing sleeves;

– AEA TECHNOLOGY (GB) for the development and testing of a folding anti-turbulence grid;

– Aluminium supply (AG3 NET) for the refurbishment project from RHENALU (F) for the sheets, FORTECH (F) and VAW (D) for the forgings, and AVIATUBE (F) for the tubes.

The contract for the construction of the reactor block was awarded to ZEPPELIN (D) on 16th September 1992.

The contract with the industrial architect, a Consortium consisting of TECHNICATOME (F), SIEMENS AG (D), and AEA TECHNOLOGY (GB), with TECHNICATOME as lead company was signed on 28th September 1992.

Forthcoming major orders for the project include the coupling sleeves and their bellows, the new reactor chimney, the painting of the reactor building, and fire prevention

Other purchases

Apart from the Reactor Division a number of important orders were placed in 1992. Notably, the manufacture of the optical part of the neutron guides H1-H2 was awarded to NEUTRONS INSTRUMENTATION (F). REYDEL (F) won the contract for the construction of the new guard post at the entrance to the common site (financed 50% by ESRF).

For the instruments, the most significant purchases were

– graphite monochromators for D20 from UNION CARBIDE (USA),

– induction coils for IN11 from BRUKER (D).

After an international call for tenders DUHAMEL (F) were chosen to develop the new ILL sample environment controller. Similarly, NORDIKO (GB) were awarded the contract for the supply of an ion source to be used for thin film deposition for the development of supermirrors.

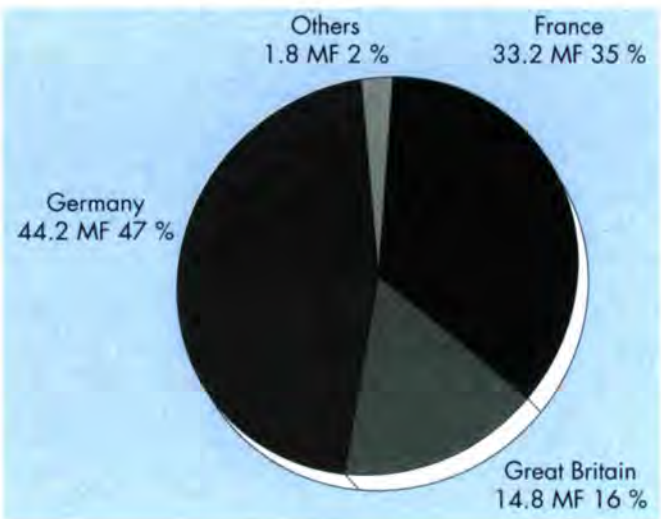
In the Computing area, workstations have been bought from the major Unix hardware suppliers - HEWLETT PACKARD, DIGITAL and SUN - with the aim of testing the equipment in line with the planned conversion to Unix.

Distribution of purchases in the member states

Considerable savings were achieved by competitive tendering for major purchases as well as by negotiating discounts with regular supppliers. Offers were compared on an exworks basis so as not to disadvantage British and German firms compared with local suppliers.

The distribution of ILL purchases (orders exceeding 50 KF) in the first 10 months of 1992 is shown in the diagram. 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.

Distribution of ILL purchases (orders > 50 kF)



Transport and Customs

The organization of the transport and customs formalities for the movements of goods across Europe requires considerable attention. After 1st January 1993, the formalities should become much simpler. In this respect, the purchasing and finance groups are currently busy preparing for the *single European market* which involves entering the new VAT numbers for all ILL's suppliers and clients as well as other modifications to the accounts and purchasing system.

Stores

In July 1992, the three ESRF storemen left the ILL stores to set up their own stores. Whilst ESRF establishes its stock of equipment, ILL stores continues to supply the whole range of items to ESRF personnel. The two institutes will aim, as far as possible, to provide complementary ranges of items held in stock, and will continue to operate a Joint Raw Material Stores.

Personnel and Human Resources

The Personnel and Human Resources Service (SPRH), consisting of two groups, Personnel Management and Human Resources, has been extremely busy for the whole of 1992, in addition to its normal work, with the preparation of special measures to adapt the staff situation to the ILL's present and future constraints. These measures include among others the drawing up of an early retirement scheme to take effect from 1 July 1993 (cf staff movements below).

Human resources

Training programme for ILL staff

In accordance with French law, 1.4 % of the ILL's total payroll 1992 is allocated to training. The Institut organises courses in various fields: languages, computing, technical fields, management etc. The aim of these courses is to help the personnel in improving and developing their professional skills, and also to assist them in their career, or in finding another post.

During the reactor shutdown, there have been many staff movements: many people have been transferred from one service to another - in particular to the Reactor Division - and sometimes needed new skills. Training was one way for them to improve their knowledge and to be more quickly operational in their new post. A total of 254 persons attended training courses in 1992.

Staff movements

At 31.12.91 there was a total of 469 staff in post, and at 31.12.92 the figure was 421, which is a considerable reduction in personnel. This is the result of the personnel policy during the reactor shutdown. After the definitive decision on the reactor shutdown, the following measures were introduced: no recruitment except in the Theory College, and for exceptional cases (in the safety area for instance) authorised by the Director ; full use of retirement at age 60 (as provided for in the Collective Agreement) ; negotiated departures in appropriate cases. In addition to these measures staff movements have been encouraged inside and outside the Institut, in the form of detachments, secondments, etc...

In 1992 the following measures were implemented as provided for in the Collective Agreement:

- **28 secondments** of staff members to other laboratories, while maintaining ILL contracts
- **9 detachments**: suspension of ILL contract to enable a staff member to sign a contract with another institute. Staff members retain the right to return.
- **7** persons have taken **unpaid leave**.
- **5** persons have taken advantage of an agreement signed by the ILL Management and the Unions on June 15, 1992 on **half-time working**.

The numerous departures in 1992 have slightly changed the breakdown by nationalities

• French	:	63.2 %	instead of 61.6 % in 1991
• German	:	16.4 %	instead of 17.5 % in 1991
• British	:	14.7 %	instead of 15.1 % in 1991
• Others	:	5.7 %	instead of 5.8 % in 1991.

The table below shows the changes in 1992.

Integration of personnel

French courses

French courses are considered as a significant element in the integration process. They were set up and organised for two main reasons: to help the new non-French staff in adapting to their professional context by learning French as soon as possible, and to permit them and their families to integrate better in the French way of life.

During the school year 1991-1992, 100 pupils attended 8 courses at different levels. These courses are open to members of other laboratories subject to availability of places. In 1991-1992 there was a considerable participation by ESRF staff (46 persons).

