ANNUAL REPORT 1990

institut Max von Laue
Paul Langevin
Grenoble - France

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All research proposals have to be submitted to the Scientific Council for approval. The Council meets twice each year and the closing dates for the acceptance of applications are:

February 15 and August 31.

The completed research proposal forms should be sent to:

Scientific Coordination and Public Relations
Office (SCAPRO)
Institut Max von Laue - Paul Langevin
156X
38042 Grenoble Cedex
France

Tel. 76 20 72 44 B. Maier
Tel. 76 20 71 79 H. Blank
Tel. 76 20 70 41 K. Mayer-Jenkins (Secretary)
Tel. 76 20 70 82 D. Dijoux (Secretary)
Telex: 320621 F

(Appropriate application forms may be obtained on request from the above office).

Under normal circumstances the ILL makes no charge for the use of its facilities. However, special equipment (other than the existing instruments, counters, standard cryostats and shielding requirements) must be provided by the user. This applies particularly to the experimental samples which must, in all cases, be provided by the user. Chemistry and Biology laboratory facilities are available for any necessary sample preparation.

The ILL makes a limited contribution towards the travel and subsistence expenses for experimentalists coming from approved laboratories in the six member countries. (Details on request).

Commercially exploitable results

Visitors and ILL scientists may occasionally be involved in experiments which have possible commercial applications. If any scientist considers that this is the case, he should get in touch with the Scientific Secretary.

Other publications available

Guide to Neutron Research Facilities, Edition 1988/89,

General Information and Regulations, Edition 1990, both available from SCAPRO.

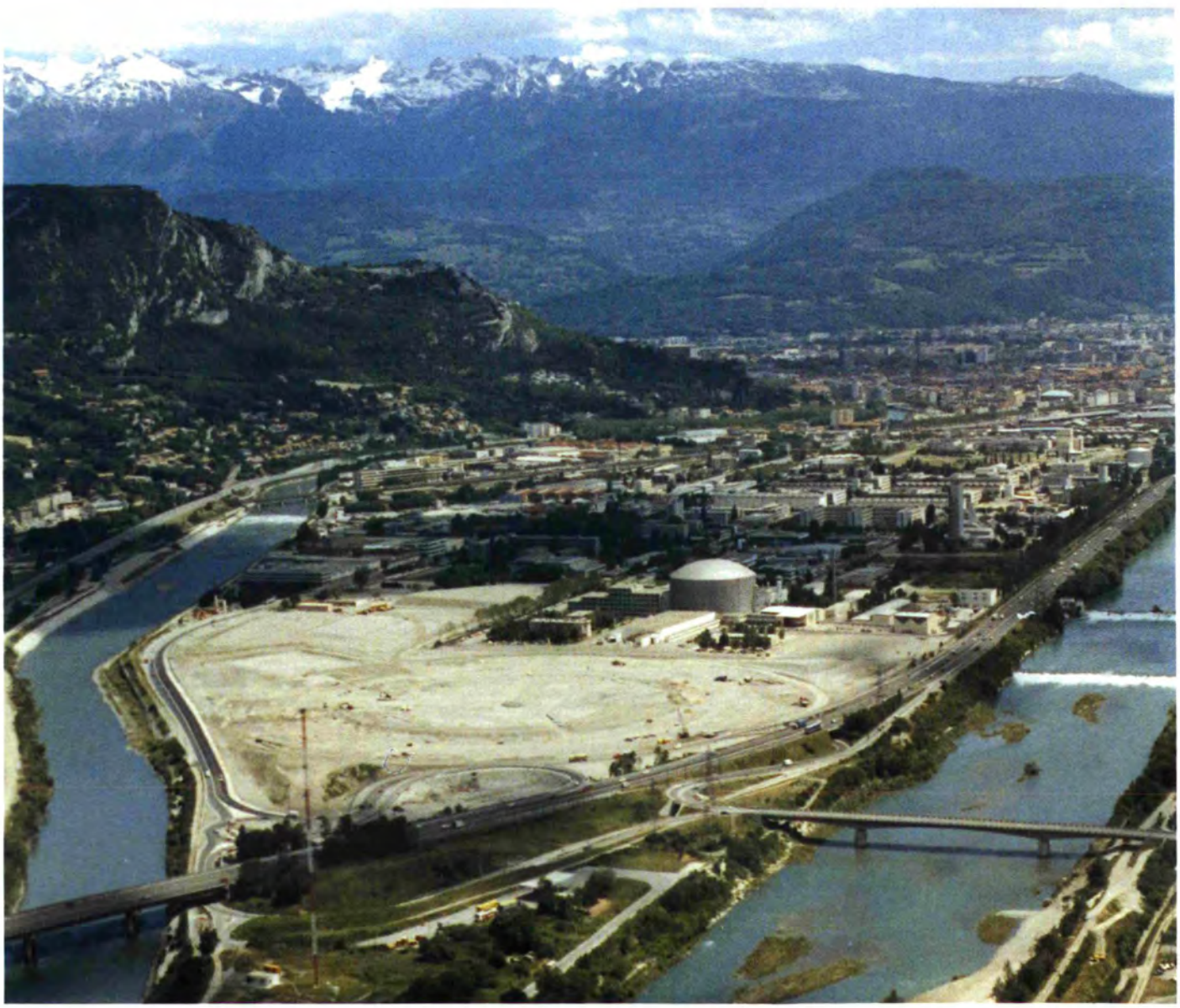
Experimental Reports and Theory College Activities 1990,

available from the ILL Library.

Front Cover:

Growth of γ-phase precipitates during "in-situ" annealing (1100°C) of a Ni-Al superalloy single crystal (results recorded by small-angle scattering on D11).

Contents



The Institut Max von Laue – Paul Langevin

The Institut Max von Laue-Langevin (ILL) at Grenoble was formally founded in January 1967, with the signature of an intergovernmental convention between France and the Federal Republic of Germany. The aim was to provide the scientific community of the affiliated countries with a unique neutron beam facility applicable in fields such as the physics of condensed matter, chemistry, biology, nuclear physics and materials science. The construction of the Institut and its high flux reactor was undertaken as a joint French-German project, with a total capital investment of 335 million FF. The reactor went critical in August 1971 and reached its full power of 57 MW for the first time in December 1971. The year 1972 saw the start-up of the cold and hot sources, the first instruments and the beginning of the experimental programme.

On January 1st, 1973 the United Kingdom joined the Institut as a third equal partner, contributing its share to the total capital investment. The corresponding intergovernmental convention was formally signed in July 1974 by the pertinent ministers from the three affiliated countries. On December 9, 1981 a protocol was signed by representatives from the three member countries which extended the agreement until 1992 and beyond unless two years' notice of termination has been given.

In December 1986, an agreement on "Scientific Membership" of Spain was signed by the ILL and the Spanish Interministerial Commission on Science and Technology for a period of five years starting on January 1st, 1987. Switzerland became another "associated scientific member" of the Institut in 1988 as well as Austria in 1990. The pertinent agreement between the ILL and the Austrian Academy of Sciences was signed in April 1990.*)

The ILL is a non-trading company under French civil law.

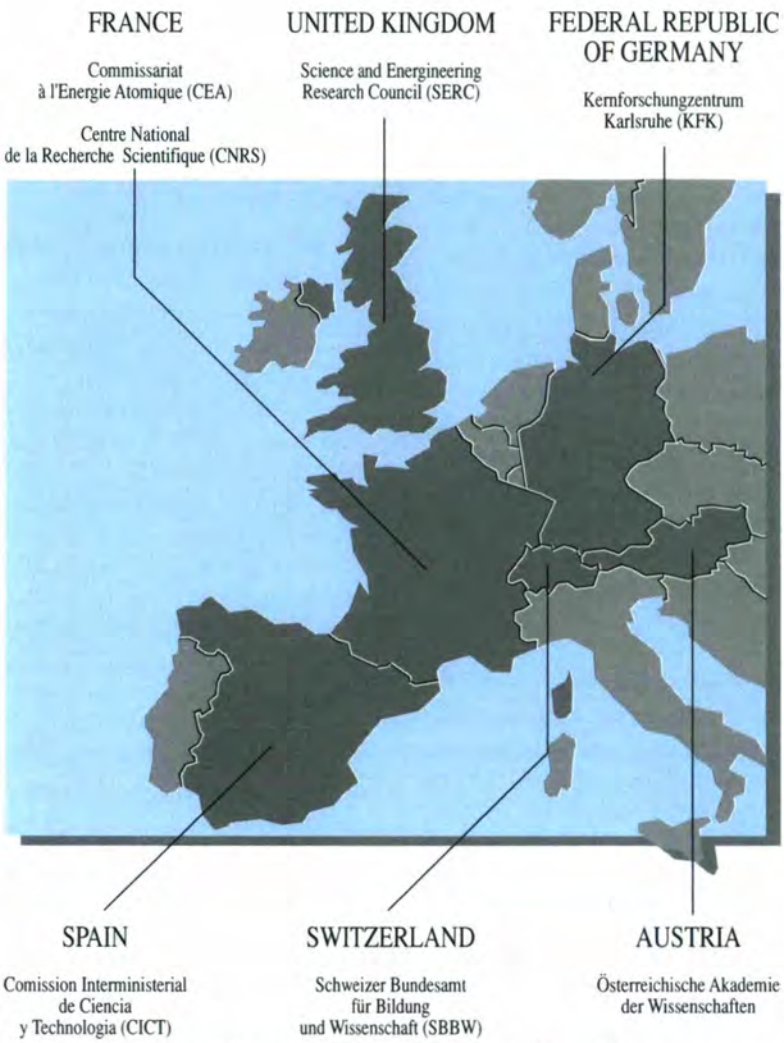
The three countries are represented by the following Associates:

- Kernforschungszentrum Karlsruhe GmbH, Germany
- Centre National de la Recherche Scientifique, France
- Commissariat à l'Energie Atomique, France
- Science and Engineering Research Council, United Kingdom.

These Associates are represented on a Steering Committee, which establishes the general rules of the management of the ILL. The Institut is headed by a Director and two Assistant Directors, all with a five year tenure, the former to be nominated alternately by the German and the British Associates, the other two by the remaining Associates. A Scientific Council, nominated by the Associates, advises the Directors on the scientific programme and on practical aspects relating to its operation. The scientific users' community of the ILL is represented in 8 subcomittees of the Scientific Council, which meet twice a year to select those research proposals which are to be carried out at the neutron beam facilities of the ILL. A further subcommittee of the Scientific Council deals with questions of instrumentation, serving as a discussion platform between the ILL and its external users. The purpose of the ILL thus differs from other research institutes in so far as it is a service institute created so that chemistry, solid state physics, fundamental and nuclear physics, biology and metallurgy specialists from laboratories in the partner countries can use the unique power of neutron techniques to broaden the attack on their problems. Designing and operating instruments and helping the visiting users to carry out their experiments is thus the principal task of the Institut's own scientists. The experimental use of the instruments by ILL staff is subject to the same approval system as their use by external teams.

*) Under these agreements Spanish, Swiss and Austrian scientists have access to the ILL facilities under the same conditions as the three member countries and have the possibility of sending two thesis students. A seat is reserved for a Spanish, Swiss and Austrian scientist in the ILL Scientific Council as well as membership in two of our sub-committees. The participation of Spain, Switzerland and Austria to the ILL Budget is limited to 1.5 % each.

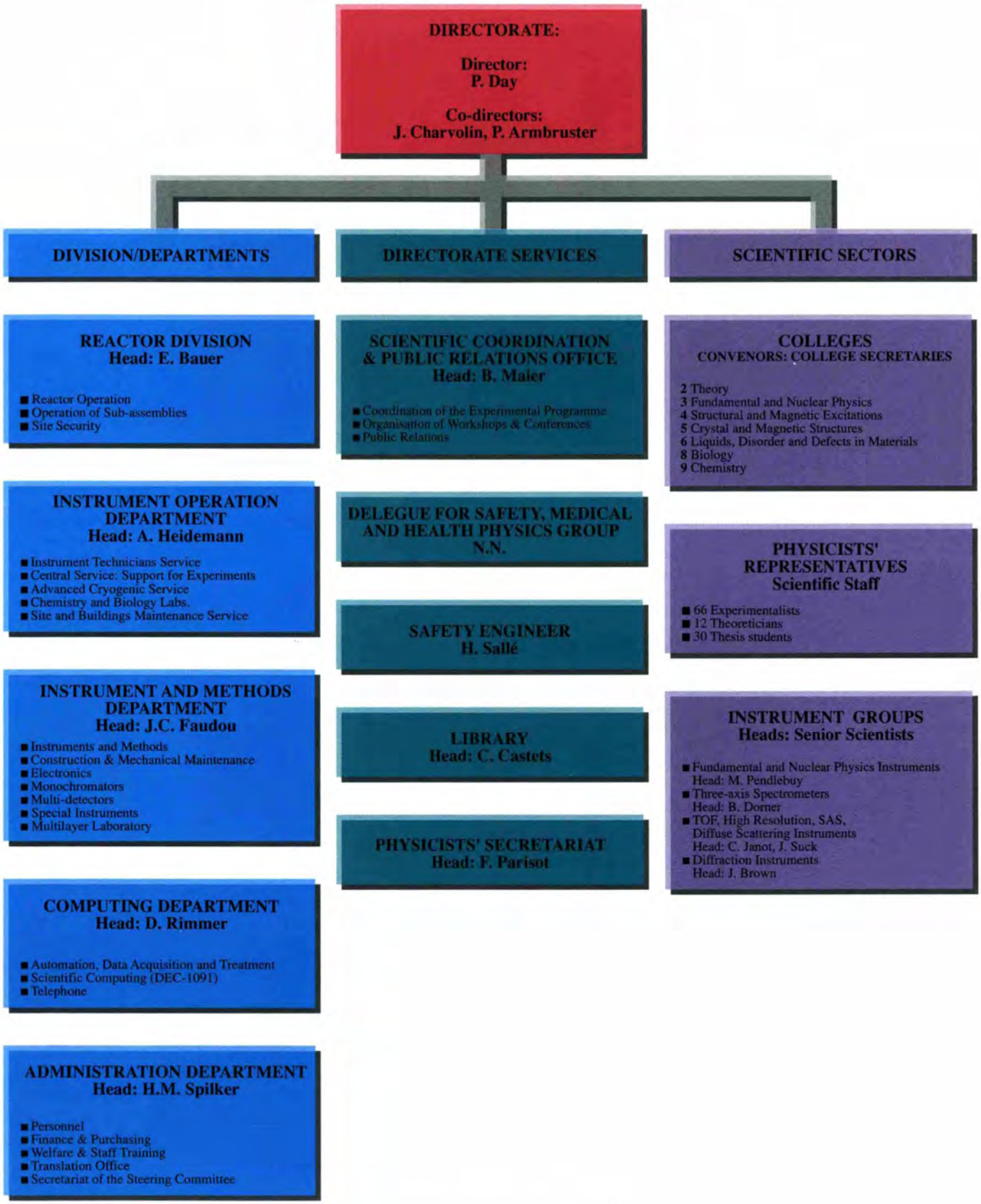
Associates of the ILL



Countries with scientific membership

Steering Committee (at its last meeting)		
❍ Hansen (BMFT)	❍ Aymar (CEA)	❍ Enderby (Univ. Bristol)
❍ Klose (KFK)	❍ Bouchard (CEA)	❍ Gray (RAL)
❍ Schunck (BMFT)	❍ Comès (CNRS)	❍ Newport (SERC)
❍ Steiner (Univ. Mainz)	❍ Sevin (CNRS)	❍ Ritzema (DES)

Scientific Council	
Plenary Session	**Subcommittees**
30 members	66 members


DIRECTORATE:
Director:
P. Day
Co-directors:
J. Charvolin, P. Armbruster
DIVISION/DEPARTMENTS
DIRECTORATE SERVICES
SCIENTIFIC SECTORS
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
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
N.N.
SAFETY ENGINEER
H. Sallé
LIBRARY
Head: C. Castets
PHYSICISTS' SECRETARIAT
Head: F. Parisot
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 Experimentalists
■ 12 Theoreticians
■ 30 Thesis students
INSTRUMENT GROUPS
Heads: Senior Scientists
■ Fundamental and Nuclear Physics 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

The exchange of documents on 2 April 1990 officializing the scientific membership of Austria between Prof. O. Hittmair, President of the Austrian Academy of Sciences, left, and Prof. P. Day, Director of the ILL.

On the occasion of Austria's scientific membership, celebrated on 2 April 1990, the Austrian Minister of Science and Research, Dr. E. Busek (fourth from left) visited the ILL. On his tour through the ILL he received explanations by Prof. Rauch (Atominstitut, Vienna) about the neutron interferometer S18.

The German Secretary of State, Dr. G. Ziller (BMFT) visited the ILL and the ESRF on 4 May 1990. In the picture he (left) receives explanations from Prof. Haensel, Director General of the ESRF (second from right), and Prof. Day, Director of the ILL (right), about the implantation of the Synchrotron in the vicinity of the ILL.

Visit of the British Select Committee on Education, Science and the Arts on 21 March 1990. The guests were guided through the ILL by Prof. P. Day, Director, and Prof. P. Armbruster, German Assistant Director.

A consistent feature of the history of the ILL is its capacity to spring surprises. For an establishment of our size (a little under 500 staff, normal budget close to 300 MF) we are a remarkably (though, it must be emphasized, necessarily) complex organization, containing numerous strands that have to be woven together for the enterprise to be fully successful. First and foremost, ILL is a powerful engine of scientific progress, a forum for the skill and creativity that designs and carries out novel experiments across an enormous range of topics: my selection of scientific highlights bears ample witness to that. ILL is also a nuclear installation, with all that this entails in assiduous observance of regulatory conditions, exactingly high standards of operation and maintenance and, perhaps most important, a careful attention to the preoccupations of the local population and their representatives. Finally, ILL is a kind of factory, making science but also hardware and equipment, with a certain hierarchical organization and the consultation and negotiating machinery to go with it. The year 1990 saw events of some significance in all three facets of the Institut's affairs.

On 2 April we had the pleasure of welcoming our sixth participating country when Prof. O. Hittmair, the President of the Austrian Academy of Sciences, signed an agreement with the Institut for Austria to become the third Scientific Member. The ceremony took place in the presence of Dr. E. Busek, Minister of Research and Technology. To make the Institut's facilities more widely known among Austrian scientists, the Academy of Sciences and ILL jointly sponsored a Workshop at Krems/Donau in September, at which ILL scientists were joined by ESRF colleagues. The occasion was also notable for the number of participants who were able to join us from the newly democratic Eastern European countries. In that context I should draw attention to the Associates' approval of a proposal that I made earlier in the year to institute an Eastern European Visiting Scientists' Programme to enable a small number of younger scientists to spend extended periods of 2-3 years working at ILL. The first two visitors, from Hungary and Bulgaria, will arrive soon. The programme will certainly help to cement ties with the Eastern European neutron scattering community and supplement the exchange programme with the USSR that has been in operation since the mid-1970's.

Five-Year Development Programme

Arguably the most important activity for the long-term future of the Institut has been to prepare the documents on the phasing, costing and presentation of the Five-Year Programme. This task has been carried out in discussion with a "Group of Experts" set up by the Steering Committee, who held meetings at ILL in July and October.

Following the suggestion of the Group of Experts, the Programme is being presented in two parts: one concerning refurbishment of major items and the other the novel departures. A first presentation of the Programme was made to the November meeting of the Steering Committee which, while endorsing the principle of an eventual Development Programme, set guidelines for a new presentation to be made in 1991.

It need hardly be said that both staff and management, as well as the many representatives of the user community consulted during its preparation, regard the introduction of a Modernization Programme as of the utmost importance for the continuing vitality of the Institut. In particular, the Scientific Council unanimously passed a resolution in favour of the proposals at its October meeting.

Reactor Operation and Experimental Programme

One of the remarkable surprises that I referred to above occurred in January, when an anomaly in the calibration of the heavy water flow in the primary cooling circuit was uncovered by the Reactor Department in the course of verifying parameters needed for a study requested by the Safety Authority. The effect of the anomaly was that the flow rate, and hence the power dissipated by the fuel element, had been underestimated by about 10 % since the first startup of the reactor. On receiving this information, the Head of the Safety Authority ordered the reactor to be shut down and called for a full report. After much hard work by the Institut, the Safety Authority accepted our case and authorized the restart of the reactor, which took place on 10 April.

I want to put on record my warmest thanks to the personnel of the Reactor Department for their extremely swift and effective work on the many complex technical issues raised. Also I want to record my appreciation for the forbearance of all the staff at the Institut during a difficult period.

Altogether 62 days of beam-time were lost. However, the opportunity was taken to change two beam tubes (H8, H10) which had been scheduled for a long shutdown due in October, which therefore was not needed. After the restart, we have been permitted to operate to the same level of fuel element burn up as before (i.e. with reactor cycles of 46 days). Thus in all we ran 4.5 cycles in 1990, giving a total of 210 days for the year, compared with 264 in 1989.

The supply of uranium is satisfactory for the time being. However, contacts with the US Authorities suggest that it is most unlikely that we shall be able to ship spent fuel elements for reprocessing for the time being. This has two consequences: first, arrangements have had to be made to store spent fuel elements at Cadarache. Secondly, it will be necessary to envisage an extra purchase of uranium in 1991 to compensate for the quantities tied up in the unreprocessed spent fuel elements.

In August there was a most unfortunate incident on the small-angle scattering spectrometer D17, in which it was found that two ILL scientists had spent a brief period in the neutron beam while aligning their sample, under the impression that the beam shutter was closed. The incident was reported to the Safety Authority. Fortunately, tests showed that there should be no significant effect on the health of those involved. Nevertheless, the incident has led us to re-examine several aspects of the induction of ILL personnel and external users into the potential hazards of working in radiation areas.

Scientific Highlights

As usual I want to draw attention to some of the more remarkable discoveries made at ILL during the year. Such choices are always difficult because of the large volume of high quality science being conducted and the enormous range of the Institut's activities. Thus my examples stretch from particle physics to molecular biology, by way of solid state physics and electrochemistry. It is hard to imagine the Director of any other laboratory in the world being faced with such a variety of work to summarize.

A new apparatus has been put into service to render even more precise the measurement of the lifetime of the free neutron. It is worth recalling that the value already determined at ILL, combined with data on the mass fraction of helium in the primordial universe, was sufficient to define the number of particle generations as 2.6 $\pm$ 0.3, even before the first experiments at the new LEP accelerator at CERN. As such large equipments price themselves further and further out of the market for experimental particle physics, experiments with neutrons will become more and more important. ILL is by far the leading facility in the world for conducting them.

Also in the realm of neutron particle physics, the team from the Universities of Sussex, Harvard, Seattle and Munich, with the Rutherford Laboratory and ILL, announced their latest estimate of the neutron electric dipole moment, an important test of charge-parity violation. The value published was $-(3 \pm 5) \times 10^{-26}$ e cm, indicating that at 95 % confidence limits the modulus of the value is less than 12×10^{-26} e.cm.

Dispersion of the phonon-roton excitation in superfluid ^4He was measured by a group from Keele, Braunschweig and ILL, including an ILL thesis student, using IN6. At the λ-point they were able to show that the roton loses its Q,ω definition.

While the microscopic mechanism of high T_c superconductivity remains a question of hot debate, experimental data to fuel the debate become more and more subtle and precise. With excellent crystals containing precisely controlled oxygen content, the CENG group have used D3B to determine the spin density distribution in $YBa_2Cu_3O_{6.99}$ above and below T_c. A very significant shift in spin density occurs, with the moment on the in-plane copper and oxygen atoms decreasing strongly on passing into the superconducting phase. In the other families of high T_c superconductors further unexpected insights continue to accumulate. For example, the Tl and Bi copper oxide systems such as $Tl_2Ba_2CaCu_2O_8$ have incommensurate structural modulations, to investigate which the methods currently applied to liquids and amorphous materials for calculating the pair distribution functions may be employed.

Turning to structural chemistry, a notable advance in techniques was the first ever determination of the rearrangement in the structure of a molecule (the nitro-prusside ion) on going from the ground state to an electronic excited state. Such a change could only be observed with neutrons since the excited state would be transformed by X-ray irradiation. Combining neutron diffraction with electrochemistry is a powerful means of observing changes in the structure of a solid during the course of a chemical reaction. When the solid in question is a proton conductor forming the positive electrode of a dry battery, the interest is more than academic. Leclanché primary batteries have been in use for more than a century but the atomic scale mechanism for the reduction of MnO2 in alkaline solution is not yet understood, and in particular, why is the process irreversible, so that the battery is not rechargeable? Using an electrochemical cell specially designed for powder neutron diffraction, it has been shown that structural defects (de Wolff disorder) in commercial MnO_2 limit the reversibility of the electrochemical process because reduction of the Mn^{4+} located in the rutile slabs leads to destruction of the lattice into small crystallites of MnOOH and $Mn(OH)_2$.

Finally, in the realm of chemistry, attention should be drawn to important new results on the dynamics of ortho and para-xylene in the ZSM-5 zeolite, which throw light on the interaction of the hydrocarbon with the alumino-silicate cage, and hence the selectivity of this important industrial catalyst. The motion of n-paraffins in the channels of urea crystals has also been clarified.

The volume and variety of neutron scattering work in structural molecular biology at ILL is impressive. In contrast, the exploitation of neutron scattering to study the dynamics of biological molecules is in its infancy. A first analysis of the incoherent inelastic scattering of neutrons by the protons in the hydrated globular protein myoglobin also shows a remarkable resemblance to that of a glass-forming liquid. This important result emphasizes the importance of density fluctuations in assisting the diffusion of O_2 through the protein matrix, and its bonding to the Fe.

The length of this section of my report, over a period of reactor operation that has certainly not been typical, is testimony to the continuing vitality and creativity of our user community and Institut scientists.

Personnel

The 1990 round of salary negotiations was a particularly difficult one. In pursuit of numerous claims that could not be met by the Management, the Unions called a series of short strikes during April and May that led to three 48-hour shutdowns of the reactor. Following these events, at the June meeting of the Steering Committee, the Management was authorized to negotiate with the Unions on the basis of the alignment of net salaries at ILL with those of the CEA. Finally, agreement was signed with the Unions on the basis of a 2 % increase in the ILL allowance, and signed at the end of June.

The Health and Safety Delegate, M. Bureau du Colombier, retired on 1 July 1990. I want to pay tribute to his contribution to safety matters over the last four years.

Two changes took place among the small group of Senior Scientists. D. Dubbers returned to Heidelberg on completion of his term as Senior Scientist in the field of Nuclear and Fundamental Physics. He is replaced by J. M. Pendlebury of the University of Sussex, who has had a long association with the neutron electric dipole moment experiment. After extensive search in the partner countries, Dr. J. B. Suck of Karlsruhe was appointed Senior Scientist in the Time-of-Flight Group. I am most grateful to Dr. A. J. Dianoux for carrying out these duties in the intervening period.

Two social events marked, in their different ways, important points in the history of the Institut. After a number of years of construction, I felt that the installations in the second neutron guide hall, ILL22, had reached a stage of development where it was appropriate to hold an inauguration of the new facility. The event also provided an opportunity to make public acknowledgment of the particular contribution to the guide hall by P. Blum, long-serving and greatly respected engineer in the Department of Instruments and Methods, by the unveiling of a small plaque in his memory.

That my Report ends with a section labelled "Personnel" certainly should not be taken as indicating the relative importance of such matters: in many ways they are the most important. The Institut is the people who work here and who make it function - scientists, technicians, administrators, secretaries etc. - on behalf of the wider community of friends and colleagues who flow through our entrance hall day by day on their way to use our instruments. 1990 was not the easiest of years for ILL but the spirit of the Institut is strong as new challenges await.

My warmest thanks to all.

It turns out that this is the last annual report I shall write as Director of ILL, having decided to accept an offer of the post of Director of the Royal Institution of Great Britain which has fallen vacant unexpectedly. The decision to leave such an excellent establishment as ILL was not easy but the opportunity to lead the oldest and most distinguished laboratory in Britain is a unique one. The ILL faces many challenges in the coming years but I have absolutely no doubt at all that it will continue from strength to strength and that its pivotal position in neutron science will be maintained. I wish my successor and all the staff of the Institut the very best for the future.

The end of the year was marked with great sadness in the Institut by the sudden death of our much valued and respected colleague John Kirby. Originally in the submarine service of the Royal Navy, one time reactor shift leader (and also part-time Father Christmas), in recent years his work in the Experimental Halls brought him into contact with many staff and visitors who greatly valued his helpfulness and commitment.

P. Day

Es ist bezeichnend für die Geschichte des ILL, dass es immer wieder Überraschungen gibt. Für eine Einrichtung unserer Grösse (ein wenig unter 500 Mitarbeiter, Normalbudget von fast 300 MF) sind wir notwendigerweise - man muss es betonen - eine recht komplexe EInrichtung, in der vielfältige Bemühungen zusammenwirken müssen, damit das Unternehmen zu einem vollen Erfolg wird. Das ILL ist zuerst und hauptsächlich eine treibende Kraft des wissenschaftlichen Fortschritts, ein Forum für die Geschicklichkeit und Kreativität, die beim Entwurf und der Durchführung neuartiger Experimente unterschiedlichster Themenkreise erforderlich sind: meine Auswahl der wissenschaftlichen Höhepunkte zeigt dies in deutlicher Weise. Ferner ist das ILL eine nukleare Einrichtung mit all dem, was dies an gewissenhafter Einhaltung der Sicherheitsvorschriften, hoher Betriebs- und Wartungsnormen und - vielleicht am wichtigsten - sorgfältiger Aufmerksamkeit gegenüber den Sorgen der Bevölkerung und ihrer Vertreter bedeutet. Schliesslich ist das ILL nicht nur ein Forschungszentrum, sondern auch eine Produktionsstätte für Ausrüstungen und Geräte, mit einer eigenen Organisation und dem entsprechenden Beratungs- und Verwaltungsapparat. Das Jahr 1990 brachte Ereignisse, die für alle drei Aspekte des Institutsbetriebs von Bedeutung waren.

Am 2. April hatten wir das Vergnügen, das sechste Mitgliedsland zu begrüssen. An diesem Tag unterzeichnete Herr Professor O. Hittmair, Präsident der Österreichischen Akademie der Wissenschaften, eine Vereinbarung mit dem ILL gemäss derer Österreich das dritte Wissenschaftliche Mitglied wurde. Die Feierlichkeiten fanden im Beisein von Dr. E. Busek, Bundesminister für Wissenschaft und Forschung, statt. Um die Einrichtungen des Instituts einem grösseren Kreis junger österreichischer Wissenschaftler bekannt zu machen, organisierten die Adademie für Wissenschaften und das ILL im September einen Workshop in Krems/Donau, an dem auch ILL-Wissenschaftler und ihre ESRF-Kollegen teilnahmen. Es war eine bemerkenswerte Veranstaltung, insbesondere auch im Hinblick auf die vielen Teilnehmer aus den jungen Demokratien Osteuropas. In diesem Zusammenhang möchte ich darauf hinweisen, dass die Gesellschafter einen von mir zu Beginn des Jahres vorgelegten Vorschlag zu einem Besuchsprogramm für osteuropäische Wissenschaftler billigten, das es einigen jungen Forschern ermöglichen soll, über einen längeren Zeitraum von 2-3 Jahren am ILL zu arbeiten. Die ersten beiden Besucher aus Ungarn und Bulgarien werden bald mit ihrer Arbeit am Institut beginnen. Das Besuchsprogramm wird sicher dazu beitragen, die Beziehungen zur osteuropäischen Gemeinde der Neutronenforscher zu festigen und das mit der Sowjetunion seit Mitte der siebziger Jahre bestehende Austauschprogramm zu ergänzen.

Fünfjähriges Entwicklungsprogramm

Die wichtigste Arbeit für die langfristige Zukunft des Instituts bestand wohl darin, die Unterlagen für den Zeitplan, die Kostenberechnung und die Darstellung des fünfjährigen Entwicklungsprogramms vorzubereiten. Diese Aufgabe wurde in Abstimmung mit der vom Lenkungsausschuss eingesetzten Expertengruppe ausgeführt.

Dem Vorschlag dieser Expertengruppe folgend, wird das Programm in zwei Teilen vorgestellt: Der eine betrifft die Erneuerung wichtiger vorhandener Einrichtungen, der andere die neuen Vorhaben. Ein erster Vorschlag für dieses Programm wurde in der November-Sitzung des Lenkungsausschusses vorgelegt, der zwar das Prinzip eines Entwicklungsprogramms befürwortete, jedoch auf einer Vorlage eines überarbeiteten Programms bei der nächsten Sitzung im Jahr 1991 bestand.

Es muss kaum betont werden, dass sowohl die Mitarbeiter, als auch die Direktion und die vielen Vertreter der während der Vorbereitung konsultierten Reaktorbenutzer die Durchführung eines Modernisierungsprogramms als wesentliche Voraussetzung dafür ansehen, die Vitalität des Instituts auch in Zukunft zu erhalten. Es ist hervorzuheben, dass der Wissenschaftliche Rat auf seiner Oktober-Sitzung einstimmig eine Resolution zugunsten der unterbreiteten Vorschläge verfasste.

Reaktorbetrieb und Experimentierprogramm

Zu den erwähnten Überraschungen zählte die Entdeckung einer Anomalie in der Eichung des Schwerwasserflusses im Primärkreislauf durch die Reaktorabteilung im Januar dieses Jahres, anlässlich der Überprüfung bestimmter Parameter für eine von den Sicherheitsbehörden angeforderten Studie. Als Folge der Anomalie war der Durchfluss und damit die Leistung des Reaktors, seit seiner ersten Inbetriebnahme um ungefähr 10% unterschätzt worden. Nach Erhalt dieser Information veranlasste die Sicherheitsbehörde eine Abschaltung des Reaktors und forderte eine ausführliche Stellungnahme. Nach eingehender Darlegung durch das Institut, akzeptierte die Sicherheitsbehörde unsere Argumentation und genehmigte das Wiederanfahren am 10. April.

Ich möchte dem Personal der Reaktorabteilung für seine äusserst schnelle und wirksame Arbeit bei der Bewältigung der vielen komplexen technischen Details danken. Weiterhin möchte ich allen Mitarbeitern meine Anerkennung für ihren Einsatz während dieser schwierigen Phase aussprechen.

Insgesamt gingen 62 Tage Strahlzeit verloren. Es wurde jedoch die Gelegenheit genutzt, zwei Strahlkanäle (H8, H10) auszuwechseln, deren Austausch ursprünglich während eines langen Reaktorstillstands im Oktober geplant war. Nach dem Wiederanfahren wurde die Genehmigung erteilt, die Brennelemente bis zum gleichen Abbrand wie vorher auszunutzen (d.h. mit Reaktorzyklen von 46 Tagen). Auf diese Weise wurden im Jahre 1990 4,5 Zyklen mit einer Gesamtzahl von 210 Tagen durchgeführt, verglichen mit 264 Tagen im Jahre 1989.

Die Uranversorgung des ILL ist zur Zeit zufriedenstellend. Nach Kontakten mit den amerikanischen Behörden ist es jedoch höchst unwahrscheinlich, dass wir in absehbarer Zeit abgebrannte Brennelemente zur Wiederaufarbeitung verschiffen können. Dies hat zwei Folgen: Erstens mussten Vorkehrungen zur Lagerung der abgebrannten Brennelemente in Cadarache getroffen werden; zweitens wird es notwendig sein, durch einen zusätzlichen Kauf von Uran im Jahre 1991 die in den nicht wiederaufgearbeiteten, abgebrannten Brennelementen enthaltenen Uranmengen auszugleichen.

Im August ereignete sich am Kleinwinkelstreuspektrometer D17 ein sehr bedauerlicher Zwischenfall, bei dem, in der Annahme, dass der Strahlverschluss geschlossen sei, zwei ILL-Wissenschaftler beim Ausrichten ihrer Probe kurzzeitig einer Bestrahlung ausgesetzt wurden. Der Vorfall wurde der Sicherheitsbehörde mitgeteilt. Glücklicherweise zeigten Tests, dass dieser keine wesentlichen Auswirkungen auf die Gesundheit der Beteiligten hatte. Dennoch hat uns dieses Ereignis veranlasst, die verschiedenen Aspekte der Information des ILL-Personals und der auswärtigen Besucher über die potentiellen Gefahren von Arbeiten in Strahlungsbereichen zu überprüfen.

Wissenschaftliche Höhepunkte

Wie üblich möchte ich auf einige bemerkenswerte Entdeckungen am ILL während des Jahres aufmerksam machen. Aufgrund der Vielfalt an wissenschaftlichen Arbeiten sehr hoher Qualität und des breiten Umfangs der Aktivitäten des ILL ist die Auswahl dieser Ergebnisse immer schwierig. Daher gehen meine Beispiele von der Teilchenphysik über die Festkörperphysik und die Elektrochemie bis zur Molekularbiologie. Es wird wohl kaum ein Direktor irgendeines anderen Labors auf der Welt damit konfrontiert, eine solche Vielfalt von Arbeiten zusammenzufassen.

Zur Erhöhung der Präzision bei der Messung der Lebensdauer des freien Neutrons wurde ein neues Gerät eingesetzt. Bekanntlich hat es der am ILL bestimmte Wert der Lebensdauer - verbunden mit Angaben über den Heliumanteil an der Zusammensetzung der Elemente im Kosmos - erlaubt, die Zahl der Teilchengenerationen auf $2,6 \pm 0,3$ einzugrenzen. Diese Aussage bestand vor den ersten Experimenten am neuen LEP-Beschleuniger am CERN. Da derartige grosse Ausrüstungen immer unerschwinglicher für die experimentelle Teilchenphysik werden, wächst das Interesse an Versuchen mit Neutronen. Das ILL ist das führende Institut auf diesem Forschungsgebiet.

Ebenso im Bereich der Elementarteilchenphysik veröffentlichte das Team der Universitäten Sussex, Harvard, Seattle und München mit dem Rutherford Appleton Laboratory und dem ILL ihren neuesten Grenzwert für das elektrische Dipolmoment des Neutrons, ein sehr bedeutender Test für die Verletzung der Ladungs- und Paritätssymmetrie. Der veröffentlichte Wert betrug $-(3\pm5) \times 10^{-26}$ e cm, was heisst, dass der Wert zu 95 % Wahrscheinlichkeit kleiner als 12×10^{-26} e.cm ist.

Die Dispersion der Phonon-Roton-Anregung in supraflüssigem 4He wurde von einer Gruppe aus Keele, Braunschweig und ILL am IN6 gemessen. Sie konnten zeigen, dass die Rotonen am λ-Punkt im Q,ω-Raum völlig unscharf werden.

Während die mikroskopische Deutung der Hochtemperatursupraleitung weiterhin ein intensiver Diskussionspunkt ist, werden die experimentellen Daten zur Belebung dieser wissenschaftlichen Debatte immer feiner und präziser. Mit hervorragenden Kristallen, die einen präzise kontrollierten Sauerstoffgehalt haben, hat die CENG-Gruppe das Diffraktometer D3B benutzt, um die Magnetisierungsdichteverteilung in $YBa_2Cu_3O_{6.99}$ über- und unterhalb Tc festzulegen. Beim Übergang zur supraleitenden Phase wurde eine starke Änderung des magnetischen Moments der Kupfer- und Sauerstoffatome in den Kupfer-Sauerstoff-Ebenen beobachtet. In den anderen Familien der Hochtemperatursupraleiter wurden weitere unerwartete Einblicke gewonnen. Zum Beispiel haben die Tl und Bi Kupferoxidsysteme wie $Tl_2Ba_2CaCu_2O_8$ inkommensurable Strukturmodulationen, zu deren Untersuchung die Methoden benützt werden können, die üblicherweise bei flüssigen und amorphen Materialien zur Berechnung der Paarverteilungsfunktionen ("pair distribution functions" - PDF) angewandt werden.

In der Strukturchemie gab es mit der allerersten Bestimmung der Änderung der Molekülstruktur des Nitroprussid-Ions beim Übergang vom Grundzustand zu einem elektronisch angeregten Zustand einen wichtigen Fortschritt bei den Messmethoden. Eine solche Änderung konnte nur mit Neutronen beobachtet werden, da der angeregte Zustand durch Röntgenbestrahlung zerstört würde.

Die Kombination von Neutronendiffraktion und Elektrochemie ist eine sehr wirksame Methode zur Beobachtung von Strukturänderungen im Festkörper während einer chemischen Reaktion. Wenn der jeweilige Festkörper ein Protonenleiter ist, der die positive Elektrode einer Trockenbatterie bildet, so geht das Interesse über den rein akademischen Bereich hinaus. Obwohl Leclanché-Primärbatterien sei über einem Jahrhundert gebraucht werden, konnte das mikroskopische Verständnis der Reduzierung von MnO_2 in Alkalilösungen noch nicht erklärt werden. Warum ist insbesondere der Prozess irreversibel, so dass die Batterie nicht wieder aufladbar ist? Unter Anwendung einer speziell für die Pulverneutronendiffraktion entwickelten elektrochemischen Zelle wurde verdeutlicht, dass Strukturdefekte (de Wolff-Unordnung) im kommerziellen MnO_2 die Reversibilität des elektrochemischen Prozesses einschränken. Es ist die Reduzierung des in den Titandioxidplatten angeordneten Mn^{4+}, die die Zerstörung des Gitters in kleine Kristallite von MnOOH und $Mn(OH)_2$ verursacht.

Im Bereich der Chemie sollte auf die wichtigen neuen Ergebnisse über die Dynamik von Ortho- und Para-Xylen in ZSM-5-Zeolit aufmerksam gemacht werden, die die Wechselwirkung des Hydrokohlenstoffs mit dem Aluminiumsilikat-Gerüst und somit die Selektivität dieses wichtigen industriellen Katalysators erklären. Die Bewegung von n-Paraffinen in den Kanälen von Urea-Kristallen wurde ebenso erklärt.