Staff complement situation in 1992
(by categories and nationalities)

	POSITION ON 31.12.91					CHANGES IN 1992 AND POSITION ON 31.12.92													
1 - CADRES	G	B	F	O	T	G			B			F			O			TOTAL		
						Recr.	Dep.	Total	Recr.	Dep.	Total	Recr.	Dep.	Total	Recr.	Dep.	Total	Recr.	Dep.	Total
SCIENTIFIC SECTOR																				
- Scientists (permanent)	14	4	5	7	30		- 2	12			4			5		- 7	7		- 2	28
- Scientists (non permanent)	15	7	10	6	38		- 4	11	+ 1	- 2	6	+ 1	- 7	4	+ 5	- 7	4	+ 7	- 20	25
- Engineers			2		2									2						2
TOTAL	29	11	17	13	70		- 6	23	+ 1	- 2	10	+ 1	- 7	11	+ 5	- 7	11	+ 7	- 22	55
OTHER "CADRES"	16	9	37		62	+ 1	- 1	16		- 2	9	+ 1	- 3	35				+ 2	- 4	60
TOTAL CADRES	45	20	54	13	132	+ 1	- 7	39	+ 1	- 3	19	+ 2	- 10	46	+ 5	- 7	11	+ 9	- 26	115
2 - THESIS STUDENTS	9	8	5	2	24		- 3	6		- 3	5		- 2	3		- 1	1		- 9	15
3 - NON CADRES																				
- Technicians	17	29	132	3	181		- 3	14		- 2	26	+ 1	- 7	126			3	+ 1	- 13	169
- Others	11	14	98	9	132		- 1	10		- 5	12	+ 3	- 10	91			9	+ 3	- 13	122
TOTAL NON-CADRES	28	43	230	12	313		- 4	24	0	- 5	38	+ 4	- 17	217			12	+ 4	- 26	291
TOTAL	82	71	289	27	469	+ 1	- 14	69	+ 1	- 10	62	+ 6	- 29	266	+ 5	- 8	24	+ 13	- 61	421

G: German, B: British, F: French, O: Others, T: Total

International education

International 'sections' within the French education system for the children of non-French parents have been running for several years in Grenoble. ILL, like ESRF, has close contacts with the schools concerned, with two aims: firstly to help foreign staff to become familiar with the education system their children are entering, and secondly to ensure that the existing system is improved. There are such international 'sections' in primary schools, at the Ecole de la Houille Blanche (German, English, French as a foreign language) and the Ecole Jean Jaurès (Italian). At the secondary level the international 'sections' are at the Collège and Lycée International Stendhal, with a Spanish 'section' opened in September 1991.

Together with ESRF, the Institut is closely following the further development of international education in Grenoble, which remains an important condition for attracting qualified staff.

Communication

The ILL magazine "La Boîte à Neutrons" was founded in 1990 and has been running successfully for three years. It is a twelve-page magazine which normally appears three times per year (except in 1992, when it was only possible to produce two issues, for economic reasons). Its main goal is to inform staff in non-specialist language about technical developments and science done at ILL, and about other topics of general interest.

Personnel Management

Salaries

A salary agreement was signed by the Management and the SA-ILL union on 12 May 1992 providing for general salary increases in 1992 as follows:

1.2 % on 1 May 1992
1.0 % on 1 October 1992
0.6 % on 1 December 1992

A meeting of the signatories will be held at the beginning of 1993 to review the application of this agreement. An adjustment may be made as a function of general economic trends and the situation of the ILL.

ESRF / ILL restaurant and cafeteria

Since 20 July 1992 a new restaurant has been available to staff in the ILL / ESRF joint building on the common site. Adjoining it a cafeteria was opened a few weeks later.

List of seminars

College 2

Theory

"Le modèle de Hubbard 1d avec interaction entre proches voisins".
J. VOÏT, ILL, Grenoble, France.

"Effet Kondo quadrupolaire".
P. NOZIERES, ILL, Grenoble.

"Théorie des multicouches supraconductrices ferromagnétiques".
A. BUZDIN, University of Moscow, Russia.

"The spin glass nature of tweed precursors in martensitic transformations".
J.P. SETHNA, Cornell University, Ithaca, New York, USA.

"Correlation functions of the one dimensional Hubbard model in a magnetic field".
H. FRAHM, TU Hannover, Germany.

"Superconducting phase transitions in a magnetic field".
K. SCHARNBERG, Univ. of Hamburg, Germany.

"Uncertainty principles, quantum fluctuations and broken symmetries".
S. STRINGARI, Univ. di Trento, Italy.

"Problems on vesicle shapes".
B. FOURCADE, ILL, Grenoble, France.

"Transport properties of anyons".
D.V. KHVESHCKENKO, Landau Inst. Moscow, Russia.

"Dynamics of spinoidal decompositions".
S. ALEXANDER, Weizmann Institute, Rehovoth, Israël.

"Strong coupling phases of two Hubbard chains generated by interchain hopping"
M. FABRIZIO, SISSA, Trieste, Italy.

"Solitons and dislocations for the current conversion problem in charge density waves".
S. BRAZOWSKII, Landau Inst. Moscow, Russia.

"Heavy fermion superconductivity".
N. GREWE, Darmstadt, Germany.

"Quantum anti-ferromagnetism in 2-d".
H. CAPELLMANN, Aachen, germany.

"The normal state transport problem in cuprates".
J. WHEATLEY, ILL, Grenoble & Cambridge, UK.

"A possible link between the local oxygen ordering and the superconducting transition temperature T_c in $Yba_2Cu_3O_{6+x}$".
J. VITTING ANDERSEN, LTPCM, INPG, Grenoble.

"Decagonal quasicrystals: where are the atoms ?".
S. BURKOV, McMaster Univ., Canada & Landau Inst., Moscow.

"Monte Carlo studies of the Haldane gap in quantum spin chains".
S.V. MESHKOV, CRTBT, CNRS, Grenoble and Inst. of Solid State Phys. Chernogolovka.

"New approach to the microscopic theory of Fermi systems".
V. KHODEL, Institute of Atomic Energy, Moscow.

"The virtual exciton mechanism of superconductivity".
M. CYROT, Lab. Louis Néel, CNRS & Univ. Joseph Fourier, Grenoble.

"Fluctuation conductivity in layered high T_c superconductors".
L. REGGIANI, Univ. di Salerno, Italy.

"The 2 dim x-y model and its application to superconductivity".
H. BECK, Univ. of Neuchâtel, Switzerland.

"Vortex liquid phase in high T_c and 2d normal Bose liquids at T = 0".
M. FEIGELMAN, Landau Inst., Moscow.

"Systèmes de fermions fortement corrélés: la limite de grande dimension comme théorie de champ moyen".
A. GEORGES, Laboratoire de Phys. Théorique, ENS, Paris.

"The dilute 2d Fermi gas: bound states and Fermi liquid theory".
I. ENGELBRECHT, Urbana, USA & ILL, Grenoble France.

"Kondo insulators".
A.J. MILLIS, Bell Labs. USA.

"Phase diagram of doped Lanthanum - Copper oxides (214): slave boson approach".
P. RISEBOROUGH, Polytech. Univ. New York, USA.

"Vortex fluctuations in layered high T_c superconductors".
K. FISCHER, Forschungszentrum Jülich, Germany.

"Anomalous dimensions far from equilibrium and the propagation of turbulence in superfluid helium".
N. GOLDENFELD, Univ. of Illinois, USA.

"Hydrodynamics of polarizable liquids".
M. LIU, Univ. Hannover, Germany.