Der Umfang und die Vielfalt der Neutronenstreuung auf dem Gebiet der molekularbiologischen Strukturen am ILL sind eindrucksvoll. Dagegen befindet sich die Nutzung der Neutronenstreuung zur Untersuchung der Dynamik biologischer Moleküle in den Kinderschuhen. Eine erste Analyse der inkohärenten inelastischen Streuung von Neutronen durch Protonen im wasserhaltigen Protein Myoglobin zeigt eine bemerkenswerte Ähnlichkeit mit einer glasbildenden Flüssigkeit. Hiermit wird gezeigt, wie die Diffusion des O2 an das Fe durch Dichtefluktuationen unterstützt wird.

Die Länge dieses Teils meines Berichts, der eine obendrein untypische Betriebsperiode des Reaktors abdeckt, beweist die anhaltende Vitalität und Kreativität unserer Nutzergemeinde und der Instituts-Wissenschaftler.

Personalfragen

Die Gehaltsverhandlungen waren im Jahre 1990 besonders schwierig. Im Zusammenhang mit verschiedenen von der Direktion unerfüllbaren Forderungen, riefen die Gewerkschaften im April und Mai zu mehreren kurzen Streiks auf, was zu einer dreimaligen Einstellung des Reaktorbetriebs von 48 Stunden führte. In der Juni-Sitzung des Lenkungsausschusses wurde die Direktion schliesslich ermächtigt, mit den Gewerkschaften auf der Grundlage einer Anpassung der ILL-Nettogehälter an die CEA-Gehälter zu verhandeln. Schliesslich wurde Ende Juni eine Vereinbarung mit den Gewerkschaften unterzeichnet, in der die ILL-Prämie um 2% erhöht wurde.

Der Beauftragte für Fragen des Strahlenschutzes, der Gesundheit und Sicherheit, Herr Bureau du Colombier, trat am 1. Juli 1990 in den Ruhestand. Ich möchte ihm meine Anerkennung für seinen während der letzten vier Jahre geleisteten Beitrag zu allen Sicherheitsfragen aussprechen.

In der kleinen Gruppe der Senior Scientists gab es zwei Veränderungen: Herr D. Dubbers kehrte nach Ablauf seiner Amtszeit als Senior Scientist auf dem Gebiet der Kern- und Grundlagenphysik nach Heidelberg zurück. Sein Nachfolger ist Herr J.M. Pendlebury von der Universität Sussex, der lange Zeit mit dem Experiment zur Bestimmung des elektrischen Dipolmoments des Neutrons verbunden war. Nach längerer Suche in den Partnerländern wurde Herr Dr. J.B. Suck aus Karlsruhe zum Senior Scientist in der FLugzeit-Gruppe ernannt. Ich bin Herrn Dr. A.J. Dianoux für die vertretungsweise Wahrnehmung dieser Aufgabe in der Zwischenzeit sehr dankbar.

Zwei weitere Ereignisse markierten auf ihre Art wichtige Phasen in der Geschichte des ILL. Angesichts des fortgeschrittenen Entwicklungsstandes der Instrumente in der zweiten Neutronenleiterhalle, hielt ich eine Einweihung der neuen Halle für angebracht. Bei dieser Gelegenheit konnte auch der besondere Beitrag von Herrn P. Blum, dem langjährigen Mitarbeiter und allseits anerkannten Ingenieur der Abteilung Instrumente und Methoden, durch die Enthüllung einer Gedenktafel geehrt werden.

Dass mein Bericht mit dem Abschnitt "Personalfragen" endet, soll nicht bedeuten, dass dieser am Ende der Wichtigkeitsskale stünde: In vieler Hinsicht ist er sogar am wichtigsten. Das Institut besteht aus Menschen, - Wissenschaftlern, Technikern, Verwaltungsangestellten, Sekretärinnen usw. - die einer grösseren Gemeinschaft von Freunden und Kollegen dienen, die tagtäglich auf ihrem Weg zu unseren Instrumenten durch unsere Eingangshalle strömen. 1990 war kein einfaches Jahr für das ILL. Der Geist des Instituts jedoch ist stark genug, um es mit neuen Herausforderungen aufzunehmen.

Allen meinen herzlichsten Dank.

Es hat sich ergeben, dass dies mein letzter Jahresbericht als Direktor des ILL ist, denn ich habe mich entschlossen, die Stelle des Direktors der Royal Institution of Great Britain anzutreten, welche unerwarteterweise freigeworden war. Die Entscheidung, ein derart hervorragendes Forschungszentrum wie das ILL zu verlassen, ist mir nicht leicht gefallen; die Gelegenheit jedoch zur Übernahme der Leitung des ältesten und renommiertesten britischen Forschungslabors ist einmalig. Das ILL wird sich in den kommenden Jahren vielen Herausforderungen gegenübersehen; ich habe aber überhaupt keinen Zweifel daran, dass es an Bedeutung zunehmen und seine Schlüsselrolle in der Neutronenforschung behaupten wird. Ich wünsche meinem Nachfolger und der gesamten Belegschaft des Institutes das Allerbeste für die Zukunft.

Das Ende des Jahres wurde im Institut von der traurigen Nachricht des plötzlichen Todes unseres sehr geschätzten und respektierten Kollegen, John Kirby, überschattet. Er hatte seine Karriere im U-Boot-Dienst der Royal Navy begonnen und war dann im ILL für eine gewisse Zeit als Leiter des Reaktorschichtdienstes tätig. In den letzten Jahren hatte er durch seine Arbeit in der Experimentenhalle Kontakte mit vielen Mitarbeitern und Besuchern, die seine Hilfsbereitschaft und sein Engagement sehr schätzten.

P. Day

Une tendance stable de l'histoire de l'ILL est sa capacité à nous surprendre. Pour un institut de cette taille (un peu moins de 500 personnes, un budget normal de près de 300 MF), nous sommes une organisation étonnamment (mais, soulignons-le, nécessairement) complexe, comprenant de nombreux fils qui doivent être tissés pour que l'entreprise réussisse pleinement. D'abord et avant tout, l'ILL est un outil performant pour le progrès scientifique, un point de rencontre pour le talent et la créativité permettant de concevoir et mettre en place des expériences originales parmi une vaste gamme de sujets : ma sélection en ce qui concerne les évènements scientifiques majeurs en témoigne. L'ILL est également une installation nucléaire avec tout ce que cela comporte comme respect strict des règlements, des niveaux exigeants de fonctionnement et de maintenance et, peut-être ce qui est le plus important, une attention particulière aux préoccupations de la population avoisinante et de leurs élus. Finalement l'ILL est une sorte d'usine fabriquant non seulement de la science mais également du matériel et des installations, avec une certaine organisation hiérarchique des organes de consultation et de négociation y afférents. L'année 1990 a été témoin d'évènements de grande importance dans chacune des trois facettes de la vie de l'Institut.

Le 2 avril nous avons eu le plaisir d'accueillir notre sixième pays partenaire lorsque le Professeur O. Hittmair, Président de l'Académie des Sciences d'Autriche, a signé un accord avec l'Institut pour que l'Autriche devienne le troisième Membre Scientifique. La cérémonie a eu lieu en présence du Dr. E. Busek, Ministre de la Recherche et de la Technologie. Pour permettre aux scientifiques autrichiens de mieux connaître les moyens existant à l'Institut, l'Académie des Sciences et l'ILL ont parrainé un "workshop" à Krems/Danube en septembre, auquel participaient les scientifiques de l'ILL ainsi que leurs collègues de l'ESRF. Cet évènement a également été marqué par le nombre de participants en provenance de nouvelles démocraties de l'Europe orientale, qui ont pu se joindre à nous. Dans ce contexte, j'aimerais attirer l'attention sur l'approbation des Associés d'une proposition que j'ai émise vers le début de l'année pour établir un Programme de Chercheurs Invités de l'Europe de l'Est permettant à quelques jeunes scientifiques de travailler sur une période de deux à trois ans à l'ILL. Les deux premiers chercheurs invités en provenance de Hongrie et de Bulgarie vont donc bientôt arriver. Il est certain que le programme contribuera à renforcer les liens avec la communauté de diffusion neutronique et complètera le programme des échanges avec l'URSS qui est en place depuis le milieu des années 70.

Plan de Développement Quinquennal

L'activité la plus importante en ce qui concerne l'avenir à long terme de l'Institut a certainement été la préparation des documents sur le planning, le coût et la présentation du Plan de Développement Quinquennal. Ce travail s'est réalisé en discussions avec un Groupe d'Experts créé par le Comité de Direction qui a tenu des réunions à l'ILL en juillet et en octobre.

Suivant la suggestion du Groupe d'Experts, le Plan peut se présenter en deux parties: l'une concernant l'aménagement des équipements importants, l'autre concernant les nouveaux objectifs. Une première présentation du Programme a été faite à la réunion du Comité de Direction du mois de novembre qui, réaffirmant le principe d'un Programme de Développement, a défini des directives pour soumettre une nouvelle présentation en 1991.

Nul besoin de dire qu'à la fois le personnel et la Direction, aussi bien que les nombreux représentants de la communauté d'utilisateurs contactés pendant sa préparation, considèrent extrêmement important l'introduction d'un Programme de Modernisation

pour la vie future de l'Institut. En particulier, à sa réunion d'octobre, le Conseil Scientifique a unanimement approuvé une résolution en faveur des propositions.

Fonctionnement du Réacteur et Programme Expérimental

L'une des surprises majeures évoquées ci-dessus a été la découverte par le Département Réacteur, en janvier, d'une anomalie dans l'étalonnage du débit d'eau lourde dans le circuit principal de refroidissement, lors de la vérification de certains paramètres nécessaires pour une étude demandée par le SCSIN. Le résultat de cette anomalie a été que le débit, et de ce fait la puissance dissipée par l'élément combustible, a été sous-estimée d'environ 10 % depuis le premier démarrage du réacteur. A la réception de cette information le Chef du SCSIN a ordonné l'arrêt du réacteur et exigé un rapport technique complet. Après un travail ardu effectué par l'Institut, le SCSIN a considéré positivement notre cas et autorisé le redémarrage du réacteur qui a eu lieu le 10 avril.

J'aimerais adresser tous mes remerciements aux agents du Département Réacteur, pour leur travail rapide et concluant devant la complexité des problèmes techniques abordés. J'aimerais également dire que j'ai apprécié la patience de tout le personnel de l'Institut pendant cette période difficile

De ce fait, 62 jours de temps de mesure ont été perdus. Cependant on en a profité pour remplacer deux canaux (H8, H10), ce qui avait été programmé pour un grand arrêt prévu en octobre et qui ne s'est donc pas avéré nécessaire. Après le redémarrage nous avons été autorisés à fonctionner au même niveau de combustion des éléments combustibles qu'auparavant (c'est-à-dire avec des cycles de 46 jours). Ainsi nous avons pu fonctionner avec 4,5 cycles en 1990, ce qui a donné un total de 210 jours pour l'année, par rapport aux 214 jours pour 1989.

La fourniture d'uranium est satisfaisante pour le moment. Cependant, après contacts pris avec les Etats-Unis, il paraît très peu probable que nous puissions envoyer les éléments combustibles brûlés pour le retraitement avant un certain temps. Cela comporte deux conséquences : d'abord des arrangements ont dû être faits pour le stockage à Cadarache des éléments combustibles consommés ; ensuite, il sera nécessaire d'envisager un achat supplémentaire d'uranium en 1991 pour compenser les quantités non disponibles dans les éléments combustibles consommés et non retraités.

En août un incident très regrettable s'est produit sur le spectromètre D17 de diffusion à petits angles, au cours duquel deux scientifiques ILL ont passé un temps assez court dans le faisceau de neutrons pendant qu'ils alignaient leur échantillon, pensant l'obturateur du faisceau fermé. L'incident a été signalé aux autorités de la sûreté. Heureusement les tests ont montré qu'il n'y aurait pas de répercussion significative sur la santé des personnes concernées. Néanmoins, l'incident nous a conduits à réexaminer divers aspects du travail en zone de rayonnement pour le personnel ILL et les utilisateurs extérieurs, avec les risques potentiels que celà comporte.

Evénements Scientifiques Majeurs

Comme d'habitude j'aimerais attirer l'attention sur quelques travaux importants effectués durant l'année à l'ILL. Ce genre de sélection est toujours difficile à faire vu le nombre important d'expériences de haute qualité scientifique réalisées ainsi que la vaste gamme des activités de l'Institut. Mes exemples vont donc de la physique des particules à la biologie moléculaire, en passant par la physique de l'état solide et l'électrochimie. Il est difficile d'imaginer le Directeur d'un autre laboratoire ailleurs dans le monde confronté à une telle variété de travaux à résumer.

Un nouvel appareil a été mis en service pour augmenter la précision de la mesure de la durée de vie du neutron libre. Il est utile de rappeler que la valeur déjà déterminée à l'ILL, associée aux données sur la fraction de masse d'hélium dans l'univers primordial, avait permis de définir le nombre de familles de particules comme 2.6 ± 0.3 avant même les premières expériences effectuées au CERN sur le nouvel accélérateur LEP. Puisque de telles grandes installations sont de plus en plus coûteuses pour la physique expérimentale des particules, les expériences avec les neutrons seront de plus en plus importantes. L'ILL est de loin , dans le monde, l'organisme en meilleure position pour les réaliser.

Dans le domaine également de la physique du neutron, l'équipe des universités de Sussex, Harvard, Seattle, Munich, du laboratoire de Rutherford et de l'ILL, a annoncé sa dernière estimation du moment dipolaire électrique du neutron, test important de la violation de parité de la charge. La valeur publiée est de - $(3\pm5)\times10^{-26}$ e.cm, ce qui indique qu'à 95 % des limites de confiance le module de la valeur est inférieur à 12×10^{-26} e.cm.

En physique de la matière condensée, la courbe de dispersion (Q, ω) de l'excitation phonons-rotons dans ^{4}He superfluide a été mesurée sur IN6 par un groupe de Keele, Brunswick et l'ILL, avec un boursier de thèse de l'ILL. Ils ont pu montrer que cette courbe se transforme en une zone diffuse au point λ.

Le mécanisme microscopique de la supraconductivité de haute T_c reste toujours un point très débattu, mais les données expérimentales se précisent de plus en plus. Avec d'excellents cristaux d'une teneur en oxygène contrôlée de manière précise, le groupe du CENG a utilisé D3B pour déterminer la distribution de densités de spin dans $YBa_2Cu_3O_{6.99}$ au-dessus et au-dessous de T_c. Cette densité varie de façon importante en passant en phase supraconductrice, le moment magnétique dans le plan des atomes de cuivre et d'oxygène décroissant fortement. Dans les autres familles de supraconducteurs à haut T_c, on continue d'obtenir un flot de résultats inattendus. Par exemple, les structures des systèmes d'oxyde de cuivre Tl et Bi tels que $Tl_2Ba_2CaCu_2O_8$ présentent des modulations incommensurables qui peuvent être observées à l'aide de méthodes habituelles appliquées aux liquides et aux matériaux amorphes pour calculer les fonctions de distribution de paires.

Si nous nous tournons vers la chimie structurale, un grand progrès dans les techniques a été la toute première détermination du réarrangement de la structure d'une molécule en partant de l'état fondamental vers un état électronique excité. Un tel changement ne peut être observé qu'avec des neutrons puisque l'état excité aurait été transformé par irradiation aux rayons X. L'association de la diffusion de neutrons avec l'électrochimie est un moyen puissant pour observer les transformations qui se produisent dans la structure d'un solide pendant le déroulement d'une réaction chimique. Lorsque le solide en question est un conducteur protonique formant l'électrode positive d'une pile primaire, l'intérêt est plus qu'académique. Les piles Leclanché sont utilisées depuis plus d'un siècle mais le mécanisme à l'échelle atomique de la réduction en milieu alcalin de leur constituant essentiel (MnO_2) n'a pas encore été compris ; en particulier, on ne sait toujours pas pourquoi le processus est irréversible, ce qui fait que la pile n'est pas rechargeable. En utilisant une cellule électrochimique spécialement construite pour la diffraction de neutrons, on a pu montrer que les défauts de structure (désordre de Wolff) sont à l'origine de la non réversibilité de la réaction électrochimique : la réduction du Mn^{4+} situé dans les blocs rutile conduit à la destruction du réseau en petits cristallites de MnOOH et $Mn(OH)_2$.

Toujours dans le domaine de la chimie, il faut attirer l'attention sur d'importants résultats concernant la dynamique de l'ortho et para-xylène dans le zéolite ZSM-5 qui met en évidence l'intéraction de l'hydrocarbone avec la cage de silicate d'aluminium, et donc la sélectivité de cet important catalyseur industriel. Le mouvement des parafines dans les canaux des cristaux d'urée a également été précisé.

La quantité et la variété des travaux de diffusion de neutrons pour décrire les structures de molécules biologiques à l'ILL sont impressionnantes. Par contre l'étude de la dynamique de ces structures par diffusion neutronique en est à ses premiers pas. Une première analyse de la diffusion inélastique incohérente des neutrons par les protons dans la protéine globulaire de la myoglobine hydratée montre également une ressemblance remarquable avec celle du liquide à l'approche d'une transition vitreuse. Cet important résultat souligne l'importance des fluctuations de densité en aidant la diffusion de O_2 par l'intermédiaire de la matrice de la protéine, pour être liées à Fe.

La longueur de cette partie de mon rapport sur une période de fonctionnement du réacteur qui n'a certainement pas été typique, témoigne d'une vitalité et créativité permanentes de notre communauté d'utilisateurs et de scientifiques de l'Institut.

Personnel

La succession des négociations concernant les salaires en 1990 a été particulièrement difficile. Après de nombreuses revendications auxquelles la Direction n'a pu répondre, les syndicats ont appelé le personnel à faire en avril et mai, une série de grèves courtes qui ont conduit à trois arrêts de 48 heures du réacteur. Suite à ces évènements, le Comité de Direction du mois de juin, a autorisé la Direction à négocier avec les syndicats, dans le cadre défini par la Convention d'Entreprise, sur la base de l'alignement des salaires nets de l'ILL avec ceux du CEA. Finalement un accord a été signé fin juin avec les représentants des syndicats sur la base d'une augmentation de 2 % de la prime ILL.

Le Délégué au Domaine Sécurité-Protection-Santé, M. Bureau du Colombier, a pris sa retraite le 1er juillet 1990. J'aimerais lui rendre hommage pour sa contribution dans le domaine de la sécurité pendant ces quatre dernières années.

Deux changements sont intervenus dans le petit groupe des Senior Scientists. M. Dubbers est reparti à Heidelberg au terme de son mandat de Senior Scientist dans le domaine de la Physique Nucléaire et Fondamentale. Il est remplacé par J.M. Pendlebury, de l'Université de Sussex, qui travaille depuis longtemps sur les mesures du moment dipolaire électrique du neutron. Après une recherche étendue dans les pays associés, Mr J.B. Suck de Karlsruhe a été nommé Senior Scientist dans le groupe Temps de Vol. Je suis très reconnaissant à Mr. A.J. Dianoux pour avoir mené à bien ces fonctions pendant cette période intermédiaire.

Deux évènements ont été fêtés, importants chacun à sa façon pour la vie de l'Institut. Après plusieurs années de construction d'instruments, j'ai trouvé que les installations dans le deuxième hall de guide de neutrons, ILL22, avaient atteint un stade de développement tel qu'il était approprié d'inaugurer ce nouveau bâtiment. Cette cérémonie a également fourni une occasion de reconnaître la contribution spécifique pour ce hall de guide de P. Blum, ingénieur très respecté, qui avait longtemps travaillé dans le Département Instruments et Méthodes ; une plaque à sa mémoire a été dévoilée.

Bien que mon rapport s'achève par le paragraphe 'Personnel' cette position dans le rapport ne veut certes pas dire qu'il traite de sujets peu importants : à bien des égards ce sont les plus importants. L'Institut se compose de personnes qui travaillent et remplissent leurs fonctions - scientifiques, techniciens, administrateurs, secrétaires, etc. - au nom de la plus vaste communauté d'amis et collègues qui affluent chaque jour dans notre hall d'entrée pour utiliser nos instruments. 1990 n'a pas été l'année la plus facile pour l'ILL mais l'Institut se sent fort dans l'attente de nouveaux défis.

Mes remerciements les plus chaleureux à tous.

Il s'avère que ce rapport annuel sera le dernier que j'écrirai en tant que Directeur de l'ILL puisque j'ai décidé d'accepter la proposition pour le poste de Directeur de la Royal Institution of Great Britain, poste déclaré vacant de manière imprévisible. La décision de quitter un excellent établissement tel que l'ILL n'a pas été facile à prendre mais l'occasion pour moi d'avoir à diriger le plus ancien et le plus prestigieux laboratoire en Grande Bretagne est unique. L'ILL aura encore de nombreux défis à relever dans les années à venir mais je n'ai absolument aucun doute sur le fait qu'il continuera à être de plus en plus performant et qu'il gardera son rôle central dans le domaine de la science des neutrons. Je souhaite à mon successeur ainsi qu'à tout le personnel de l'Institut mes meilleurs voeux pour l'avenir.

La fin de l'année a été tristement marquée par le décès de notre collègue très apprécié et respecté John Kirby. Venant du service des sous-marins de la Royal Navy, il a travaillé comme chef de quart au réacteur (il a également fait office de Père Noël), puis ces dernières années son travail dans les Halls Expérimentaux lui ont permis d'avoir des contacts avec énormément de personnes, dont les visiteurs, qui ont beaucoup estimé son aide et son engagement.

P. Day

Over the last year the two institutes have devoted considerable effort to the transfer of the British and German teachers in the international sections at the Houille Blanche Primary School and the Lycée Stendhal (secondary school) to the French educational system. With the new school year in September 1990 it was finally established that all the teachers, who had previously had contracts with ILL and ESRF, are now given contracts with the "Recteur de l'Académie" (Director of Education) for Grenoble, the appropriate French authority.

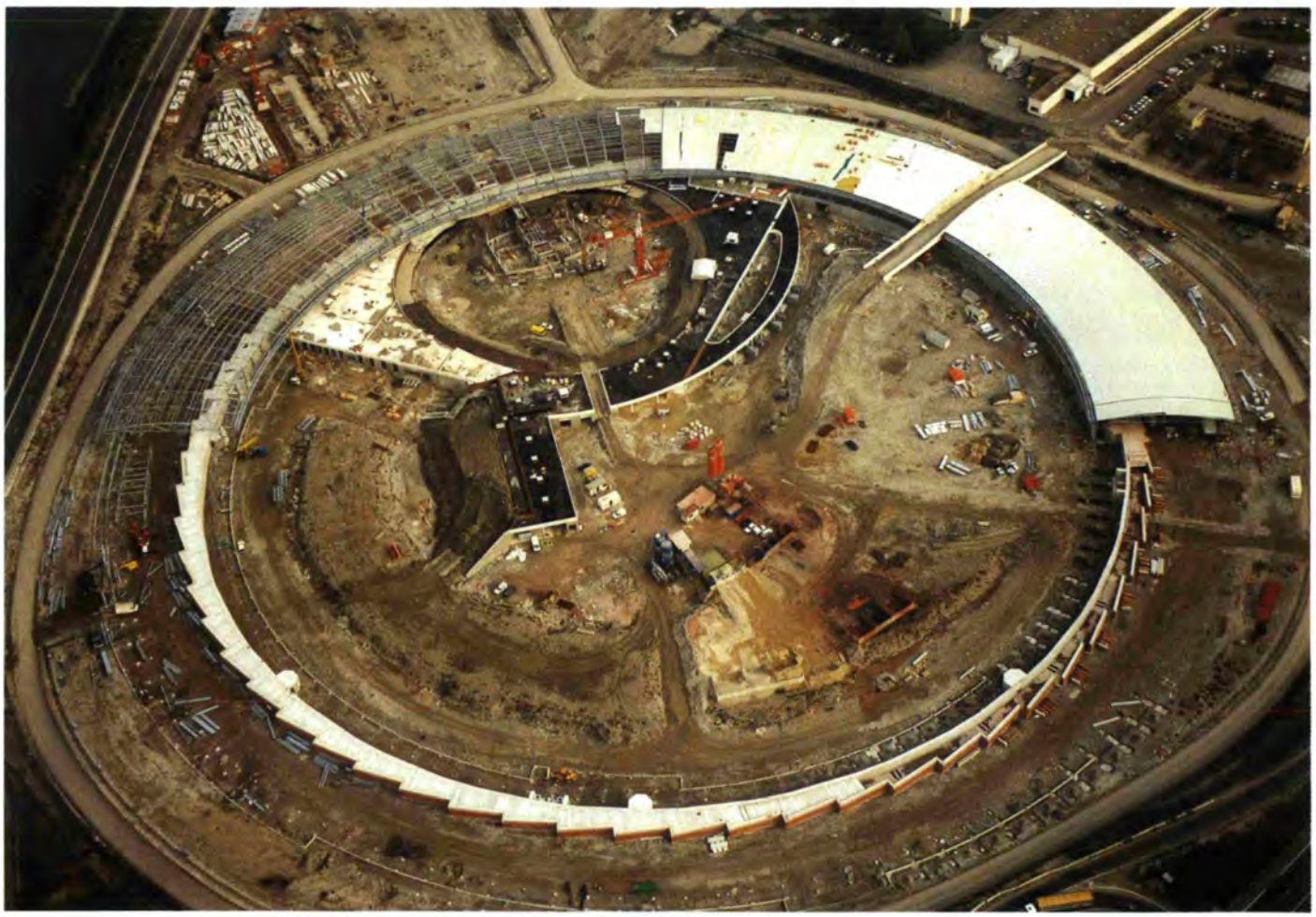
The two institutes have set up a joint working group to work out the conditions for the future control of access to the common site and are currently having discussions with the French authorities on the physical protection of the common site. In these discussions ILL and ESRF are working on the principle that the unity of the site and circulation without constraints between the two institutes must be ensured.

Negotiations are currently taking place between the two institutes and the unions at ILL and ESRF on the conditions for a joint medical service.

The tenders received by ESRF for the construction of the joint ILL/ESRF building have been evaluated and the contract with Léon Grosse, BETEG, for the construction of the buildings has been signed. The building will be completed in the second half of 1992.

The discussions on the Modernisation Programme have indicated various possibilities, desirable in the long term, for cooperation between the two institutes. A workshop on Neutron Optics showed clearly that there are numerous opportunities for cooperation in the fields of monochromators, mirrors and thin layers. This is particularly true for the methods of characterising these products. The stock of instruments for analysis is almost identical. Sample environment and characterisation in the two institutes need similar facilities. A joint laboratory could be the first step in this collaboration. The two institutes are investigating how a closer collaboration in the computing sector could be organised.

P. Armbruster



Aerial view of the ESRF construction site. The picture shows the first contours of the 844 m storage ring and the adjacent ring of the experimental hall. The synchrotron tunnel and the preinjector building can be seen on the upper part of the photograph.

Theory

Members of the College

J. Chalker
B. Fourcade
P. Holdsworth
D. Janssen
I. Jolie
M. Lavagna
P. Nozières
D. Núnez-Regueiro
N. Schopohl
E.F. Shender
J. Solyom
M. Uwaha
J.T. Voit
D. Waxman
A. Würger.

Introduction

The scientific activities within the Theory College cover condensed matter physics and nuclear physics.

In accordance with the composition of the college the majority of its members work in the field of condensed matter physics. Here a wide range of topics is studied and includes rotational tunnelling, rheology of suspensions, capillarity effects, polymer systems, magnetism, classical as well as high temperature superconductivity, quantum fluids, the theory of strongly correlated Fermi systems.

The activities in nuclear physics include Gamma Ray Induced Doppler broadening, the theory of odd-odd nuclei, the many body problem in nuclear matter.

Scientific Trends and Highlights in 1990

Condensed matter physics

J. Chalker has been mainly concerned with Anderson localisation of electrons in disordered semiconductors. One focus has been the interpretation of experiments on the integer quantum Hall effect, which probe localisation via the temperature dependence of Shubnikov de Haas oscillations. A second topic has been the consequences for transport of the fractal nature of wave functions near a mobility edge.

Bertrand Fourcade worked on problems related to the shape of a vesicle. The general question is to know what is the evolution of a closed vesicle under the action of an external stimulus. His work concentrated on the phase diagram as well as on the characterization of the boundary lines.

In the past year P.C.W. Holdsworth completed a numerical study of random bond and random field disorder in two-dimensional orientational glasses. He proposed a neutron scattering experiment here at ILL to test this work, using an adsorbed mixture of Nitrogen and Argon on a graphite substrate. Also he began simulations on anisotropic ferromagnets, and frustrated antiferromagnets.

M. Lavagna continued her studies of strongly correlated Fermi systems using the slave-boson method. She extended the range of validity of previous work to include not only charge but also spin fluctuations and calculated in detail the effect of gaussian fluctuations around the mean field solution. At low temperature she showed how one can relate the theory to a Fermi-liquid picture.

P. Nozières worked towards an explanation of experiments carried out by the Marseille group (Métois, Heyraud) which show evidence for elastic deformations of a thin graphite film in contact with a drop of liquid lead.

The theory of the phenomenon takes into account the weak capillary forces which exist at a liquid-solid interface and become more important for thin films.

P. Nozières devoted part of his time to lecturing on

(1) The theory of interfacial instabilities

(2) The theory of strongly correlated fermions.

In his lecture series (2) he emphasized the atypical physical nature of the 1-dim case. In particular he discussed in depth the 1-dim Hubbard model with its exactly known Bethe Ansatz solution. He elucidated the nature of the elementary excitations of the system as composite entities, which could be dissociated into 'holons' and 'spinons', and pointed out that the interesting question of how to generalize what can be learned from the exactly solvable 1 dim system to two and higher dimensional systems has presently no conclusive answer.

M.D. Núnez Regueiro continued her studies on a charge transfer model for high T_c superconductors. The model proposed for hole-doped CuO_2 and BiO_3 based systems has been shown to allow pairing of the electrons in the CuO_2 layers.

Neutron diffraction has shown the peculiar behaviour of RMn_2 systems : complex magnetic orderings where magnetic and non magnetic Mn sites coexist and unusual dependence with external parameters. A first model including the instability of the Mn moments in a frustrated lattice has been proposed by M.D. Núnez Regueiro in collaboration with R. Ballou and C. Lacroix (CNRS).

N. Schopohl and D. Waxman studied the interface that exists between the A and B phases of superfluid ^{3}He. Working in the framework of quasiclassical theory they made predictions for the magnetic influence that the interface would have on quasiparticle excitations. For example, a moving A-B interface generates magnetization and there is experimental evidence for this in work carried out by S. Boyd and G. Swift in Los Alamos. A complete calculation for a moving interface is far more complex than a static interface. The reason for the complexity arises from the additional time dimension introduced into the problem and the associated inelastic Andreev-scattering at the A-B phase boundary. The end product of their efforts was to find an exact solution to the moving interface problem for sharp order parameter profiles and to predict the velocity

dependence of the magnetization accompanying the moving interface. They are continuing to work on this subject.

J. Solyom studied the difficult problem how to calculate explicitly the correlation functions of the Bethe Ansatz soluble models. Also he investigated the effect of a twist in the boundary condition for the 1-d Heisenberg model and established a relationship to Haldane's conjecture about integer and half-integer spin chains.

M. Uwaha continued his studies together with Y. Saito and S. Seki on the theory of aggregation growth in a lattice gas. He also investigated the vicinal surface of solid ^{4}He, where physical properties like stiffness and mobility are attributed to the occurrence of steps on a facet. In ^{4}He these steps can be looked at as moving elastic strings which, however, are coupled due to interference effects of the superfluid flow field. As a result there exists an effective interaction proportional to T/d at finite temperature T, where d denotes the step distance.

J. Voit initiated work on the spectral properties of a Luttinger liquid. Together with D.K. Campbell he also investigated a continuum field theory of the commensurate-incommensurate transition in interacting 2 D electron systems.

A. Würger continued his collaboration together with A. Heidemann (also at ILL) and A. Hüller (Univ. Erlangen) on rotational tunnelling. Also he investigated the nuclear spin conversion of methyl groups.

Nuclear Physics

Jan Jolie pursued the experiments using the **G**amma **R**ay **I**nduced **D**oppler broadening (GRID) method on the two-axis flat crystal spectrometer GAMS4 in close collaboration with College 3. The most important results were obtained in two heavy nuclei, ^{196}Pt and ^{168}Er. Both are considered to be representative for two different kinds of nuclear collective motion : a γ-soft nucleus and a rotational nucleus. The aim of the experiments was to test to what extent the theoretical interpretations are valid at higher excitation energy.

He also continued his work on the theory of odd-odd nuclei as more experimental data became available recently. The transfer reaction amplitudes for the pick-up reactions 197Au(d,t) and 197Au(He^3, α) performed at the T.U. München were compared to predictions. They show a reasonable agreement with the theory taking into account the complex structure of heavy odd-odd nuclei. The same agreement holds for the calculated electromagnetic transition rates between the negative parity states in ^{198}Au and ^{176}As in comparison with branchings measured at the ILL. The strength of the supersymmetric approach lies in the almost parameter free description of complicated nuclei.

Dietmar Janssen collaborated with the group of H. Börner on the possibility of obtaining information concerning the constants of the weak interaction by measuring the doppler broadening of a γ-line emitted after β-decay. He studied how the lineshape of the γ-line can yield information on the helicity of the neutrino. Also, he developed a new self consistent RPA theory, where the fermion character of the particle-hole excitation can be preserved completely.

Secretary: H. Schopohl

Nuclear and Fundamental Physics

Members of the College

K. Balog
H.G. Börner
D. Dubbers
P. El-Muzeini
H.R. Faust
E. Gutsmiedl
S. Judge
J. Klora
B. Krusche
J. Last
W. Mampe
U. Mayerhofer
M. Pendlebury
S. Robinson
P. Schillebeeckx
F. Schorr
M. Tschernitz
A. Williams

External Members and Guests

Yu. Abov (ITEP, Moscow)
P. Ageron (ILL)
M. Asghar (CEN Alger)
M. Baldo-Ceolin (Padova)
J. Blachot (CENG)
L. Bondarenko (KIAE, Moscow)
R. Bongratz (TUM)
R. Casten (Brookhaven, USA)
M. Chouder (Sussex)
G. Danilyan (ITEP, Moscow)
H. Denschlag (Mainz)
S. Dewey (NIST-USA)
W. Drexel (ILL)
R. Gähler (TUM)
P. Geltenbort (ILL)
K. Gobrecht (ILL)
R. Golub (HMI)
F. Gönnenwein (Tübingen)
K. Green (RAL)
H. Günther (Heidelberg)
M. Harder (Brighton)
B. Heckel (Seattle)
D. Janssen (Dresden)
J. Jolie (ILL)
J. Kalus (Bayreuth)
E. Kessler (NIST-USA)
I. Kilvington (RAL)
R. Kossakowski (Annecy)
E. Krüger (PTB)
S. Lamoreaux (Seattle)
H.M. Lauber (Heidelberg)
P. Liaud (Chambéry)
P. Lieb (Göttingen)
V.I. Morozov (KIAE, Moscow)
A. Nastoll (Karlsruhe)
W. Nistler (PTB)
A. Oed (ILL)
R. Oliver (ILL)
A.K. Petukhov (LNPI, Leningrad)
G. Puglierin (Padova)
N. Ramsey (Harvard, USA)
H. Rauch (Vienna)
H.J. Roth (Heidelberg)
S. Schründer (TUM)
K. Smith (Sussex)
A. Steyerl (Rhode Island, USA)
D. Thompson (RAL)
J. Van Klinken (KVI, Groningen)
G. Vivier (Grenoble)
C. Wagemans (Mol)
W. Weirauch (PTB)
T. Winkelmann (Braunschweig)
J. Wulff (Braunschweig)
P. Yaidzhiev (Sofia)
A. Zeilinger (Vienna)

Summary

The study of hadronic matter at low excitation energies is oriented increasingly towards the elucidation of basic problems rather than to the determination of bulk properties. This trend is seen in a decreasing number of proposals concerning nuclear spectroscopy (elaboration of complex level schemes following neutron capture), and in an increasing activity for the understanding of questions like the existence of two phonon excitations in nuclei, on fine structure effects in hadronic decay modes, on the study of properties of exotic n-rich nuclei along the astrophysical rapid neutron capture process paths and on parity violating and time reversal violating amplitudes in the decay of the neutron as well as in large systems. This trend away from study of bulk properties of nuclei led to the conversion of the instrument PN8 into an 'S'-facility and the classification of the heavily subscribed cold polarized neutron beam SN7 into a scheduled instrument, now PN7.

Apart from the running of the instruments scheduled in College 3, a considerable effort was put in by our members to develop the projects for the ILL's second modernisation programme:

- a new GAMS-crystal spectrometer, using an innovative two axis bent crystal geometry
- addition of a third field on the mass spectrometer LOHENGRIN
- installation of an intense positron source
- neutron optical image of a cold source
- zero field spin echo spectrometer.

In the course of the year 3 members left the College, having come to the end of their 5 years contract: D. Dubbers took over a professorship at the Technische Universität München. S. Robinson went to the Tennessee Technological University and P. Geltenbort is now managing the detector group of the ILL.

The successful work of H. Börner in developing high resolution γ-ray techniques was honoured by the "Röntgenpreis" of the University of Giessen. W. Mampe and D. Dubbers received the "Stern-Gerlach Preis" of the Deutsche Physikalische Gesellschaft for their precise determination of the neutron lifetime, the neutron β-decay asymmetry and the weak interaction coupling constants for the neutron.

Scientific Trends and Highlights in 1990

Development of scientific tools

On the instrumentation side progress is manifold in College 3: The big ionisation chamber on the mass spectrometer **Lohengrin** is increasingly used for the detection of light particle emission in fission at energies of about 2 MeV/amu. The high resolution allows for a use of much larger windows on the chamber reaching 20 cm. Also, a large area time of flight detector is being developed and tested by a research group from the Technische Universität München. The detector can use about 6 cm of the focal length and is equipped with a position sensitive anode.

On the γ-ray spectrometer **GAMS** the GRID technique, which allows lifetime measurements of nuclear levels in the femto-to-picosecond region was pushed to its extreme limits by applying the method to heavy nuclei. A slowing down model specific to the GRID measurements has been developed and is being continuously tested by dedicated experiments. This year the application of the model to polyatomic compounds was tested experimentally.

This accounts for both the mass dependence of the slowing down model, and its dependence on different stoichiometric compositions. Fig. 1 shows some of the results obtained for Cl-compounds. By scanning Doppler broadened profiles in α-Fe_2O_3 and β-Fe_2O_3 effects of the crystallographic structure were studied. Statistical models and semi-empirical prescriptions have been developed to determine the initial recoil distribution of the nucleus after γ emission in cases where side-feeding by unknown γ-cascades constitutes the major limitation of the accuracy of the GRID lifetimes. On the experimental side we worked to increase the range of measurable lifetimes with GRID by lengthening the slowing down time of the recoiling nucleus. For instance zeolite cage structures were used to contain the target.

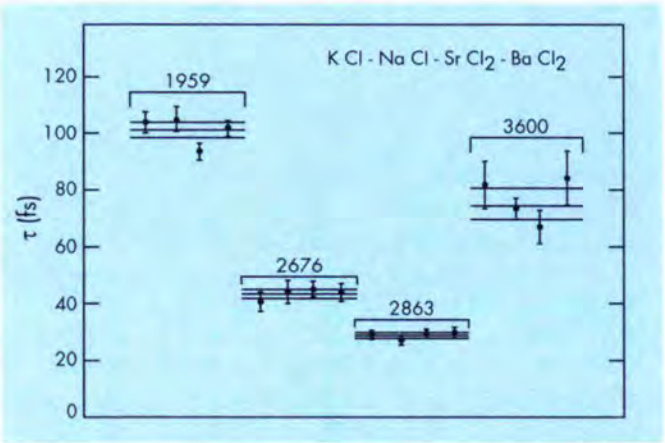


Fig. 1: Consistency of the lifetime values obtained for the same transition in ^{36}Cl, but from different chemical compounds, measured on GAMS4.

On the β-spectrometer **BILL** an experimental programme is under way to test the reliability of theoretical conversion coefficients for pure transitions. This is not only important in ensuring the use of the right screening function in the calculations, especially for higher shell conversion, but also for reliability in extracting small penetration matrix elements appearing in hindered transitions.

In order to perform an experiment on the electron neutrino helicity at the ultra high resolution γ spectrometer GAMS4, a prototype polarimeter for circularly polarized gamma rays was tested on the **PN7** beam, where, by polarized n-capture on nuclei with O^+ groundstate a polarized γ-beam was produced. On this beamline also some effort has been devoted to the development of a flux concentrating neutron optical element for cold neutrons (Heidelberg-ILL).

On various beam positions studies have been undertaken to discern systematic errors in different experiments. Therein falls the investigation of the penetration depths of neutrons in a Si single crystal which effects the accuracy of the determination of the constant h/mn, performed by the PTB group from Braunschweig.

The measurement of the neutron lifetime by ultra-cold neutron storage requires the knowledge of loss mechanisms which are not due to its decay. This year, for the first time after twenty years development of storage experiments, it has been possible to make precise measurements of the way in which the loss rate of stored neutrons depends on their kinetic energy (ILL-Sussex). The results agree with the theory on which one has had to rely almost entirely up to now, except for energies just below the Fermi potential, where some slight warming of the UCN during storage may manifest itself. This slight warming has also been detected in other experiments designed specifically to look for it. This work has exploited the recently developed ultracold neutron gas monochromator (Fig. 2).

In another experiment the cold **H17** beam has been used for experiments to measure the spectrum of upscattered neutrons derived from UCN stored in superfluid Helium (Hahn-Meitner Institut-ILL). A temperature of about 1K was chosen for the helium to give significant upscattering from the helium excitations. Some differences have been seen compared with the spectrum expected on the basis of the momentum independent three phonon interaction.

Survey of results of experiments

The classical domain of the study of the nuclear Hamiltonian via the establishment of level schemes was followed on the bent crystal γ-ray spectrometer GAMS 1,2,3, on the beta spectrometer BILL, on the pair spectrometer PN4 and on the correlation facility H22F. 'Standard' spectroscopy was applied to ^{137}Cs (Belgrade-ILL) and ^{197}Hg on GAMS, to ^{51}V and ^{52}V (Göttingen-ILL) on PN4, which was also used in a Compton suppression mode, and to ^{172}Yb (Tübingen-ILL) and ^{156}Gd (Munich-ILL) on the correlation facility. On the BILL spectrometer classical conversion electron spectroscopy was

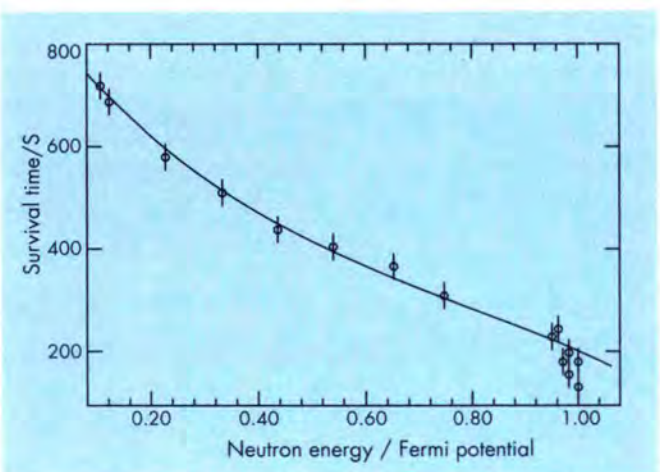


Fig. 2: Comparison between theory and experiment for the energy dependence of the survival time for stored UCN.

performed in ^{80}Br (Tübingen-ILL) and ^{112}Cd. Furthermore an exhaustive measurement of the decay scheme of ^{144}Nd was performed on this instrument. These studies aim at the comparison of the level schemes with nuclear model predictions, with special weight on odd mass nuclei. Apart from the Nilsson model and the particle-vibration coupling model, detailed comparison is possible with the interacting boson model, extended to include the coupling of one or two fermions.

The nucleus ^{112}Cd is considered to be an important testing ground for the U(5) limit of the boson part of the model, and the ILL experiments contribute to a considerable effort to understand this nucleus including also different kinds of nuclear reactions, performed elsewhere. The nucleus ^{144}Nd is being studied with respect to levels at higher excitation energies, where mixed symmetry states, as a new class of nuclear excitation, should appear.

The electromagnetic interaction in nuclei was studied on the GAMS4-spectrometer performing GRID-measurements (Gamma ray induced Doppler broadening). This technique allows the determination of nuclear lifetimes down to the femto-second domain and was applied to ^{196}Pt (ILL-BNL-Rutgers) and ^{168}Er (ILL-BNL-ISN). The first nucleus should belong to the 0(6) dynamical symmetry limit and the second to SU (3) of IBA. In ^{196}Pt the lifetime of the 0_3^+ state was established as $\tau > 1.86$ psec in perfect agreement with the O(6) picture. In ^{168}Er the existence of 2 phonon excitation in deformed nuclei was strongly supported by lifetime measurements of the decay of the $K^\pi = 4^+$ bandhead to the 2^+ level of the γ-band (Fig. 3). The transition rate was determined to be of the same order of magnitude as the gamma-to-ground state transition and confirms the two phonon character of the $K^\pi = 4^+$ band. This solves a longstanding debate whether the Pauli exclusion principle forbids the existence of multiphonon states in deformed nuclei, as was suggested by some theoretical predictions.

Hadronic decay modes are investigated on the LOHENGRIN-spectrometer, on Cosi Fan Tutte and the beam position H22D. On the latter instrument the reaction cross sections of ^{138}La(n, α), ^{184}Os (n,α) and ^{187}Os (n,α) were determined using a dedicated detector telescope (Ghent-ILL). The results give values which are two to three orders of magnitude smaller than expected from statistical model calculations. Special attention has been given to the reaction ^{36}Cl (n,p) and ^{35}Cl(n,p), which have some importance to astrophysics. The cross section was accurately determined.

Search for binary decay modes including light nuclei (from ^{6}Li to ^{32}Si) continued on the LOHENGRIN spectrometer (Tübingen-Darmstadt-Bordeaux-ILL). Heavy cluster activity has been seen in the spontaneous decay of several actinides but so far no clear signal for cluster decay following neutron capture in actinides has been detected.

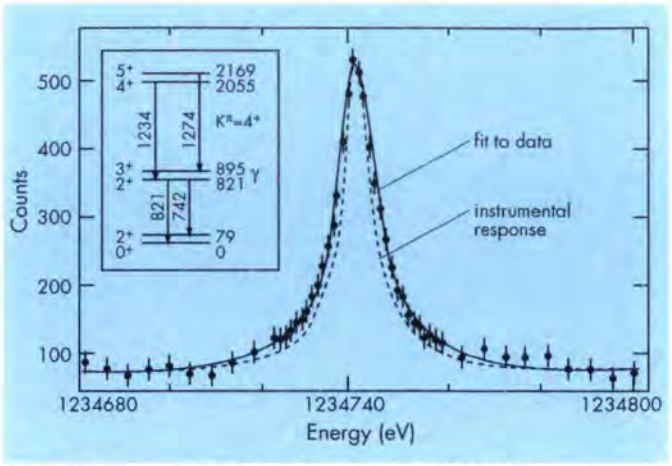


Fig. 3: The Doppler profile obtained for the 1234 keV $K^\pi = 4^+ \rightarrow 2\gamma$ transition in ^{168}Er. The dashed line represents the instrumental response function of GAMS4.

The study of the binary nuclear fission process continued on LOHENGRIN and Cosi Fan Tutte. On the former instrument nuclear charges as high as Z = 52 could be determined with the large ionisation chamber and results in symmetric fission of ^{250}Cf have been obtained (Mainz-ILL). The data evaluation will give an answer how the unchanged nuclear charge density reverses sign near the Z=50 closed shell and to what extent this closed proton shell influences the fission probability. On Cosi Fan Tutte the analysis of data from ^{232}, ^{235}U(n,f) and ^{239}Pu(n,f) (Alger-Bordeaux-Tübingen-ILL) continued. From the data evidence is collected for an enhanced emission of paired fragments also at low kinetic energies. The experiments reveal a surprising reappearance of structure in the mass distributions at low kinetic energy and an increased odd even effect for the fragment charge.

The light particle accompanied fission process was investigated on LOHENGRIN and H22D. On H22D the neutron induced ternary fission of 229Th(n,f) has been partially investigated using solid state detectors (Ghent-ILL). On LOHENGRIN the large ionisation chamber was employed to determine yields in ternary fission for particles heavier than ^{12}C for the reaction ^{241}Am(2n,f) (Tübingen-Darmstadt-Bordeaux-ILL) and ^{249}Cf (n,f) (Mainz-ILL). The quality of the data is shown in Fig. 4, where a mass over ionic charge ratio of 3 was selected, giving a snap shot of the particles ranging from ^{9}Be to ^{24}Ne which are recorded. Fig. 5 shows the energy distribution for ^{21}F and ^{24}Ne being emitted in ^{241}Am (2n,f), for selected charge states. Fig. 6 shows ^{14}C distribution in ternary fission of ^{249}Cf(n,f) measured for all relevant charge states. It was found that ^{14}C emission in ^{249}Cf increases more than a factor of 16 in comparison to ^{235}U(n,f), a surprising fact with respect to the ternary α-yield, which for both isotopes is comparable. The measurements of ternary fission yields in 241Am (2n,f) for light particles below ^{12}C using a special solid state detector arrangement has been completed in 1990.

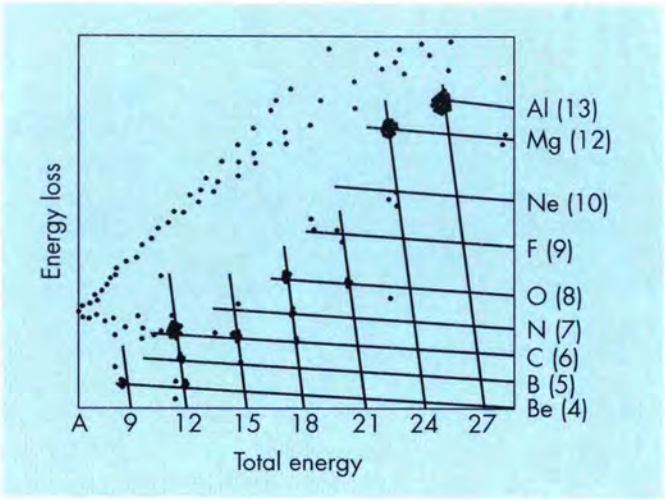


Fig. 4: Ionisation chamber data obtained on the LOHENGRIN mass spectrometer. The scatter plot shows the energy loss versus the total energy, which is proportional to the nuclear charge, of ternary particles from $^{249}Cf(n,f)$.

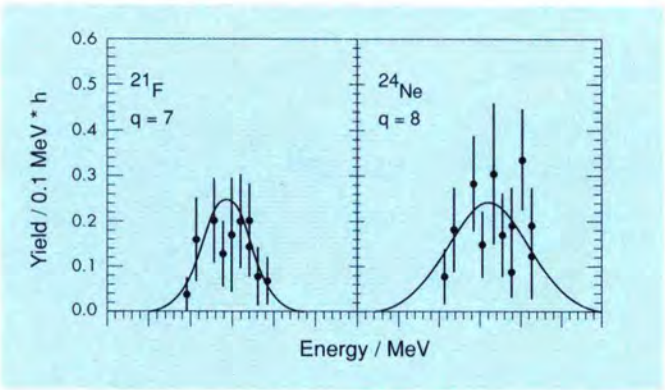


Fig. 5: Energy distribution of ^{21}F and ^{24}Ne from tripartition of ^{241}Am (2n,f), measured on LOHENGRIN.

Angular momentum induced in hadronic decay was measured for selected mass splits in ^{249}Cf(n,f) via the population of isomeric states (Mainz-ILL). The data evaluation will establish the dependence of the creation of angular momentum as a function of the kinetic energy of the single fragment.

The weak interaction is being investigated with respect to the determination of the weak coupling constants g_V and g_A, with respect to the question of the photon-to-baryon ratio in the universe and with respect to the astrophysical neutron rapid capture process. Here the weak interaction determines the β-halflives of nuclei along the r-process paths.

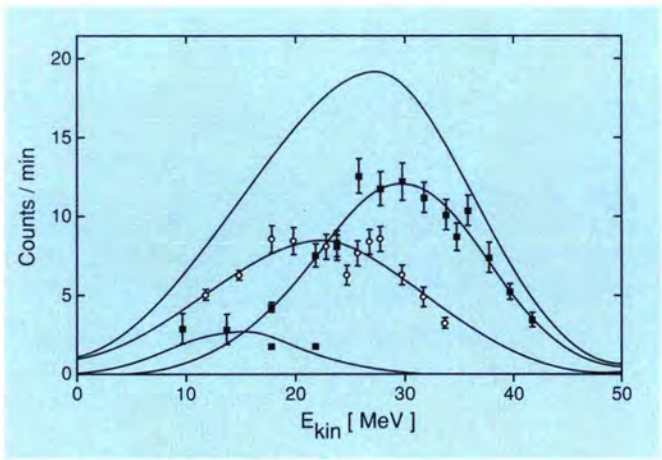


Fig. 6: ^{14}C yield from ternary fission of $^{249}Cf(n,f)$ for ionic charge states $q = 6^+, 5^+$ and 4^+.

Early in the year a new neutron lifetime experiment using stored UCN and Fromblin liquid coated metal surfaces was carried out (Kurchatov Institute, Moscow and ILL). The storage vessel is not closed to UCN at the top and is always open to the vacuum pumps (Fig. 7). Stored UCN are held in by gravity. The rates of disappearance of neutrons are compared for an empty vessel and for the vessel with a perforated lining added. The lining increases the wall area by a known fixed factor in all regions of the vessel so that the comparison allows the wall induced losses to be deduced. The experiment was repeated at three different wall loss rates by choosing different temperatures. The preliminary result is τ_n=883(3)s.

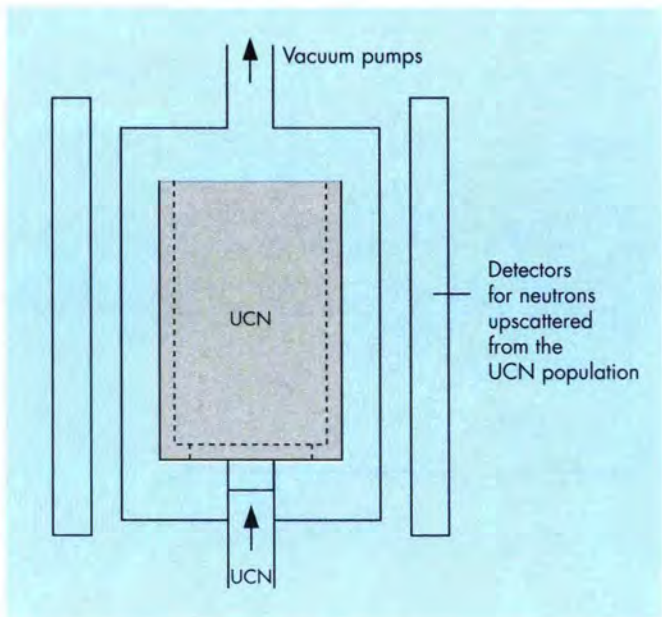


Fig. 7: The Kurchatov-ILL neutron lifetime experiment.

Also this year the data processing was completed for the Sussex NIST neutron lifetime experiment which was carried out last year on the PN7 beam using a technique where trapped decay protons are counted. The result is τ_n=893.6(5.3)s.

For further comparison we may quote the recent result τ=887.6(3.0)s from the ILL experiment of W. Mampe et al. using UCN storage in a variable geometry liquid coated glass vessel.

At the level of **fundamental interactions and elementary particles**, experiments are directed towards the determination of parity and time reversal violating amplitudes, the search for evidence for new particles and the test of quantum mechanics.

The largest and best established **P-odd amplitude** is the correlation coefficient A in polarized neutron decay. It describes the angular distribution of the decay electrons relative to the neutron spin direction. A measurement of this quantity which, for the theoretical understanding of weak interactions, is very important, was undertaken by the Annecy-ILL collaboration. The scientists employed a helium filled Time Projection Chamber in coincidence with a plastic scintillator counter to record trajectories and kinetic energy of decay electrons (PN7). Analysis of the event data is under way.

P-odd amplitudes in hadronic decay have been determined by measurement of the angular distribution of fission products in relation to the neutron spin. A group from LNPI-Gatchina investigated light fragment emission in binary fission of ^{229}Th, ^{233}U, ^{249}Pu, ^{237}Np and ^{241}Am (Fig. 8). A similar experiment on ^{233}U was performed by scientists from the University of Tübingen. Their goal is to measure the asymmetry as a function of various fission parameters, particularly in the cold fission regime. In a separate experiment the P-odd asymmetry in ternary fission was compared with that of binary fission of ^{233}U. Here the heavy fission fragments are detected in coincidence also with an emitted α-particle. The measurements were carried out by a group from the Institute of Theoretical and Experimental Physics in Moscow.

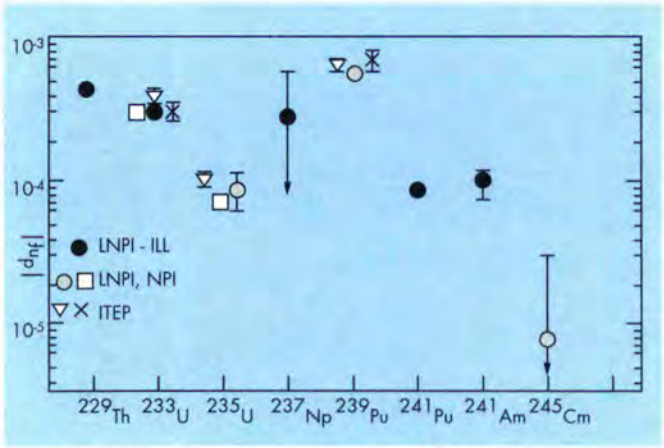


Fig. 8: Results of various experiments performed at the ILL to determine the parity violating amplitude in hadronic decay processes.

T-odd amplitudes may be detected in neutron decay correlation measurements and in the search for an electric dipole moment of the neutron. With the former technique the so-called R-coefficient in neutron decay is determined by measuring a possible decay asymmetry in a combination of three vectorial quantities - electron spin, electron momentum and neutron spin (Annecy-ILL). The experiment is in progress. Along the line of the determination of T reversal violation through the measurement of the neutron electric dipole moment, progress has been made on two fronts: The old EDM machine was rebuilt this year in preparation for measurements with increased sensitivity (Sussex-ILL-Washington-Harvard). The main changes introduced are a factor of ten increase in the neutron storage volume, and a new magnetometer which will monitor the nuclear precession of ^{199}Hg atoms stored in the same chamber as the neutrons.

On the second front, ideas for a new generation experiment to measure the neutron EDM were sketched by R. Golub and S.K. Lamoreaux. The line of thought of the new idea employs the storage of ultra-cold neutrons in superfluid ^{4}He. ^{3}He is dissolved in the ^{4}He liquid in a small amount and acts simultaneously as UCN polarizer and UCN analyzer, as agent for detecting the UCN and as the magnetometer. For this last function an oscillating magnetic field dressing would be used to equalize the spin precession rates of the ^{3}He nuclei and the neutrons. Without the dressing the precession rates differ by about 10%.

Baryon number violating amplitudes are searched for in the neutron-antineutron oscillation experiment. The experiment was running during the year. (Padova-Pavia-Heidelberg-ILL). No clear signal indicating a violation of the baryon number in this process was observed, which puts the lower limit of the oscillation period to $\tau_{osc} > 7.10^7$s. To increase the sensitivity of the experiment still further, a continuous effort is being made to decrease the influence of external magnetic field perturbations and to increase the detector efficiency. The experiment will run for 6 more reactor cycles.

The search for **new particles** continued on the β-spectrometer BILL with the Bhabha scattering experiment, in collaboration with the GSI Darmstadt. The existence of a neutral particle with a mass of 1.8 MeV/c^2 has been postulated at the GSI to explain the observation of mono-energetic coincident positron-electron pairs in heavy ion collisions. The particle could also be created in an electron-positron collision at the appropriate centre of mass energy, the recoiling neutral particle would then decay into an electron-positron pair. No evidence has been found in Bhabha scattering to support the existence of a new particle, and the experiments of the ILL have set its lower lifetime limit to $7x10^{-12}$s (see box). In a second experiment on BILL a manifestation of neutrino mass in β-decay was searched for. A target of ^{176}Lu was irradiated for eight days to produce a highly active (50 Ci) source of ^{177}Lu. The latter

nuclide decays by emitting a beta ray with an end-point energy of 500 keV and has a halflife of 7 days. It was therefore possible to measure the β-spectrum during the ten days shutdown after the end of the reactor cycle. For the moment no indication of the existence of a massive neutrino was found.

The tests of fundamental laws of **quantum mechanics** continued on the beam-line H18, with the diffraction of cold neutrons (λ=20Å) on macroscopic slits (TU München and Atominstitut Wien). The measurement is in excellent accordance with theory and proved that the rigorous diffraction theory for neutrons is correct.

Alongside the ultracold neutron outlets of the vertical (TGV) source is a very cold (100 Å) beam used for neutron optics experiments by the Vienna-Munich-ILL collaboration. A grating interferometer with transmission gratings is currently being developed. After early tests using a 2 μm grating constant, the emphasis has been on providing more efficient isolation against vibrations and thermal influences. A special cabin has been set up around a bench and the levelling system for the optical table has been improved.

Following this, new gratings with 1 μm grating constants have been tested successfully and found to meet the requirement for a new set up which will soon be used to measure the phase shift of neutron waves due to the Earth's gravity.

Applied and interdisciplinary science

On the LOHENGRIN spectrometer the long-standing effort continued to measure the end-point energies of β-spectra from neutron-rich fission products. In particular the region around the closed N=50 neutron shell has been investigated (University of Braunschweig). At the same instrument a Studsvik/CENG collaboration measured average γ and β yields for various fission chains containing refractive elements inaccessible with ISOL-systems. The results are used as input for heat calculations of nuclear power reactors.

The prompt gamma facility of H22E was used by geologists from the University of Grenoble in collaboration with the ILL to study the light element distribution in Himalayan leucogranites from two new intrusions. Neutron activation analysis was used to determine rare earth, trace and LIL elements on a variety of rocks from different environments. Notably, samples from the geodynamic domaine of the Andean Cordillera have been investigated. Measurements were made on andesites and dacites from several active volcanoes to determine the sources and evolution of Andean magmatics from the Central Volcanic Zone. Cooperation for these measurements was with the University of Grenoble and ORSTOM, Paris.

Secretary: H. Faust

Astrophysics

The elemental abundance in the solar system for masses heavier than ^{56}Fe is supposed to have been created by two distinct processes: the s-process, short for slow process, and the r-process, short for rapid process. The s-process is defined as the capture of neutrons by stable or long lived isotopes and by their subsequent β decay. In the s-mechanism each step involves the gain of one nuclear charge unit, until the element ^{209}Bi is reached. The α instability which sets in beyond this isotope brings the slow neutron capture process to an end. Whenever a closed shell is approached in the s-process, the extra stability implied leads to an increased elemental abundance showing up as 's' peak yield in the Fig. 9.

The rapid neutron capture process proceeds via a different mechanism: in a presumed explosive stellar event as the side of the r-process the intensity of the neutron flux is extremely high (10^{28} ncm^{-2}s^{-1}) for a short time (2s). Neutron capture starting from ^{56}Fe proceeds very rapidly, leaving no time for the intermediate isotopes formed to decay. The process stops when the closed N = 50 neutron shell far away stability is reached, the reason being that the neutron binding

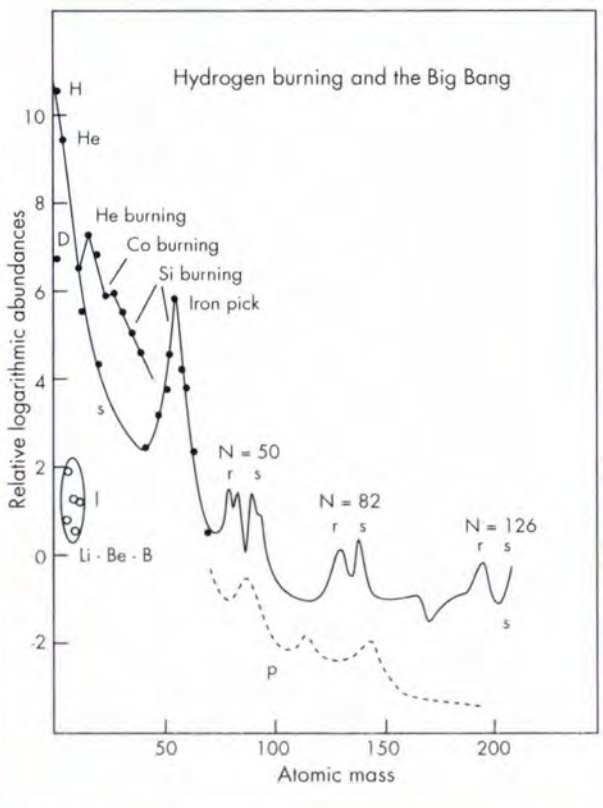


Fig. 9: Relative abundances of elements in the solar system, decomposed into the various processes. The N=50 r-peak is subject to investigations on the LOHENGRIN spectrometer.

energy, on crossing the magic shell, drops considerably and an equilibrium builds up between (n,γ) and (γ,n) reactions in the 'hot' stellar atmosphere. A hiatus is reached where β decay must occur first before any other neutron may be captured.

After freezing out of the process these very n-rich nuclei decay back by numerous β decays to stability. The result is a strong enhancement of solar abundances in 'r' peaks on the left of the 's' peaks in Fig. 9. Another consequence is that thorium and uranium isotopes can be created, which are important to us now as a source of nuclear energy. The region of the nuclear chart where the very first part of the r-process is assumed to take place, is shown in Fig. 10, the main elements of interest being iron, cobalt, nickel, copper and zinc. To reproduce the abundance curve by calculation, input parameters to models have to be known, the most important are the lifetimes, the masses, the delayed neutron emission probabilities and the properties of low-lying excited states. Obtaining these nuclear parameters presents a challenging problem: the production, identification and spectroscopy of exotic nuclei which have up to 14 neutrons in excess of their stable isotope.

Reversing the process of nuclear synthesis by using the thermal neutron induced fission reaction of U and Pu isotopes, we have been able to identify very neutron rich species along the r-process paths. These isotopes are extremely rare, having abundances as low as 10^{-9} compared to 'standard' fission.

In a special set-up of the ionisation chamber used on LOHENGRIN it has been possible to implant the isotopes into Si detectors, using the last 6 MeV of kinetic energy of the particles at the very end of their ionisation track. By looking into the time correlations between the incoming identified ion and its subsequent β decay it is possible to determine its halflife. In this way the decay of ^{71}Ni, ^{72}Ni, ^{73}Ni, ^{74}Ni, ^{74}Cu, ^{75}Cu, ^{68}Co, ^{69}Co and ^{68}Fe have been measured (Table 1). The outcome of the experiment is that the halflives of these nuclei on the r-process paths have been found to be much shorter than assumed previously in the calculation for the elemental abundances. This is especially true for the isotopes ^{68}Co, ^{69}Co and ^{68}Fe. The results suggest that the r-process calculations should be redone in this region. The mass limit of the isotopes which contribute to the abundance peaks must be displaced towards the stability line in the Co-Fe region.

Whereas the understanding of the r-process gives us information about elemental distribution above Iron, and therefore about later stages in the development of the universe, where the iron 'seed' was already formed, the value of the neutron lifetime provides information about the very beginning. In the standard big bang model light element abundances depend both on the number of existing neutrino families and the neutron lifetime. This year the number of families of quarks and leptons including neutrinos was determined with a great accuracy by the experiments on the Z° decay at the LEP accelerator at CERN. With their results the neutron lifetime and the information on the light element abundance (helium for example) give an estimate of the baryon-to-photon ratio of the universe. This ratio is very uncertain from direct observations and at the same time it is of great interest because it gives the very small asymmetry in the numbers of particles and antiparticles which must have existed in the early fireball of the universe. Without this asymmetry there might now be only radiation and no matter ! Early speculation by Sakharov related this asymmetry to the violation of time reversal in the fundamental interactions.

The accepted range of baryon-to-photon ratio in Fig. 11 is derived from various neutron lifetime experiments at the ILL which have continued to give further results during the last year as described in the College 3 report section. These new lifetime results lead to a baryon to photon ratio between 2×10^{-10} and 6×10^{-10}.

		T 1/2 (S)
Cu:	74	1.46 (0.25)
	75	1.35 (0.40)
Ni:	71	1.95 (0.38)
	72	2.05 (0.50)
	73	0.86 (0.15)
	74	1.07 (0.5)
Co:	68	0.18 (0.10)
	69	0.27 (0.05)
Fe:	68	0.10 (0.06)

Table 1: Measured halflives for Cu, Ni Co and Fe isotopes.

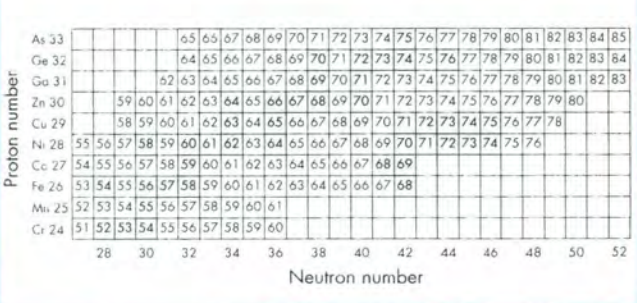


Fig. 10: Part of the chart of nuclides showing the region of the very beginning of the r-process paths. Shaded isotopes are stable, dotted ones are produced in the fission process of U and Pu. The halflives of underlined isotopes has been determined on LOHENGRIN.

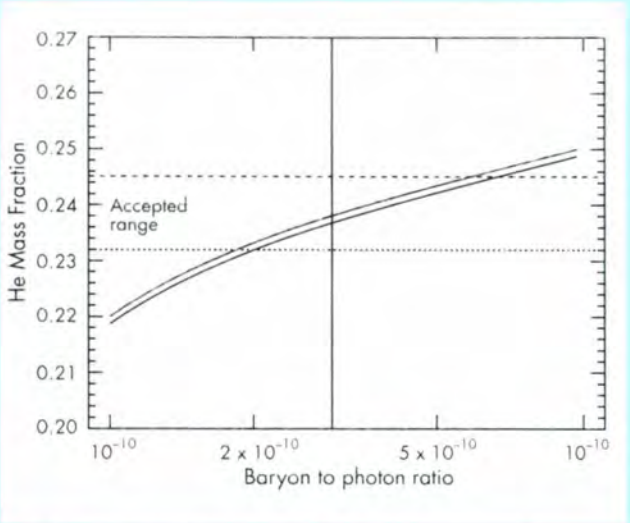


Fig. 11: The shaded band shows the relation between the Helium mass fraction in the primordial universe and the present baryon-to-photon ratio as determined by the value of the neutron lifetime and its uncertainty. It seems that the baryon to photon ratio has to be between $2x10^{-10}$ and $6x10^{-10}$. The calculation assumes that there are three types of neutrinos.

Experiments with neutron induced positron sources

K. Schreckenbach

The development of an intense positron source at the ILL was prompted by a recent and intriguing problem in particle physics, the investigation of which required a beam of positrons in the MeV range, monoenergetic and tunable in energy. The problem was posed by the observation of correlated narrow positron and electron lines in heavy ion reactions at the GSI, Darmstadt. These monoenergetic e^+e^- lines could be evidence for an as yet unknown neutral object of short life-time (experimental range 10^{-20} to 10^{-10} s) and with an invariant mass of about 1.8 MeV, decaying freely in e^-e^+ pairs. If this should be the case the time reversed reaction, e^+e^- scattering (Bhabha scattering), would also be able to produce this exotic particle. This has been the subject of our investigations.

A conventional way to search for a very short-lived object is to measure the cross section in the collision of particles in dependence on the centre of mass energy. The production of a new particle with immediate back decay into the original ones would yield a similar signature in the detection system to that of elastic scattering. In our case the experimental evidence for a particle formation would just be a resonance like peak in the Bhabha scattering cross section at the total centre of mass energy equal to the particle rest mass.

For the Bhabha scattering experiment we used a positron beam interacting with the electrons in a metal foil. To achieve a centre of mass energy of 1.8 MeV the kinetic energy of the positron beam must be around 2.2 MeV. How can one produce positrons in this energy range at a reactor and create out of them a monoenergetic beam of variable energy ?

The basic idea employed was to use pair creation in the absorption of high energy prompt gamma rays from the neutron capture reaction, i.e. the conversion chain neutron —> gamma-ray —> e^+e^- pairs. Placed in the high neutron flux at the target site of the BILL beta spectrometer a strong positron source with a continuous spectrum was available. The spectrometer served as momentum selector and formed a monochromatic, tunable positron beam. Its intensity closely follows the neutron flux at the source.

The energy release in the neutron capture reaction is typically 6 to 10 MeV and it is normally shared between several gamma ray transitions cascading down from the capture to the ground-state.

A significant fraction of the neutrons can be captured with target nuclei of high capture cross-section. Thus the number of gamma-rays produced can be similar or even higher than the available number of neutrons. The positrons are produced when the gamma-rays undergo pair-production in the (n,γ) target itself and/or in a separate converter material. An element of high nuclear charge is favourable since the pair production cross-section is approximately proportional to Z^3. The resulting positron energy spectrum depends primarily on the gamma-ray spectrum. However, it is modified by the energy loss and scattering of positrons in the target.

For an optimum production of positrons in the range 2 to 3 MeV the gamma-ray energy must be around 6 MeV, since 1 MeV is needed for the e^+/e^- rest masses and the kinetic energy is shared about equally between the particles. The reaction $^{48}Ti(n,\gamma)^{49}Ti$ with 7.8 barn cross-section provides such gamma-rays at the average rate of 0.8 gammas per captured neutron in the range 6.4 to 6.8 MeV. The final source used at BILL was composed of a 3 mm thick plate of natural titanium, area 50 x 100 mm^2, covered by a plate of 0.25 mm thick platinum as a high Z material. The positrons were momentum selected by the double focussing iron core magnets of the spectrometer, yielding in the energy range 1...3 MeV $3x10^5$ e^+/s per 1 cm in the 10 cm long focal plane. Numerical calculations have shown that the positron flux cannot be increased by more than a factor of two by using thicker Ti and Pt layers. However this increase would cause too high a gamma-heating of the source at the target site.

With this positron beam two types of experiments were performed in collaboration with the GSI (Fig. 1). Positrons were scattered at a 4.7 mg/cm^2 thick beryllium foil suspended in the focal plane of the spectrometer. In the first experiment the foil was directly viewed by two rows of Si(Li) detectors. A scattering event triggered two detectors in coincidence with a sum energy close to the incoming positron energy. The multidetector device provided stable measurement conditions and used the dispersion in the focal plane for optimum energy resolution. In the second experiment one detector row was shielded from the scattering foil. We were looking for longer lived objects, which might be produced in the target, and then decay behind it in free flight. The normal elastic scattering events could be suppressed by more than three orders of magnitude, but the arrangement is only sensitive to lifetimes longer than 10^{-12} s corresponding to a flight path of the relativistic object of about 0.4 mm.

The results could only be interpreted in terms of an energy integrated cross-section. In fact, the hypothetical resonance would show up in the laboratory system with a minimum width of about 30 keV, caused by the centre of mass transformation of the momentum spread of the electrons in the beryllium foil. This width would be even larger for heavier elements. The result from the GSI indicated that we should search for a much narrower particle decay width. Thus the intensity of the resonance line observed is spread over the experimental resolution. The limits derived from our experiments are shown in Fig. 2.

The unitarian limit for reaction cross-sections is applicable for the present events and tells us the theoretical height of the hypothetical resonance:

$$\sigma_R^{max} = 4\pi\lambda_R^2 \cdot \frac{2J+1}{(2s_1+1)(2s_2+1)}$$

$$\lambda_R = 2h/(M_R^2 - 4m_e^2)^{1/2}$$

where M_R denotes the particle mass, J the total angular momentum of the particle and si the spin of the leptons.

The unitarian limit for the integral cross-section for a J=0 particle is shown in Fig. 2. Our data exclude the lifetime range shorter than 10^{-11} and our more recent experiment (evaluation in progress) achieved a sensitivity up to 10^{-10} s. A further gain in sensitivity in our method could be achieved only with thicker scattering foils. But the result would become ambiguous,

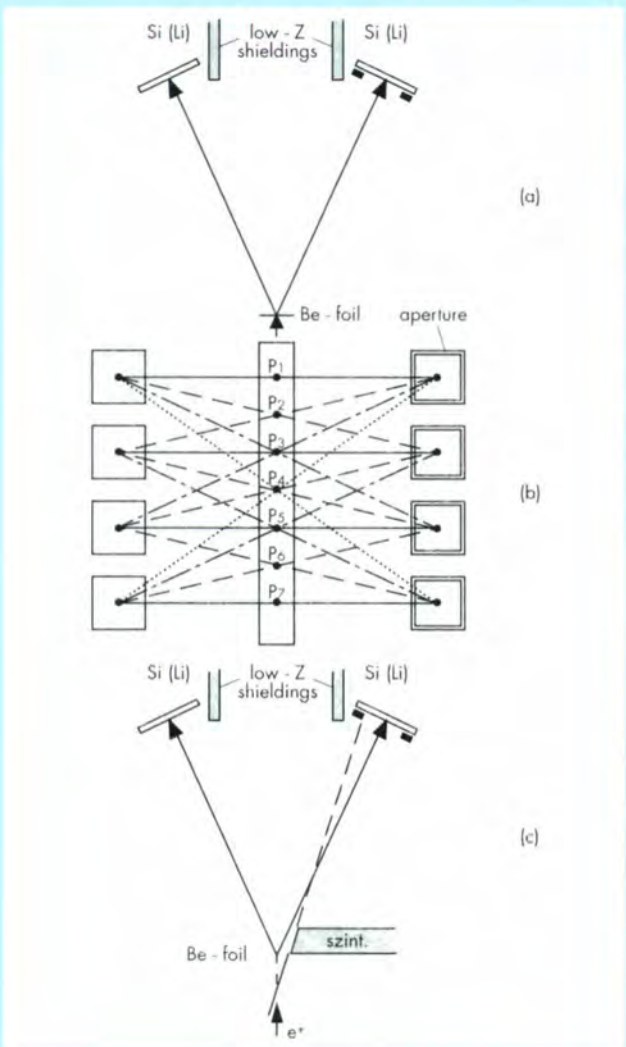


Fig. 1: Arrangement for the Bhabha-scattering experiments in the focal plane of the BILL beta spectrometer. (a) Unshielded view on the scattering foil; (b) illustration of the grouping of scattering points; (c) shielding of elastic scattering events.

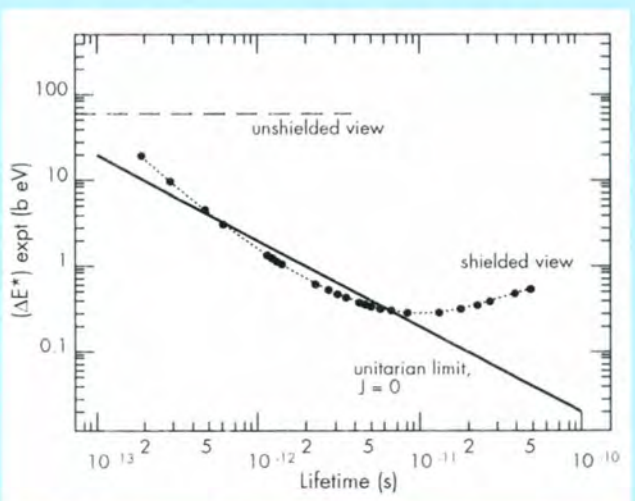


*Fig. 2: Experimental limits compared to the unitarian limit for a J=0 particle. The region **above** the dotted/dashed line is excluded by the experiment.*

since an extended object may disintegrate prior to its decay when passing through a thick layer of matter.

Our result goes beyond the specific GSI problem and tells us that no 1.8 MeV particle exists, even if composed, which decays with a partial lifetime shorter than 10^{-11} s into e^-e^+. This limit is more general and more precise than that derived from the (g-2) magnetic moment anomaly of the electron. It results from high precision experiments on (g-2) with stored electrons compared with theoretical calculations taking into account all known particles which couple to the electron. An additional particle would change the electrons g value through its virtual emission-absorption loop.

It should be noted that the positrons passing the focal plane of the BILL spectrometer could be easily focussed together. This would lead to a spot of about 5x10 mm^2 comprising $2x10^6$ positrons per second at MeV energies with an energy spread of 1.5 %, thereby constituting an excellent beam for solid state physics studies of bulk materials.

A new generation of positron sources

Following the experience with the positron source for the Bhabha experiments we considered the potential of our method for a source of slow positrons (eV to few keV range) as frequently used in atomic and solid state physics. In these sources fast positrons are slowed down in a moderator and emitted from its surface with an energy corresponding to a positive workfunction of the moderator for positrons. The positron spectrum from the Ti-Pt arrangement is not optimum for this purpose since it is too energetic. A much better choice would be cadmium as a (n,γ) source and tungsten as a γ-e^+ converter and moderator. The thermal neutron capture in natural cadmium is completely dominated by the $^{113}Cd(n,\gamma)^{114}Cd$ reaction with a cross section of 26,000 barns. The measured and calculated positron spectrum for a Cd-W sample is compared in Fig. 3.

The theoretical limit for the conversion yield of neutrons into slow positrons is given by the absorption of all gamma-rays in the converter and by the minimal losses in the moderation process. The calculated fast positron yield is 0.6 e^+ per captured neutron for the Cd/W combination. In the slowing down process of the fast positrons to eV energies the losses are in the order of a factor two. Thus one neutron can yield in principle 0.3 slow positrons.

Unfortunately typical moderators strongly annihilate slow positrons. The diffusion length in W for instance is only about 500 to 1000 Å. Thus the moderator must be split in thin foils and the emerging slow positrons collected and accelerated into a beam. With present techniques the slow positron extraction yield into a beam is hardly better than 10^{-3} per fast positron. On the other hand large neutron flux areas are available at a reactor and therefore the intensity of a positron source is mainly limited by the requirement that the slow positrons produced must be collected from a large area into a small beam cross section. We have discussed focussing devices or drift tubes. The estimates are very promising and point towards slow positron fluxes which are orders of magnitude higher than available at present. New generations of positron beam experiments would become possible.