"Pseudo-gaps and Bags in High T_c materials".
R. SCHRIEFFER, N.H.M.F.L., Tallahassee, Florida, USA.

"Van der Waals like interaction of domain walls".
A. LEVANYUK, ILL and Inst. of Crystallography, Moscow, Russia.

"Phase transitions in the vicinity of incipient tricritical points".
A. LEVANYUK, ILL and Inst. of Crystallography, Moscow, Russia.

"The third order optical nonlinearity of metal-halogen complexes and polymers".
Xin SUN, Fudan Univ. Shangai, Japan.

"Courants permanents, paramagnétisme orbital et rigidité spectrale dans les systèmes mésoscopiques".
G. MONTAMBAUX, Phys. Solides, Orsay, France.

"Electron-phonon interaction in doped Mott-Hubbard insulators: freezing electron correlations".
J. ZAANEN, AT & T Bell Labs, USA.

"Is there a universal wetting agent ?"
J. TREINER, IPN, Orsay, France.

"De l'ordre au chaos: propriétés génériques de quelques surfaces libres".
C. MISBAH, ILL, Grenoble, France.

"Phase transitions in the half filled Hubbard model".
P. KOPIETZ, M.P.I. Stuttgart, Germany.

"Larmor precession in superfluid ^{3}He: new ordered state of condensed matter".
G. VOLOVIK, Institut Landau, Moscow & CRTBT-CNRS, Grenoble, France.

"Exact results for a Hubbard model with linear dispersion".
F. GEBHARD, Univ. Marburg, Germany.

"Approches numériques pour des systèmes de fermions fortement corrélés".
J.C. ANGLES D'AURIAC, CRTBT, CNRS, Grenoble.

"Infinite dimensions as mean-field theory for disordered and interacting systems".
R. VLAMING, Univ. Aachen, Germany.

"The "antiferromagnetic" state of the heavy-fermion superconductor URu_2Si_2: Is it really antiferromagnetic or something more exotic ?"
M. WALKER, Univ. of Toronto, Canada & ILL, Grenoble, France.

"Theory of a superconductor with a tricritical point".
I. FOMIN, Institut Landau, Moscow, Russia.

College 3
Fundamental and nuclear physics

"Structure of high spin states in ^{87}Nb".
A. JUNGCLAUS, ILL, Grenoble, France.

"Performance of microstrip detectors".
A. OED, ILL, Grenoble, France.

"Magmatic processes at destructive plate margins".
R. OLIVER, ILL, Grenoble, France.

"Photon scattering experiments using polarized Bremsstrahlung".
C. WESSELBORG, University of Giessen, Germany.

"Recent developments for silicon based monochromators".
A. MAGERL, K.D. LISS, ILL, Grenoble.

"The problems and achievements in investigating cascade gamma-decay of heavy-nuclei compound-states".
A.M. SUKHOVOY, Dubna, Russia.

"Nuclear structure investigations in Gd 156".
J. KLORA, ILL, Grenoble & TU München, Germany.

"Transmutation of fission products and transuranium by high energy neutron".
H. HARADA, Brookhaven National Lab., New York, USA.

"Transmutation of fission products".
H. TAKASHITA, Brookhaven National Lab., New York, USA.

"Weak vector coupling constant from neutron beta-decay and possible indication on the right-handed currents".
A. SEREBROV, Leningrad Nuclear Physics Institute, Russia.

"Experiments at the Institute of Nuclear Researches - Meson Factory Division - Academy of Sciences of Russia".
V.M. LOBASHEV, Moscow, Russia.

"On the importance of (n,p)-,(n,α)- and fission reactions in stellar nucleosynthesis".
C. WAGEMANS, Geel, Belgique.

"Fission modes and related emission processes".
H. MÄRTEN, Univ. Dresden, Germany.

"Développement d'un nouveau système de détection pour le spectromètre Lohengrin".
M. HESSE, Univ. Dresden, Germany.

"GRID profiles determined from molecular dynamics channeling calculations".
D. JANSSEN, Univ. Dresden, Germany.

"A new high energy scale"
V. KADYSHEVSKY, JINR, Dubna, Russia.

College 4
Structural and magnetic excitations

"High temperature thermodynamic properties of metals".
G. GRIMVALL, Royal Institute of Technology, Stockholm, Sweden.

"Dipole-dipole renormalisation of the spin hydrodynamics in ferromagnets. Polarised neutron studies of the spin-correlation tensor".
B. TOPERVERG, LNPI, Gatchina, Russia.

"The cross-section of neutron coherent inelastic scattering".
J. KULDA, ILL, Grenoble.

"Lattice dynamics of sapphire".
H. SCHOBER, ILL, Grenoble.

"Neutron scattering and μSR: Complementary techniques ?".
B. CYWINSKI, Univ. of Reading, U.K.

"How important is the Kondo effect in Ce-Al_2-evidence from new measurements of the ordered moments".
E.M. FORGAN, Univ. of Birmingham, U.K.

"Phonon gap in commensurate methane and light domain-walls".
T. MOLLER, ILL, Grenoble, France.

"Paramagnetic spectral response in heavy fermions and valence fluctuation systems".
A. MURANI, ILL, Grenoble, France.

"Evidence of magnetic domains in reentrant spin glasses by neutron depolarisation".
I. MIREBEAU, CEN Saclay, France.

"The advanced neutron source".
J.B. HAYTER, Oak Ridge National Laboratory, USA.

"Neutron scattering in UPd_2Al_3".
A. KRIMMEL, ILL, Grenoble, France.

"Inelastic magnetic neutron scattering in metallic and semiconducting 4f compounds".
A. SEVERING, ILL, Grenoble, France.

"Development of Be-monochromators".
F. MÜCKLICH, MP.I. Stuttgart, Germany.

"Experience of a physicist using Unix in everyday life".
C. NAIRN, Dept. of Engineering Science, Oxford, U.K.

"Neutron scattering studies of a low carrier Kondo system".
M. KOHGI, Tohoku Univ. Japan.

"The separation of magnetic and phonon scattering: A novel technique".
S. DAKIN, ILL Grenoble, France.

"The Jahn-Teller (pseudo Jahn-Teller) origin of structural phase transitions in condensed media. Relation to ferroelectricity and superconductivity".
I. BERSUKER, Acad. Sci. Moldova, Kishinev, Russia.

College 5
Crystallographic and magnetic structures

"Applications of neutron and synchrotron scattering to magnetic and non-magnetic phase transitions"
J.K. COCKCROFT, Univ. of Durham, U.K.

"From Landau-Theory to Landau-Numbers: Linking diffraction with thermodynamics".
W. SCHMAHL, Technische Hochschule, Darmstadt, Germany.

"Magnetic excitations and fluctuations in the S = 1. one dimensional antiferromagnet NENP".
L.P. REGNAULT, CEN-Grenoble, France.

"Monochromators: new solutions to old problems".
T. VOGT, Brookhaven Nat. Lab., Upton, NY, USA.and ILL, Grenoble, France.

"Spin glass dynamics above tg: Relaxation and damage spreading".
I.A. CAMPBELL, Physique des Solides, Orsay, France.