The present article summarizes several recent papers:

H. Tsertos, C. Kozhuharov, P. Armbruster, P. Kienle, B. Krusche and K. Schreckenbach, Phys. Rev. D40 (1989) 1397

S.M. Judge, B. Krusche, K. Schreckenbach, H. Tsertos and P. Kienle, Phys. Rev. Lett. 65 (1990) 972

K. Schreckenbach, B. Krusche, W. Triftshäuser and G. Kögel, "A High Flux on-line Source of Moderated Positrons", Proposals for the "3ème souffle", in technical report ILL 90IL21T

B. Krusche and K. Schreckenbach, Nucl. Instr. Meth. A295 (1990) 155.

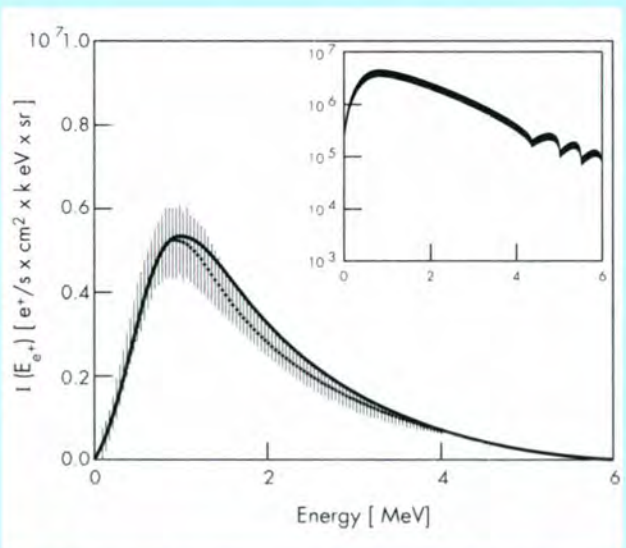


Fig. 3: Fast positron spectrum measured at BILL for Cd as (n,γ) source and 0.1 mm tungsten as converter. The solid line represents the calculation. The experimental results are shown by the error bars. About 10^{13} n/cm^{2}s were captured.

Structural and Magnetic Excitations

Members of the College

M. Alba	J.E. Lorenzo Diaz
K. Al Usta	J. Mesot
L. Andersen	A. Magerl
R. Bateson	W. Marshall
J. Bossy	J.L Martinez
T. Brückel	T. Möller
R. Currat	A.P.Murani
S. Dakin	H. Mutka
B. Dorner	L. Needham
B. Fåk	W. Petry
B. Farago	O. Schaerpf
T. Fernandez	B. Schmid
S. Hayden	H. Schober
A. Krimmel	A. Severing
H.J. Lauter	C. Vettier
J.F. Legrand	M. Vrtis
A. Lied	C.M.E. Zeyen

General Summary

In 1990 as in the past three years, a huge amount of work and beam time was devoted to studies on high-T_c superconductors, but this has not prevented further research in other fields such as normal superconductors, heavy fermions and low dimensional systems.

This year 1990 will be remembered as a period of high turn-over of physicists in college IV with the departure of many eminent members such as C. Vettier, S.M. Hayden, H. Godfrin, V. Frank and the arrival of new physicists, L. Needham, B. Fåk and J. Bossy. The college has done its best to fulfil its task despite a slightly heavier overload in these changing conditions.

Scientific Trends and Highlights in 1990

Lattice Dynamics and Structural Phase Transitions

This is a very active domain, work can be divided into 3 main categories: dynamics of incommensurable phases, soft phonons in simple metallic structures and phonon density of states in superconductors. In the past year, progress was made in these three domains but in this annual report we shall focus on examples drawn from the last two .

γ-tin

Recently measurements were made on the phonon spectrum of metallic γ-tin (substitutional solid solution $Sn_{0.8}In_{0.2}$) [1]. This crystallographic modification of tin has an unusual simple hexagonal (SH) structure with one atom per primitive cell. The existence of a number of low frequency modes in the γ-tin phonon spectrum reflects low stability of SH structure.

The soft transverse phonon mode at q = (1/2 0 1/2) (L-point at the Brillouin zone boundary) relates the SH to the well-known β-Sn (white tin) structure.The phonon frequencies of the L-point mode do not reveal any dramatic change between 100 and 370 K (the last value is 50 K below the melting point). The temperature dependence of the frequency seems to have a small step in the range between 140 K and 310 K where additional elastic intensity appears with hysteresis (reminiscent of a "central peak"). Otherwise, the overall tendency is a slight decrease in frequency strongest near the melting point (Fig. 1).

Superconductors

The discovery of superconductivity in lamellar copper oxide materials has led to a huge amount of experimental and theoretical effort to understand the mechanism of high T_c superconductivity. Neutron scattering techniques, which can probe lattice and spin modes, are appropriate to probe both spatial and temporal fluctuations which could induce coupling leading to superconductivity. Several groups have embarked upon the investigation of lattice modes, while other have concentrated on the magnetic properties of single crystals.

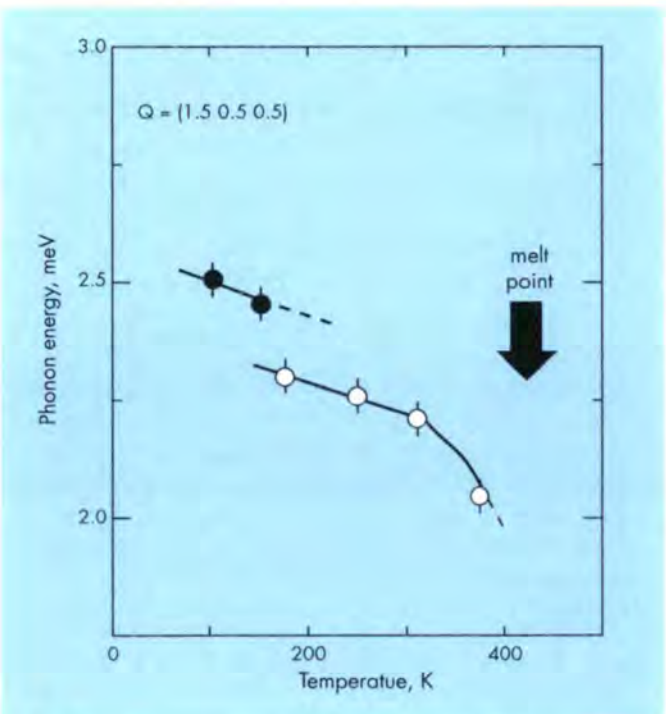


Fig. 1: Temperature dependence of the energy of the L-point phonon mode in γ-tin. Full and open symbols are obtained in presence of an intense elastic peak and without it.

Phonon partial density of states in $YBa_2Cu_3O_{6.97}$

Experiments on determination of the Cu atom partial density of vibrational states of the ceramic samples $YBa_2Cu_3O_{6.97}$ have been performed by using the isotopic contrast method in neutron inelastic scattering. The neutron cross-section is proportional to the factor σ/M. This factor for Cu^{65} is 0.223 barn/a.u.m. and for Cu^{63} 0.0825 barn/a.u.m. In this case the difference between the spectral distributions found for two samples $YBa_2Cu_3O_{6.97}$ with these isotopic compositions will thus be proportional to the Cu atom partial density of vibrational states.

The Cu atom vibration spectra in the superconducting sample (T_c = 92 K) have been measured at three temperatures: 300, 95 and 80 K with the cold neutron focussing TOF spectrometer IN6 (Fig. 2). It changes little as the temperature decreases below T_c. The cut-off energy is 40 meV at all temperatures. However, the intensity of the peak at energy E = 15 meV increases as the temperature decreases from 300 K to 35 K. Such behaviour indicates that it is associated with anharmonic Cu atom vibrations. Recently it was noted that this peak increases when the oxygen concentration decreases [2] and it was suggested that this band corresponds to the Cu_1 atom vibrations in the chains Cu_1-O_4.

Magnetism

As in the case of lattice dynamics, recent work in magnetism can be separated in three major domains: superconductors, low dimensional physics and critical dynamics in model compounds.

Spin dynamics in the superconducting and normal states of $YBa_2Cu_3O_{6+x}$.

During the last year, attention has been focussed on metallic samples with T_c = 60 K to study the magnetic response in the normal and in the superconducting states. The experiment was carried out on the IN8 three-axis spectrometer. The dynamic magnetic correlations have been clearly observed with very short correlation length down to 1.6 lattice unit for x = 0.69. This correlation length has been found to be independent of temperature and energy [3]. The energy dependence of the magnetic response is markedly different from what has been observed in the antiferromagnetic materials. No sharp spin wave-like excitations exist any more but a rather broad response extends towards higher energy as the oxygen content is increased. In the superconducting state, the opening of a gap in the magnetic susceptibility has been demonstrated (Fig. 3). Furthermore, some superconducting correlations persist up to $T \approx 2T_c$. In the normal state, the Cu spin dynamics is dominated by the presence of carriers which renormalize the energy scale down to a characteristic energy related to the density and mobility of carriers. Further work is under way to characterize the magnetic response and the coupling to carriers in 90 K $YBa_2Cu_3O_{6+x}$ superconductors.

A transition from a local moment spin glass to a marginal Fermi liquid

$La_{2-x}Ba_xCuO_4$ is in an insulating antiferromagnet for x = 0. On doping, the three dimensional magnetic order is destroyed and there is a metal-insulator transition at $x \approx 0.05$ followed by the onset of superconductivity at $x \approx 0.15$.

The magnetic fluctuation spectrum of a nearly metallic single crystal of $La_{1.95}Ba_{0.05}CuO_4$ has recently been

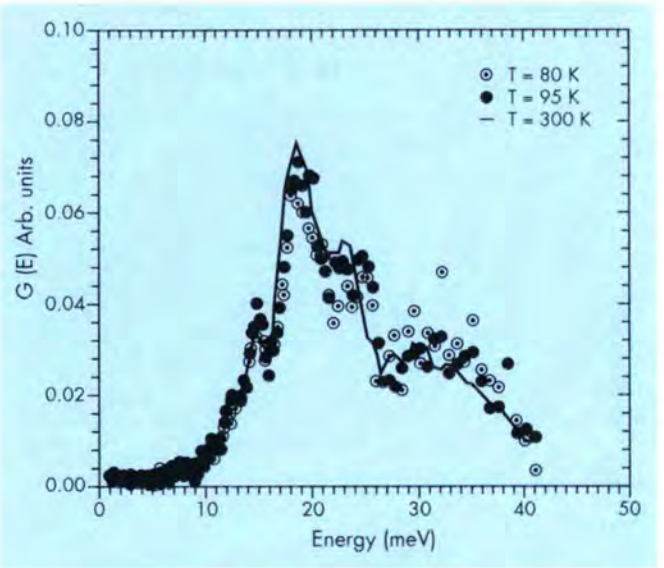


Fig. 2: Partial density of states of the Cu atom vibrations in $YBa_2Cu_3O_{6.97}$ as determined by isotopic contrast method at temperatures of 80 K, 95 K and 300 K.

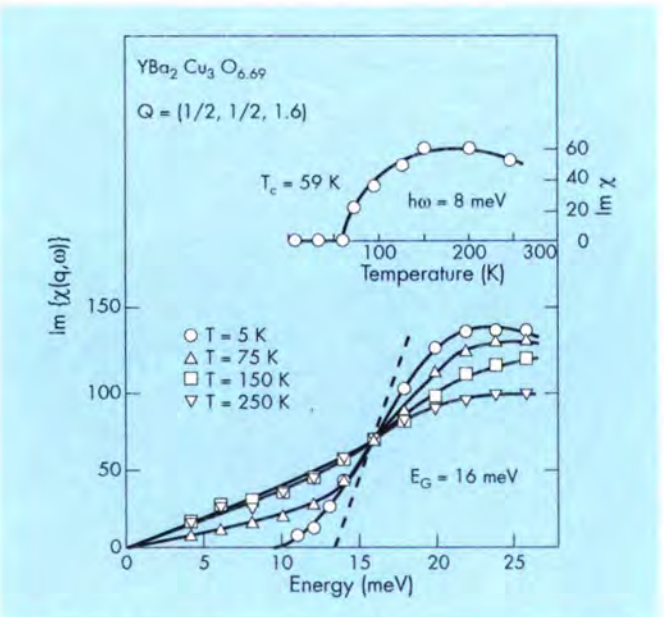


Fig. 3: $Im\{\chi(q,\omega)\}$ (in arbitrary units) as a function of energy for $YBa_2Cu_3O_{6.69}$ at temperatures above and below T_c. The energy gap at 16 meV in the excitation spectrum persists above T_c.

investigated [4]. The 'cold', 'thermal' and 'hot' sources at the ILL permit experiments to be performed over a wide range of energy. Some results are shown in Fig. 4 as constant energy scans as a function of in-plane momentum q through antiferromagnetic zone centres.

At low temperatures ($T \leq 8$ K) the sample forms a novel two-dimensional antiferromagnetic 'spin-glass' with microdomains of typical size 20 Å frozen on long time scales (as can be seen in the $h\omega = 0$ scan). On warming, the lifetime of these antiferromagnetic clusters becomes shorter and the 'elastic' peak disappears, as shown by the temperature dependence of the magnetic intensity. Such freezing phenomena in spin-glass systems were first studied with neutrons at the ILL by Murani and co-workers [15].

Our experiments also demonstrate a strong coupling of charge and spin degrees of freedom: there is a dramatic increase in the magnetic fluctuation rate $\hbar\Gamma$ near the resistance minimum associated with the cross-over from low-temperature insulating to high-temperature metallic behavior. A particularly interesting finding is that in the latter regime, $\hbar\Gamma \sim 1/3\ k_B T$, characteristic of the recently proposed "marginal Fermi liquid" [5] which may exist in the normal state of high-T_c superconductors.

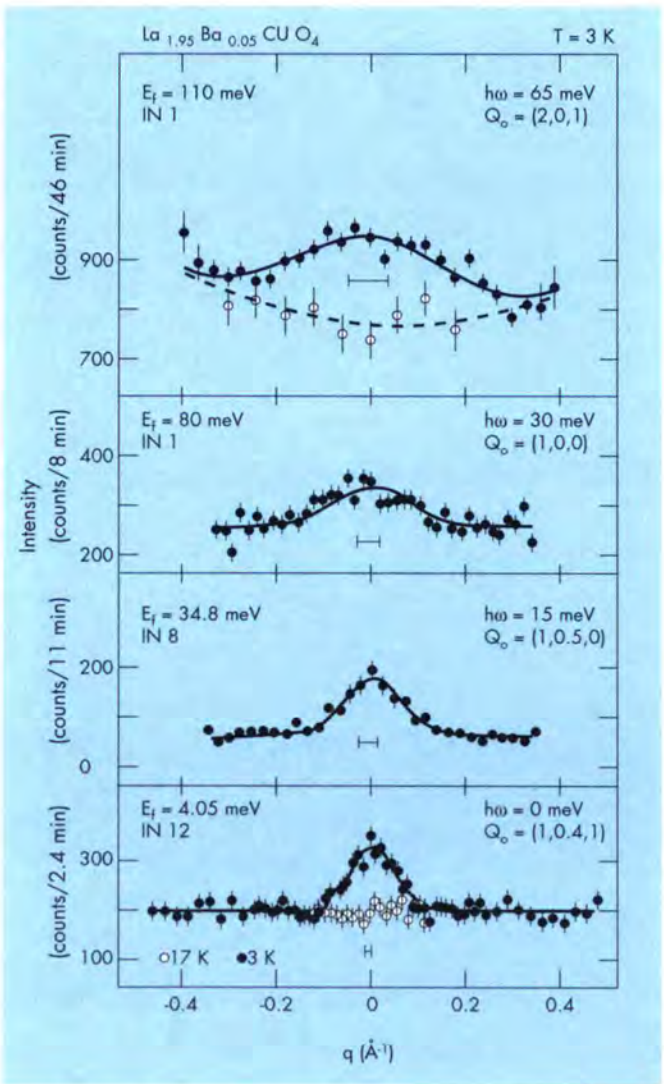


Fig. 4: Constant energy scans on TAS instruments on cold, thermal and hot sources through the 2D antiferromagnetic zone centre in $La_{1.95}Ba_{0.05}CuO_4$ showing broad magnetic scatttering.

The Haldane gap

As first predicted by Haldane [6], one-dimensional Heisenberg antiferromagnets with integer spin S show a finite energy gap, E_G, in their excitation spectrum. This quantum effect is found to be maximum for the S = 1 case where $E_G \approx 0.41\ |J|$ where J is exchange between adjacent spins.

$AgVP_2S_6$ with V^{3+}, S = 1 chains has been examined in the context of the Haldane ground state [7]. The gap for magnetic excitations has been determined to be $Eg = 27 \pm 1$ meV by TOF measurements on polycrystalline samples on the IN4 instrument.

A modelling of the powder averaged TOF spectra was undertaken in order to overcome the lack of single crystal measurements. A simple one-dimensional model can fully account for the observed features in a wide range of incident energies from 17 to 650 meV (measurements were also made on the HET instrument at RAL). The full analysis gives a spin-wave velocity of $C = 150 \pm 10$ meV and independently a dynamic correlation length of $x = 5.5 \pm 1$. This compares very well with the expected relation $x = C/Eg$. In spite of the strong intrachain coupling, J = 550 K, the measurements on D1B have shown that this quasi-one-dimensional system does not order down to T = 2 K, which is in agreement with the disordered 1D character of the Haldane ground state.

NENP ($Ni(C_2H_8N_2)_2NO_2(ClO_4)$) is a good realization of a one-dimensional antiferromagnet with |J| equal to 47 K. However, it exhibits some magnetic anisotropy. Easy-plane D and in-plane E crystal field anisotropies lead to different values of the gap for the three different polarizations of the excitations. From the values of the three gaps, it was found that $D/|J| = 0.17$ and $E/|J| = 0.02$. A magnetic field applied perpendicular to the chain axis was predicted [9] to induce a phase transition corresponding to the softening of the energy gap of in-plane modes polarized along the chain axis. Experiments carried out on the IN12 three-axis spectrometer [8] have confirmed the theoretical predictions. Although the maximum value of the applied field was 10.33 T, slightly less than the predicted critical value 11.8 T, data shown in Fig. 5 demonstrate the softening of the mode with polarization perpendicular to the field, while the other in-plane mode is not affected.

Polarized neutrons

The separation of the longitudinal from the transverse susceptibility can be achieved by the use of polarized neutrons. If the spin fluctuations are parallel to the

polarization **P** of the neutrons and **P** perpendicular to Q, then the scattered neutrons maintain their spin state. A small vertical guide field at the sample position directs **P** perpendicular to Q. If the substance is ferromagnetic and the vertical field strong enough to saturate the magnetisation of the sample, then the Non Spin Flip (NSF) cross-section is directly proportional to the longitudinal susceptibility X_L (Q). The Spin Flip (SF) cross-section in turn is proportional to the transverse susceptibility. The situation is very different if the saturating field is applied horizontally parallel to Q. Then all magnetic scattering is confined to the SF channel. Only transverse fluctuations contribute, while longitudinal ones are invisible. This technique is illustrated in the next two paragraphs.

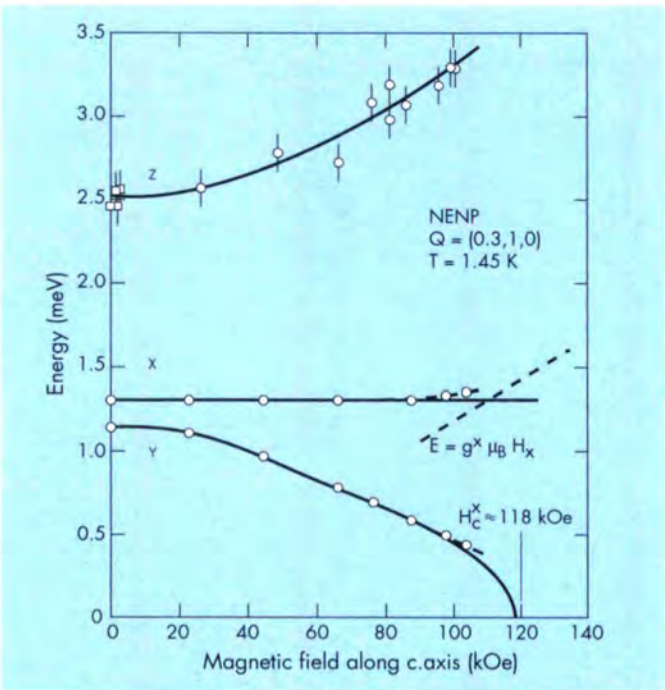


Fig. 5: Effect of applied magnetic field perpendicular to chain axis (z) on NENP. (x) denotes the field direction. The continuous lines correspond to calculations by I. Affleck [9].

Kosterlitz-Thouless phase transition

The 2-dimensional Heisenberg ferromagnet with planar (XY) anisotropy is expected to undergo a "Kosterlitz-Thouless" (KT) phase transition, due to the unbinding of pairs of spin vortices. Near to the critical temperature, increasing vortex numbers are predicted to cause rapid renormalisation of long-wavelength spin wave energies and diffusive central peak scattering; the experimental signature of the KT phase transition.

These predictions were tested in the quasi 2D-XY ferromagnet Rb_2CrCl_4 in polarized neutron experiments on IN12 and IN14 [10]. The in-plane dynamic critical scattering (Spin Flip and Non Spin Flip) of Rb_2CrCl_4 was measured at small wave-vectors q near to the "rod" of diffuse scattering characteristic of 2D correlations. A small field (H = 0.2 T) was applied to the sample within the easy (XY) plane of magnetization, to define the spin direction and to prevent neutron depolarization.

At T_C (~52 K) the in-plane scattering was clearly separated into a Lorentzian central peak (NSF) due to longitudinal diffusive spin fluctuations and "sharp" transverse spin waves (SF; Fig. 6a). At higher temperatures the SF scattering could only be fitted with the inclusion of a central peak, which was found to reach maximal intensity at ~60 K (Fig. 6b). Theoretical calculations [11] predict that such a central peak arises from vortex diffusion. The data were insufficiently accurate to confirm the predicted squared Lorentzian peak shape, but an order-of-magnitude calculation of the peak width gave good agreement with theory.

"Forbidden" (i.e. NSF) spin waves at finite q were also observed for the first time, indicating regions in which the local spin direction is perpendicular to the field. Final

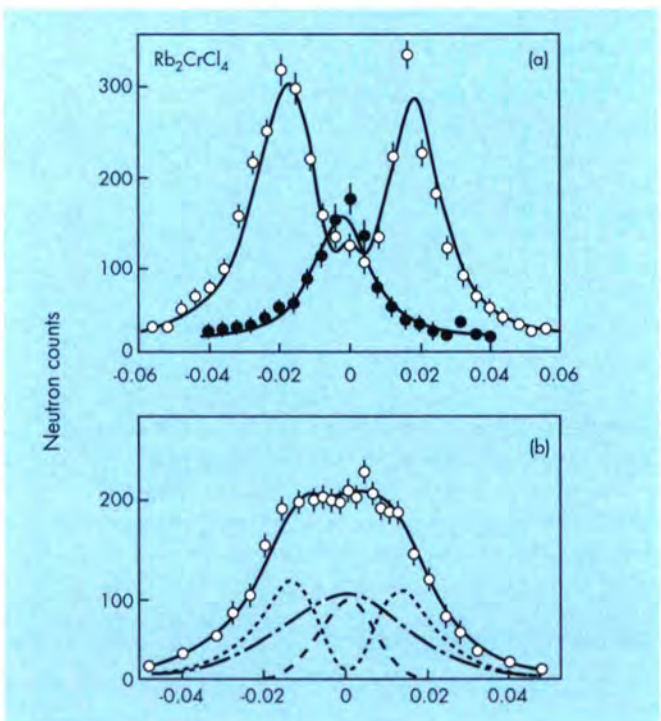


Fig. 6:
a) NSF (closed circles) and SF (open circles) scattering at T =51 K, q = 0, B = 0.2 T. The continuous lines are fits to the data of theoretical dynamic scattering functions convoluted with the experimentally determined resolution function, plus background and incoherent scattering determined separately.
b) SF scattering at T =60 K, q = 0, B = 0.2 T. The continuous line is a fit to the data comprising sharp spin waves (short dash) and a squared-Lorentzian central peak predicted to arise from vortex diffusion (dot dash), plus separately determined nuclear incoherent scattering (long dash).

confirmation of the existence of vortices rests to some extent on the formulation of a more complete theory of diffusive critical scattering in such a system.

Longitudinal fluctuations

The experiment on critical dynamics of EuS [12] was performed on the triple axis spectrometer IN12 working at fixed final energy E_f of 3.13 meV, and equipped with the polarization analysis setup to separate the longitudinal from the transverse susceptibility (guide field on sample H = 5 x 10^{-4} T). In order to compare the experimental result, the parametrized magnetic cross-section calculated in the Mode Coupling theory using the Lorentzian approximation [13] was used:

$$S_\alpha(\mathbf{q},\omega) = 2k_B T \chi_\alpha(q,T) \frac{1}{\pi} \frac{\Gamma_\alpha}{(\hbar\omega)^2 + \Gamma_\alpha^2} \qquad (1)$$

This cross-section was convoluted with the 4-dimensional resolution function for the present configuration of IN12. The q-dependence of Γ_L demonstrates that the longitudinal fluctuations are significantly suppressed for $q < q_d$, where dipolar effects become significant.

To provide a direct comparison with the Mode Coupling theory, all fitted Lorentzian linewidths of the longitudinal fluctuations were normalized to the (hypothetical) linewidth of the isotropic system at T_c,

$$\Gamma_T(q,T_c) = Aq^{2.5}, \qquad (2)$$

and these are shown in Fig. 7 plotted against the scaled inverse correlation length κ/q, using for κ the theoretical value 0.55 Å^{-1} $(T/T_c\text{-}1)^{0.69}$. Also indicated are the dynamic scaling functions of the Mode Coupling theory [13] for the three different temperatures under investigation depending on the dipolar scaling variable $q_d/k(T)$ (solid line Fig. 7). This representation does not involve any free parameters and is in agreement with the theory within the experimental error.

Disordered ferromagnets

Dilute AuFe samples (AuFe 18 % and 16 %) close to xc (xc = 15.5 Fe at %), the threshold between the ferromagnetic and the spin glass phase, have a strongly disordered ferromagnetic phase below Tc and a coexistence of ferromagnetic and spin glass behaviour below Tg [15] at lower temperatures .

The critical scattering of these disordered ferromagnets was measured at Tc in a wide range of q extending from 0.03 up to 0.2 Å^{-1} [14]. The combination of at least an elastic (Gaussian) and a quasi-elastic (Lorentzian) contribution was necessary to account for the experimental S(q,ω) vs. ω spectra at Tc (respectively 93 K and 144 K for AuFe 16 % and 18 %) as well as at high temperature (up to 250 K used as a paramagnetic reference).

The width of the quasi-elastic Lorentzian follows at T_c the same scaling law as a function of q mentioned above for the pure compound EuS (eq. 2) but with a slightly varying dynamical exponent z (Fig. 8): z(AuFe 18 %) = 2.48 ± 0.1 and z(AuFe 16 %) = 2.2 ± 0.1 .

At all temperatures the relative weight of the elastic component increases with increasing q and with decreasing temperature: the elastic intensity increase between 250 K and Tc varies between 2.5 and 1.4 in the q-range from 0.1 Å^{-1} to 0.2 Å^{-1} . Such a strong temperature dependence implies that, at Tc a very important fraction of the elastic peak is of magnetic origin. This would distinguish these disordered ferromagnetic samples from usual ferromagnets such as EuS, where at T_c the magnetic intensity is only described by eq. 1 and 2.

Secretary: M. Alba

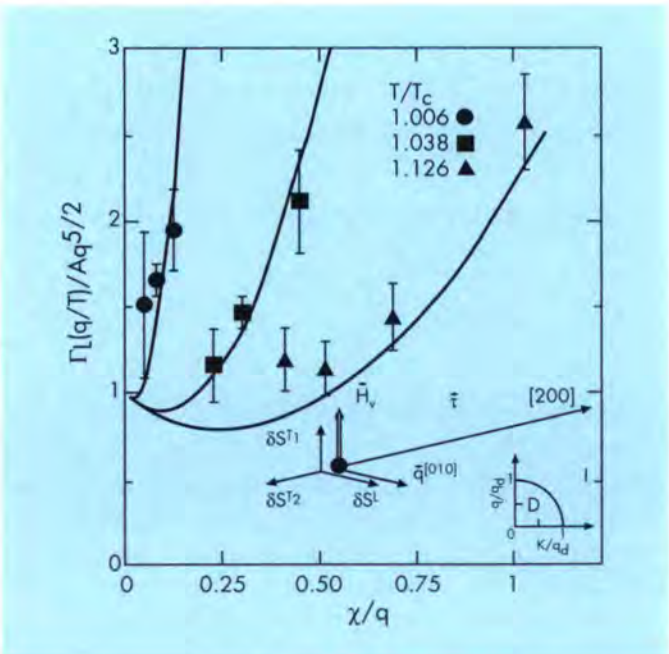


Fig. 7: Comparison of the longitudinal linewidth in the Lorentzian approximation normalized to $Aq^{2.5}$ with A = 2.1 meV Å$^{5/2}$ to the dipolar dynamic scaling function predicted by mode coupling calculation with qd = 0.245 Å^{-1} for EuS. Inset shows the scattering geometry used in the experiment.

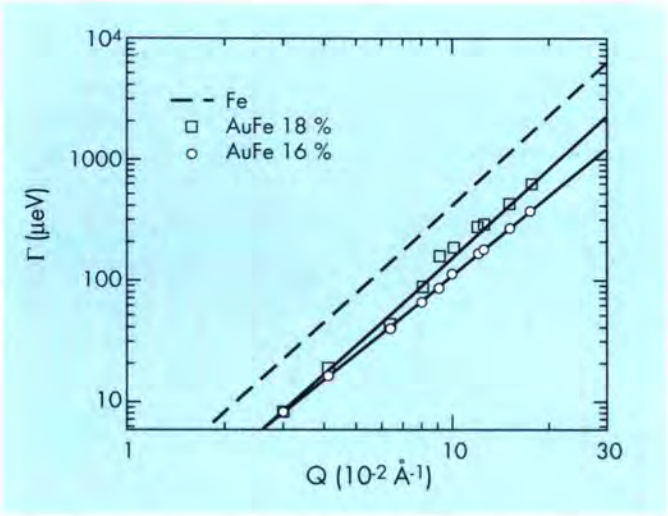


Fig. 8: Widths of quasi-elastic Lorentzian scattering at T_c as a function of q in AuFe. Continuous lines correspond to the scaling law Aq^z with z = 2.48 and 2.2 for AuFe 18 % and 16 % respectively. The dotted line corresponds to the width of quasi-elastic Lorentzian in pure Fe with z = 2.5.

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Inelastic Neutron Scattering and lattice dynamics

H. Schober and B. Dorner

Asked about what can be done with inelastic neutron scattering many scientists would spontaneously answer: One determines phonon dispersion curves.

Although the main scientific activity in inelastic scattering has shifted to the field of magnetic excitations and magnetic critical phenomena, the field of structural dynamics still covers a wide range of investigations not only in crystalline materials but also in amorphous and liquid states as well as substances of intermediate order such as polymers.

Here we would like to give some examples of recent developments in the classical domain of structural dynamics, i.e. the determination and interpretation of phonon frequencies and eigenvectors. This field was pioneered by B.N. Brockhouse in the fifties and let to a world wide activity in the sixties and seventies.

Phonons are elementary excitations of a crystal arising from the collective movement of the ions. For each wave vector there are 3r different modes of vibrations where r is the number of atoms in the primitive cell. The frequencies and eigenvectors of these modes are entirely determined by the interactions between the ions of the crystal.

The experimental determination of these frequencies and as far as possible the determination of their eigenvectors provides therefore the basis for the construction of microscopic models of atomic interactions.

As the intensity (visibility) of a certain mode is solely determined by its eigenvector, its experimental determination becomes more complicated the lower the symmetry and the higher the number of atoms in the primitive cell of the substance under investigation. This arises because the lower symmetry imposes less constraints on the eigenvectors. Therefore the investigation of phonons has so far mainly been limited to highly symmetric crystals having not more than two atoms per primitive cell.

The advent of the high T_c superconductors has shown that the knowledge of phonon dispersions is highly desirable also for more complicated structures. This is only possible if the experiment and the models used to interpret the data advance simultaneously. The first experimental results allow the construction of a crude model. This model predicts the frequencies and visibility of the modes enabling the continuation of the experiment, which in turn leads to a refinement of the model and so on.

As mentioned above, a complete investigation of the lattice dynamics of a crystal requires the determination of the frequencies as well as the eigenvectors. So far, however, nearly exclusively frequencies have been measured. Whilst the frequencies are simply taken from the position of the measured peaks, the determination of the eigenvectors makes it necessary to determine the intensities of the particular mode in many zones of reciprocal space. We will show later how the knowledge of a few eigenvectors can be decisive in selecting the most appropriate lattice dynamical model from several which describe the phonon frequencies with comparable quality.

First, we wish to present ongoing investigations on quartz (SiO_2) and sapphire (Al_2O_3). These materials are of particular interest because they contain the highly polarizable oxygen ion. H. Bilz devoted much of his effort to study this polarizability and it plays an essential role in many theories attempting to explain high T_c superconductivity.Through a combined theoretical and experimental effort as described above, we were able to determine the frequency as well as the symmetry of nearly all the phonon branches for certain high symmetry directions in quartz and sapphire [1].

It has turned out that existing models of the rigid ion type adjusted to fit only the low frequency part of the dispersion curves neither reproduced the frequencies nor the intensities of the higher branches. There was no way of substantially improving these models without introducing highly unphysical interactions. Only after allowing for the polarizability of the oxygen ion by using a simple shell model were we able to reproduce the experimental results satisfactorily (see Fig. 1).

There is no single set of short range interactions but a variety of shell models which reproduce the experimental results equally well. All of them indicate a rather high charge on the oxygen ion. In the case of quartz as well as sapphire we get values in between 1.5 and 1.8 elementary charges. We therefore conclude that the oxygen ion is very close to a O^{2-} configuration. The oxygen charge is, however, strongly screened giving effective charges of 1.0 e - 1.2 e for all models.

Contrary to what could be expected we found neither a positive influence of valence forces on the reproduction of the dispersion curves nor could we adjust bond charge models to the experimental data.

Although our models are rather crude they clearly indicate that the lattice dynamics of quartz and sapphire, at least for the investigated high symmetry directions, are dominated by the screened Coulomb interactions together with simple repulsive potentials between nearest neighbour ions. Quartz can therefore not be treated as a

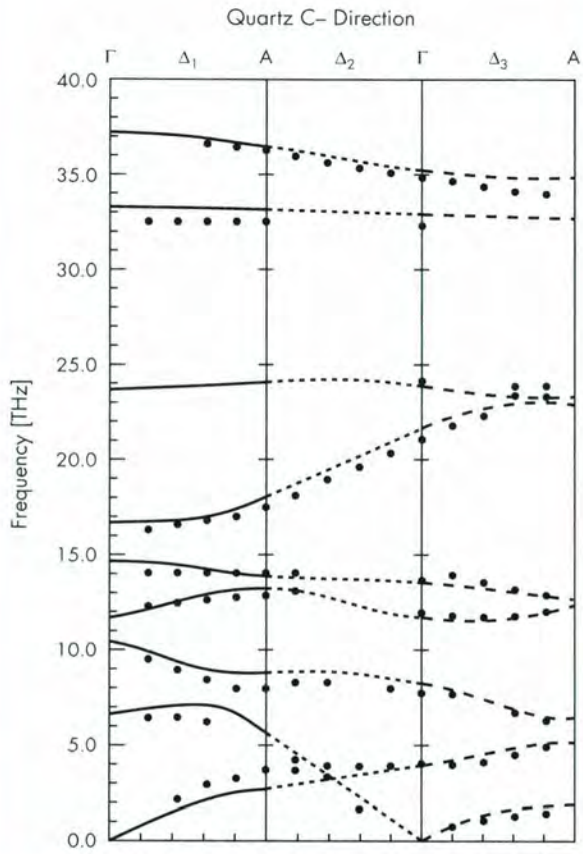

Fig. 1 Dispersion curves of α-quartz at 25 K. The experimentally determined frequencies are described by a 9 parameter shell model. The 3 irreducible representations have been unfolded for clarity.

covalent crystal nor can sapphire be considered a molecular crystal.

We want to point out that it appears absolutely necessary to measure at least two different symmetry directions. In particular in the case of sapphire, models which were adjusted only to the data of the first measured direction, poorly reproduced the frequencies of the other directions.

Although the measured intensities helped us in constructing the lattice dynamical models, we have not yet undertaken a detailed eigenvector determination.

In the case of GaAs not only have the phonon dispersion curves been measured with higher precision and for more symmetry directions but, in addition, the eigenvectors at 2 symmetry points the X- and L-points have been determined [2].

Eight different lattice dynamical models have been adjusted to the data. Two of them, the rigid ion and deformable dipole model, were ruled out because the eigenvector at the L-point was predicted completely incorrectly. A shell model with 14 parameters reproduced the eigenvectors and also most of the frequencies very well but there were discrepancies around the W-point (see Fig. 2). A bond charge model with only 6 parameters showed an equally good overall agreement but with discrepancies for frequencies at the zone centre and the X-point. Therefore it was not surprising that the eigenvector at the X-point was not predicted correctly by this model. Summarising, this analysis showed that the experimental data now available for such an important substance such as GaAs can not be explained satisfactorily by any existing lattice dynamical model.

If one replaces the two different atoms in the structure of GaAs by two identical ones, such as Si, one obtains the diamond structure. In contrast to GaAs, in Si the eigenvectors at the L-point are fixed by symmetry and the eigenvectors of the longitudinal modes in the L direction (Γ-L) are fully determined if one knows the phase angle describing the relative motion of the two sublattices. This phase angle has been determined experimentally [3]. An eigenvector determination represents a delicate experimental study because spurious effects may contribute to the intensities and falsify the results. In the case of Si there exists a sum rule for the intensities of the longitudinal modes which we used to check the experimental results. In addition, we compared the observed widths of the peaks with predictions from resolution calculations (see Fig. 3).

Four model calculations were available which described the phonon dispersion comparably well: a full quantum mechanical density-response calculation (DR); a semi-quantum mechanical partial-density model (PDM); and a phenomenological valence force field

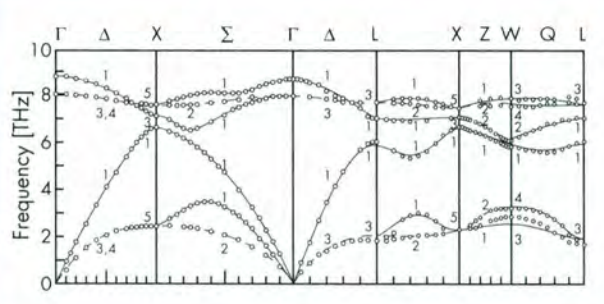

Fig. 2 Dispersion curves of GaAs at 12 K. The experimentally determined frequencies are described by a shell model. The arabic numbers indicate the group theoretical irreducible representations.

model (VFFM) as well as a phenomenological bond charge model (BCM). As can be seen from Fig. 4 only the bond charge model can reproduce the experimentally determined phase angle of the eigenvector. This shows that the knowledge of the eigenvectors can play a decisive role in the evaluation of different lattice dynamical models. Needless to say that a fundamental understanding of the lattice dynamics of Si is highly desirable.

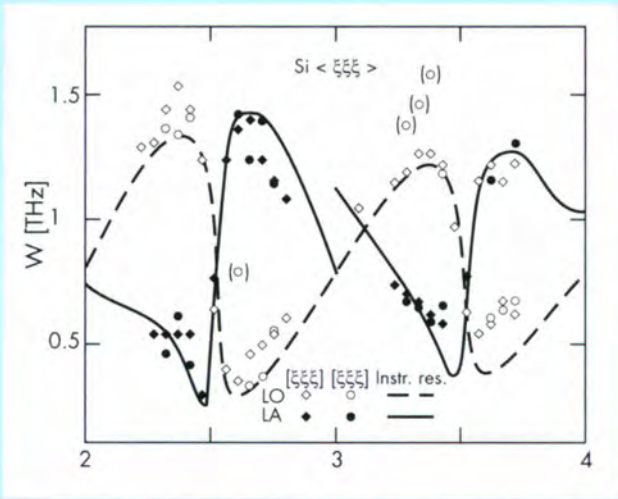

Fig. 3 Spectral line widths. Symbols, experimental widths; lines, line widths as calculated from the instrument resolution. Data in brackets are not used for the evaluation of the phase angle φ of the eigenvector.

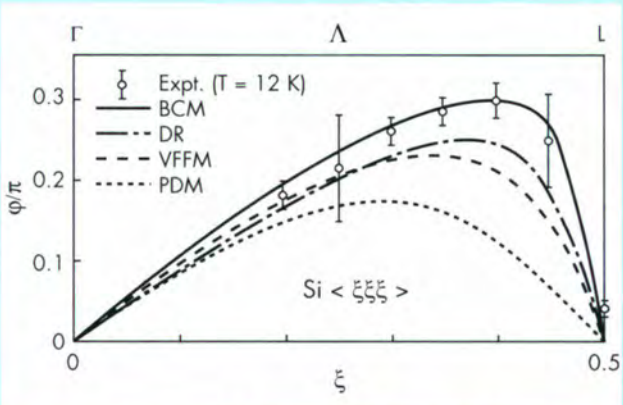

Fig. 4 The phase angle φ of the eigenvectors of the longitudinal modes in Λ-direction for Si. The 4 curves represent predictions by different models.

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Crystal and Magnetic Structures

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Introduction

The year 1990 has been the one of forced reactor shut-downs. These events produced some problems concerning the normal schedule of the experiments. Another consequence has been the shortening of the available beam time for the february proposals. Many good proposals have not been accepted due to this fact. However, the number of experiments and submitted proposals to the sub-committee of october have increased.1824 days were requested for college 5, only 862 could be allocated.

Scientific Highlights in 1990

Advances in Powder Diffraction Data Analysis

Since the beginning of the year 1990 the new computer program FULLPROF, developed at the ILL, has been available. Apart from the standard multiphase nuclear Rietveld refinements (X-rays and neutrons), the program has many other important features of which we point out three: (i) refinement of commensurate magnetic structures, (ii) full account for anisotropic broadening of Bragg peaks due to microstrains and (iii) "pattern matching" of the full diffraction pattern without prior knowledge of the crystal structure of the compound.

(i) The magnetic structure refinement is performed considering the magnetic part as a separate phase in which the appropriate constraints (using the parameter codes) have to be introduced. For instance the scale factor, the magnetic and the chemical unit cell, and the magnetic atom positions have the same parameter number as their nuclear counterpart but with the appropriate multiplicative factor. As an example of magnetic structure refinement Fig. 1a shows good agreement between observed and calculated patterns for $Ho_2Cu_2O_5$. The magnetic structure can be described by a propagation vector k=[0 1/2 0] and the magnetic modes: $\{G^{(1)}_x+G^{(2)}_x,\ A^{(1)}_y-A^{(2)}_y,\ C^{(1)}_z+C^{(2)}_z\}$ and $\{A^{(1)}_x+A^{(2)}_x, 0, 0\}$ for the two Ho sites and for the two Cu sites in the chemical unit cell respectively.

(ii) The anisotropic broadening of the Bragg peaks due to strains is taken into account using a generalized formulation of microstrains in terms of cell parameter fluctuations and correlations. As an example we give in Fig. 1b part of the diffraction pattern of Pr_2NiO_4 at 1.5K on D2B. In this case the microstrains are due to a phase transition from Bmab to $P4_2/ncm$ at 120K, the low temperature phase is tetragonal on

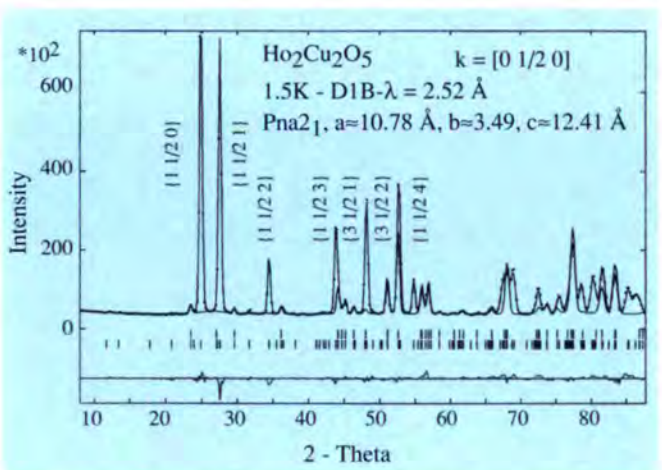


Figure 1 (a). Diffraction pattern of $Ho_2Cu_2O_5$ obtained at 1.5K on D1B. The nuclear diffraction pattern plus background are included in the plot as a suplementary continuous line. The second row of reflection markers corresponds to the magnetic reflections.

average but locally orthorhombic [Pccn, $a_l = a_T(1-\varepsilon_l)$, $b_l = a_T(1+\varepsilon_l)$] the microstrain parameter being $\varepsilon^2 = \langle\varepsilon^2_l\rangle$. The broadening of the peaks is described by the formula given in the figure.

(iii) The method of "pattern matching" consists of estimating the integrated intensities of an unknown structure without using the least squares optimization. The method is applied by iterating the formula given by Rietveld to calculate the "observed" integrated intensities in order to introduce the nuclear R-factor. To be used successfully, this method requires a good estimation of the cell parameters, background and profile parameters. At variance with the Pawley approach (constrained least squares) the "pattern matching" method is much more stable and less computer time consuming. In Fig. 1c we give the diffraction pattern corresponding to YIG as taken on D20 for $\lambda = 1.36$ fitted with the present procedure.

The "pattern matching" method can be applied, in addition to the conventional Rietveld method, just to estimate the R factors coming only from the model for the profile parameters.

Crystallography of Non Magnetic Systems

Physintercalation of alkanes in caesium graphitides

Graphite is a host structure which can be intercalated by various atoms or molecules. The resultant compound has the property of structuring in stages, i.e. the intercalated species fill one interlayer every n graphite planes, where n is the stage of the compound. Non polar molecules (H_2, N_2, methane, n-alkanes, etc) can be reversibly intercalated in alkali graphitides. Since the sorption involves both an increase of the c parameter and van der Waals interactions, we call it PHYSINTERCALATION.

The evolution of the reaction between n-alkanes and CsC_{24} or CsC_{36} was investigated by real-time neutron diffraction on the D1B diffractometer at the ILL. The data in Fig. 2 shows that the intercalation of n-hexane in the 2nd stage CsC_{24} yields a mixture of a 2nd stage ternary and a 1st stage "CsC_8", whereas in the 3rd stage CsC_{36} only a pure 2nd stage ternary is found. The area density of the caesium is smaller in the ternary layer than in the starting binary layer due to either the formation of binary domains rich in alkali metal (CsC_8) or to the stage lowering produced on passing into the ternary phase. This particular behaviour must be correlated with calculations of Madelung energy of 1st stage alkali graphitides, which shows that an increase in

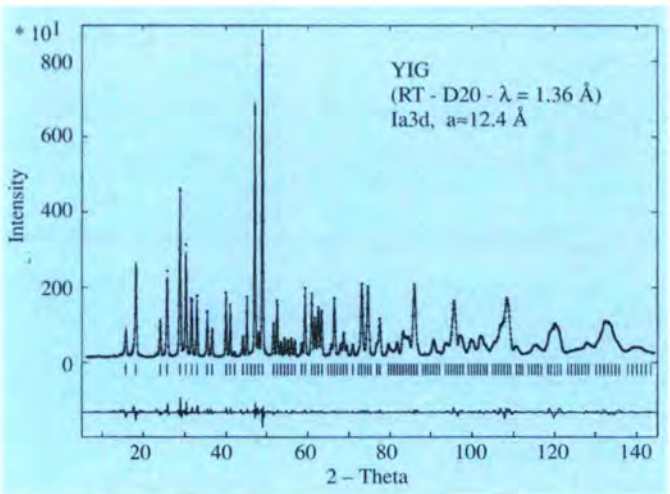
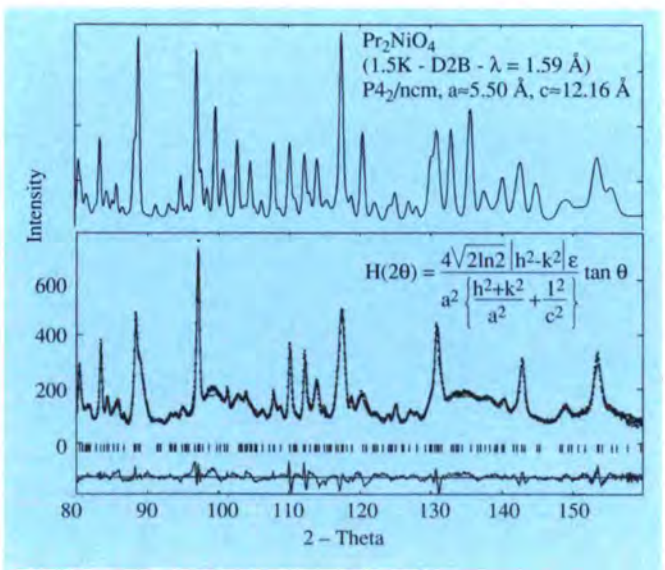


Figure 1 (c). Diffraction pattern of YIG obtained at room temperature on D20. The calculated profile is obtained without a structural model using the "pattern matching" procedure.



Figue 1 (b). Part of the diffraction pattern of Pr_2NiO_4 obtained at 1.5K on D2B. At the top of the figure, the calculated profile with $\varepsilon = 0$ shows the dramatic effect of microstrains in the width of the Bragg peaks.

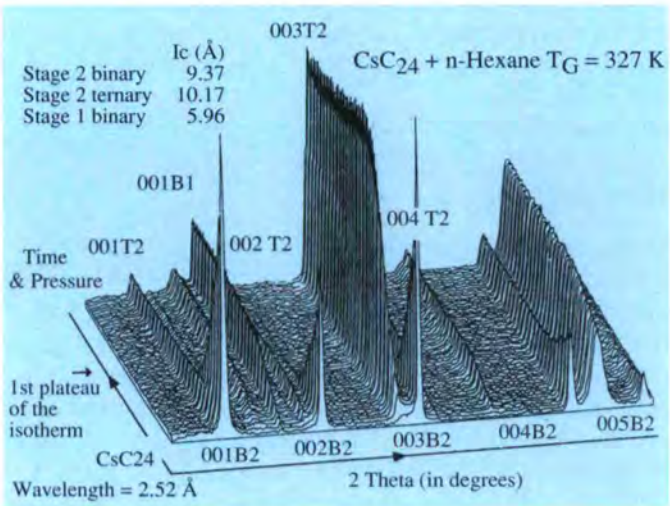


Figure 2. 3D plot of diffraction patterns of CsC_{24} + n-hexane as a function of time and pressure.

the interlayer distance always involves an increase in the C/M ratio for maximum stability.

The process of intercalation in graphite intercalation compounds is little known. Hypothetical models are proposed but no experimental methods are suitable for confirming this process. In the case of our first investigation, no realistic model is available to explain the structural juxtaposition and size of 1st stage binary and 2nd stage ternary domains.

Considering the diffusion of large molecules in the interlayer space of graphite intercalation compounds from the edges, we could predict an expulsion of the Cs ion around the middle of the grain. A neutron topographic study carried out on S20 with a CsC_{24} highly oriented pyrolytic graphite platelet, intercalated into n-pentane allowed the spatial observation of the phases within the samples. It can be seen in Fig. 3 that the 1st stage CsC_8 and 2nd stage ternary domains are superimposed. Moreover the middle of the platelet does not correspond to a diffracting domain. This is proof that the molecules diffuse from the edges of the sample. The fact that the expelled Cs ions stay near the ternary structures, may be explained by the formation of kinks minimizing the elastic constrain of the layer plane.

Why are manganese dioxide batteries not rechargeable?

The form of manganese dioxide known as γ-MnO_2 is the active component of Leclanché primary batteries. Although these batteries have been used for more than a century, the structure of MnO_2 and the atomic scale mechanism of their reduction in alkaline batteries were not yet understood. In particular the origin of the non-reversibility of the reaction $MnO_2 + H^+ + e^- \longrightarrow MnOOH$, which implies that such batteries are not rechargeable, has not been unambiguously identified. Using a new method of characterization of the defect structure of γ-MnO_2 two commercial samples were selected for *in situ* investigation by real time neutron powder diffraction : i) an international reference sample (IBA-11) whose structural arrangement is close to that of the mineral ramsdellite and ii) a commercial sample (Sedema-WSA) whose structure can be described as a stochastic stacking of single (rutile-like) and double (ramsdellite-like) layers of edge-sharing octahedra [MnO_6]. Using an electrochemical cell designed for neutron powder diffraction, the potentiostatically controlled reduction of these two samples from MnO_2 to MnOOH was monitored on D1B and D20 with a time resolution of 10 and 30 minutes respectively. In spite of the rather bulky sample environment, it was possible to analyse the data (Fig. 4) by profile refinement using the new program FULLPROF. The results show, for the first time, that the structural transformations taking place in γ-MnO_2 during battery discharge depend *qualitatively* on the *quantity* of defects in the starting material; they also provide evidence that the reduction proceeds through three different stages and that the reversibility of the electrochemical process in action in Leclanché batteries is fundamentally limited by the structural defects present in most commercial samples of MnO_2. (Collaboration with Université J. Fourier and INPG, Grenoble)

Charge transfer and superconductivity in $YBa_2Cu_3O_{6+\delta}$

One of the most cited papers on superconductivity in 1990 was the CNRS-ILL-Bell laboratories experiment of Cava *et al.* [1] which showed that Tc in $YBa_2Cu_3O_{6+\delta}$ was directly related to charge transferred to the conducting CuO-planes by oxidation of the intermediate 'charge reservoir' CuO-chains.

Fig. 5, where the valence charge was calculated from the Cu-O bond lengths measured on D2B, shows that Tc follows the same functional dependence on oxygen content,

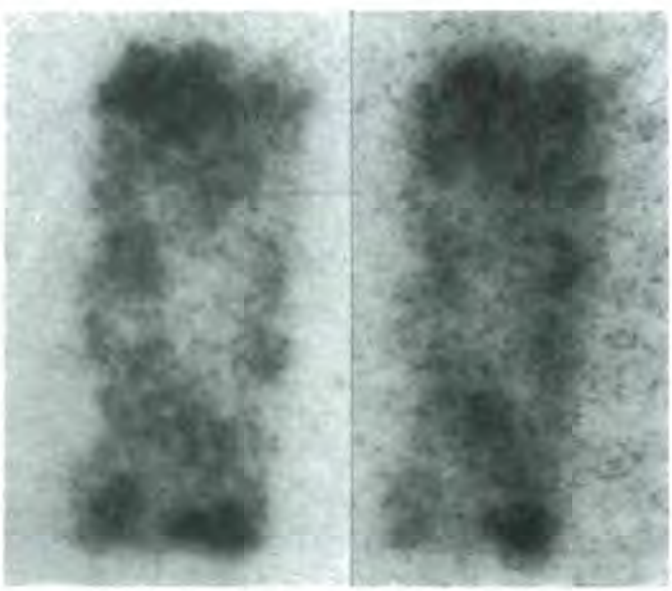


Figure 3. Topographs of the superimposition of the 1st stage binary CsC_8 (at left) and 2nd stage ternary domains (at right).

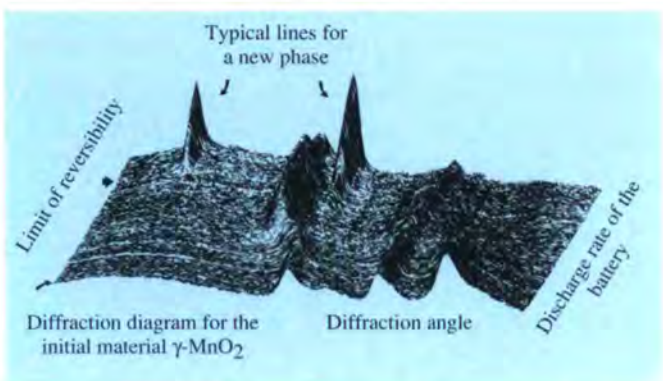


Figure 4. 3D plot of diffraction patterns of γ-MnO_2 as a function of time.

including the famous 60K plateau. The neutron work emphasized the importance of the 'apical' oxygen atom which connects the CuO-planes to the 'charge reservoir' layers in many of these superconductors. Of particular interest is that it was just this 'apical' oxygen atom that was so important in Bednorz and Müller's original idea for copper oxide superconductors; this neutron structural work has helped revive interest in non-magnetic explanations of superconductivity.

Later in 1990, these measurements were extended by a Zürich-Grenoble experiment to investigate anomalies in the length of the c-axis near δ=0.9. The c-axis contracts with oxidation, due to the shortening of the copper to apical oxygen length, but for δ<0.9, the c-axis was found to expand again (Fig. 6). The reason was shown to be an increased 'buckling' of the conducting Cu-O plane, due to the oxygens moving further out of the plane of the coppers. This effect may help explain why T_G plateaus at 90K in $YBa_2Cu_3O_7$, whereas in very similar materials it can go much higher.

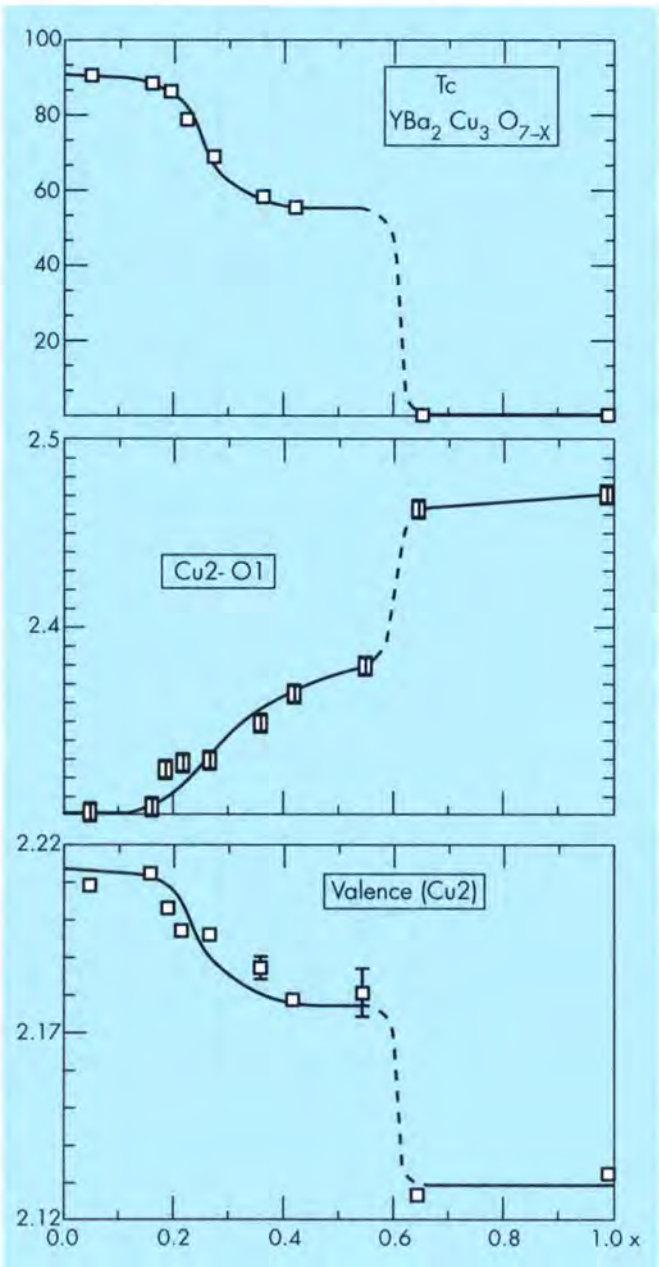


Figure 5. The ILL-D2B results of Cava et al. [1] showing the Tc of $YBa_2Cu_3O_{6+\delta}$ as a function of x (a) reflected in the changes in the Cu2-O1 apical distance (b), implying charge transfer to the conducting Cu2 planes with oxidation and decreasing x (c).

References

[1] Cava R J, Hewat A W, Hewat E A, Batlogg B, Marezio M, Rabe K, Krajewski J J, Peck Jr. W F & Rupp Jr L W (1990) Physica C, 165, 419.

[2] Kaldis E, Fischer P, Hewat A W, Karpinski J, & Rusiecki S (1991) Physica C (to be published).

Neutron diffraction up to 2000 K

The main interest of the work was the investigation of structural changes of some high-melting oxides and silicates. Samples used were :

- ZrO_2, a compound with a great variety of applications in the ceramics industry

- $ZrSiO_4$, a mineral which plays an important role in geochronology, refractory research and, due to its ability to accept Uranium and Thorium as cations, as a simulator for radiation damage occurring in nuclear waste containers.

Since all these materials change their behaviour in absence of oxygen, there is great interest in examining these compounds at high temperatures in air. This was carried out with the 'mirror furnace' from the crystallographic institute in Munich (see ILL Annual Report 1989). This furnace made it possible to carry out powder and single crystal

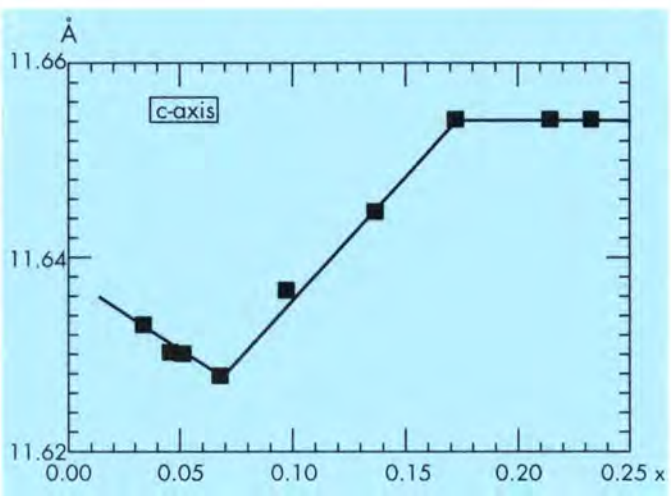


Figure 6. The ILL-D2B results of Kaldis et al. [2] showing the anomalous behaviour of the c-axis of $YBa_2Cu_3O_{7-x}$ due to increased buckling of the CuO-plane, which may be associated with the 90K plateau in Tc.

experiments on D2B and D19 up to 2000 K in air thus reflecting the real behaviour of all these samples during their applications.

a) Single crystal studies :

The use of D19 with the 'mirror furnace' gave us the possibility of examining physical effects which have not previously been observed due to the lack of both the advantages of a nearly background-free furnace and a large PSD, like that of D19 :

In the case of $ZrSiO_4$ the annealing process of the heavily distorted lattice was observed from room temperature up to 2000 K using natural minerals. A few reflections were measured every 100 K showing a remarkably fast annealing process around 1200 K.

Beside this qualitative analysis some temperature points (room temperature, 800 K, 1573 K, 1823 K) were used for a complete data collection with following structure analysis yielding interesting results of higher order temperature coefficients reflecting the static disorder of the material. Fig. 7 shows probability density functions of the oxygen in zircon with the tendency of minima in direction to the neighbouring cations at room temperature due to strong static disorder. The disappearance of these minima at higher temperatures can be explained by the decrease of static disorder at higher temperatures and the shift of the function towards the Si cations by a start of rotational processes of the tetrahedra due to a growing misfit between the polyhedral units.

A second project was the investigation of the monoclinic to tetragonal (martensitic) phase transition in ZrO_2. For this purpose some very rare baddeleyite crystals were used to get information about temperature and the widely discussed orientation of the new phase in relation to the old monoclinic one. Fig. 8 shows the rise of a tetragonal peak next to the old monoclinic peak within the short interval of 10 K proving the single crystal character of the transformation and showing the importance of a large PSD for such experiments. Further structural studies generated a simple orientational connection between the two phases.

b) Powder diffraction:

The powder experiments were mainly carried out on D2B. The good collimation of the instrument was useful in retaining aluminium peaks from the detectors.

In order to examine the structural properties of $ZrSiO_4$ up to 1900 K powder patterns were measured every 100 K and after 1400 K in steps of 50 K. Rietveld analysis of the data brought many new and unexpected features of the structure, e.g. a displacive phase transition near 1200 K.

The question of the decomposition temperature was also solved since at 1850 K the first peaks of tetragonal ZrO_2 rise.

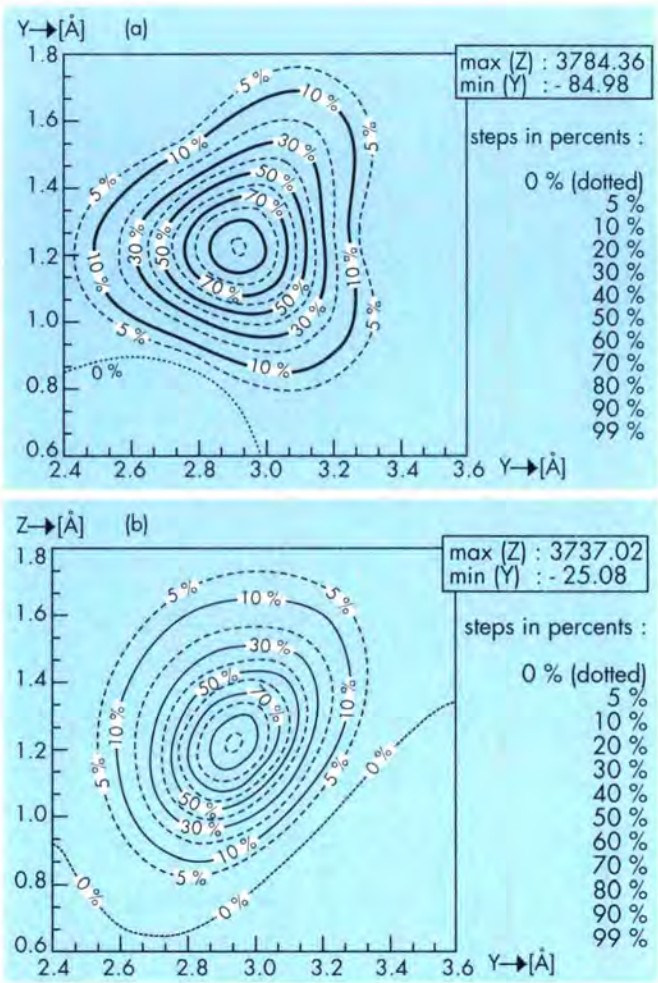


Figure 7. Probability density function of oxygen in zircon at room temperature (a) and 1823 K (b).

Location of hydrogen atoms in large metal carbonyl clusters

Studies of hydrogen derivatives of polynuclear metal carbonyl compounds are of interest because their reactions and structures may be relatively easily studied and they provide the closest molecular analogues to the processes that occur on bulk metal surfaces during important catalytic processes such as hydrogenation. Additionally they are novel materials of as yet untapped potential ; for example, recent work shows that the large cluster dianion $[Os_{10}C(CO)_{24}]^{2-}$ supported on inert matrices catalyses hydrogenation of olefins.

Several modes of H-atom bonding to cluster surfaces have been established from X-ray and neutron diffraction studies, and these include examples of the ligand bonded to from one to as many as five metal atoms. The first H-atom to be discovered inside a carbonyl cluster was in the monoanion $[HRu_6(CO)_{18}]^-$; the overall close-packing of the carbonyl ligands provided evidence that a surface location would be impossible and therefore an interstitial site at the centre of the Ru_6 octahedron was proposed, and this

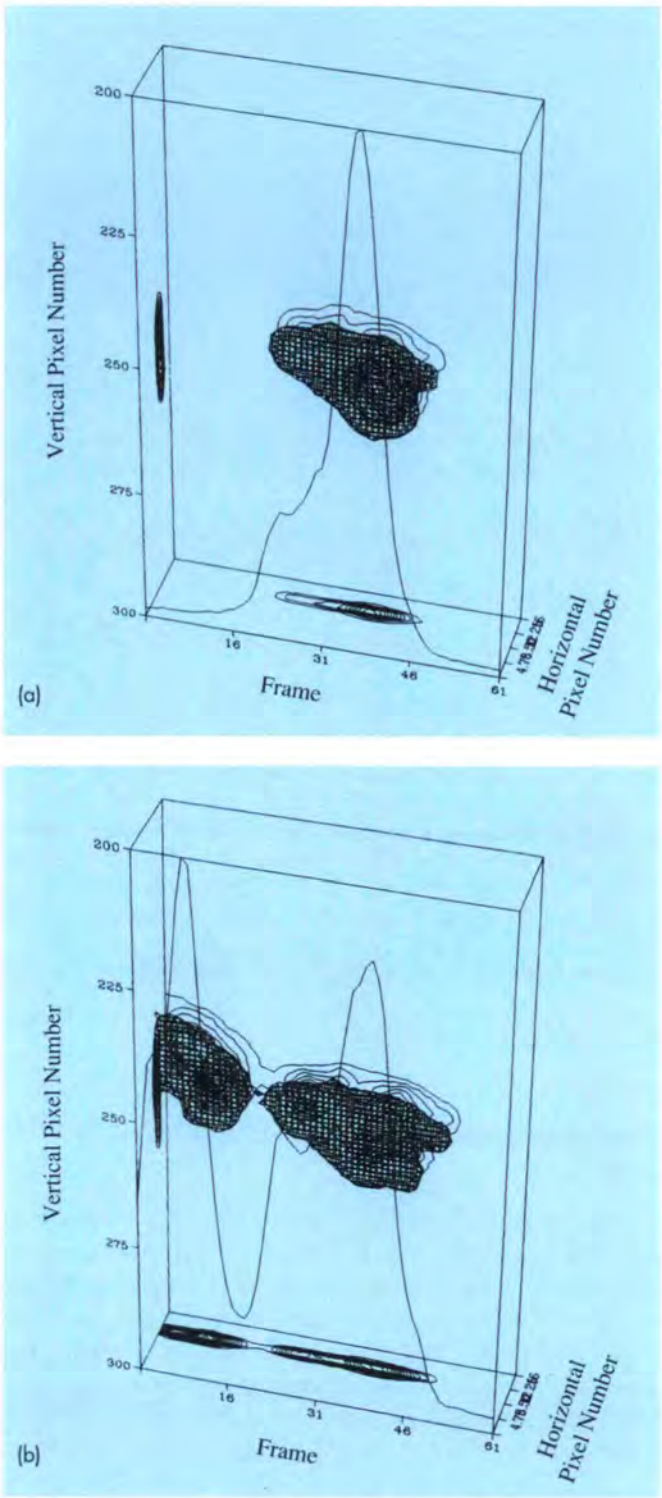


Figure 8. Omega scan of the 1 0 4 reflection of ZrO_2 (monoclinic) before (a) and during (b) the transition (1300 K and 1310 K) with the appearance of a tetragonal peak at a lower omega angle.

was subsequently confirmed by neutron work at ILL. Based on similar arguments, of virtual close-packing of the carbonyl array covering the cluster surfaces, internal locations have been proposed for H-ligands in a number of large clusters of osmium or ruthenium, all of which have giant tetrahedral metal cores which can be envisaged as tetracapped octahedra.

The first neutron diffraction study (on D19) of one of these decametal species, the $[N\{P(C_6H_5)_3\}_2]^+$ salt $[H_4Os_{10}(CO)_{24}]^{2-}$, has unexpectedly shown that all four hydrogen ligands are on the cluster surface, two in edge-bridging μ_3-sites in the centre of the large triangular faces of the metal core. A 50:50 disorder of one of the μ_2-H atoms was apparent, and has been interpreted as indicating an equal distribution throughout the crystal of two isomers of $[H_4Os_{10}(CO)_{24}]^{2-}$, (A) and (B), illustrated in Fig. 9a and 9b. A 50:50 disorder of carbonyl CO (82) adjacent to the two bridged edges provides support for this model.

The H-atoms are in particularly congested sites on the cluster surface and those bridging the central Os_3 triangles are overlapped by the van der Waals radii of the surrounding carbonyl ligands (see Fig. 9c and 9d). The apparent tolerance for very close H...C(carbonyl) contacts (range 1.953 to 2.241 Å for the shortest distances to each H-atom) reduces the value of the usual criterion applicable to indirect location of H-atoms in smaller molecules. The success of this experiment in establishing H-atom locations, unpredictable from the X-ray data, demonstrates an essential role for neutron diffraction in the chemistry of large hydrido clusters. (Collaboration with The Polytechnic of North London and Cambridge University).

First neutron diffraction observation of oxygen ordering in 123 high Tc single crystals

It is well established that the high temperature superconductivity in $YBa_2Cu_3O_{6+\delta}$ results from the electronic structure of the basal CuO planes. While the well ordered compound with δ=0 is insulating, superconductivity appears at higher oxygen concentrations due to the introduction of highly mobile holes in the in-plane oxygen orbitals. Electron microscopy indicates that the ordering of the oxygen atoms within these basal planes is a crucial parameter for the superconducting transition temperature T_C. So far however, the oxygen ordering has not been observed with neutrons except for the trivial case of the end members with δ=0 and δ=1. Neutron diffraction studies are crucial for a definite understanding of the connection between oxygen ordering and superconductivity, since only this method combines the spatial resolution with the sensitivity to bulk properties.

We have carried out a single crystal neutron diffraction study of a δ=0.35 sample on the four-circle triple axis spectrometer D10. Superstructure reflections have been found in the (hk0) layer which have been indexed in an eight times larger superlattice cell $2\sqrt{2}\,a \times 2\sqrt{2}\,a \times c$ (diagonal).

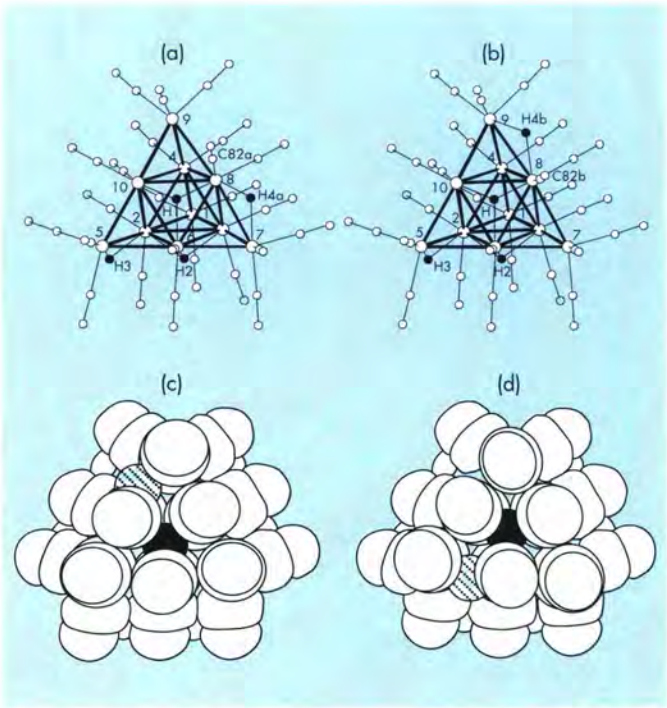


Figure 9. (a) and (b). The two isomers, (A) and (B), of $[H_4Os_{10}(CO)_{24}]^{2-}$, differing mainly in the position of one of the four hydrido ligands (filled circles), observed in the $[N\{P(C_6H_5)_3\}_2]^+$ salt. Space filling views of isomers (A) of the two large triangular faces that contain hydrogen atoms in μz-sites (filled atoms).

From the negligible intensity variation between 300K and 410K > T_N = 390K we conclude that these peaks are not of magnetic origin. Their intensities are about 10^4 to 10^5 times smaller than for the main Bragg peaks. Since these superlattice peaks appear at commensurate positions (e.g. (1/2, 1/2, 0)), special care was taken to determine the higher order contamination of the neutron beam (8.10^{-5} for λ/2 at λ = 2.36Å) and to exclude a Renninger effect. For this task, the combination of four circle geometry and analyzer proved essential.

The measured structure factors of the superlattice reflections could well be reproduced with a model of the basal plane oxygen ordering as shown in Fig. 10: "half-filled" CuO chains alternate with "quarter-filled" chains. Thus each oxygen atom has oxygen vacancies as first and second neighbours. However, only 15 % of the oxygen atoms in the basal CuO layer take part in the long range order which explains the difficulties to observe this superstructure.

In conclusion, we have reported the first neutron diffraction observation of oxygen ordering in a $YBa_2Cu_3O_{6.35}$ compound. Theoretical calculations of the oxygen ordering phase diagram have now to be extended to explain the observed superstructure. Thus interaction energies can be determined between the oxygen atoms which are the charge-reservoir for the superconducting carriers.

Crystallography of Magnetic Systems

Investigating the magnetic structure of $MnWO_4$

$MnWO_4$, space group P2/c, is known to order antiferromagnetically below 14 K /1/. Susceptibility measurements on one of our powder samples confirmed this result, but in addition to the usual antiferromagnetic behaviour two minima occur, at 12 K and 7 K respectively. They show that there are at least two magnetic transitions in the given temperature range.

The specific heat versus temperature curve, measured on our single crystal has three anomalies which are indicative of three, not necessarily magnetic, phase transitions.

A similar curve was already obtained by Landee et al. /2/, who measured the specific heat of a $MnWO_4$ powder sample, which was pressed to a pellet.

Neutron powder diffraction experiments were carried out on D1B. In the temperature ranges of 1.2 K -7.5 K and 7 K - 13 K respectively, two different magnetic phases were detected.

The low temperature phase could be refined with a model given by H. Dachs, E. Stoll and H. Weitzel /1/. These authors found by neutron diffraction on a single crystal that at 4.2 K the magnetic structure of $MnWO_4$ has a periodicity, which in direction of the a-axis is four times that of the crystal lattice, the other two lattice constants being doubled. The magnetic moments are collinear in the a-c-plane.

The preceding, so far unknown, magnetic phase does not have a periodicity in reciprocal space, which could be expressed in simple rational fractions of the nuclear periodicity. The propagation vector, which was found from the peakpositions of the powder pattern, by means of a method described by B.M. Knapp, F. Sinclair and C. Wilkinson /3/, is **q** = (- 0.205, 0.495, 0.457).

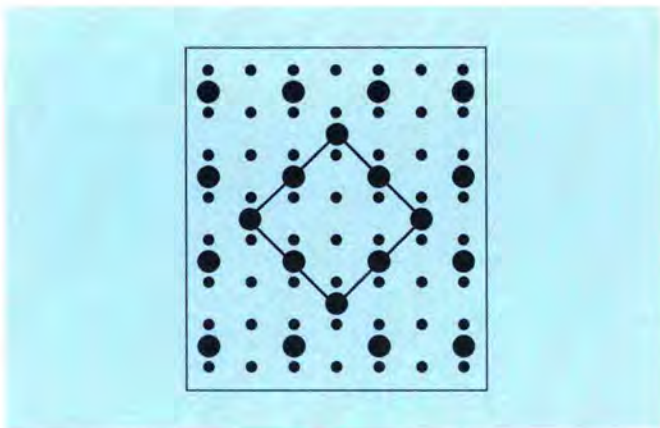


Figure 10. Derived oxygen superstructure in the basal plane of $YBa_2Cu_3O_{6.35}$. Small circles represent Cu, big circles represent O atoms. Also shown is the diagonal superstructure unit cell of dimensions $2\sqrt{2}\,a \times 2\sqrt{2}\,a \times c$.

Now single crystal experiments have to follow, in order to search systematically reciprocal space for satellites of the form **K±q**, **K** being a reflection of the nuclear structure.

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/1/ H. Dachs, E. Stoll, H. Weitzel, Z. Kristallogr. 125, 120-129 (1967)

/2/ C.P. Landee, H.F. Westrum, J. Chem. Thermodynamics 8, 663-674 (1976)

/3/ B.M. Knapp, F. Sinclair, C. Wilkinson, J. Appl. Cryst. 7, 370-372, (1974)

Incommensurate magnetic short range order in MnS_2

Valuable information about magnetic interaction parameters and the mechanism of magnetic phase transitions can be obtained from neutron scattering investigations of spin correlations in the paramagnetic phase. This has already been exemplified in the ILL Annual Report for 1989. Here we want to present the system MnS_2 as a particularly interesting example of a face centred cubic antiferromagnet which is well known to be inherently frustrated. Mn^{2+} ions in MnS_2 have a spherically symmetrical $^6S_{5/2}$ ground state. The peculiarity of this system is that it undergoes a first order phase transition into a type III single k antiferromagnetically ordered phase. The aim of our neutron scattering investigations on the four circle triple axis spectrometer D10 was to elucidate the nature of this unusual first order phase transition.

Using D10 in two axis mode, we verified in Q-scans along the main symmetry directions that the diffuse scattering above T_N was not centred at the antiferromagnetic propagation vector, but instead shifted to an incommensurate position $\mathbf{k} = (1, k_y, 0)$. The component k_y increases continuously from $k_y = 0.40$ at T = 115 K to $k_y = 0.44$ at a temperature just above $T_N = 48.2$ K. At the first order phase transition k_y locks into a commensurate value of 1/2 (Fig. 11). Such a temperature dependence of the incommensurate modulation has to our knowledge been observed for the first time in a magnetic system. Even just above T_N, the spatial correlations extend over little more than one unit cell ($\xi = 8$Å). Using the analyzer we showed that the inverse time correlations also decrease linearly with decreasing temperature from 2.9 THz at 150 K to 0.16 THz at T_N.

In order to obtain information about the magnetic interactions that drive the magnetic fluctuations to the incommensurate positions, we have performed calculations of the diffuse intensity distributions in the framework of the mean field and the quasistatic approximations. Fig 12 shows a comparison between the measured diffuse intensity in the (001) plane and a calculation using the values $J_1 = -2.60$ K, $J_2 = -0.60$ K and $J_3 = 0$ for the isotropic exchange interactions up to the third neighbours. Clearly, the

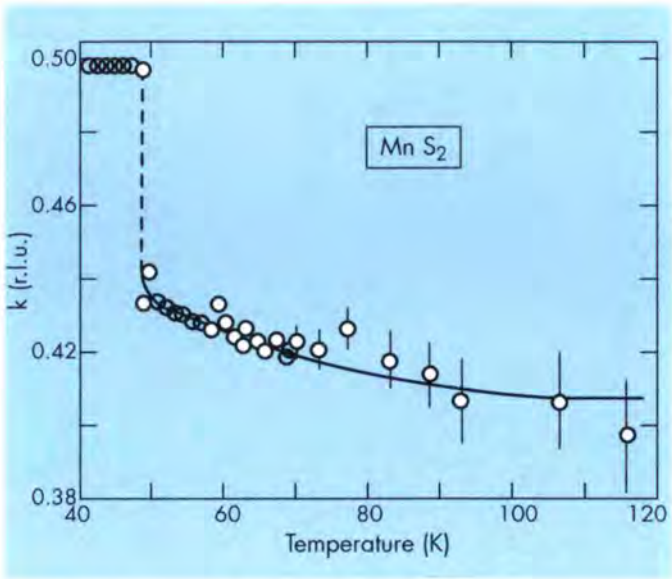

Figure 11. Temperature variation of the incommensurate component of the vector at which the diffuse magnetic neutron scattering is centred.

calculation reproduces the main features of the magnetic diffuse scattering very well, but fails to predict the incommensurate positions. The magnetic diffuse scattering is rather sensitive to small changes of the exchange parameters: a larger value of J_2 as was proposed in the literature leads to additional fluctuations characteristic of type II order, while by changing J_3 to -0.3 K only spin fluctuations characteristic of the type I antiferromagnetic structure are observed. Thus we learn from the diffuse scattering investigations that due to the particular values of the exchange integrals and the inherent frustration a strong competition of different types of antiferromagnetic order take place in MnS_2. In order to explain the centring of the diffuse scattering maxima at incommensurate positions anisotropic exchange interactions have to be considered. It is known that these can shift the maxima of the diffuse scattering to incommensurate positions as has been demonstrated in UAs.