College 6
Liquids, disordered materials

"Light scattering experiments at the solid-liquid interface during freezing and melting".
J.H. BILGRAM, ETH Zürich, Suisse.

"Complementarity of X-ray and neutron techniques in small angle scattering studies of porous materials".
J. DORE, Univ. of Kent, Canterbury, U.K.

"Brillouin spectroscopy studies of orientational glasses".
R. JIMENEZ, Univ. des Saarlandes, Saabrücken, Germany.

"Vibrational and electronic properties of quasicrystalline systems".
H. BOETTGER, TU Magdeburg, Germany.

"Low frequency Raman spectoscopy and nanostructure of disordered materials".
A.P. SOKOLOV, Inst. of Automation and Electrometry, Novosibirsk, Russia.

"Investigation of magnetic fluctuations in La_2CuO_4 using D7".
O. SCHÄRPF, ILL, Grenoble, France.

"Nanometric multilayers for soft X-ray and neutron optics".
P. BOHER, Laboratoire d'Electronique Philips, Limeil Brévannes, France.

College 8
Biology

"The multiwavelength anomalous diffraction method (MAD) with synchrotron radiation. Instrumentation at LURE, methodology and application to the determination of macromolecular structures".
R. FOURME, LURE, Université Paris-Sud, Orsay, France.

"Recognition in protein synthesis and the mechanism of the action of the risobomal elongation factors".
K.H. NIERHAUS, MPI für Molekulare Genetik, Berlin, Germany.

"Structure and function of the iron centre of ribonucleotide reductase".
M. FONTECAVE, LEDSS, Université Joseph Fourier, St. Martin d'Hères, France.

"Small angle scattering studies on chromatin high-order structure".
V. RAMAKRISHNAN, Brookhaven Nat. Lab., Upton, NY, USA.

"The structure of ribosomal protein S5 and histone H5: Applications of the MAD method, and implications for nucleic acid binding".
V. RAMAKRISHNAN, Brookhaven Nat. Lab., Upton, NY, USA.

"Structure and function of porin from the outer membrane of Rhodobacter capsulatus".
W. WELTE, Institut für Biophysik and Strahlenbiologie, Freiburg, Germany.

"The structures of two porins from E.coli; examples of membranes channels formed by β-barrels".
S.W. COWAN, Univ. Basel, Biocenter, Switzerland.

"Microtubular dissipative structures and biological auto-organisation".
J. TABONY, CEN-Grenoble, France.

"Genes coding for proline-rich proteins in plants".
P. PUIGDOMENECH, Conseil Sup. d'Investigacions Cientifiques, Barcelona, Spain.

"The problem of hydration forces between amphiphilic surfaces. Can neutron scattering help to solve it ?"
V.I. GORDELIY, Lab. Léon Brillouin, Saclay, France and Lab. of Neutron Physics, Dubna, Russia.

College 9

Chemistry

"Polymer dynamics in solutions and gels".
E. GEISSLER, Laboratoire de Spectrométrie Physique, Saint Martin d'Hères, France.

"The effects of polymers on colloidal suspension stability".
F. LAFUMA, Ecole Supérieure de Physique et Chimie, Paris.

"Sitewise electron transfer in mixed valence solids by dielectric relaxometry: manganese (VI/VII), metal hexacyannometallates and others".
D. ROSSEINSKY, Univ. of Exeter, U.K.

"Statistical conformations of substituted polyacetylenes in solution".
J.P. AIME, L.C.P.C. Université de Bordeaux, France.

"Phonon lifetimes in molecular crystals".
S. CALIFANO, European Lab. for Non-Linear Spectroscopy, Florence, Italy.

"The vibrations of hydrogen bonds, recent INS results".
J. TOMKINSON, Rutherford Laboratory, ISIS Facility, U.K.

"Structural studies of aggregation in ionic polymers".
C. WILLIAMS, LURE, Orsay, France.

"Gelation or precipitation ?"
B. CABANE, CEN-Saclay, France.

"The glass transition".
G. WILLIAMS, Swansea, U.K.

"Using properties of the charge density to characterize atomic and molecular interactions".
K.E. LAIDIG, Cambridge University, U.K.

"Structure and interactions in inorganic gel systems".
J. RAMSAY, CNRS-Villeurbanne, France.

"C_{60}, the celestial sphere that fell to earth".
H. KROTO, University of Sussex, Brighton, U.K.

"Probing the physico-chemical properties of solid inclusion compounds".
K.D.M. HARRIS, University of St. Andrews, Scotland.

"The Jahn-Teller effect".
Issac BERSUKER, Institute for Quantum Chemistry, Moldavia.

Thursday colloquium

"Orbital magnetism from itinerant electrons".
G.H. LANDER, Inst. for Transuranium Elements, Karlsruhe, Germany.

"Chaos spatiotemporel d'ondes de surface excitées paramétriquement".
S. FAUVE, Ecole Normale Supérieure, Lyon, France.

"Disordered phenomena in organic solids as studied by spectral hole burning".
J. FRIEDRICH, Bayreuth University, Germany.

"From seaweed to trees: Botanics of crystal growth".
H. MÜLLER-KRUMBHAAR, KFA, Jülich, R.F.A.

"Theory of non-adiabatic superconductivity".
L. PIETRONERO, Università "La Sapienza" Italy.

"Neutron scattering and computer simulation".
G.R. KNELLER, IBM France & CEN, Saclay, France.

"On the free energy of crystal surfaces".
H. Van BEIJEREN, Utrecht University, Pays-Bas.

"High temperature: Superconductivity is gapless".
Laszlo MIHALY, State University of New York, Stony Brook, USA.

"Observation expérimentale des courants permanents dans un anneau GaAs-AlGaAs".
A. BENOIT, CRTBT, CNRS, Grenoble, France.

"White dwarf stars as quantum crystals: the Coulomb lattice at stellar conditions"
N. ASHCROFT, Cornell University, USA and LEPES, CNRS, Grenoble, France.

"Approche expérimentale de la physique des milieux granulaires: modèle du tas de sable".
E. CLEMENTS, Univ. de Paris VI, France.

Conference Contributions

ABINGDON, UK: European Workshop on Neutron Scattering at High Pressures - 1992/03/19-21

CHATTOPADHYAY T. Effects of hydrostatic pressure on modulated magnetic phases.