In conclusion we have shown that the first order phase transition in MnS_2 can be understood as a lock-in transition from incommensurate magnetic short range order into a commensurate long range ordered phase. We demonstrated the strong competition between different types of magnetic order due to the inherent frustration of an fcc antiferromagnet and propose values for the exchange parameters. An anisotropic exchange interaction can be identified to be the origin of a shift of the diffuse scattering to incommensurate positions. Thus MnS_2 is a nice example of how magnetic interactions as well as the driving forces for the phase transition can be determined from neutron scattering studies of the paramagnetic diffuse scattering.

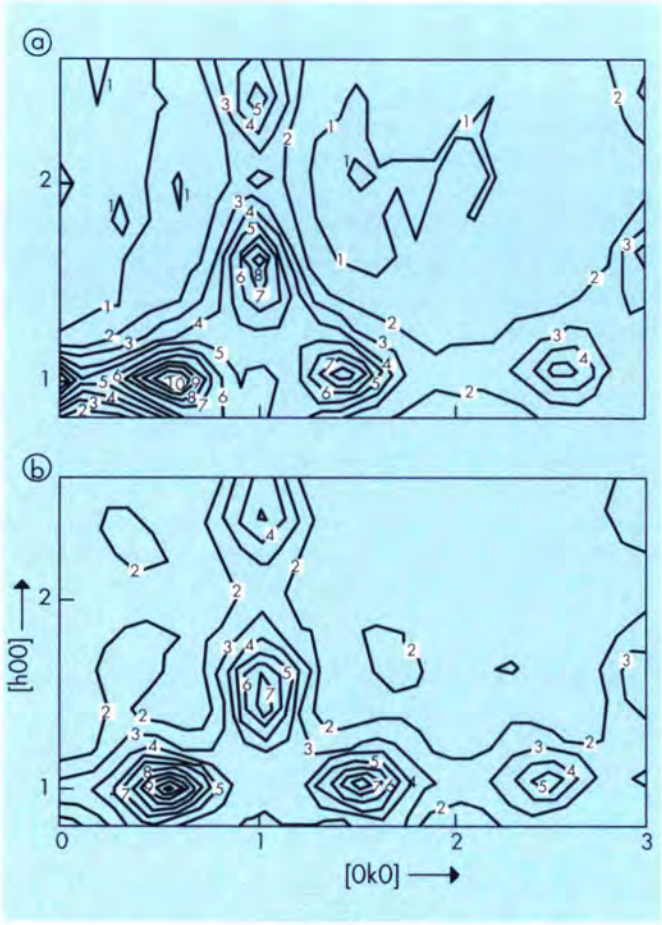

Figure 12. Contour plot of the magnetic diffuse intensity in the (001) plane. To suppress nuclear background, the difference 65 K - 200 K is plotted. Measurement (a) and a calculation (b) with J_1 = -2.60 K, J_2 = -0.60 K and J_3 = 0 are shown for comparison. Convolution with the resolution function was taken into account.

Anisotropic spin correlations in CuO above the Néel temperature

Intense interest in the valence, bonding and magnetism of square planar coordinated copper-oxygen planes has been engendered by their presumed importance in the high-temperature superconductors. Pure CuO provides an opportunity to study the magnetic properties of square planar Cu^{2+} coordinated by oxygen in a relatively simple system: a complete understanding of the magnetic properties of CuO may indicate whether magnetic mechanisms actually play any role in the hole pairing in the high-temperature superconductors. The magnetic properties of CuO are very similar to those of $YBa_2Cu_3O_6$. In both compounds the susceptibility exhibits only a minute anomaly at T_N and continues to increase at higher temperatures, eventually reaching a broad maximum which suggests that they may be similar to low-dimensional Heisenberg antiferromagnetic systems. The spin-wave velocities in both compounds have been reported to be exceptionally large. The magnetic moments of the Cu ions are significantly reduced from the full moment of Cu^{2+}, presumably due to the spin fluctuations which are typical of low-dimensional systems. It is perhaps more surprising to find low-dimensional behaviour in CuO than in the insulating analogues of the high temperature superconductors, since the exchange paths in CuO are far less anisotropic than in the distinct two-dimensional crystal structures of the high T_c superconductors. However, recent specific heat and magnetization investigations suggest that CuO behaves in fact like a quasi-one-dimensional antiferromagnet. In the following we report a neutron study of diffuse critical scattering from a single crystal of CuO, which provides new information about the detailed microscopic nature of its magnetic anisotropy. Fig. 13(a) shows Q-scans parallel to **k** at several temperatures close to T_N. Diffuse peaks were observed above T_N and these rapidly decrease in intensity as the temperature is increased. The continuous curves fitted to the data above T_N are of Lorentzian form, convoluted with the Gaussian resolution function determined from a similar scan below T_N (the variation of magnetic form factor of Cu^{2+} ions over the scan range was taken into account). Fig. 13(b) shows similar Q-scans perpendicular to **k** and the corresponding Lorentzian fits. The resolution function parallel to k is much broader than that perpendicular to k and has a width comparable to that of the diffuse scattering peaks. This caused difficulties in the convolution procedure and the widths of the diffuse scattering peaks are effectively resolution-limited close to T_N. The inverse correlation lengths $k_{//}$ and $k_{\perp}$ obtained by fitting the peak shapes of the scans parallel and perpendicular to k, respectively, are shown in Fig. 13(c). Despite the large uncertainties in $k_{//}$, the anisotropy in the correlation length is clearly seen, since at 230 K the correlation length along (1, 0, 1) is 50-60 Å whereas along (1, 0, -1) it is at least 300 Å. The correlation length parallel to (1, 0, 1) decreases with increasing temperature linearly in the temperature range from 230 to 234 K, being reduced by a factor of two at the latter temperature. This value, some 30 Å, then appears to be retained to 240 K, but it cannot be determined with good accuracy at these higher temperatures due to the poor counting statistics. Surprisingly, the correlation length of ~300 Å along (1, 0, -1) does not change significantly with temperature in the interval from 230 to 237 K, but then decreases at higher temperatures.

It is to be noted that O-Cu-O chains with a bond angle of 146° exist approximately along this direction. The present neutron investigations indicate that above T_N these chains are still strongly correlated and the magnetic susceptibility therefore continues to increase above T_N. The correlations persist up to about 450 K, at which temperature the susceptibility eventually starts to decrease.

Magnetic structures of holmium in an applied magnetic field

In the absence of an applied field, the complex magnetic structure of metallic holmium results from the competition between exchange and crystal-field interactions. Just below the ordering temperature T_N ≈32 K, the magnetic moments are confined by the crystal-field anisotropy to lie in the basal plane, forming a ferromagnetic sheet. The exchange

interaction and the lowest-order crystal field terms favour the formation of a magnetic spiral,with a wavevector **q** which is in general incommensurate, so that the moments in successive layers along the **c**-axis rotate. As both the exchange and crystal field are temperature dependent, the spiral wavevector decreases with decreasing temperature. On cooling below approximately 90 K the higher-order terms in the crystal field produce a series of long-period, commensurate structures, which consist of regions of the low-temperature structure separated by spin slip phases. At $T_c \approx 18$ K there is a first order transition to a ferromagnetic cone phase with the basal plane moments described by a wavevector **q**o = 1/6**c***. The magnetic ordering in holmium is probably the best known example of a structure exhibiting spin slips (or spin discommensurations) arising from competing interactions. Evidence for the existence of spin slips in holmium came from diffraction studies using both X-rays and neutrons. The spin-slip model also provides an explanation for the anomalies seen in ultrasonic, specific heat and thermal expansion measurements.

The neutron diffraction studies have recently been continued with investigations using the D10 triple-axis spectrometer of the effect on the magnetic structure of further competing interactions: magnetic fields applied along the c-axis or along an easy direction in the basal plane.

Unexpectedly a **c**-axis field has the effect of suppressing the onset of the commensurate cone phase found at low temperatures in zero field. Instead a number of spin-slip structures are observed, some of which are similar to those found in the zero-field spiral phase, while the others are new structures. A typical scan with the wavevector transfer varied between (001) and (002) for a field of 2 T at a temperature of 4 K is shown in Fig 14. In contrast to the zero-field diffraction experiments, where a continuous variation with temperature of the spiral wavevector **q** of a single magnetic phase was observed, the diffraction patterns

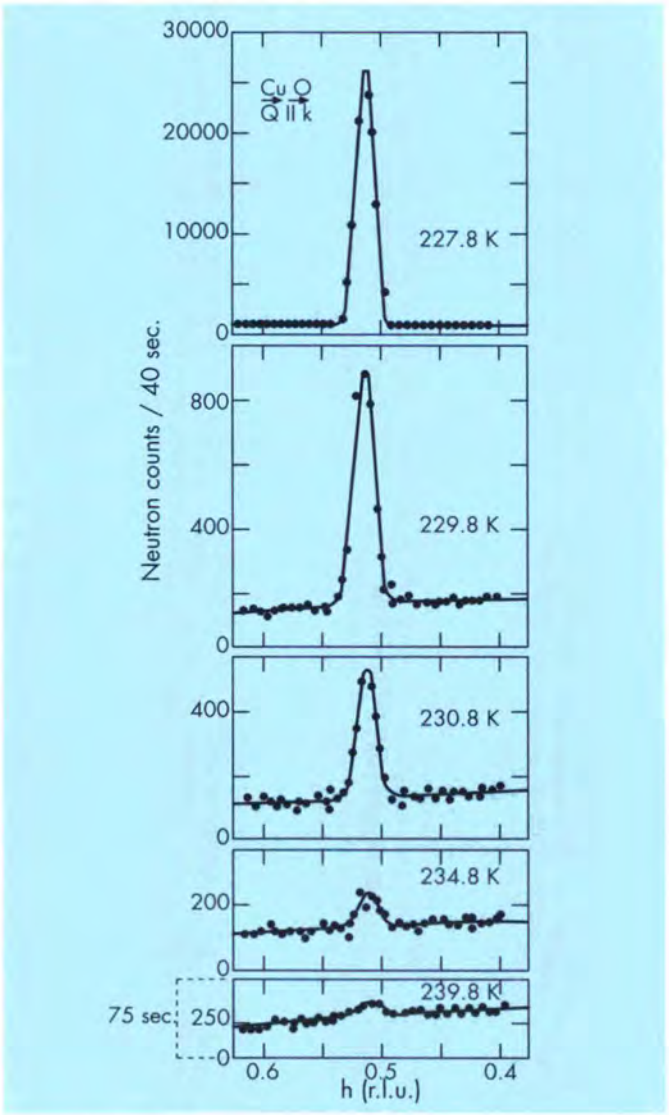

Figure 13. (a) Q-scans parallel to the propagation vector of CuO close to T_N.

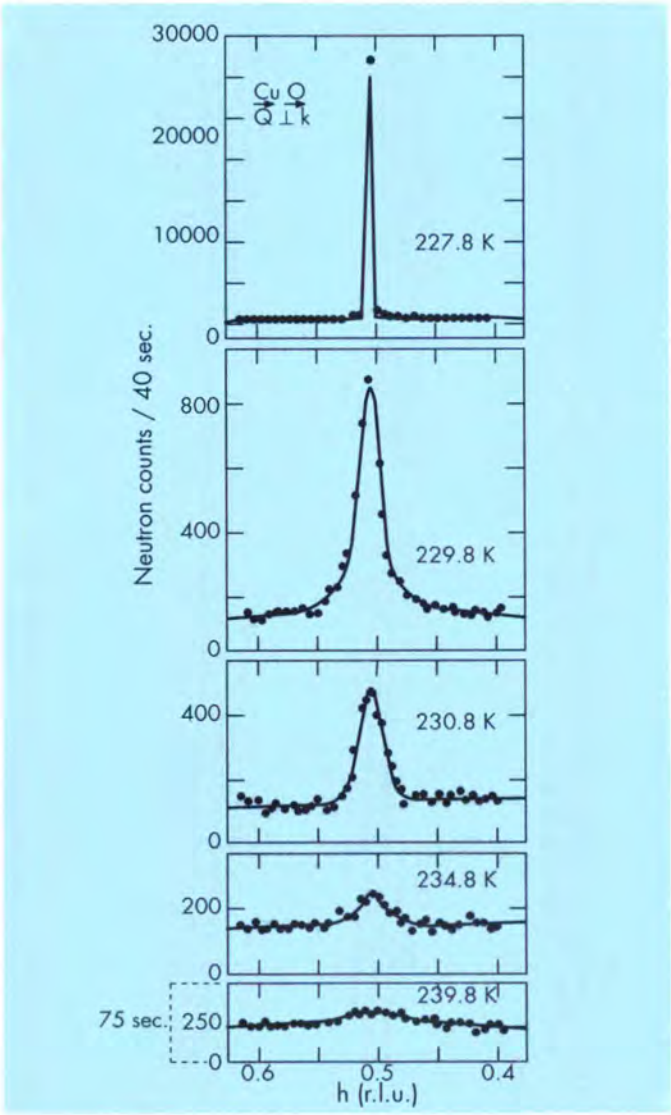

Figure 13. (b) Q-scans perpendicular to the propagation vector of CuO close to T_N.

may be interpreted as arising from structures with two (or more) co-existing spin-slip phases. Moreover below ≈ 15 K the wavevector is always commensurate and forms a devil's staircase with increasing field. The field and temperature dependence of the wavevectors is summarized in Fig. 15.

It was believed from earlier experiments that the application of a magnetic field along an easy direction in the basal plane of holmium produced a first-order transition from the spiral phase to ferromagnetic alignment at low temperature. However, these new experiments have shown that an applied field up to 1 T along an easy direction has a similar effect to a **c**-axis field: spin-slip structures with distinct rather than continuous spin-slip spacings, and the moments remain locked into a given structure over a wide temperature range. At higher easy-axis fields and temperatures the magnetic structure passes through the "helifan" structures predicted by Jensen and Mackintosh, and a fan structure before aligning ferromagnetically.

Detailed analysis of a few of the lock-in spiral structures both in a **c**-**q** axis field and in an easy-direction field has shown the presence of a basal plane moment, which may explain their stability. The rich variety of structures observed in holmium results from the delicate energy balance between exchange interaction, crystal field, and applied field.

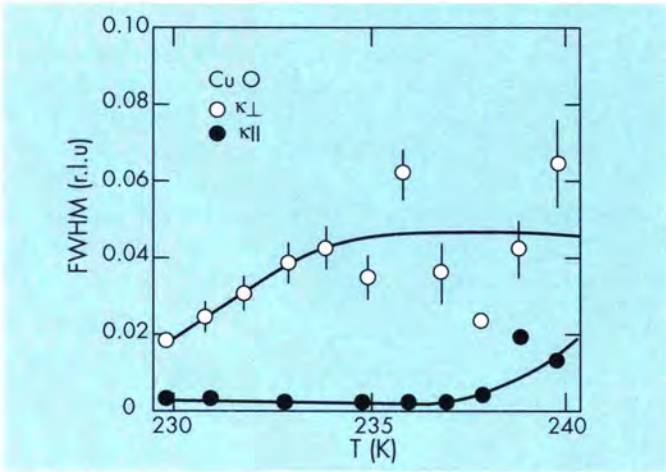

Figure 13. (c) temperature variation of the inverse correlation lengths of CuO parallel and perpendicular to the propagation vector above T_N.

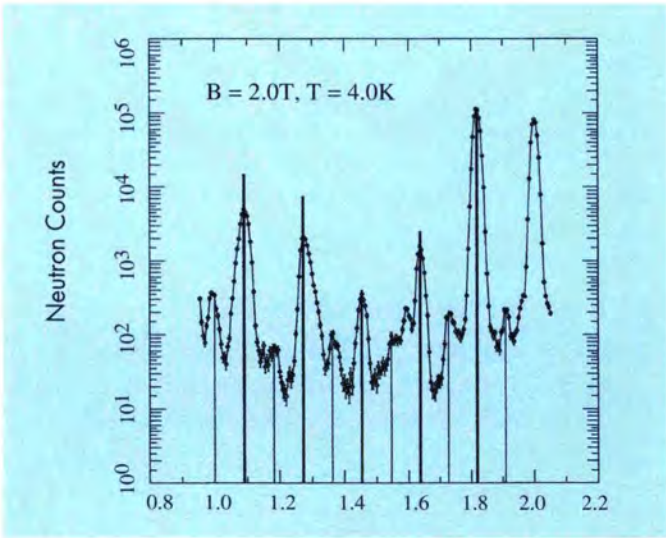

*Figure 14. The neutron scattering observed for holmium in a scan of the neutron wavevector transfer along [001] at 4.0 K, with a 2.0 T field applied along the **c**-axis. The vertical lines show the position of peaks with **q** = (n/11)**c***: the length of the thick lines represent the measured intensities from the **q** = (2/11)**c*** structure in zero field; the position of the thin lines indicate the n odd peaks which are attributed to breaking of the equivalence of the two holmium sub-lattices by the applied field.*

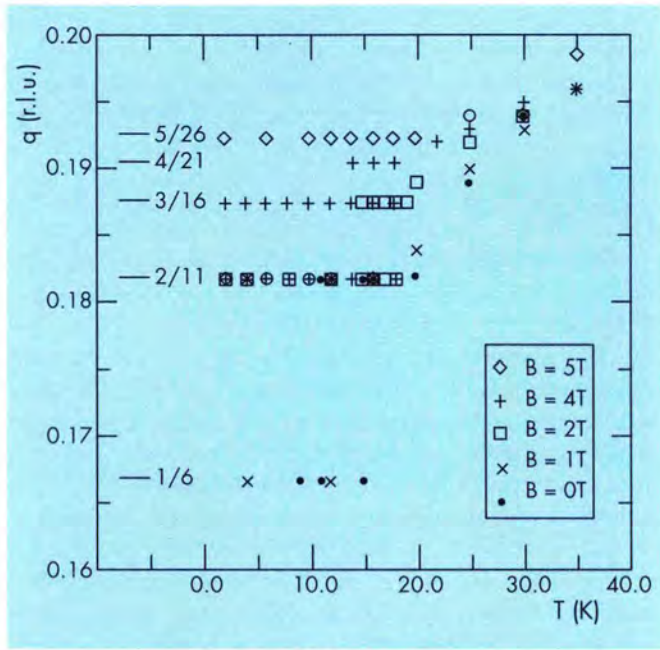

Figure 15. The temperature dependence of the magnetic spiral wavevectors in holmium at different applied c-axis fields.

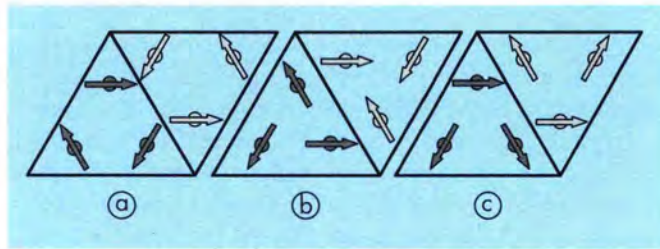

*Figure 16. [001] projection of three possible magnetic structures for Mn_3Sn which give identical intensities for neutron scattering from powder samples. The arrows indicate the relative orientations of the spins on the Mn atoms. The heavily shaded atoms are displaced by **c**/2 with respect to the lightly shaded ones. Zero field neutron polarimetry shows that the correct structure is (C). It was not possible to determine whether the spins are parallel to the {100} directions, as shown, or to the {120} directions.*

Magnetic structure determination using Zero Field Neutron Polarimetry

The traditional method for determining magnetic structures is by measurement of the position and intensities of the magnetic Bragg reflections. In this method the orientations of the magnetic moments with respect to the crystal axes are deduced from the dependence of the scattered intensity on the angle between the direction of the magnetic moments and the scattering vector. This approach is rather indirect and may be subject to ambiguities; a more direct and less ambiguous method of determining the magnetic moment directions in antiferromagnetic crystals is to use polarised neutron scattering with polarisation analysis to determine the absolute direction of the magnetic interaction vector **Q** for one or more magnetic reflections. The zero field neutron polarimenter CRYOPAD[1] which can be installed on IN20 provides a particularly convenient means by which the direction of **Q** for individual Bragg reflections may be determined and the very significant improvements made in the operation of CRYOPAD[1] over the past year have enabled some of this potential to be realised. This is demonstrated by using as examples three different problems which it has allowed us to solve.

The triangular spin structure adopted by Mn_3Sn presents an intriguing problem. The compound has the hexagonal DO_{19} structure and orders magnetically at 420K to a structure in which the spins on the three manganese sub-lattices are arranged in an equilateral triangle[2]. The three different arrangements shown in Fig. 16 all give rise to magnetic scattering of equal intensity in powder patterns. The structures differ in their symmetry and hence in the number of different domains which are allowed. (A) retains the full symmetry of the nuclear structure (6/mmm) and has only 180° domains, (B) with point group (6/m) has additional domains related by the missing mirror plane while (C) which is orthorhombic (mmm) has three trigonally related domains each with its 180° partner making six in all. If the symmetry related domains are equally or nearly equally populated it is not possible to distinguish between these three structures from measurements of the intensity of magnetic scattering even using single crystals and even if the 180° domains are unequally populated. In polarisation analysis measurements the presence of domains with different directions of **Q** depolarises the scattered beam. Measurement of the magnitude and direction of the neutron polarisation scattered by some h0l reflections of a single crystal of Mn_3Sn shows unequivocally that there must be three trigonal domains present and hence that the correct structure is (C). So long as the trigonal domains are almost equally populated it is not possible to tell whether the moments are parallel to {100} or {120} directions.

Cr_2O_3 is a member of a group of magneto-electric compounds with antiferromagnetic structures having identical magnetic and nuclear unit cells in which the crystallographic centre of symmetry reverses the spin direction. Such structures give rise to magnetic scattering which is 90° out of phase with the nuclear scattering and to a consequent rotation of the polarisation of scattered neutrons in the plane containing the incident polarisation and the scattering vector. The direction of the rotation depends on the absolute orientation of the magnetic moments with respect to their ligand environment, and if this environment is polar the two opposite orientations are distinguishable and may have different energies. Only a polarimeter such as CRYOPAD in which all three components of polarisation are measured can be used to investigate this effect. Our observations show that in Cr_2O_3 the configuration in which the magnetic moment points towards the smaller of the two equilateral triangles of near neighbour oxygen atoms is largely predominant right up to the Néel temperature.

Between its Néel temperature of 230K and the lock-in transition at 213K CuO has an incommensurate magnetic structure with propagation vector τ =(0.506,0,-0.483). A study based on single crystal integrated intensity measurements[3] suggested a helical rather than an amplitude modulated structure. The best fit to a structure of monoclinic symmetry was one in which the magnitude and direction of the copper moments is given by a function of the form:

$$\mathbf{S} = \mathbf{S_1} \cos 2\pi (\tau \cdot \mathbf{R}) + \mathbf{S_2} \sin 2\pi (\tau \cdot \mathbf{R})$$

where **R** is the radius vector to any copper site and $\mathbf{S_1}$ and $\mathbf{S_2}$ are perpendicular vectors in the **a-c** plane. $S_1/S_2 \sim 2$ and $\mathbf{S_1}$ is inclined at ~33° to **c** in obtuse β. Since the sensitivity of magnetic intensities to the orientation of the axes of the helix is not high, this structure has been re-investigated using CRYOPAD. The results of polarisation analysis of 6 different h0l reflections confirm the helical structure but show very clearly that one axis ($\mathbf{S_1}$) of the elliptical envelope of the spiral is parallel to b while the other ($\mathbf{S_2}$) lies in the a-c plane at 28(1)° to c in obtuse b with S_1/S_2=1.034(5). It should be emphasised that the scattered polarisations expected for models with spins in the a-c plane and those with a b-axis component are qualitatively different, which makes polarimetry a particularly suitable tool for solving this type of problem.

[1] Tasset F (1989), Physica B **156-157** 627

[2] Zimmer G J and Kren E (1973) Magnetism and Magnetic Materials 1972 (AIP Conference Proceedings **No 10**, American Inst of Phys, New York p 1379

[3] Forsyth J.B., Brown P.J. and Wanklyn B.M.(1988) J. Phys.C **21** 2917

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Measurement of magnetic anisotropy using polarised neutrons

J. Brown

One of the key parameters determining the suitability of permanent magnet materials for device applications is the anisotropy constant K_1. Transition metal ferromagnets have rather low values of $K_1 (<10^6 \text{erg cm}^{-3})$ and for device applications they have largely been replaced by mixed rare-earth transition metal compounds such as $SmCo_5$ and $Nd_2Fe_{14}B$ in which the 3d element maintains a high Curie temperature while the the rare-earth element increases the anisotropy. Compounds containing 5f actinide elements exhibit even more anisotropic magnetic behaviour than the analogous compounds containing 4f elements, but the size of this anisotropy has never been measured.

Traditionally anisotropy parameters have been obtained using bulk magnetisation and magnetic torque measurements. These techniques require large single crystals machined to rather accurate shapes and, if the anisotropy is large, very high magnetic fields. The use of polarised neutron diffractometry provides an alternative method of obtaining K_1 which can give not only bulk anisotropy parameters but also show up differences in the anisotropies associated with different atomic sites. It has the advantage of giving the actual moment directions rather than their projection on that of the applied field. The principle of the method is to mount the crystal on the diffractometer so that the applied field direction is parallel to a general crystallographic direction rather than to an axis of symmetry so that the application of the magnetic field breaks the crystal symmetry. The symmetry is broken because with such a mounting there is a unique direction amongst the set of crystallographically equivalent "easy" axis directions, which is that lying closest to the applied field. The magnetisation will lie somewhere in the plane between this "easy" direction and the field direction at an angle determined by the anisotropy constants and the field strength. Under these conditions the vector character of the interaction of the neutron with atomic magnetic moments leads to different magnetic structure factors, and hence to different polarised neutron "flipping ratios" for crystallographiclly equivalent reflections. The method consists in measuring the "flipping ratios" of sets of such equivalent reflections and then fitting the data by varying the assumed magnetisation direction to obtain that which most nearly restores equivalence between values calculated from the "flipping ratios", under that assumption, of the scalar part of the magnetic structure factors.

This technique has been used to measure for the first time the giant magnetic anisotropy in uranium sulphide. A magnetic field of 4.6 T was applied along a direction approximately 26° from one of the "easy" {111} axes. The precise direction of the aligned moments and their magnitude were determined as a function of temperature from measurement of the "flipping ratios" of sets of strong low angle reflections. From 5 to 140K the moment was found to be locked along the {111} axis closest to the field but at higher temperatures it starts to rotate towards the field. The aligned moment does not become parallel to the field direction until 195K some 17K above the Curie temperature. The value of the anisotropy constant K_1 has been deduced from these results and is plotted against the reduced moment $\mu(T)/\mu(T=0)$, which is an implicit function of temperature, in Fig. 1. The straight line extrapolation suggested by theory leads to a value of K_1 of ~ 10^{10} erg cm^{-3} at 0K.

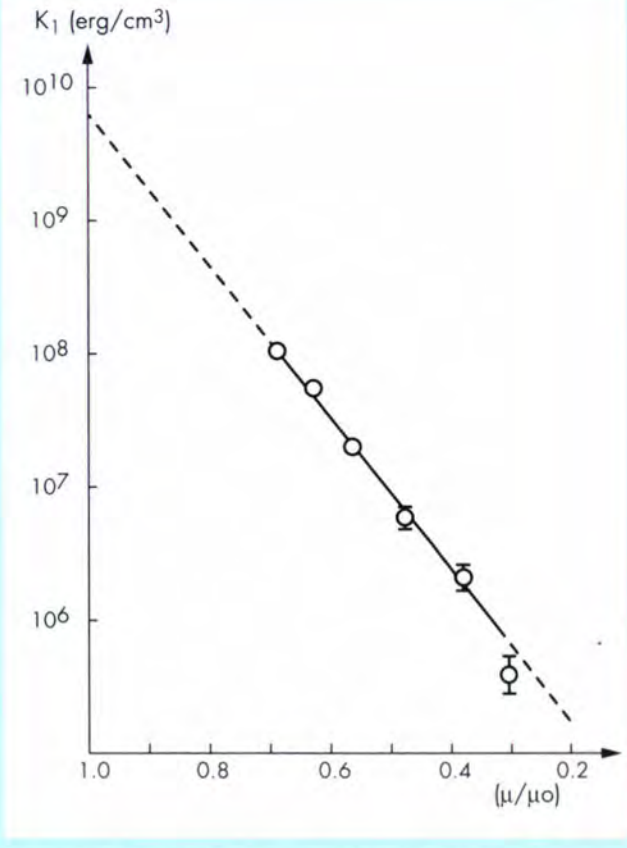

Figure 1. The anisotropy constant K_1 of US, obtained from polarised neutron measurements, plotted as a function of the reduced moment.

Liquids, Disordered Materials and Metal Physics

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Summary

In the following we will give a rapid and limited view on the very active and broad field of college VI scientific work. Instead of being a statistically representative collection the aim is to point out just a few outstanding examples and to show the variety of subjects treated. Definitely the mainstream of the work in our college is still the structure and dynamics of disordered and glassy substances that count for more than one third of the proposals submitted. The various liquid systems, their structure and excitations are, as usual, well represented and we can note the increasing number of investigations in extreme experimental conditions, high temperatures and pressures. The problems of metallurgy, alloys, precipitation, diffusion are of constant interest. Among the important developments not mentioned explicitly below we can recall the productive efforts on quantum liquids and on quasicrystals for example.

Scientific trends and highlights in 1990

The dynamic structure factor of expanded liquid alkali metals

The main interest in the study of expanded liquid alkali metals is to find out how the structure, dynamics and effective interaction potential change during the expansion of the liquid metal from the melting point towards its critical point (critical data e.g. for caesium T_c = 1924 K, p_c = 92 bar, d_c = 0.38 g cm^{-3}; for rubidium: T_c = 2017 K, P_c = 124 bar, d_c = 0.29 g cm^{-3}. Near the liquid-vapour critical point, the change from a liquid metal to a nonmetal takes place, as can be inferred from measurements of the electrical conductivity, magnetic susceptibility and optical reflectivity. The occurrence of the metal-nonmetal transition implies that the interatomic forces must exhibit drastic changes when the liquid metal is expanded and the metal nonmetal transition is approached.

Recently the static structure factor S(Q) of expanded liquid caesium from the melting point up to its critical point was measured on the D4B-diffractometer. Characteristic changes of the microscopic structure, such as the distance (Winter et al. 1987, 1988) and number of nearest neighbours have been obtained and measurements of the isothermal pressure derivative of S(Q) over the whole liquid range provided valuable information about three-body correlations and the validity of model potentials. The results showed that the nearly-free electron model fails at relatively high densities of about three times the critical density, which can be explained by the starting decrease in the screening of the ion cores during the expansion of the liquid metal towards its critical point. In order also to obtain information about the dynamics of the expanded liquid alkali metals, such as the self-diffusion coefficient and collective excitations, the dynamic structure factor $S(Q,\omega)$ of liquid rubidium has now been measured up to 1900 K using the IN6 TOF-spectrometer (Pilgrim, Winter, Hensel, Morkel, Gläser, Mutka). Fig. 1 shows as an example some data of $S(Q,\omega)$ for liquid rubidium at T = 1400 K. Interesting, characteristic phonon-like side peaks in liquid rubidium are seen even up to this temperature of 1400 K. The corresponding dispersion relation of the collective modes, which has been evaluated from the longitudinal current correlation function, is also shown in the figure. We find a dispersion curve which resembles that of liquid rubidium measured by Copley and Rowe (1974) at 320 K. This indicates that at these conditions of temperature and density (about three times the critical density) the ion-ion interaction of liquid rubidium is still controlled by the dynamics of the electron sea of the liquid metal. These new quantitative results obtained at extreme conditions of temperature and pressure present a real challenge for new theories describing the single particle and collective dynamics of atoms in expanded liquid metals.

Structural changes in a liquid near melting

Detection of structural changes in a liquid close to the melting point (T_m) is a long-standing problem. Recent observation (McGreevy and Van der Lugt) near T_m for Rb has shown that the crystalline diffuse scattering and the liquid structure factor are very similar indicating that the short range structure in the crystal and in the liquid are almost identical. However, while the height of the structure factor maximum increases slightly from T_m + 1 to T_m + 0.20 as would be expected, it decreases below T_m + 0.20. This anomaly and the structural changes involved are being further investigated.

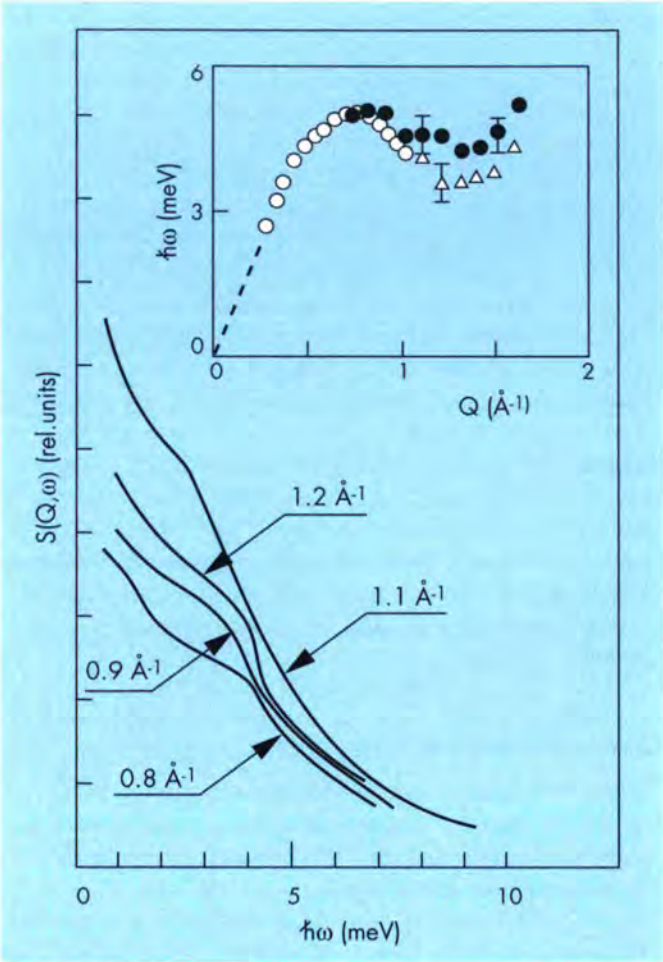

Fig. 1: The dynamic structure factor S(Q,ω) of liquid rubidium at T = 1400 K (inset : the dispersion relation ħω(Q) of the collective modes (o at the melting point , Δ at 1100 K, ● at 1400 K).

Plastic crystal phase in a metal alloy

Quasielastic scattering on IN6 (Price, Saboungi, Reijers, Kearley, White) has revealed that the intermediate phase of the intermetallic alloy CsPb is a plastic crystal characterized by jump reorientations of Cs_4Pb_4 structural units. The wave vector variation of elastic and quasielastic intensities is well reproduced by a simple model of independent structural units jumping between the four orientations observed in the crystal at room temperature. This represents the first observation of a plastic crystal phase in a metal alloy.

Collective excitations in a dense molecular liquid : SO_2

The collective properties of liquid sulphur dioxide have been studied by means of inelastic, triple-axis neutron spectroscopy on IN8 (Bermejo, Martínez, Garcia-Hernandez, Martín-Marero, Monpeán, Enciso, Batallán). This liquid was chosen for two reasons: first, it constitutes an optimal representative for this class of liquids due to its low melting point and relatively simple molecular structure. The liquid structure is well known from a recent neutron diffraction study, where it was shown that the range of strong orientational correlations (coherence length) extends up to 20 Å; and second, it is a nearly pure coherent scatterer for neutrons, a fact that will provide good counting statistics, nearly free from incoherent contributions.

A set of spectra measured at a temperature just above the melting point is shown in Fig. 2. Noticeable inelastic intensities indicate the presence of propagating modes below 0.70 $Å^{-1}$ at T = 210 K. The continous lines correspond to fits using a model scattering law which makes use of the viscoelastic approximation and has been shown to provide reliable results when analysing triple-axis spectra for liquid methanol and heavy water.

Water and solvated species at high temperatures and pressures

Structure factors were measured for heavy water at various T and P up to 400°C, 1630 bars (Neilson, Howell, Stockford, Chieux). The results show significant changes accompanying the application of P and T : in the region of the critical point the results are characterized by a rise in the small angle scattering and the disappearance of a shoulder on the high k side of the main peak centred at 2 $Å^{-1}$. These observations are taken as evidence of the breakdown of the H-bond network at high T and the onset of "normal" liquid behaviour. With applied pressure (up to 550 bar) a low atomic fraction of a few parts in a thousand of Argon could be solubilized in heavy water. The isotopic substitution of Ar was nevertheless used (Neilson, Broadbent et al.) in an attempt to reach the local atomic environment of Ar from the scattering difference between ^{36}Ar and ^{nat}Ar samples. A rather well defined $G_{Ar}(r)$ could be obtained which shows a conformation of about 20 ± 4 water molecules around the Ar atom. It is anticipated that this work will be extended to include studies of the hydrophobic effect where the salt phenomenon is known to occur, e.g. in aqueous mixtures of salts and proteins.

Isotopically enriched (Ni enrichment) samples of a 1.2 molal Ni SO_4 solution were also studied as a function of applied P,T. The difference function $\Delta N_i(k)$, which describes the structure around a Nickel ion, showed a dramatic modification between ambient conditions and T = 300° C, P = 1000 bar. In fact, a total disruption of the Ni^{2+} hydration shell and the establishment of ion-pairing is observed.

Iron in aqueous solutions

Work on aqueous solutions is now extending from room temperature studies of the Li^+, Cl^-, $Ni2^+$ environment to ions with more complicated hydration shells. A particularly suitable candidate for neutron diffraction is iron in aqueous solutions (Herdman, Neilson), since it exhibits changes in oxidation state, hydrolysis, polymerization and complexes with anions, all of which involve changes in the water

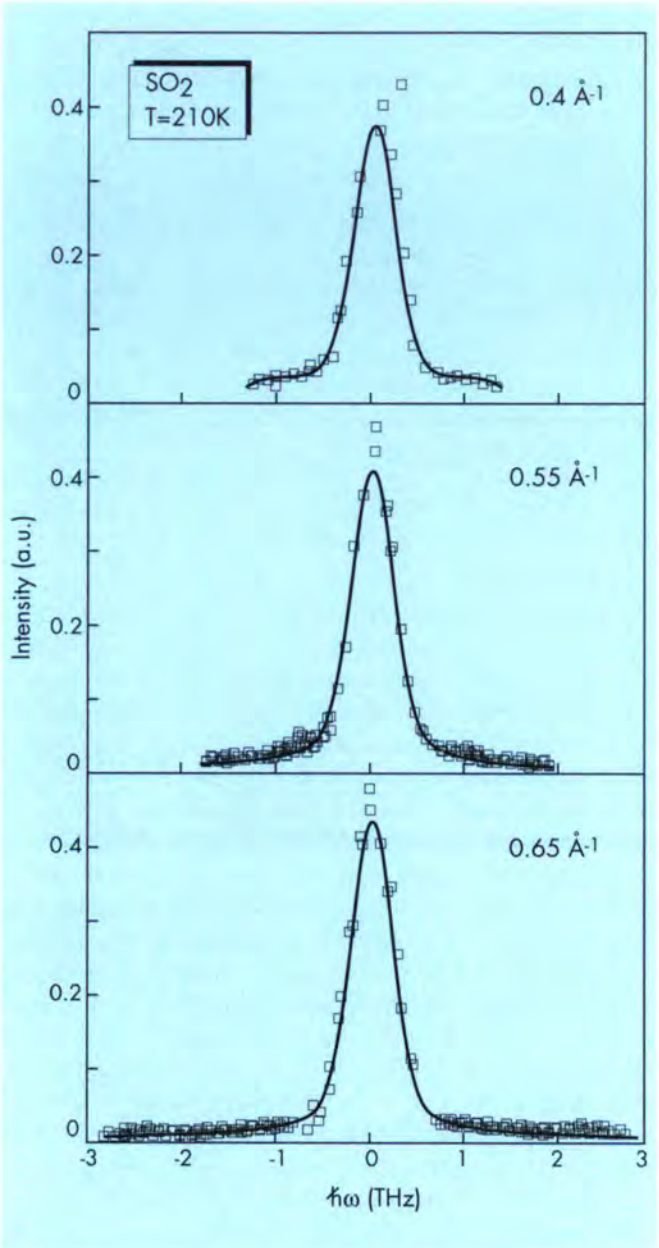

Fig. 2: Corrected spectra for selected momentum-transfer values. Open squares represent experimental intensities and the continuous lines are fits to the model function.

hydration structure. Samples heated during preparation, deviated from the expected hexaqua coordination : in the case of iron perchlorate ($n_O = 6$ and $n_D = 10$) due to hydrolysis, in the case of iron nitrate ($n_O = 5$, $n_D = 9$) due to polymerization. For comparison, samples prepared at R.T. gave the expected hexaqua ion ($n_O = 6$, $n_D = 12$). Ferrous instead of ferric ion is also immediately apparent from changes in the Fe-O and Fe-D distances (e.g. Fe-O goes from 2.0 to 2.1 Å).

Vibrational dynamics of liquid and glassy electrolytes

LiCl aqueous ionic solutions have been extensively studied and are structurally well characterized in the various equilibrium or metastable thermodynamical states. They are therefore appropriate for detailed vibrational dynamics investigations. Intermolecular motions of water have been obtained (Dupuy et al.) from inelastic neutron scattering measurements for saturated aqueous solutions of Li Cl, RH_2 D (R = 6 and R = 4). Bending (~7 meV), stretching (~ 25 meV) and libration (~ 90 meV) modes were investigated as a function of H_2 D content and compared with the frequency distribution for pure water. The stretching motion which is independent of concentration, is much better resolved at low T than in the liquid state where the two other modes overlap with it significantly as in pure water. In the glassy and super-cooled states, an additional band appears near 36 meV which, on warming, is progressively overlapped by the librational band. Clearly in this system where H-bonding competes with other interactions, the study of the glass transition itself will benefit from studies combining structural characterization of water with its surroundings and measurements of the extended vibrational density of states in the range of the stretching motion.

Geometry of small molecules in molecular solids

Neutron scattering at high momentum transfer is commonly used for the determination of intramolecular parameters of molecular liquids. It could also be applied to the determination of the geometry of small molecules or of well defined (strongly bonded) local configurations in solids. The geometry of the ammonia molecule in $Ca(ND_3)_6$, a compound which shows proton disorder at liquid Helium temperature (molecular glass) and rapid reorientational motion of the ammonia groups above 40K, has been obtained from diffuse scattering measurements at large momentum transfer (up to 23 $Å^{-1}$). It is found (Damay, Leclercq, Chieux) that the overall structure of the gaseous ammonia is preserved in solid and liquid ND_3 as well as in the Ca $(ND_3)_6$ compound at all temperatures investigated. This accurate and direct determination should be seen as a complement to the molecular structure refinement which is quite difficult to achieve in powder diffraction.

Crystal field excitations as a probe for order and relaxation in an amorphous metal

Changes of bond orientational order during structural relaxation in the amorphous metallic compound $PrNi_5$ have been investigated using the high sensitivity of of the crystal field splittings of the magnetic rare earth ion to the local atomic environment. While the low temperature neutron inelastic scattering spectrum (measured on IN4, Alekseev, Klementjev, Lazukov, Orlov, Sadikov, Suck)) of $PrNi_5$ is dominated by two very pronounced and sharp CF peaks at 4 and 13 meV (two other are unresolved in the foot of the elastic peak) the spectrum of the amorphous compound shows just a smooth, continuous magnetic intensity distribution in the same energy range. The shape of the

magnetic spectrum of amorphous $PrNi_5$ can be described by a model based on a perturbed crystal only if in addition to a **bond length** variation a **bond angle** variation is assumed. One can expect that due to structural relaxation in the vicinity of crystallization, indications of CF peaks should appear on the smooth spectrum if the environment of the Pr ion approaches the hexagonal structure of the crystal. Surprisingly, even after relaxation as close as $0.97T_X$ to the crystallization temperature T_X, no sign of CF peaks was observed. One has to conclude that even though the bond lengths may change during structural relaxation of this amorphous metal the changes in bond angles are not sufficiently pronounced to induce locally crystal-like environment for the Pr atoms. That change seems to happen more abruptly very near to or at T_X (see Fig. 3).

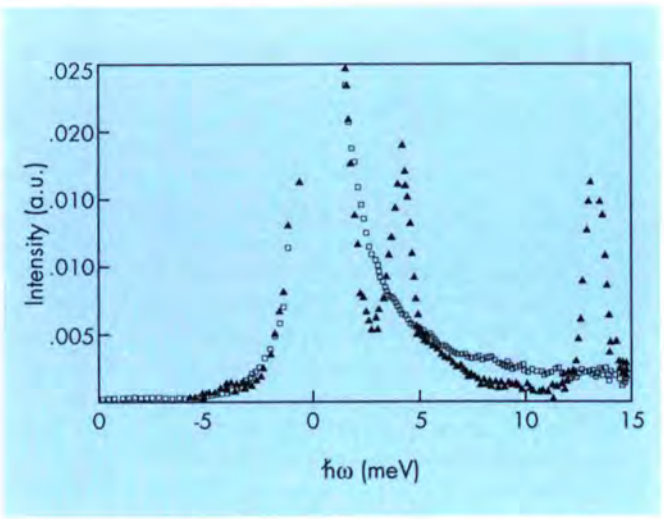

Fig. 3: Inelastic neutron scattering from crystalline (open squares) and amorphous (black triangles) $PrNi_5$. In the amorphous material the characteristic CF peaks are replaced by a continuous distribution of magnetic intensity. No peak structure was observed even after structural relaxation at $T = 0.97T_X$, where T_X is the crystallization temperature.

Silicate glasses

The spatial distribution of Ca and other so-called "network-modifying" ionically-bonded elements in alkali and alkaline-earth silicates is an open question - a random distribution determined solely by macroscopic parameters such as composition and density being the general assumption. Isotopic substitution of Ca in $(CaO)_{48.0}$ $(SiO_2)_{49.0}$ $(Al_2O_3)_{30}$ silicate glass, gives directly, from a double difference experiment, the Ca-Ca distribution (Gaskell et al.). It confirms that a Ca-Ca first neighbour distance at 0.38 nm corresponds to a typical value of crystals and the peak in $G_{ca}(r)$ at 0.64 nm gives a clear indication that the cation environment is octahedral with interconnexion through edge linkages. All these features are consistent with the notion that Ca lies within regions where the structure, although distorted, approximates to cubic close-packing. The presence of a well-defined local structure around such elements has extensive implications for medium-range organization. Briefly, in close-packed glasses (or in the close-packed regions of silicates and other oxide glasses) the occurrence of local ordering around atoms such as Ca that are highly interconnected, is a *consequence* of a well-developed medium-range structure.

In-situ backscattering study of oxygen precipitation in Silicon

The study of oxygen precipitation in silicon wafers is a matter of acute technological interest that has been examined with continuous effort by small angle scattering (D11, Stewart, Messoloras et al.). A new opening in the field is an unconventional application of the backscattering instrument IN10 for studying *in-situ* lattice deformation due to oxygen precipitation in silicon single crystals (Liss, Magerl, Schneider, Zulehner). The integrated reflecting power and lattice parameter variations, associated with the strain fields due to the the oxygen precipitates, were recorded as a function of temperature and annealing time from room temperature up to 1500 K. In high purity float zone crystals the reflecting power remains characteristic of perfect crystal up to 1200 K. On the contrary, Czochralski grown crystals with about 10^{18} oxygen atoms cm^{-3} show a steep increase in reflectivity starting at 1160 K and reaching a maximum at 1350 K, and annealing out slowly at 1456 K. The method allows the investigation of massive samples (up to 10 cm thickness) which may be of interest for technical applications.

Pressure dependence of the hydrogen diffusion in Nb at low temperatures

The pressure dependence of the Hydrogen diffusion in Nb was investigated by quasielastic neutron scattering at the instrument IN14 (Stuhr, Wipf, Vettier, Dorner, Schober) with an incident neutron wavelength of 5.98 Å. The experiment was carried out with a constant Q-scan with $\vec{Q} = 1.62$ Å^{-1} in [110]-direction. The upper part of Fig. 4 shows the spectra of the sample under a hydrostatic pressure of 5 kbar and 1 bar. The continuous lines in these figures are fits to the spectra each made with two Lorentzian lines with fixed ratios for the intensities and the linewidths according to a Chudley-Elliott model for the jump diffusion of the hydrogen (intensity ratio 3.2, width ratio 2.49). The data points in the lower part of the figure below show the difference between the two spectra. The fits yield a pressure induced reduction of the diffusion coefficient D of (2.5 ± 8.5) % with a mean value of $D = 0.83 \cdot 10^{-6}$ cm^2/sec.

Tunnelling of hydrogen in rare-earth metals

Hydrogen dissolved in hcp rare earth metals is known to exhibit unusual short range ordering, which apparently stabilizes the alpha phase at much lower temperatures than

in other metal-hydrogen systems, and which leads to a variety of interesting physical properties. Quasielastic scattering studies of hydrogen dynamics in these systems have shown that long range diffusion is rather slow but at the same time there is a more rapid proton diffusion between near neighbour sites along the c-axis. Further studies of the temperature dependence of this localised motion in scandium and yttrium (IN5 and IN6, Anderson, Berk, Rush, Udovic, Barnes, Magerl, Richter) reveal that the quasielastic line width has a pronounced minimum near 100 K and rises at lower temperature with an approximate T^{-1} dependence, indicative of nonadiabatic behaviour that can be associated with weak coupling of a quantum two state system. The simultaneous determination of the elastic incoherent structure factor may be interpreted in terms of labile and nonlabile hydrogen configurations in a manner consistent with recent estimates of pairing and activation energies in these systems.

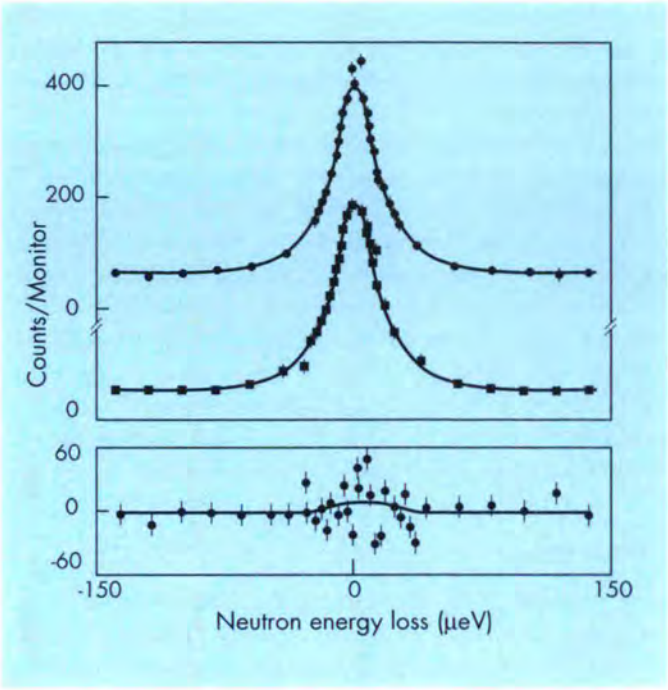

Fig. 4: Pressure dependence of quasielastic scattering in NbH_X: the lower curve is the difference between the 5 kbar and 1 bar results.

Local structure and dynamics in high-T_c superconductors

A notable feature in the structural data of $Tl_2Ba_2CaCu_2O_8$ high T_c superconductors is the difference in pair distribution functions (PDF) when either calculated from standard crystallography analysis or measured directly using methods currently applied to non-crystalline materials (liquids, amorphous alloys, etc.). The former gives the time averaged PDF while the latter results in the instantaneous PDF. In particular, in the crystallography determined structure the Tl-O distance is 2.73 Å while this distance is clearly split at 2.4 and 3.0 Å in the measured PDF. To clear up this apparent discrepancy the IN1 triple-axis instrument was used in two different modes without and with energy analysis (Egami, Toby, Janot). In the first case the directly measured PDF shows an anomalous temperature dependence on the pair distances at 3.4 and 3.8 Å in the vicinity of T_c corresponding to the Cu-Ba and Tl-Tl pairs with a departure from what is expected from the measured phonon-DOS as determined by inelastic neutron scattering. In the second case using IN1 as an "elastic diffractometer", the elastic scattering intensity S(Q,0) has been measured within the resolution of the analyser; the Fourier transform of S(Q,0) is the average density-density correlation function, which is slightly different from the instantaneous PDF in that the dynamic correlations are missing. The largest difference is found in the height of the peak at 3.4 Å, the very peak which showed an anomaly. This difference is temperature dependent and increases below T_c. It clearly suggests that the observed anomaly of dynamic nature - the opening of the superconducting gap - drastically alters the lattice dynamics (see Fig. 5).

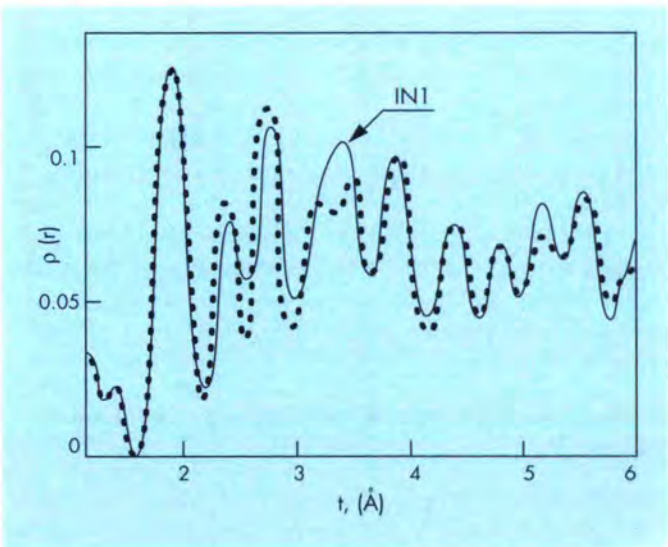

Fig. 5. Elastic pair-density correlation of $Tl_2Ba_2CaCu_2O_8$ at 70 K (solid line) compared to the instantaneous pair distribution function obtained by pulsed neutron scattering (Argonne) at 80 K (dotted curve). The peak at 3.4 Å is notably higher when the dynamic correlations are missing.

Secretary: H. Mutka

Towards a new understanding of the glass-liquid transition

W. Petry

In general the structure of a glass does not differ from the structure of its liquid. If no structural changes occur during the transition of a liquid to its glassy state the question arises whether it is justified to speak of a glass-liquid transition. Modern theories show a way out of this dilemma. In the mode coupling approach [1] the glass transition is seen as a critical slowing down of **relaxations** at a critical temperature T_c above the calorimetric glass transition temperature T_g. Density fluctuations are considered as the most relevant low frequency excitations in a liquid. The evolution of the density correlator is given by a damped oscillator equation with memory. The equation is closed by specifying the friction kernel again as a functional in the density correlator. The resulting nonlinear coupling of density modes enhances the effective friction and induces structural freezing-in at T_c. The transition to the frozen-in or nonergodic state is expected to exhibit universal features largely independent of the specific glass material.

The high resolution neutron spectrometry as established at the ILL with a time window from 10^{-8} to 10^{-13} s and a Q-range from 0.05 to 5 Å^{-1} covers exactly the range where the critical slowing down should be observed. In the last 3 years experiments on different glass formers such as salts ($Ca_{0.4}K_{0.6}(NO_3)_{1.4}$ [2]), van der Waals liquids (α-trinaphtylbenzene [3], ortho-terphenyl (OTP) [4], polymers (polybutadiene (PB) [5]) and biological glasses (myoglobin (MG) [6]), have been performed and exhibit a remarkable accord with the mode coupling concept. To show this we focus on a few crucial points:

1) The relaxations are expected to split into **two time regimes** which follow different scaling laws and which are separated by a critical frequency ω_ε which again depends on temperature. Reformulating the scattering law S(Q,ω) as a normalized compressibility $\hat{\chi}''(\hat{\omega})$ a simple relationship is predicted [7]

$$\hat{\chi}''(\omega) = (b\hat{\omega}^a + a\hat{\omega}^{-b})/(a+b) \qquad (1)$$

with $\hat{\chi}''(\omega) = \chi''(Q,\omega)/\chi''(Q,\omega_\varepsilon)$

$$\chi''(Q,\omega) = \omega.S(Q,\omega)$$

$$\hat{\omega} = \omega/\omega_\varepsilon$$

which depends only on one quantity, because the critical exponents a, b are coupled via the Γ function

$$\Gamma^2(1-a)/\Gamma(1-2a) = \Gamma^2(1+b)/\Gamma(1+2b) = \lambda \qquad (2)$$

The measured normalized susceptibilities $\hat{\chi}''$, of OTP, PB, myoglobin and the normalized scattering law $S(Q,\hat{\omega})$ of $Ca_{0.4}K_{0.6}(NO_3)_{1.4}$ are shown in Fig. 1. Clearly the observed relaxations separate into two time regimes which follow different scaling laws. The closer the temperature to T_c the larger the frequency range covered by the two scaling laws. From the experimental point of view it is important to note that the dynamic range shown in Fig. 1 has to be covered by two different methods such as backscattering or spin echo for the slow α-relaxations and time-of-flight for the fast β-relaxations. The von Schweidler parameter *b* which governs the slower α-relaxations of the viscous liquid can be determined quite confidently, whereas the scaling parameter *a* which describes the fast β-relaxations is very sensitive to details of the deconvolution procedure. Partially, this may explain the discrepancy between the set of **measured** parameters *a, b* and their connection via eq. (2).

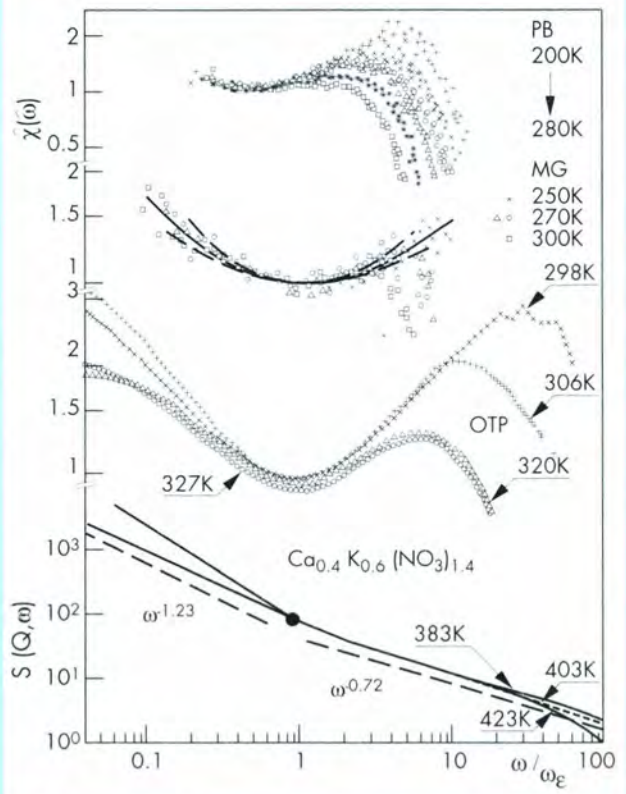

Fig 1. Normalized dynamical susceptibility χ'' of glass formed at $T \geq T_c$. For $Ca_{0.4}K_{0.6}(NO_3)_{1.4}$ the scattering law S(Q,ω) is shown.

2) With increasing temperature the fast and localized motions gain in importance and disintegrate at the critical temperature T_c in long range diffusional motion or structural relaxations. These structural relaxations are expected to show a universal behaviour and to follow the time-temperature shift principle. Fig. 2 shows measurements of the intermediate scattering law S(Q,t) which probes directly the density fluctuations $\phi(Q,t)$. In Fig. 2 relaxations measured at different temperatures above T_c have been normalized to a common master curve by dividing the time scale by a relaxation τ_c which stems from macroscopic viscosity η data

$$\tau c(T) \infty \eta(T)/T \quad (3)$$

The master curves, i.e. the structural relaxations of the different glass formers fit perfectly well to a stretched exponential

$$S(Q,\hat{t}) = A(Q).e^{-(\hat{t}/\tau(Q))^{\beta(Q)}} \simeq f_Q^c - hQ(t/\tau_c)^b \quad (4)$$

which again is a convenient parametrization of the von Schweidler law (right side of eq. (4)) predicted by the mode coupling approach.

3) In the case that the two processes are well separated in time, the long time limit of the β-process is identical to the short time limit of the α-process and can be interpreted as a non-ergodicity parameter, i.e. as a measure of the frozen-in (glass forming) state.

The theory predicts a square root decay down to a constant f_Q^c

$$f_Q(T) = \begin{cases} f_Q^c + h_Q C_o \sqrt{\dfrac{T_c - T}{T_c}} & \text{. weak T-dependence} \\ f_Q^c & \text{. weak T-dependence} \end{cases} \quad (5)$$

Hence $f_Q(T)$ should show a distinct cusp at T_c. The experimental problem is to match the condition of integration over the slow α-relaxations when measuring this quantity. Fig. 3 gives examples, either measured by spin echo or backscattering. There is clear evidence of a discontinuity of $f_Q(T)$ at a $T_c > T_g$, but evidently the anomaly at T_c is smeared out over a certain temperature region.

To summarize, the neutron measurements of the density relaxation in the glassy and viscous state present the picture of a glass transition defined by its dynamical behaviour. At low temperature the glass is frozen-in on a long time scale. As the temperature rises localized and fast relaxations become more and more activated and can be seen as dynamical precursors of the glass transition at

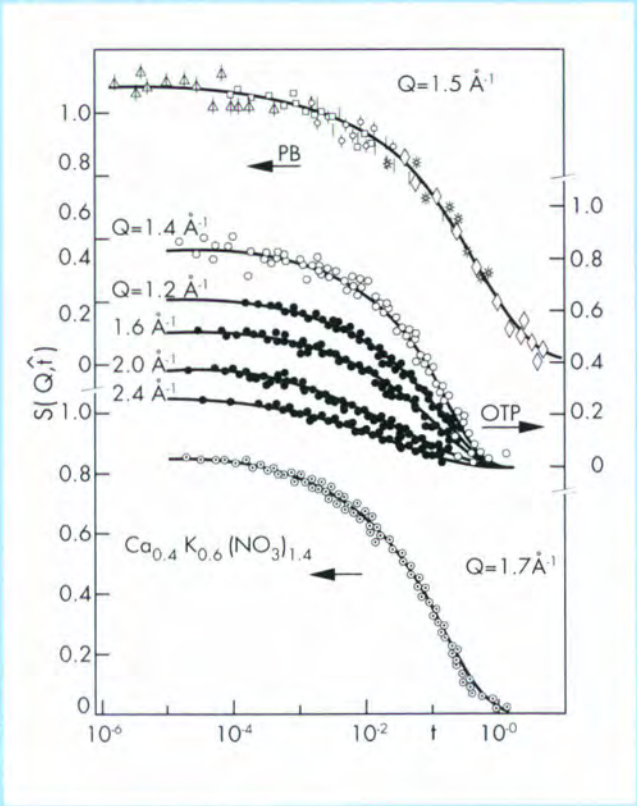

Fig 2. Decay of the density fluctuations $\phi(Q,t)$ in the viscous regime measured via the incoherent (●) and/or coherent (o) intermediate scattering law. Fits by means of a stretched exponential are shown.

Tc where this "rattling in a cage" disintegrates into long range and structural relaxations. Typically T_c lies some tens of a degree above the calorimetric T_g. Scaling predictions of the mode coupling theory for this transition scenario are at least qualitatively confirmed.

Some critical points which need further consideration have to be noted :

- What is the exact scaling parameter a for the fast localized relaxations, i.e. does eq. (2) holds exactly ?

- What is the physical nature of the smearing out of the non-ergodicity parameter at T_c (see also [7]).

- How far strong or network glass formers like Se or silica glass do follow the picture above presented of a glass-liquid transition in simple fragile glass formers (see also [8]).

	T_g(K)	T_c(K)	β at $S(Q)_{max}$	a	b
$Ca_{0.4}K_{0.6}(NO_3)_{1.4}$	333	366(4)	0.58	0.28	0.23
polybutadiene	181	216(5)	0.45(1)	–	0.26(3)
O-terphenyl	243	290	0.61	0.31	0.52(1)
myoglobin	-	195(10)	-	0.33(5)	0.64(1)

Table: Critical temperature T_c, stretched exponential β and scaling parameters *a*, *b* as evaluated from measurements of the density fluctuations in glasses by neutron spectrometry [2-6]. These independently measured quantities fulfill eq. (2) only partially.

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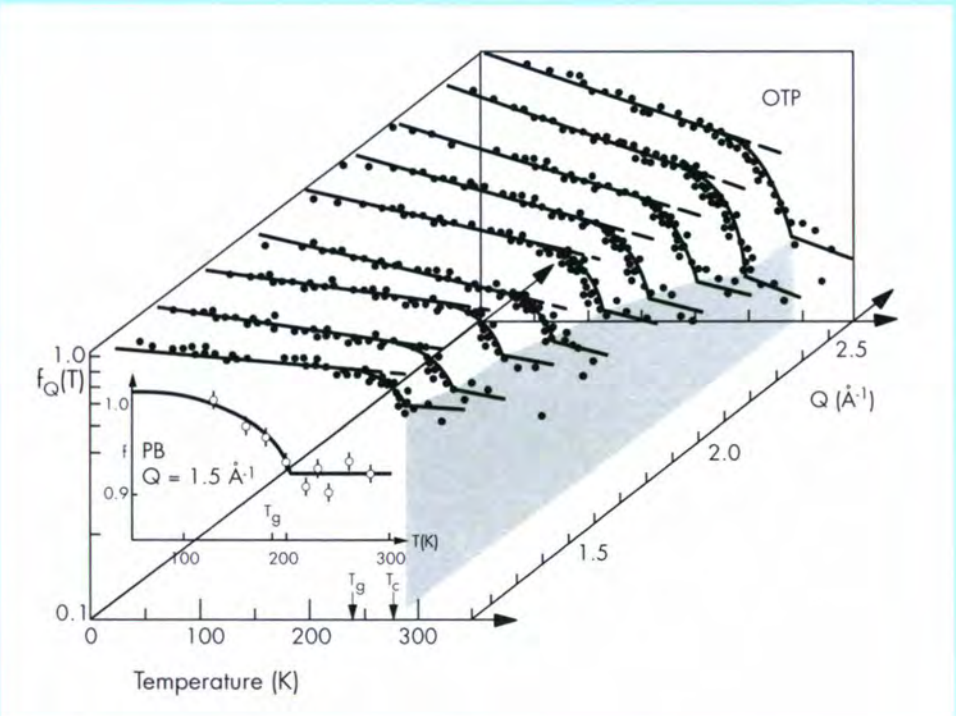

Fig. 3. Structure factor $f_Q(T)$ as a gauge of the frozen-in (glass forming) state.

Biological Structures and Dynamics

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Introduction

The last few years have seen a change in emphasis in biological studies employing neutrons. Part of this is clearly related to the explosive increase in three-dimensional structural information obtained with X-ray crystallography, and the neutrons serve typically as a follow-up, either by solution studies of conformational changes or macromolecular assemblies or by further low-resolution analysis of disorder regions employing single crystals and contrast variation. Dynamical studies of these complex systems also find inspiration in the growing mass of structural information, and although still in their infancy, show promise of rapid progress.

The demand for beam-time has remained constant, and as usual the request for small-angle scattering measurements is high. This created a number of problems during the autumn scientific council due to reduced allocation of beam time on D11, where a replacement of the collimation system is planned for the spring of 1991. When this has been accomplished, the situation should return to a normal large overload. Another instrument in demand is D16, indicating an increased use of neutrons for the study of various aspects of membrane structure.

The college continues to suffer from space problems, partly due to the arrival of new scientists on the second floor of ILL 20, and partly due to the need for shorter term housing of students. At present all offices are full, and the only hope for relief is an extension of the building as found in the proposal for a modernization programme. Fortunately, the high density of personnel in the building as a whole, which for the major part belongs to the EMBL, has only helped to enrich the scientific life. Below are outlined some of the year's main scientific activities of the ILL physicists, their long term visitors and students.

Scientific Trends and Highlights in 1990

Techniques

A scattering experiment in biology often requires considerable sample preparation. At the ILL this has resulted in a growing activity in the field, at present mainly supported by long term visitors (CNRS Grenoble), and an example is the work on the expression of Adenovirus fibre.

The Adenoviruses constitute a family of non-enveloped viruses with icosahedral symmetry. The penetration of the virus into the cell is mediated by an interaction between one of the virus structural proteins, called fibre, and the cell receptor. The fibre is an elongated protein protruding from the 5-fold vertices of the virion. It is trimeric and is organized in the form of a shaft, whose length varies with virus serotype, with a C-terminal knob, interacting with cellular receptors. The purpose of the study is to determine the structure of the fibre and to understand the molecular basis of its interaction with the receptor.

In order to obtain large quantities of the fibre necessary for these studies it was decided to express fibre in the prokaryotic expression system. The proteins of two different serotypes : adenovirus 2 (Ad2) and adenovirus 3 (Ad3) were expressed in *Escherichia coli* as stable insoluble proteins. They were solubilized in 6 M urea and purified on several chromatographic columns with the subsequent slow removal of urea. The final soluble product was studied with biochemical methods such as protein gel analysis, chemical crosslinking, gel filtration, proteolysis as well as biophysical methods such as electron microscopy and small angle neutron scattering.

Both recombinant fibres trimerize spontaneously upon expression. The trimer of Ad2 fibre has, however, a less

compact structure than the native trimeric fibre and has a high propensity for precipitation from solution. On the contrary, Ad3 fibre preparation consists of a population of particles with the characteristic morphology and size of the Ad3 trimeric native fibre. Small angle neutron scattering gives a molecular weight consistent with a trimeric fibre and a radius of gyration consistent with the dimensions derived from electron microscopy (see Fig. 1). Recombinant Ad3 fibre protein will be used for the crystallization assays and for the fibre/cellular receptor interaction studies.

Although small-angle scattering with neutrons is now a well established technique, there are still some very interesting new developments. One of these is the triple isomophous substitution (TIS) method as proposed by Pushchino scientists for the study of complexes in solution. The method has been tested extensively on the *Escherichia coli* EF-Tu complexes (Pushchino USSR, EMBL Grenoble and ILL) and its advantages and limits are now published. Currently, this approach is being applied to the *Escherichia coli* 30S ribosomal subunit (Yale University and ILL).

There is also a continued interest in instrument development in the college. Major constituents of the mechanics of the new small-angle scattering instrument D22 such as collimator, detector tube and protection were installed during the year, and the velocity selector and detector were ordered.

More preliminary work was done on the Quasi-Laue diffractometer, which is part of the proposal for a modernization programme. A considerable effort was invested in the theory of interpretation of spectra by members of the EMBL, who participate in the development of this idea, and simultaneously a small, high resolution position sensitive detector was constructed (collaboration with LAPP, Annecy) to test this in practice.

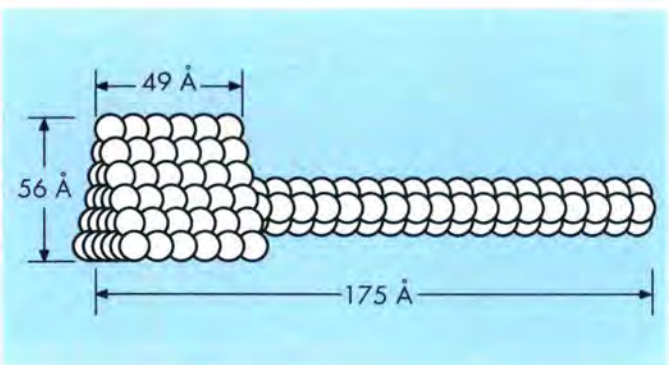

Figure 1. Model of recAd3fib used for calculating the radius of gyration. The model is described by 252 spheres of diameter 10.6 Å. Its dimensions are derived (a) for the head from electron microscopy (56 x 49 Å) and (b) its overall length (175 Å) such as to be compatible with the radius of gyration observed by neutron scattering.

Protein-nucleic interactions and protein synthesis

Two of the reasons why neutrons are so useful for determining biological structures is that first they make it possible to distinguish between the two main components of biological macromolecules, nucleic acids and proteins, and secondly they are sensitive to the deuterium content of both these components, which is easily changed by growing micro-organisms (bacteria, yeast, etc.) in solutions containing heavy water. Several biologically relevant molecules either consist of both chemical classes (such as ribosomes, made of proteins and RNA), or they form complexes containing both (like RNA polymerase (RNAP) together with DNA).

In all living cells the genetic information is contained in DNA, which are long chain molecules usually in the form of 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 blueprints in the form of chains of messenger RNA (mRNA) are produced. This duplication process is catalyzed by the enzyme RNAP which has an elongated triangular shape as determined by neutron small-angle scattering. RNAP, which has a molecular weight of 450 000, consists of relatively large subunits a_2, b, and b', and a factor s which acts only temporarily.

Over a period of several years, the spatial arrangement of RNAP and of its subunits, isolated and in complexes with the A1 promoter, a well-defined DNA fragment, and with the mRNA originating from it, has now been studied *in situ* by neutron small-angle scattering (collaboration between MPI, Martinsried and ILL).

Recently, a DNA fragment was constructed which had a binding site for a repressor molecule on it, and, at a well-defined distance on the opposite side, a promotor, i.e. a binding site for RNAP. (Repressors control the transcription of DNA, i.e. they can switch it on and off). RNAP is asymmetric, and the distance of the centre of gravity to the DNA axis had been determined previously. Therefore, it was possible to find out how the RNAP molecule is oriented with respect to the direction of transcription by determining the distance between the centres-of-gravity of repressor and RNAP, knowing the location of the binding sites of both molecules on the DNA. The distance value of 150 Å which was obtained by neutron scattering is compatible with the larger side of RNAP pointing towards the end of the DNA molecule, like an open pair of scissors (see Fig. 2 page 81).

Finally, 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) from *Escherichia coli* 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).

A long-term project (MPI für Molekulare Genetik, Berlin and the ILL) aims at establishing a three-dimensional map of the components of the 50S subunit in order to contribute to a better understanding of the structure/function relationship. Some of the proteins in the small (30S) subunit (S1 to S21) have been included in the investigation.

The method used consists in incorporating selected pairs of protonated single proteins into "glassy ribosomes", ribosomal particles reconstituted from isolated partially deuterated ribosomal proteins and RNA which are both rendered quasi-invisible for neutrons by a buffer solution with high D_2O content. The small-angle neutron scattering curves from these particles can be interpreted in terms of the distances between the proteins.

The aim of the study is to produce a map of the three-dimensional arrangement of the majority of the 50S proteins on the basis of the table of protein distances. This model is to serve as a scaffold for locating the sites which are important for the function of the ribosome. More than 130 pair-distance measurements in the 50S subunit have been performed to date, some of them repeatedly. A closer inspection of them has revealed so far about 80 distances which can be considered of sufficient quality and internally consistent in the model-building process. The current measurement programme is intended to verify several further distances using samples obtained by an an improved preparation technique. This will improve the interconnectivity of the distance table so that a reliable map of 12 to 13 proteins can be expected soon, followed by a map of about 24 proteins within a few years.

In more recent years single crystals of this protein factory have also been obtained (MPI in Berlin and Hamburg and the Weizmann Institute), and the three-dimensional structure determination of this super-molecule has been started. Several different ribosomal particles have been used, and the one most suitable for neutron diffraction is the 50S subunit from *Halobacterium marismortui*. As a first step low resolution single crystal neutron diffraction experiments are carried out to distinguish between the protein and the RNA domains. The contribution from the different domains can be mapped out by contrast variation. The solvent in the crystal is exchanged with partially deuterated solutions of a scattering power corresponding to different components, and for each contrast a set of diffraction data is measured.

The diffraction measurements have been carried out at the ILL on the biological diffractometer DB21 since 1986. Because of the small size and the variable quality of the crystals these experiments are very time consuming and difficult. So far an almost complete data set in 100 % D_2O solution to 30 Å resolution and an incomplete set in H_2O have been collected.

To extract structural information from these data *ab initio* phasing methods for low resolution data have been developed. They contain 3 steps, namely a normalization procedure of the data followed by direct method phasing and finally a sorting procedure which identify the best density maps among all those generated by direct method analysis. In the case of the 100 % D_2O data a density map coherent with the model obtained by electron microscopy of the ribosome was found, and there might even be more information available as two levels of density were found which can be interpreted as protein and RNA.

The first results are very exciting, but it is obvious that at this stage further confirmation of the validity of this map is urgently needed, so experiments and data treatments are still going strong. In parallel, members of the ILL also collaborate with the ribosome teams in Hamburg and at the Weizmann Institute on the phasing of the X-ray data.

Beyond the transcription of DNA and the protein synthesis other studies related to proteins interacting with DNA/RNA are carried out in the college, and in recent years the recA protein has been a target of much interest. The recA protein of *Escherichia coli* mediates the exchange of homologous strands of DNA, a process of fundamental importance in genetic recombination. The exchange takes place through a stoichiometric binding of recA protein to DNA during which the DNA is stretched by approximately 50 %. A number of different complexes are active in these processes, recA protein with single-stranded DNA, with double stranded DNA and also polymeric forms of the recA protein itself. Moreover the structure of these complexes varies depending on the presence or absence of cofactors such as ATP whose hydrolysis is necessary for the strand exchange reaction to take place.

Neutron small angle scattering studies (Edinburgh, EMBL Grenoble and ILL) have shown that the complexes can be divided into two categories: compact filaments typified by the recA self polymer, and the stretched complex such as observed with single or double-stranded DNA in the presence of $ATP_\gamma S$ (a non-hydrolyzable analogue of ATP). Recently it was shown that the ATPase activity could be induced in the absence of DNA by the presence of high salt concentrations. Small angle scattering results have subsequently shown that this activity is correlated with a structural change analogous to that observed on the addition of DNA, i.e the stretched form can be induced by the presence of salt alone. The conformations of the various complexes are illustrated in Fig. 3. The recent determination of the crystal structure of the recA monomer combined with the neutron scattering results should allow further details of the protein-protein and protein-DNA interactions to be elucidated.

Protein-membrane interactions and hydrophobic proteins.

The solution of the structure of bacteriorhodopsin, the protein that functions as a light driven proton jump in the purple membrane of *Halobacterium halobium*, is a

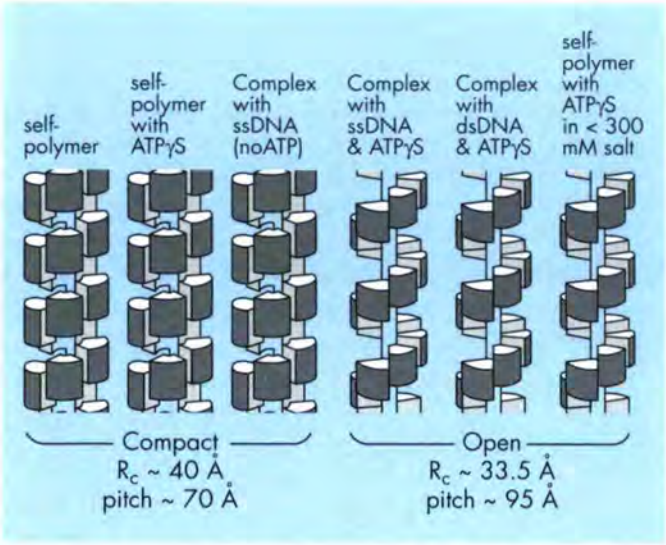

Figure 3. Diagram of the active state and the inactive stage of recA protein as determined by neutron scattering in solution (ss = single stranded, ds = double-stranded).

wonderful example of the complementarity of modern methods in structural molecular biology - in this case low-dose electron microscopy and neutron diffraction on specifically deuterated samples. The main features of the structure are now known, but further neutron diffraction experiments are addressing specific questions concerning functional aspects in native and mutant membranes (IBPC Paris, MRC Cambridge, Freie Universität Berlin, MPI Martinsried, CNRS Grenoble, University of Barcelona and ILL). Inelastic neutron scattering studies of the membrane dynamics in different conditions have shown interesting correlations between the mean square amplitudes of the motions and the functional behaviour of the protein.

Two different classes of membrane proteins have been crystallized over the last few years. The first structure to be solved by X-ray crystallography was that of the photosynthetic reaction centre from the purple bacterium *Rhodopseudomonas viridis*, the trans-membrane part of which was composed largely of a-helices. Recently the X-ray structure of Porin from the bacterium *Rhodobacter capsulatus*, has been determined, revealing a completely different secondary structure composed mainly of b-sheet. Porin is a protein which allows the selective passage of polar molecules up to a cut-off value of molecular weight about 600.

In all cases these membrane proteins have been crystalized by "classical" techniques after solubilisation in detergent. The detergent 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. Neutron diffraction, where there is very high contrast between D_2O and detergent, has already allowed an investigation of the detergent organization in the reaction centre crystals (Munich and ILL; see Annual report 1989). A study has now been undertaken on the crystals of Porin (Freiburg and ILL) to locate the detergent in these crystals. The crystals diffract neutrons strongly to ~12Å resolution and should soon provide clues to the detergent-protein interactions in this system.

Protein-lipid interactions are important in membranes and also in the soluble lipoproteins found in the serum as transport proteins or in eggs as storage proteins. Lipovitellin is a storage protein found in a number of vertebrates and has some genetic similarity to serum lipoproteins such as human apolipoprotein B-100 which is found in low density lipoprotein particles (LDL). The X-ray analysis of the protein/lipid complex, isolated from oocytes of the lamprey, revealed a complex structure of supercoiled α-helices and a series of β-sheet structures surrounding a cavity in the molecule, but no electron density attributable to lipid. Neutron diffraction studies on these crystals (Minneapolis and ILL) have demonstrated that the lipid is in fact located in the cavity region. The recently determined amino acid sequence of the protein will soon allow a detailed analysis of the protein-lipid interactions to be made.

In collaboration with long term visitors from the CNRS and Université Joseph Fourier, Grenoble, a study has also been undertaken on hydrophobic interactions involving small proteins from plants. The ultimate goal is to learn more about the interactions between the hydrophobic part of the protein and the surrounding water, a subject that is well suited for neutron diffraction. The first protein chosen for this study is from soy-bean. It has a molecular weight of 8300 and crystallizes well. The action of the protein, which is found in the surface of the grain, is not yet known, but studies of proteins of this kind (collaboration with INRA, Nantes) indicate that it might be part of the defence system of the grain. Further interest in this protein derives from the fact that it is member of a newly observed group of proteins with a common, characteristic core of four sulphur bridges, which exhibit a number of different functions.