GOBRECHT K., MELESI L., MCINTYRE G.J. High-pressure facilities at the Institut Laue-Langevin. (Invited paper)

ABINGDON, UK: ESSS Meeting - Instrumentation and Techniques for the European Spallation Source - 1992/03/24-27

TIMMINS P.A. Scientific horizons in structural biology. (Invited talk)

ANTIBES/JUAN-LES-PINS, France: 11th International Conference on Vacuum Metallurgy - 1992/05/11-14

EISENHANS O., BOENI P., GRIMMER H., BUFFAT P., LEIFER K., ANDERSON I. Thin films for neutron optics. (Poster)

AUTRANS, France: 48 hours of Structural Biology - 1992/09/15-16

TIMMINS P.A. Neutron crystallography of a lipoprotein lipovitellin. (Invited talk)

BAD SCHANDAU, Germany: Verbundtreffen der Arbeitsgemeinschaft Forschung mit Neutronen - 1992/03/29-04/01

DORNER B., FÅK B. Linienformen, Anregungsenergien und Summenregeln für inelastische Neutronenstreuung von Phononen. (Poster)

HINRICHS K., BRÜCKEL T., KNORR K., PRANDL W. Percolation like behaviour in amorphous spin glasses $(Mn_xCa_{1-x})_3Al_2(SO_4)_3$. (Poster)

JERICHA E. Perfect crystal neutron storage. (Poster)

RITTER C. Elastische Neutronenstreuung an Kupferchrom-chalkospinellen. (Poster)

SUCK J.-B. Brillouin Streuung mit Neutronen an ungeordneten Systemen. (Invited talk)

TRAMPENAU J., LAUTER H.J., TAUB H., LEIDERER P. Krypton physisorbiert in der kommensurablen Phase auf Graphit: Phononengap und quasielastische Streuung. (Poster)

WUTTKE J. Zeitkorrelationen im Glasbildener Orthoterphenyl. (Talk)

BAD-HONNEF, Germany: Training Course on Modern Methods in Radiation Measurements and Dosimetry - 1992/11/23-27

OED A. Microstrip proportional counters. (Invited talk)

BERLIN, Germany: 18th IUPAC International Conference on Thermodynamics and Statistical Physics - 1992/09/18

BERMEJO F.J., MARTINEZ J.L., MOMPEAN F.J., GARCIA-HERNANDEZ M. Low frequency excitations in molecular glasses.

BERNKASTEL-KUES, Germany: Conference on Nuclei far from Stability IV and Atomic Mass and Fundamental Constant IX - 1992/07/19-24

BERNAS M., CZAJKOWSKI S., SIDA J.L., DESSAGNE P., MIEHE C., PUJOL C., ARMBRUSTER P., BRISSOT R., BOCQUET J.P., FAUST H., KOZHUHAROV C., GEISSEL H., HANELT E., MÜNZENBERG G., VIEIRA D., AUDI G., LEE J.K.P. New very neutron-rich isotopes of Ni, Co and Fe.

BOMBANNES, France: 2nd European Workshop on Neutron-, X-ray and Light Scattering as an Investigative Tool for 'Soft' Condensed Matter - 1992/05/31-06/06

CHARVOLIN J. Cubic structures with large cells: from metals to amphiphiles.

LINDNER P., ZEMB T. Scattering experiments under external constraints.

BOSTON, USA: MRS (Materials Research Society) Meeting Fall '92 - 1992/11/30-12/04

FRICK B. Short time dynamics of polymers near the glass transition, investigated by inelastic neutron scattering. (Poster)

BRISTOL, UK: Polymer Colloids - 1992/03/30-04/01

LINDNER P., RIEGER J., DIPPEL O., HÄDICKE E., LEY G. Crystals made of close packed polymeric spheres. A small angle neutron scattering study. (Contributed paper)

CANTERBURY, UK: Third Euro-American Conference in the UK on Functional Polymers and Biopolymers - 1992/10/07-11

GABRYS B., SCHAERPF O., PFEIFFER D.G. Polymers studied with spin polarized neutrons. (Contributed paper)

CHÂTEAU DE BONAS, France: NATO ASI - Chemical Physics of Intercalation II - 1992/06/28-07/08

VOIT J. Charge transport and percolation in conducting polymers.

CHICAGO, USA: American Department of Energy Panel Meeting on Advanced Neutron Sources - 1992/09/08-10

PENDLEBURY J.M., GREENE G.L., SEESTROM S.J., WERNER S.A. Neutron Sources and Applications Review: Section on Fundamental and Nuclear Physics.

DARMSTADT, Germany: International Conference on the Physics of Transition Metals - 1992/07/20-24

JANOT C. Structure and properties of quasicrystals. (Invited paper)

DOUCY, France: Réunion du GDR Films Moléculaires Flexibles - 1992/04

CHARVOLIN J. Structures cubiques micellaires.

DRESDEN, Germany: International Conference on Solid State Chemistry - 1992/10

SALINAS-SANCHEZ A., SAEZ-PUCHE R., GARCIA-MATRES E., MARTINEZ J.L., GARCIA-MUNOZ J.L., RODRIGUEZ-CARVAJAL J. Relative structural stability of R_2BaMO_5 (R=Rare Earch, M=Cu, Ni).

DRESDEN, Germany: XXIIth European Symposium on the Dynamical Properties of Solids - 1992/10

SCHOBER H. Lattice dynamics of α-quartz and sapphire. (Invited talk)

DUBNA, Russia: International Seminar on Structural Investigations at Pulsed Neutron Sources (ISSI) - 1992/09/01-04

DORNER B. Eigenvector determination - a dynamical structure determination. (Invited talk & Abstract)

EL ALGARBE, Portugal: 2nd Italy-Portugal-Spain (IPS) Inorganic Chemistry Symposium - 1992/03

MARTINEZ J.L., GARCIA MUNOZ J.L., RODRIGUEZ-CARVAJAL J. X-ray and neutron diffraction studies of R_2BaCuO_5 oxides (R = Sm, Eu, Gd, Dy, Ho, Er, Tm, Yb, Lu and Y).

ENSCHEDE, Holland: 14th European Crystallographic Meeting - 1992/08/02-07

BAUMBACH G.T., PIETSCH U., METZGER H., SEIFFERT W., ROBINSON I.K., RHAN H. Identification of an enlarged quantum well in semiconductor superlattices by grazing incidence X-ray diffraction.

FUESS H., CZJZEK M., KIRSCHHOCK C., KLEIN H., VOGT T. Structure and dynamics of aromatic molecules in zeolites.

OLOVSSON I., MCINTYRE G.J., PTASIEWICZ-BAK H. Bonding deformation and superposition effects in the electron density. (Invited talk)

PEBAY-PEYROULA E. The structure of a hydrophobic protein from soybean. (Poster)

GIARDINI NAXOS, Italy: European Physical Society - Condensed Matter Division, Conference on Neutron Scattering from Liquid matter - 1992/09/15-18

BERMEJO F.J., CHAHID A., GARCIA-HERNANDEZ M., MARTINEZ J.L., MOMPEAN F.J., CRIADO A. Neutron inelastic scattering from molecular liquids and glasses.

CHAHID A., BERMEJO F.J., GARCIA-HERNANDEZ M., MARTINEZ J.L., MOMPEAN F.J. Dynamical properties of plastic and liquid oxygen.

MOMPEAN F.J., BERMEJO F.J., CHAHID A., GARCIA-HERNANDEZ M., MARTINEZ J.L. Dynamical behaviour of liquid deuterium.

MUTKA H. A dedicated instrument for thermal neutron Brillouin scattering design and simulation.

WUTTKE J. Relaxation and phonons from viscous and glassy orthoterphenyl. (Talk)

GÖTEBORG, Sweden: International Conference on Synthetic Metals - 1992/08/12-19

BARANOWSKI D., VOIT J., BÜTTNER H. Electron-libron-coupling in polyaniline.

GRENOBLE, France: HERCULES Course -1992/02/24-04/10

MARTINEZ J.L. Layers-multilayers-superlattices.

TIMMINS P.A. Virus structure. (Invited talk)

GRENOBLE, France: Journées des Polymères et des Colloïdes - 1992/04/14-15

CHARVOLIN J. Structures cubiques micellaires.

PALMERI J. Polymerized membranes. (Poster)

TERECH P. A new class of living polymers in organic solvents. (Talk)

GRENOBLE, France: ILL-ESRF Workshop Partial Structures Factors - 1992/09/10-11

JANOT C., BOISSIEU M. DE, BOUDARD M., DUBOIS J.M. Partial structure factors of quasicrystals.

GRENOBLE, France: Physique en Clips - 1992/12/14-15

PALMERI J. Polymerized membranes. (Talk)

HITACHI, Japan: Neutrons in Biology Meeting - 1992/09/04-05

TIMMINS P.A. Low resolution neutron crystallography of large macromolecular assemblies. (Invited talk)

INDIANAPOLIS, USA: Spring Meeting of the American Physical Society - 1992/O3/16-20

PETRY W. Quasielastic neutron scattering through an orientational glass transition. (Invited paper)

VOIT J. Charge transport and percolation in conducting polymers.

IRSEE, Germany: International Symposium on "Metastable Phase Formation in the Solid State" - 1992/07/27-31

SUCK J.-B. Dynamical properties of rapidly quenched $Al_{94}Si_6$ solid solution. (Talk & Abstract)

KARLSRUHE, Germany: Conference: Nuclei in the Cosmos - 1992/07/06-10

CZAJKOWSKI S., BERNAS M., ARMBRUSTER P., FAUST H., BOCQUET J.P., BRISSOT R., DESSAGNE P., MIEHE C., PUJOL C., AUDI G., LEE J., KOZHUHAROV C., GEISSEL H., HANELT E., MÜNZENBERG G., VIEIRA E. β-decay half-lives of neutron-rich isotopes of Fe, Co, Ni involved in the beginning of the r-process.

KYOTO, Japan: Rare Earths 1992 - 1992/06/01-05

HÖLSÄ J., ANTSON O., MUTKA H., PORCHER P. Crystal structure and crystals fields of NdOF: a neutron study. (Poster)

LA COLLE-SUR-LOUP, France: Journées de la Diffusion Neutronique - 1992/05/12-14

CURRAT R., EVEN J., BERTAULT M., TOUDIC B., CAILLEAU H., MOUSSA F. Etude par diffusion de neutrons des transitions d'un cristal polymerisable: pTS-. (Poster)

GELTENBORT P., OED A. L'anode à micro-bandes: un nouvel élément de construction pour compteurs proportionnels de haute résolution.

LA PLAGNE, France: Symposium on Surface Science - 1992/03/15-21

LAUTER H.J., PASYUK V.V., BLAND J.A.C., PETRENKO A.V., JOHNSON T.M., DEN BROEDER F.J.A. Magnetic moment in a CoPd ultra-thin film studied by polarized neutron specular reflection.

LILLE, France: SFP 3èmes Journées de la Matière Condensée - 1992/09/02-04

BAUMBACH G.T., GERFFROY O., GIVORD D., OTANI Y., PANNETIER B., SANTOS A.D., SOUCHE Y. Propriétés magnéto-optiques d'un réseau bidimensionnel de particules amorphes de Gd-Co.

PALMERI J. Polymerized membranes. (Poster)

LOCTUDY, France: Transphase IV - Colloque d'Expression Française sur les Transitions de Phases - 1992/05/25-29

CURRAT R., LORENZO-DIAZ J.E., MONCEAU P., LEVY F. Transitions de phase et excitations de basse fréquence dans les composés $(MSe_4)Ni$. (Invited paper)

DORNER B., SCHMID B., VISSER D., STEINER M. Transformation de phase dans $CsFeBr_3$ sous champ magnétique externe. (Invited talk)

PETRY W. Gel des mouvements relaxationnels à la transition vitreuse dans les verres structuraux et orientationnels. (Abstract)

SANDONIS J. Observation par topographies au rayonnement synchrotron de la coexistence de phases au point triple de MnP. (Talk)

MADRID, Spain: 12th International Symposium on the Reactivity of Solids - 1992/10

FERNANDEZ-DIAZ M.T., RODRIGUEZ-CARVAJAL J., MARTINEZ J.L. Structural characterization of $Nd_2NiO_{4+\delta}$.

GARCIA-MATRES E., RODRIGUEZ-CARVAJAL J., MARTINEZ J.L., SALINAS-SANCHEZ A., SAEZ-PUCHE R., ALONSO J.A. Magnetic properties and polymorphism in one-dimensional oxides R_2BaNiO_5.

SAEZ-PUCHE R., FERNANDEZ F., MORALES A., FERNANDEZ-MARTIN F., MARTINEZ J.L Phase transitions and magnetic properties of $RCaCrO_4$ oxides (R=Rare Earth).

MAINZ, Germany: 1. Jahrestagung der Deutschen Gesellschaft für Kristallographie - 1992/06/09-12

SCHNEIDER J.R., BOUCHARD R., KOUPTSIDIS S., SCHMIDT T., LISS K.D., MAGERL A., MADAR R. K-space characterization of imperfect single crystals by means of a 3-crystal diffractometer for high energy synchrotron radiation.

THEIRY D., CHATTOPADHYAY T., MCINTYRE G.J., VON SCHNERING G. Strukturen beim Phasenübergang: α-$TlGaSe_2$ (paraelektrisch) β-$TlGaSe_2$ (ferroelektrisch).

MARSEILLE, France: First European Symposium on X-ray Topography and High Resolution Diffraction - 1992/07/08-10

BAUMBACH T., GAILHANOU M., MARTI U., CARLIN J.F., RUDRA A., ILEGEMS M. Four crystal-six reflection X-ray diffraction of III-V multilayer gratings.

KULDA J. Recent developments in extinction theories. (Invited talk)

KULDA J. Extinction in thin crystals. (Poster)

REJMANKOVA P., BARUCHEL J., KULDA J. X-ray diffraction on α-$LiIO_3$ crystals in presence of electric field. (Poster)

SANDONIS J. Observation by synchrotron radiation topography of the phase coexistence at the triple point in MnP. (Talk)

MONTEREY, California, USA: International Conference on Martensitic Transformations - 1992/07/20-24

PETRY W. Dynamic and Static Precursors of Displacive Transformations. (Abstract)

MONTPELLIER, France: European Workshop on Glasses and Gels - 1992/01/29-31

PREVEL B., JAL J.F., DUPUY J., CHIEUX P., DIANOUX A.J., LEGRAND J.F. Vibrational dynamics and structural relaxation in aqueous electrolyte solutions in the liquid, undercooled liquid and glassy states. (Poster)

MONTPELLIER, France: Ecole Thématique sur les Effets de Gradients Internes dans les Semiconducteurs - 1992/09/10-11

LISS K.D., MAGERL A., MADAR R. Diffraction rayons X à haute énergie sur des cristaux massifs Si-Ge.

MONTPELLIER, France: Réunion Française de Ferroélectricité - 1992/09/25

CURRAT R., PARLINSKI K., VETTIER C., ALEKSANDROVA I.P., ECKOLD G. Effet de la pression hydrostatique sur les phases modulées de Rb_2ZnBr_4. (Poster)

NEW YORK, USA: 7th International Conference on Phonon Scattering in Condensed Matter - 1992/09

ANDRES A. DE, TABOADA S., MARTINEZ J.L., SAEZ-PUCHE R. Phonons and luminescence processes studied by Raman spectroscopy in high T_C-related oxydes.

MARTINEZ J.L., BERMEJO F.J., GARCIA-HERNANDEZ M., ALONSO J., MOMPEAN F.J. Collective excitations in a molecular glass.

PRIETO C., CHAHID A., GARCIA-HERNANDEZ M., BERMEJO F.J., MARTINEZ J.L. Temperature dependence of the sound velocity in a polar liquid: SO_2.

PARIS, France: 12ème Rencontre de Physique Statistique - 1992/01/30-31

PALMERI J. Polymerized membranes. (Talk)

PARIS, France: Comité de Direction du GDR Films Moléculaires Flexibles - 1992/05

CHARVOLIN J. Approche topologique des systèmes de films.

PARIS, France: Conference: Origin and Evolution of the Elements - 1992/06/22-25

CZAJKOWSKI S., BERNAS M., SIDA J.L., ARMBRUSTER P., FAUST H., DESSAGNE P., MIEHE C., PUJOL C., AUDI G., LEE J.K.P., KOZHUHAROV C., GEISSEL H., MÜNZENBERG G. AND THE FRS GROUP. Investigation of very neutron-rich Fe, Co and Ni isotopes encountered along the r-process path.

PAVIA, Italy: Societa Italiana de Fisica. LXXVIII Congresso Nazionale - 1992/11/05-10

FIONI G., FAUST H.R. Determinazione della distribuzione di carica nucleare nella fissione spontanea del ^{248}Cm. (Talk)

PERM, Russia: IVth Inter-Republican Symposium on Residual Stresses: Simulation and Control - 1992/06/30-07/3

KOSCIS M. Neutron strain measurement experiences at the Institut Laue-Langevin, Grenoble, and Laboratoire Léon Brillouin, Saclay.

PONTA DELGADA - SAO MIGUEL, Portugal: NATO-ASI Molecular Spectroscopy: Recent Experimental and Computational Advances - 1992/08/30-09/11

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. (Poster)

PRAGUE, Czechoslovakia: 12th European Conference on Condensed Matter - 1992/04/06-09

ANDRES A. DE, TABOADA S., MARTINEZ J.L., SALINAS-SANCHEZ A., SAEZ-PUCHE R. Light scattering from R_2BaMO_5 oxydes with R=Lanthanide and M=Co, Ni or Cu.

FRICK B. Short-time dynamics of polymers near the glass transition - investigated by inelastic neutron scattering. (Invited talk)

GARCIA-MATRES E., MARTINEZ J.L., RODRIGUEZ-CARVAJAL J., ALONSO J.A., SALINAS-SANCHEZ A., SAEZ-PUCHE R. Structural characterization and polymorphism in R_2BaNiO_5 (R=Y, Yb. Tm, Er, Ho, Dg, Dy) studied by neutron diffraction.

HAYDEN S.M., AEPPLI G., CANFIELD P.C., CHEONG S.W., CLAUSEN K.N., FISK Z., HUNDLEY M.F., MASON T.E., MARTINEZ J.L., MOOK H.A., RYTZ D. Magnetic excitations in the high-T_c superconducting systems.

READING, UK: Neutron Scattering - 1992/04/02-03

HARRISON A., CLARKE S.J., MASON T.E., VISSER D., MCINTYRE G.J., SCOTT C.A., CLAUSEN K.N. Neutron and μsr studies of two-dimensional quantum antiferromagnets.

VISSER D., MCINTYRE G.J., KEEN D.A., SHEARMUR T., MORRISON A. Magnetic ordering in the 1D antiferromagnet $CsMnI_3$ - A study using SXD and D16.

REGENSBURG, Germany: Verhandlungen der Deutschen Physikalischen Gesellschaft, Früjahrstagung Festkörperphysik - 1992/03/16-20

BARANOWSKI J., VOIT J., BÜTTNER H. Elektron-Libronen-Kopplung in Polyanilin.

CHATTOPADHYAY T. Resonante Magnetische Röntgenstreuung in $EuAs_3$. (Talk)

DORNER B., FÅK B. Linienform, Anregunsenergien und Summenregeln für inelastische Neutronenstreuung von Phononen. (Contributed talk)

FRICK B., RICHTER D. Niederfrequente Anregungen in einem nicht-fragilen polymeren Glas: Polyisobutylen. (Contributed talk)

SCHMID B., DORNER B., VISSER D., STEINER M. Korrelationen im Singulet Grundzustandssystem $CsFeBr_3$ in Abhängigkeit von Temperatur und Magnetfeld. (Contributed talk)

SCHOBER H., STRAUCH D., DORNER B. Gitterdynamic von Saphir. (Poster)

SUCK J.-B. Dynamische Eigenschaften der ikosaedrischen Legierung $Al_{71}Pd_{19}Mn_{10}$.

SUCK J.-B., EGELSTAFF P.A., ROBINSON R.A., SIVIA D.S., TAYLOR A.D. Experimentelle Bestimmung der Dispersion kollektiver Schwingungen in einem amorphen Festkörper.

ROUEN, France: Réunion de la Société Française de Microscopie électronique - 1992/07

CHARVOLIN J. Cristaux de fluides.

SALZBURG, France: Spring Meeting of Nuclear Physics Sections - 1992/02/24-28

AIT SALEM M., GEHRKE P., GÖNNENWEIN F., GRAF U., KAUFMANN J. Energy loss and straggling of fission fragments in C, Ni and Au foils. (Poster)

BOUCHENEB, ASGHAR M., GELTENBORT P., OED A. Phenomenon of cold fission for $^{229}Th(n_{th},f)$ and $^{239}Pu(n_{th},f)$. (Poster)

GEHRKE P., GÖNNENWEIN F., MÖLLER A., OED A., GELTENBORT P. Stop-detector for TOF measurements on ions using microchannel plates.

GELTENBORT P., OED A. Recent results of position sensitive gas counters with microstrip anode for neutron detection. (Poster)

GRAF U., GÖNNENWEIN F., GELTENBORT P., DANILYAN G.V., BONDARENKO L. Parity-nonconservation in nuclear fission of $^{233}U(n_{th},f)$. (Poster)

GROSS M., FIONI G., FAUST H.R. Improvement of the Lohengrin spectrometer by using a focusing magnet. (Poster)

MAYERHOFER U., BÖRNER H.G., JOLIE J., ULBIG S., WILLIAMS A., SCHRECKENBACH K., WHITE D. Discussion of an alternative installation of the PN2 (BILL) electron spectrometer at an external beam of the ILL. (Poster)

SAN DIEGO, California, USA: SPIE's 1992 International Symposium on Optical Applied Science and Engineering - 1992/07/19-24

ANDERSON I. From 1 to m: the development of supermirrors. (Invited talk)

ANDERSON I., ELSENHANS O., BÖNI P., FRIEDLI H.P., GRIMMER H., BUFFAT P., LEIFER K. Thin films for neutron optics. (Contributed paper)

GELTENBORT P., OED A. Features of microstrip proportional counters.

GELTENBORT P., OED A., JACOBE J., FELTIN D. Thermal neutron position-sensitive detectors used at the Institut Laue-Langevin.

LUKAS P., VRANA M., MIKULA P., KULDA J. Instrumentation for strain measurements using cylindrically bent perfect crystals.

MIKULA P., LUKAS P., KULDA J., STRUNZ P., VARONV J., WAGNER V., SCHERM R., ALEFELD B., REINARTS R. Unconventional double bent-crystal (DBC) diffractometer equipped by a position sensitive detector.

SCHELLERHAU, Germany: XXIInd European Symposium on the Dynamical Properties of Solids - 1992/09/27-10/01

DORNER B. Anomalies of the acoustic phonons behavior in disordered perovskite-like crystals. (Poster & Abstract)

DORNER B., SCHMID B., PETITGRAND D., REGNAULT L.P., STEINER M. Neutron scattering from $CsFeCl_3$ in an external magnetic field. (Poster)

PETRY W. Neutron Scattering near the Transition to the Glassy State.

TRAMPENAU J., LAUTER H.J., LEIDERER P., TAUB H. Dynamics of physisorbed krypton on graphite.

SENDAI, Japan: Sendai Conference on "Correlated Electrons" - 1992/09

LANDER G.H. Neutron and synchrotron X-ray scattering experiments on actinides. (Contributed paper)

SINGAPORE: Inaugural Conference of the Asian Crystallographic Association - 1992/11/13-16

OLOVSSON I., MCINTYRE G.J., PTASIEWICZ-BAK H. Bonding deformation and superposition effects in the electron density. (Poster)

ST. ETIENNE, France: 8ème Colloque International. Investigation des Métaux et Nouveaux Matériaux - 1991/11

BASTIE P., BELLET D., ROYER A., BARUCHEL J. Two non destructive techniques for the investigation of single grain turbine blades: γ-ray diffractometry and neutron topography.

ST. LOUIS, USA: 4th International Conference on Quasicrystals - 1992/04/31-05/06

SUCK J.-B., KLEIN T., PARES G., FOURCAUDOT G., CYROT-LACKMANN F. Atomic dynamics of icosahedral $Al_{62}Cu_{25.5}Fe_{12.5}$ and tetragonal $AL_{70}Cu_{20}Fe_{10}$: A comparative study using neutron inelastic scattering. (Contributed paper)

SUCK J.-B. Generalized vibrational density of states of icosahedral $Al_{71}Pd_{19}Mn_{10}$. (Contributed paper)

THESSALONIKA, Greece: 6th International Conference on Intergranular and Interface Boundaries in Materials - 1992/06/21-26

GRIMMER H., BOENI P., FRIEDLI H.P., ANDERSON I., LEIFER K., BUFFAT P. Growth and investigation of Ni/Ti multilayers. (Talk)

TOKAI-MURA, Japan: First Neutron Symposium JAERI - 1992/12/16-18

ZEYEN C.M.E. Polarized neutrons by Zeeman splitting: applications. (Invited talk)

ZEYEN C.M.E., NISHI M., KAKURAI K. A versatile spin-echo option for Ponta at the JRR-3M reactor. (Poster)

TSUKUBA, Japan: BSR92 Tsukuba - 1992/08/30-09/04

TIMMINS P.A. Low resolution neutron crystallography of lipoproteins and membrane proteins.

UPPSALA, Sweden: International Symposium on Metal-Hydrogen Systems, Fundamentals and Applications - 1992/06/08-12

GYGAX F.N., AMATO A., ANDERSON I.S., RUSH J.J., SCHENCK A. Study of μ^+ localization and diffusion in Sc and $ScH_{0.05}$. (Contributed paper)

LEISURE R.G., SCHWARZ R.B., MIGLIORI A., TORGESON D.R., SVARE I., ANDERSON I.S. Resonant ultrasound investigation of rare-earth metal-hydrogen materials. (Contributed paper)

UDOVIC T.J., RUSH J.J., BERK N.F., ANDERSON I.S., DAOU J.N., VAJDA P., BLASCHKO O. Neutron spectroscopic comparison of rare-earth/hydrogen α-phase systems. (Contributed paper)

VIENNA, Austria: 8th International Conference on Liquids and Amorphous Metals, LAM8 - 1992/08/31-09/05

JANOT C. Structure of Quasicrystals. (Invited seminar)

JANOT C., BOISSIEU M. DE, BOUDARD M., CURRAT R., QUILICHINI M., HENNION B., GOLDMAN A. Phonons in Al-Pd-Mn Quasicrystals. (Talk)

SUCK J.-B. Dynamic properties of glasses and quasicrystals. (Invited seminar)

VILLENEUVE D'ASCQ, France: Troisièmes Journées de la Matière Condensée de la SFP - 1992/09/02-04

BARUCHEL J. Coexistence de phases hélimagnétique-ferromagnétique-éventail dans MnP étudiée par topographies aux neutrons et au rayonnement synchrotron. (Invited seminar)

WUTTKE J. Diffusion quasiélastique des neutrons autour de la transition vitreuse. (Talk)

VILLIGEN, Switzerland: Workshop über Instrumentierung der Spallationsneutronenquelle SINQ am Paul Scherrer Institut - 1992/03/16-20

Invited Experts: ANDERSON I., DORNER B., GELTENBORT P., HEWAT A.W, MAY R., PETRY W., SCHÄRPF O., VOGT T.

WINDSOR, UK: International Workshop on Quasielastic Neutron Scattering - 1992/04/06-07

BERMEJO F.J., CHAHID A., GARCIA-HERNANDEZ M., MARTINEZ J.L., MOMPEAN F., ENCISO E. Neutron quasielastic scattering from molecular liquids and glasses.

CHAHID A., GARCIA-HERNANDEZ M., BERMEJO F.J., MARTINEZ J.L., ENCISO E. Quasielastic neutron scattering from condensed oxygen.

DIANOUX A.J. Future directions in quasielastic neutron scattering. (Invited talk)

SCHAERPF O. Polarization analysis techniques for quasielastic neutron scattering. (Invited talk)

Workshops organized or sponsored by the ILL in 1992

Bombannes, France., May 31- June 6, 1992.
2nd European Workshop on Neutron X-ray and light Scattering in Colloidal and Polymeric Systems
Organizers: P. LINDNER, T. ZEMB

La Colle-sur-Loup, France, May 12-14, 1992.
Journées de la diffusion neutronique.
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Other publications available

- Guide to Neutron Research Facilities, Edition 1988/89

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