As the structure of the hydrophobic protein from soy-bean is not known, a structure analysis was undertaken, and during the year the necessary X-ray work was carried out involving determination of some heavy atom derivatives. This exercise has now given an electron density map, which is presently being interpreted, and work has been undertaken to produce crystals large enough for neutron diffraction. At the same time a continuation has been started involving a crystallization effort of other similar proteins.

Protein-protein interactions and muscle structure

It is well known that small angle neutron scattering is a powerful technique for the study of interactions in solution between macromolecules of different scattering density - such as nucleic acid-protein complexes, protein-detergent

complexes or complexes with specifically deuterated components. This was discussed above in some detail. But neutrons also have valuable advantages for the characterisation of interactions between macromolecules and solvent molecules, and between macromolecules of similar scattering density as in protein-protein complexes. It is very useful to study such interactions as a function of solution conditions and, by using neutron radiation, widely different conditions (obtained by varying temperature, salt concentration, pH etc.) are easily examined while maintaining a good signal to noise ratio.

Solvent interactions play an important role in protein folding and the particle formed by a protein and associated solvent molecules has been named its "solution particle". Proteins from halophilic bacteria have extensive solvent interactions and are only stable in highly concentrated salt solutions. They are useful models for the study of the correlation between stability and the structure of solution particles (CNRS Grenoble, Weizmann Institute and Tel Aviv University, BARC and ILL).

Denaturants such as guanidinium hydrochloride have been used for decades in protein folding studies, but their mechanism of action remains poorly understood. In neutron scattering experiments on hen egg-white lysozyme, it has been possible to follow simultaneously and quantitatively the interaction of the denaturant with the protein and its unfolding. This provided data for testing different mechanistic models of unfolding by the action of denaturants (University of Oregon, CNRS Grenoble and ILL).

Protein-protein interactions are of great importance in a number of biological processes, and are themselves very sensitive to solution conditions. Examples of protein-protein interactions on which neutron scattering experiments have been performed this past year include muscle structure, the complement cascade in the immune system, and the histone core particle in nucleosomes.

Nucleosomes, the fundamental units of chromatin, are made up of a histone octamer core and DNA. Novel histone octamers, in which the "unstructured" N-termini of the native proteins were removed by selective proteolysis with clostripain, have been characterised and they appear to be very good models for the protein-protein interactions in the native nucleosome core (CNRS Montpellier and ILL). The complement cascade involves a large number of protein-protein interactions, a few of which have been described structurally in solution (CEN-Grenoble, University of Florida and ILL).

Thin filaments of vertebrate muscle consist of polymerized helical filaments of actin (F-actin) around which is wound two strands of the filamentous protein tropomyosin. Conflicting models exist to explain the switching mechanism which is activated by binding of Ca^{2+} ions to a third protein called troponin. In one case a large radial movement of the tropomyosin is predicted whereas in the other case the switching is explained by an azimuthal movement of the tropomyosin. Preliminary small angle scattering experiments have been carried out (San Francisco and ILL) using thin filaments reconstituted from hydrogenated actin and fully deuterated tropomyosin to try and distinguish between the two models. Measurements in 41% D_2O, where the actin is invisible, permitted the measurement of the cross-helix separation of the two deuterated tropomyosin strands and suggest that the radial separation changes rather little between the resting and active states.

Secretary: M.S. Lehmann

Molecular Spectroscopy, Surfaces and Mesophases

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Summary

The number of proposals submitted to College 9a has declined over the last year. This is, in large measure, due to the large number of neutron reflectivity experiments that are now being considered in other subcommittees, rather than being indicative of a general trend. It should be noted, however, that the number of proposals relating to problems concerning mainstream chemistry was small. This reflects the diversity of other topics studied within the College, ranging from surface studies to molecular spectroscopy, from intercalation systems to electron transfer (to mention only a few), with quasielastic scattering, inelastic scattering, powder diffraction, and small angle scattering being amongst the experimental probes employed. Here we highlight some of the advances made in the last year in the area of chemistry, spectroscopy and surfaces.

Scientific Highlights in 1990

Inclusion compounds

Zeolites are well known as one of the most important classes of industrial catalyst, but because it is so difficult to study the dynamics of molecules within zeolites using optical spectroscopic techniques, relatively little is understood about their catalytic activity. Klinowski (Cambridge) proposed recently that shape selectivity is a key factor in determining the products of processes such as the catalytic conversion of methanol to higher hydrocarbons. Preliminary experiments on the instrument IN5 on xylenes (1,2-1,3-or 1,4-dimethylbenzenes) contained at low concentration within the zeolite (ZSM-5), seem to bare out this theory. For example, quasielastic scattering at high temperature indicates a larger dynamic motion for para-xylene (1,4-dimethylbenzene), than for ortho-xylene. This is in agreement with steric considerations which suggest that ortho-xylene cannot pass along the zeolite channels, whereas the meta and para analogues are not so strongly constrained. At low temperature, the very weak host - guest molecular interaction is confirmed for para-xylene by a distribution of tunnelling levels below about 0.3 meV. As tunnelling is very sensitive to small changes in the potential, it could prove a good probe for the host-guest interactions within systems of industrial importance.

Another system which initially attracted the attention of two groups working independently ((Boysen, Frey (Munich), Blank and Kearley (ILL); and Guillaume, Sourisseau (Bordeaux) and Dianoux (ILL)) and more recently working together as a rare German, French, British collaboration) are urea-paraffin inclusion compounds. Urea has straight hexagonal channels which can isolate alkane chains in their all-trans conformation, providing a model for more complicated hydrocarbon systems of scientific and technological importance. These semi-oriented urea chlatrate inclusion compounds have been studied intensively by vibrational spectroscopy. This is because of the "insulated" environment of the alkane, and because of a motional broadening found in the antisymmetric C-H stretching modes. Whole body librational motions of the alkane seem to be responsible for these broadening effects. Although these compounds have come to be regarded as one of the best systems for testing band broadening theories, studies via Raman peak widths tend to be complicated because both the internal mode force constants and bond polarizabilities vary with the torsional angle of the alkane molecule within its cage. Studies by inelastic neutron scattering have been made on hexadecane, nonadecane and dodecane in deuterated urea and peaks due to large amplitude vibrations have been seen at energies of the order of 1 meV. By using semi-oriented samples at appropriate sample orientations, the motions parallel or perpendicular to the main chain axes can be analyzed. For example, for the urea/dodecane system with the long axis either transverse or longitudinal to Q, these peaks dominate in the longitudinal direction (Fig. 1). This resolves the long standing problem as to whether these peaks are translational or rotational in origin. (In this case we can say that they are translational).

Molecular dynamics of benzene: hexafluorobenzene (update)

Investigations on IN4, IN5, IN6 and IN13 of the temperature dependence of the quasielastic and inelastic scattering of the van der Waals solid Benzene: Hexafluorobenzene, have showed that in the lowest temperature phase of this solid the molecules are able, if they have sufficient thermal energy, to undergo a six-fold reorientational motion (Fig. 2). These quasielastic measurements have given the height of the barrier to reorientation to be 98 ± 5 meV per molecule. This is quite a deep potential and is capable of supporting a number of bound levels, to which and from which it is possible, with the indiscriminate selection rules of inelastic scattering, to observe discrete transitions.

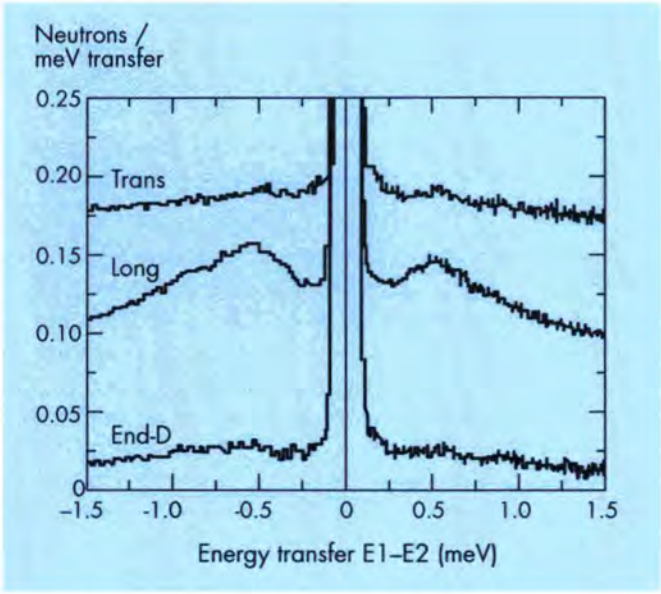

Fig. 1: Dodecane in urea (measurements recorded on IN5).

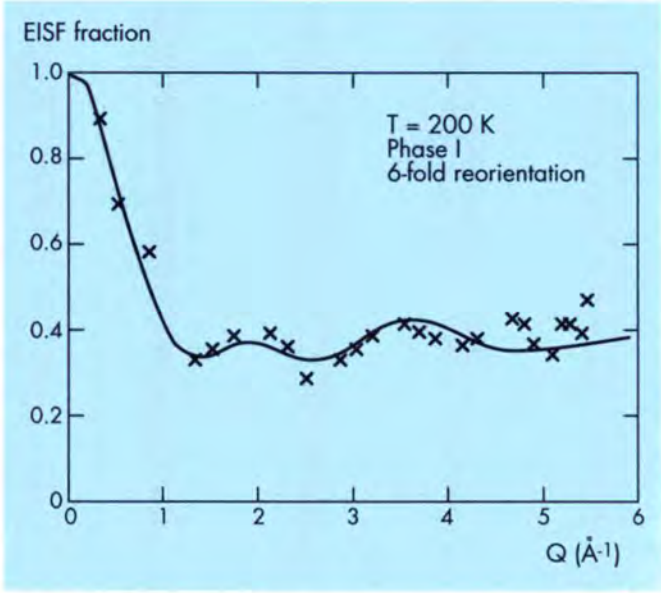

Fig. 2: EISF of benzene: hexafluorobenzene, recorded on IN13 and fitted to a six-fold reorientational jump model.

A harmonic analysis of the inelastic spectra recorded at successively higher temperatures reveals that the spacing between the benzene and hexafluorobenzene rings in a dimer and the spacing between such dimers changes continuously. Indeed, we go from a situation of distinct individual dimers at low temperature to one of equidistant molecules at a temperature corresponding to the first phase transition seen in this material. A picture of quadrupole induced dipole moments has been suggested as the driving force for the change in molecular spacings. At low temperature each dimer has an induced dipole moment whose mutual interactions contribute to the lattice energy. As the molecules become equidistant (loss of dimer character), these induced dipole moments vanish with a consequent reduction in the strength of the intermolecular potential.

Depth controlled grazing angle neutron diffraction - a promising technique for sub-surface studies

Physisorbed and chemisorbed species on substrates such as graphite continue to attract attention within College 9a and early successes of the study of neutron reflection profiles from solid-liquid interfaces (see last year's annual report) have made this a well established and important technique. A new instrument, dedicated to depth-controlled grazing angle scattering experiments promises to augment these existing techniques, and make significant contributions to the study of surface magnetism. Until recently, the experimental determination of structural properties across an interface has been almost exclusively attacked by X-rays, mainly because of the availability of brilliant synchrotron sources. Neutron scattering under the condition of total external reflection does have advantages over X-rays mainly because the magnetic photon cross-section is extremely low. Thus the evanescent neutron scattering technique, as it is called, promises to be highly competitive in this area.

The scattering geometry of the evanescent wave diffractometer involves neutrons glancing on the sample surface at an angle α_i of about 5 mrad, such that the majority are specular reflected. A small part of the evanescent wave field inside the crystal sample is Bragg scattered and a detailed scattering profile along the grazing exit angle α_f is recorded by a position sensitive detector (see Fig. 2 of

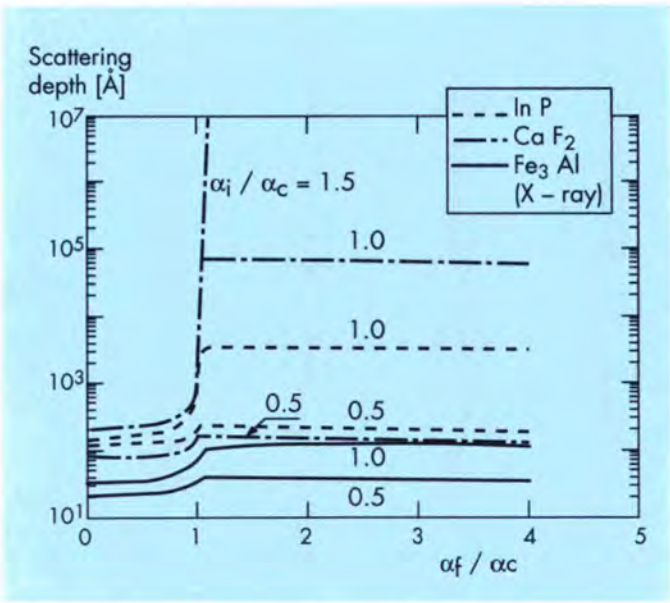

Fig. 3a: Calculated scattering depth profiles as a function of the exit angle for various incident angles and samples (α_c = critical angle).

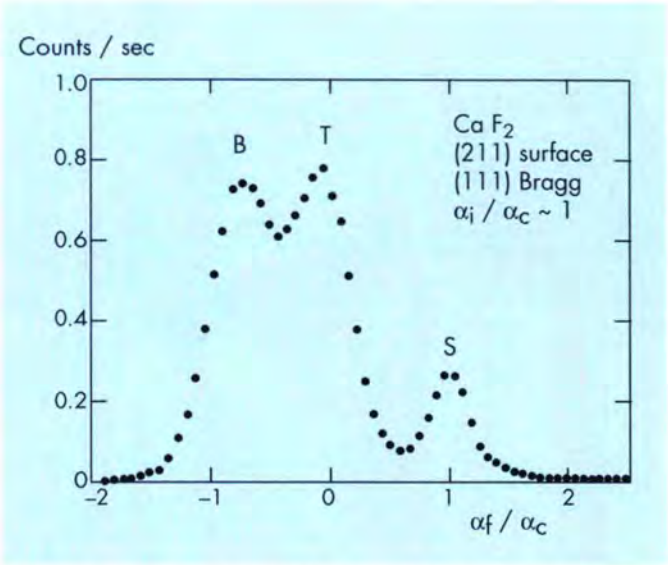

Fig. 3b: α_f-profile of the (111) Bragg reflection from a CaF_2 (211) surface observed under grazing incidence angle of $\alpha_i/\alpha_c \approx 1$.

Instrument Group "Special Instruments"). The first experiments carried out with this set up on the instrument EVA have yielded information at scattering depths between 100 Å and macroscopic lengths, depending on the system studied and the exact scattering geometry used (Fig. 3a). This technique allows structural information to be obtained at sub-surface crystal layers. The α_f profile from CaF_2 (Fig. 3b) was obtained for an incident angle of $\alpha_i = \alpha_c$ (the angle of critical reflection), and shows three different contributions: the expected pure surface peak at $\alpha_f = \alpha_c$ (marked "S" in the figure), the diffracted peak at $\alpha_f = 0$ (peak "T", (111) reflection, corresponding to a scattering depth of about 100 Å), and also a contamination from bulk scattering from the sample (peak "B").

One other experiment worth mentioning here (and to be performed in 1991) concerns molecular beam epitaxy which is to be used to deposit $Ga_{(1-x)}Al_{(x)}As$ layer by layer on GaAs, with x varying from layer to layer so that the index varies in a controlled manner perpendicular to the layers. In this way the theoretical prediction of a singularity in the neutron reflection coefficient in layer systems of this type at the critical angle, α_c, will be tested.

Secretary: R. White

Neutron rotational tunnelling spectroscopy as a probe of the electronic details of a novel chemical bond

J. Eckert, G.J. Kubas and R. White

The observation that some metal complexes bind hydrogen in molecular form was one of the past decade's most significant fundamental discoveries in inorganic chemistry [1]. Not only do these molecular hydrogen complexes contain an entirely new chemical bond, namely the first stable intermolecular coordination of a σ bond, they may also be viewed as arrested reaction intermediates in the oxidative addition of hydrogen to the metal. Significant activation of the H-H bond is indicated by a drastically lowered H-H stretching frequency for these compounds (around 2700 cm^{-1}, as opposed to 4400 cm^{-1} for free H_2) and a concomitant lengthening of the H-H bond from 0.74 Å to typically 0.82 Å (determined by neutron diffraction). These observations lead to the hope that one may be able to follow this reaction coordinate by synthesizing various complexes with different degrees of H-H bond activation. In order to be able to do this the factors that govern the binding of the molecular hydrogen ligand (referred to as "dihydrogen") must be understood. It is therefore highly desirable to have a probe of the electronic details of the dihydrogen-metal bond. We have achieved this by relating rotational barriers for the dihydrogen ligand measured with neutron scattering techniques to appropriate theoretical calculations for an increasing number of these compounds where either the metal centre or the other ligands on the metal are varied.

Dihydrogen binding to the metal

The manner in which the molecular hydrogen ligand binds to the metal (Fig. 4) is thought to be analogous to olefin binding: electrons from the bonding σ orbital of the hydrogen molecule are donated to an unoccupied symmetric hybrid orbital on the metal. This is accompanied by "backdonation" of electrons from metal orbitals to the antibonding σ* orbital of H_2. In both cases the H-H bond is weakened while the H-M interaction is strengthened. The factors that govern these electron flows are the electronic state of the metal itself and the influence of the other ligands of the metal on the state of the former. While the former interaction does not give the metal-dihydrogen bond a directional property (for rotation about the M-H_2 axis), the backdonation from an antisymmetric orbital on the metal into the σ* orbital does. Thus the rotational barrier for the dihydrogen ligand may be expected to be sensitive to the latter electronic interaction.

One would not normally expect neutron scattering techniques to be able to probe these details directly or

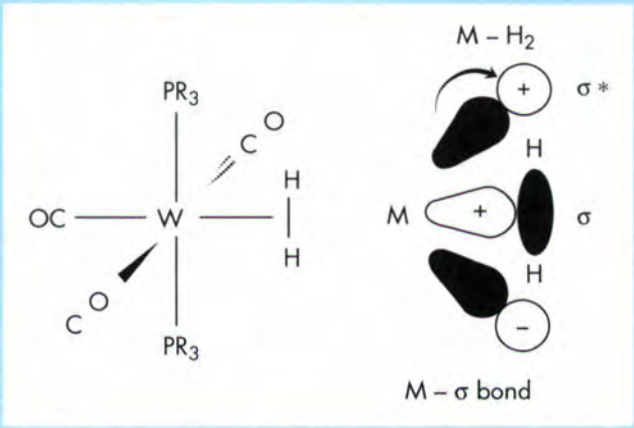

Fig. 4 Dihydrogen binding to the metal.

with great sensitivity. However, the fact that the interaction between H_2 and the metal is relatively weak, and that the rotational constant, B, of H_2 is very large (about 7.4 meV or 60 cm^{-1}) combine to make rotational tunnelling spectroscopy (along with measurements of the torsional transitions) by neutron scattering an effective probe of the electronic details of this novel chemical bond.

Contributions to the barrier for dihydrogen rotation

Inelastic neutron scattering experiments have been carried out at the ILL (IN5 and IN6) and at LANSCE, Los Alamos National Laboratory (FDS), to obtain the rotational energy levels of the dihydrogen ligand. The results can be interpreted in the simplest terms, namely planar reorientation in a potential of predominantly two-fold symmetry. Barrier heights for this rotation may thereby be derived [2]. At this point one must attempt to determine if this barrier has its origin mainly in the electronic interactions, or if non-bonded interactions (e.g. van der Waals forces) between the H_2 ligand and the other atoms play a significant role as well. In an earlier set of experiments we obtained rotational tunnelling spectra on three of the original Kubas complexes. They are of the form $M(CO)_3(\eta^2\text{-}H_2)(PR_3)_2$ (Fig. 5), where M = W, Mo and R = Cy (cyclohexyl), i-Pr (isopropyl). These measurements demonstrated that the barrier to dihydrogen rotation is largely determined by the direct electronic interaction between the hydrogen molecule and the metal: the measured rotational tunnel splitting changed by a factor of three when exchanging Mo with W, but only by some 20 % on replacement of PCy_3 with $P(i\text{-}Pr)_3$. This conclusion was strongly supported by sophisticated theoretical calculations (ab-initio, Fenske-Hall), which reproduce both the trends and the magnitudes of the observed barriers remarkably well. Another type of calculation (molecular mechanics) that

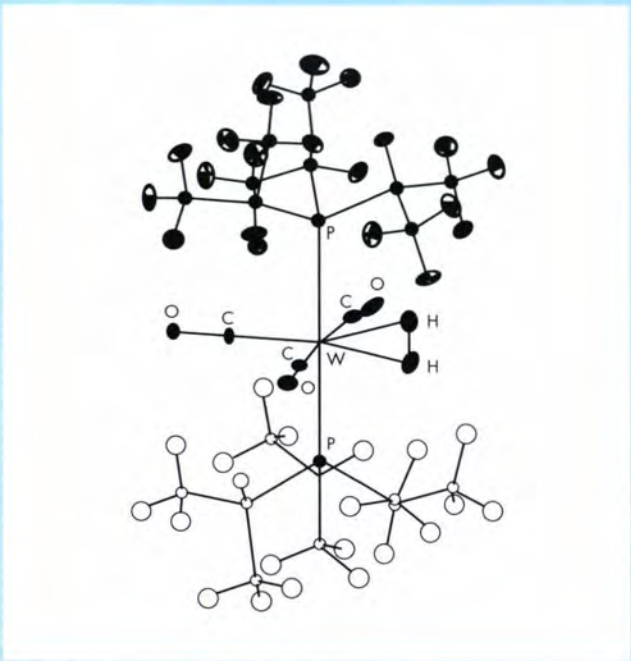

Fig. 5 Neutron structure of $W(CO)_3(P\text{-}(iPr)_3)_2(H_2)$ at 30 K.
H-H = 0.82(1) W-P = 2.491(5) W-C= 1.954(5) (trans)
W-H = 1.89(1) W-P = 2.500(5) W-C = 2.010(5) (cis)
W-C = 1.997(5) (cis)

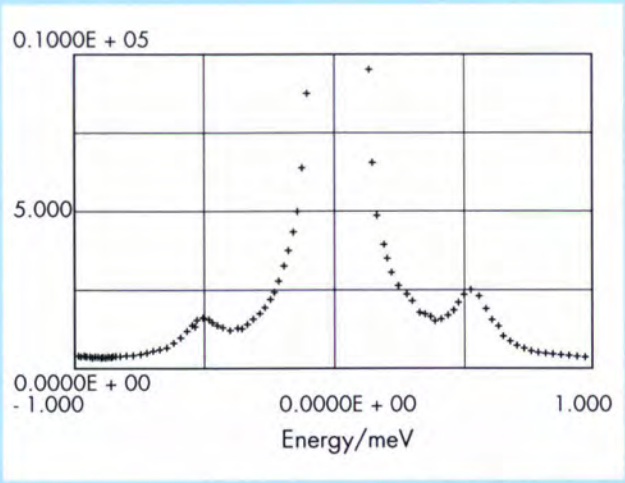

Fig. 6 Measurement of the transition metal-dihydrogen complex $Cr(CO)_3(H_2)(PCy_3)_2$ at 5 K.

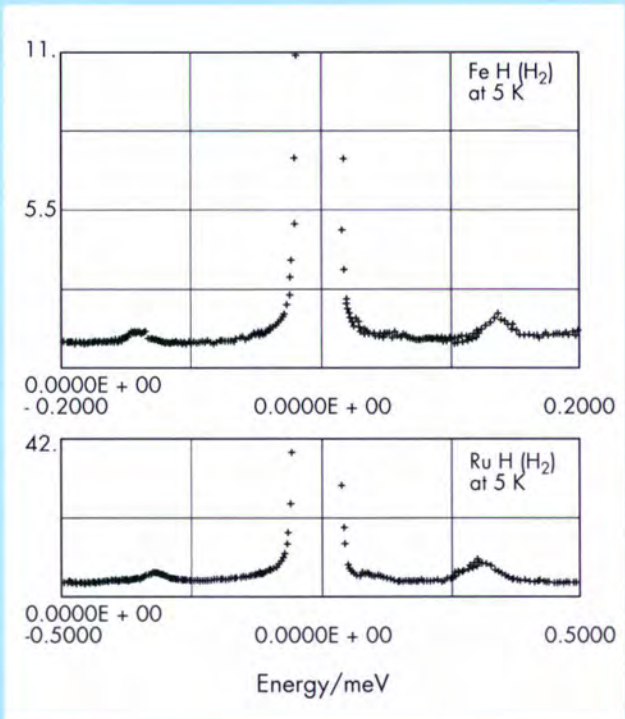

Fig. 7 Measurements of two complexes $[FeH(H_2)(PPh_3)]BPh_4$ and $[RuH(H_2)(PPh_3)]BPh_4$ recorded on IN5.

treats primarily non-bonded interactions was found, on the other hand, to drastically overestimate the effect of changing the phosphine ligands on the barrier to dihydrogen rotation.

Factors in stable dihydrogen binding

We have recently collected data (Fig. 6) on the missing member of the column of transition metal dihydrogen complexes, namely $Cr(CO)_3(\eta^2\text{-}H_2)(PCy_3)_2$. This complex is known to be the least stable of the three (Cr, Mo, W). Unlike the other two complexes it looses H_2 instantly when in solution at 1 atm of H_2 pressure (stable under about 20 atm of H_2), but can be isolated in the solid state. Accordingly, the Cr complex was found to have the lowest barrier to dihydrogen rotation among the three (tunnel splitting of 530 μeV, vs. 330 μeV for the Mo and 110 μeV for the W compounds). This observation is in agreement with the known trend of metal-ligand bond strength down a column in the periodic table.

In another set of recent experiments (IN5, shown in Fig. 7) for two complexes of the form $[MH(\eta^2\text{-}H_2)(PPh_3)]BPh_4$, where M = Fe, Ru, the observed rotational tunnel splittings (142 μeV for Fe, 330 μeV for Ru) suggest the opposite ordering in metal-hydrogen interaction in this column of the periodic table. This observation is, however, in agreement with a similar one by Morris and collaborators based on NMR studies in solution of the exchange between the dihydrogen and trans-hydride ligands [4]. They also found that the Os analogue has the strongest metal-hydrogen interaction in this column. The latter observation is in accord with our results for the W, Mo, Cr group and the general notion that the third-row transition metals are the best π-donors, and do therefore interact most strongly with the σ*

orbital of H_2. This, of course, frequently leads to heterolytic cleavage of the H-H bond, as is the case for most Re-complexes, for example. Our experimental observation that the Ru complexes interact less strongly with the dihydrogen ligand than their Fe analogues can similarly be attributed to the Fe unexpectedly being a better back-donor than Ru in these cases. The electronic reason for this is not understood, and further investigations to this end are needed.

Similar considerations apply to the effect of the other ligands of the metal on dihydrogen binding. Ligands that are very electron rich lead to more backdonation from the metal, and stronger H_2 binding. This can, of course, also lead to H-H bond cleavage and dihydride binding. We have, for example, studied two Mo-complexes, $Mo(CO)_3(\eta^2\text{-}H_2)(PCy_3)_2$ and $Mo(CO)(\eta^2\text{-}H_2)(dppe)_2$, and found a much higher barrier to rotation (i.e. stronger M-H interaction) for the latter. Two factors are likely to be responsible for this: first, the carbonyl ligands are good π-acceptors, and therefore reduce the degree of backbonding in the former compound. Second, the additional phosphines in the latter complex increase the degree of backbonding (M-H interaction), but not quite to the point of breaking the H-H bond.

Weakly bound dihydrogen ligands and the H-H stretch

Among the molecular hydrogen complexes we have examined with neutron scattering techniques the compound $FeH_2(\eta^2\text{-}H_2)(PEtPh_2)_3$ has the largest rotational tunnel splitting (about 800 μeV) [5]. This would suggest that the H-H bond is less activated in this complex than in the others. On the other hand, it is also known to have a very low ν(HH) of approximately 2400 cm^{-1}. Furthermore, an IR study [6] of dihydrogen complexes of the same W, Mo, Cr group with CO ligands only (i.e. $M(CO)_5(\eta^2\text{-}H_2)$), that are stable only at low temperatures in rare gas matrices, found H-H stretching frequencies which indicate a different order of H-H bond activation from what we inferred in the same series (with different ligands) from the rotational tunnelling measurements. Furthermore, a recently discovered, very labile V-dihydrogen complex (in rare gas matrix) was also found to have a surprisingly low ν(HH) [7]. These apparently contradictory observations seem to suggest that the H-H stretch is not simply a measure of the degree of backdonation since σ donation will also weaken the H-H bond. The barrier to dihydrogen rotation, on the other hand, would seem to primarily reflect the former, as rotation about the σ(H2)-to-metal alone would not give rise to such a barrier. These considerations would then lead to the conclusion that the balance between σ donation and π-σ^* backdonation for achieving dihydrogen coordination may vary, or, to put it in other words, there may be different paths towards oxidative addition of hydrogen to the metal.

Much work remains to be done on these systems before the details of this novel and very fundamental chemical bond are fully understood. Nonetheless, even at the present stage it must be considered truly remarkable to what level of detail of this bond inelastic neutron scattering studies have been able to provide some insight.

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Large Molecules

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Scientific Highlights in 1990

Surfactant organogels

Thermotropism and gelation: case of a binuclear copper complex in cyclohexane

A binuclear copper(II) complex of a ramified C8 fatty acid $Cu_2(O_2C_8H_{15})_4$ exhibits both liquid crystalline thermotropism and gelation ability of some apolar organic solvents. The thermotropism is that of a discotic phase (hexagonal array of linearly stacked molecules). In previous studies on surfactant organogels (hydroxystearic acid: see Annual Report 89 and on a steroid/cyclohexane system: see Annual report 88), this situation has also been noticed. With this new organometallic gelator we want to detail the structural connections between the aggregates of the thermo reversible gels and the former discotic state.

Numerous techniques have been devoted to the study of the liquid-crystalline state. Incoherent quasielastic neutron scattering (IQNS using the high resolution backscattering spectrometer IN10, see Annual Report 1989) has detailed the motions of the outlying alkyl chains along the directions of the columns in fibres of a laurate derivative. Concerning the aggregation and gelation processes, we observe that these alkyl chains (length, ramification) play a fundamental role (obtaining or not of aggregates and/or gel phases, their stability). We are studying the small angle neutron scattering (D16, D17, D11 spectrometers) of various systems (solutions and gels) of the bicopper complexes of fatty acids. A typical rod-like, behaviour (without detailing the flexibility and finite length effects) has been observed. The corresponding radii of gyration are comparable to the intercolumnar spacings in the related liquid crystalline state. Without prejudging the cross-section size and shape, this suggests that the mechanism of molecular association in the gel phase could be an electronic superexchange between the oxygen atoms of the carboxylate groups of one molecule and the free octahedral sites on the copper ions in neighboring molecules as it is for the liquid-crystalline phase. The exhaustive data treatment is in progress but these preliminary results indicate a strong correlation between the structural features of the thermotropic and gel phases (ILL, CEN-Grenoble, ULP Strasbourg) .

Polymerlike reverse micelles

In contrast to aqueous micellar systems, reverse micelles at moderately high values of surfactant concentration and molar ratio of water to surfactant, w_o, are generally believed to have a droplet-like structure. However, we recently discovered the formation of gel-like, viscoelastic reverse micellar solutions in the system lecithin/organic solvent/water. Their unusual polymerlike properties were explained with a water-induced one-dimensional micellar growth into very long and flexible cylindrical reverse micelles. At low values of w_o, the micelles are small and the solutions have static and dynamic properties which are typical for classical micellar or colloidal solutions. At high values of w_o, the micellar size can be extremely large, and the micelles have polymer-like properties. We thus have a unique system which shows a characteristic sphere-to-rod transition normally observed in aqueous solutions only.

A first series of SANS experiments on D11 with lecithin/cyclohexane reverse micellar solutions at $w_o = 4.0$ and $w_o = 8.0$ supported our model and gave excellent agreement with the light scattering results. We were able to obtain very interesting results both for the local cylindrical structure and the micellar flexibility. The light and neutron scattering data were consistent with the presence of flexible cylindrical reverse micelles in solution of lecithin and cyclohexane. Due to the fact that it was possible to work at very low volume fractions even for values of $w_o = 8.0$ close to w_o, max, where the micellar contour length is extremely large, we were able to study overall size, flexibility and local micellar structure within the Q-range accessible to light and neutron scattering. For $Q < 0.025$ nm^{-1} the scattered intensity I(Q) is dominated by the finite overall length of the particles, and we were thus able to determine the radius of gyration R_g of the micelles. For 0.035 nm$^{-1} < Q < 0.14$ nm^{-1}, a Q^{-2} decay could be observed for I(Q), which permitted a characterization of the micellar flexibility. At large Q values ($Q > 0.15$ nm^{-1}), I(Q) is controlled by distances over which the reverse micelles are rod-like rather than flexible coils and the asymptotic Q^{-1} limit is recovered, from which the local cylindrical structure was investigated.

The results from scattering experiments with lecithin/cyclohexane solutions thus permitted us for the first time to study directly individual structural properties of the reverse micelles present in these solutions, and we confirmed the postulated model of flexible rodlike aggregates.

(Zürich CH, University of Tennessee USA, Rutherford Appleton Laboratory UK, ILL F).

Comparison between static and hydrodynamic lengths in polymer solutions: effect of cross links

Measurements on polydimethyl siloxane/toluene with D11 showed that the static correlation length ξ is longer in the fully swollen gel than in solution (Figs. 1 and 2). The gel

spectra display a static large-scale structure plus a solution-like component. The intensity of the later is in agreement with the macroscopic swelling pressure of the gels (Macromolecules, in press).

A corresponding comparison was performed on IN11 with two incident wavelengths, 8.7 and 5.7 Å, and scattering angles in the ranges 2° to 13°, and 8.5° to 19° respectively. For the collective diffusion mode ($Q\zeta<1$) the diffusion coefficient D_C in the gel is smaller by about 30 % than in the solution (Fig. 3); in the universal Zimm region ($Q\zeta>1$) the two relaxation rates become indistinguishable. These results are consistent with static observations both of osmotic swelling pressure and of the correlation length shown in Fig. 2 (University J. Fourier, Grenoble, ILL, ELTE Budapest).

Polymer reptation

Recently new experimental results (PRL 64 1389 (1990) Richter et al.) have shown clear experimental evidence for deviation from the Rouse scaling in polymer melts, where the intermediate scattering function $I(q,t)/I(q,0) = f_r(x) \cdot f_r(x)$ being a universal function of a single parameter $x = \sqrt{W_0^4 q^4 t}$. This deviation from scaling supported the de Gennes reptation concept, where with the appearance of an intermediate length scale (the tube diameter d_t) the scaling breaks down.

We tried to get more insight into the origin of this intermediate length scale by measuring:

1. The temperature dependence of d_t applying Neutron Spin Echo spectroscopy.

2. R_G by SANS.

3. G°, the plateau modulus by rheological measurements.

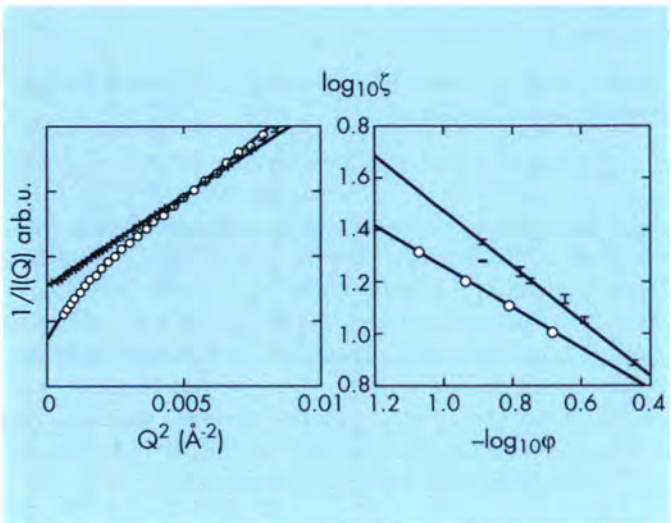
Surprinsingly d_t showed a much greater temperature dependence than any of the other parameters (Fig. 1). According to the Doi-Edwards theory of viscoelasticity d, $G° / c_\infty \rho T$ should be temperature independent. Instead we find a high temperature dependence for T<500K and it seems to become constant only above this, where both d_t and G° become independent of T (Exxon, Jülich, ILL) (see Fig. 4).

Stiff polymers

Mixtures of stiff and flexible polymers exhibit a very high resistance to mechanical, thermal and chemical stress. An example of this behaviour is Polyetherketones (PEK) blended with other polymers. Because of the poor solubility of the stiff components their characterization is very difficult.

Recently we were able to investigate the chain conformation of a Polyetherketone by means of small angle neutron scattering (SANS). We prepared deuterated species of PEKEKK, a linear polymer which consists of phenylene units linked by ether and ketone groups. SANS experiments were done with blends of protonated and deuterated polymer at D11 and D17. The covered Q-range was $0.006 < Q / Å^{-1} < 0.3$ at a wavelength of 10 Å. Fig. 5 shows the (absolute) scattering curve of PEKEKK in the Kratky representation and the scattering function of Yamakawa fitted to the data. Following this first analysis, PEKEKK may be described as a persistence chain with a statistical chain element b of about 30 Å. Compared with PMMA for example (b = 13 Å), the stiffness of the main chain is increased. (Mainz, ILL).

Secretary: B. Farago



Figs. 1 and 2. Zimm plott and concentration dependence of the static correlation length of the fully swollen PDMS gel (dotted line) and solution (full line).

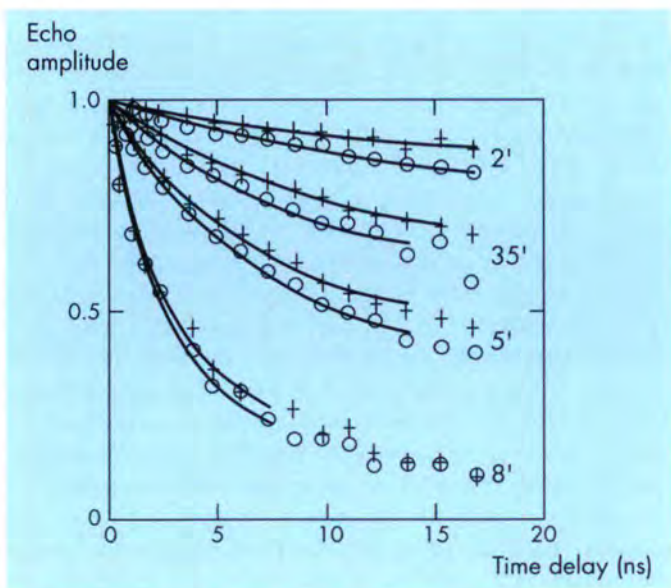


Fig. 3. The intermediate correlation function in the small q region of the gel (open symbols) and of the solution (crosses).

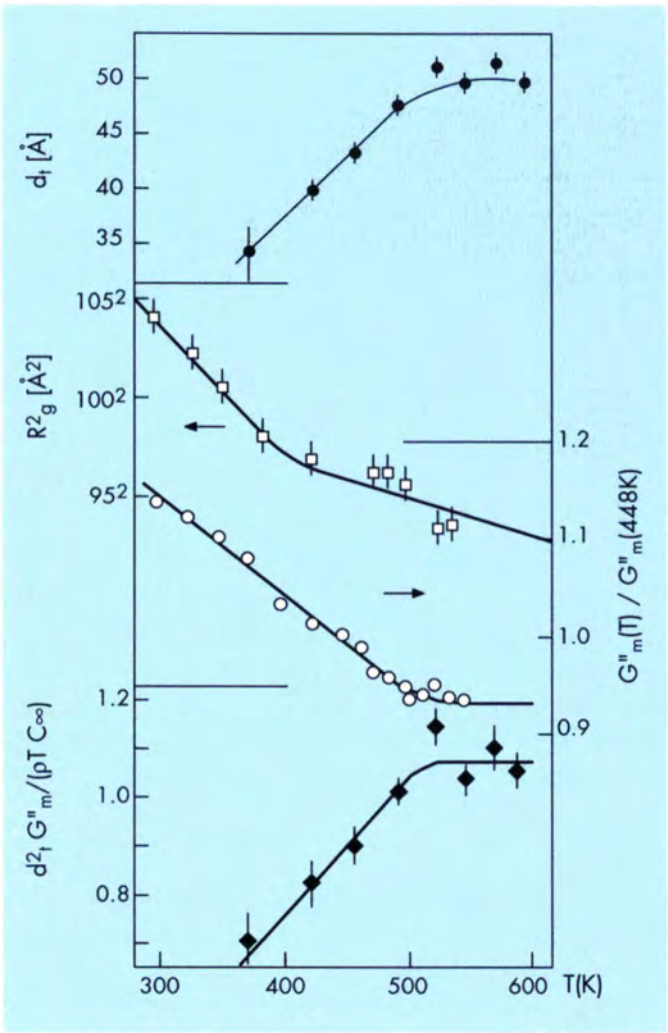


Fig. 4. Tube diameter dt, radius of gyration R_G, $G''_mT/G''_m(448K)$ and $d_t^2/G''_m/\rho TC_\infty$ as a function of temperature

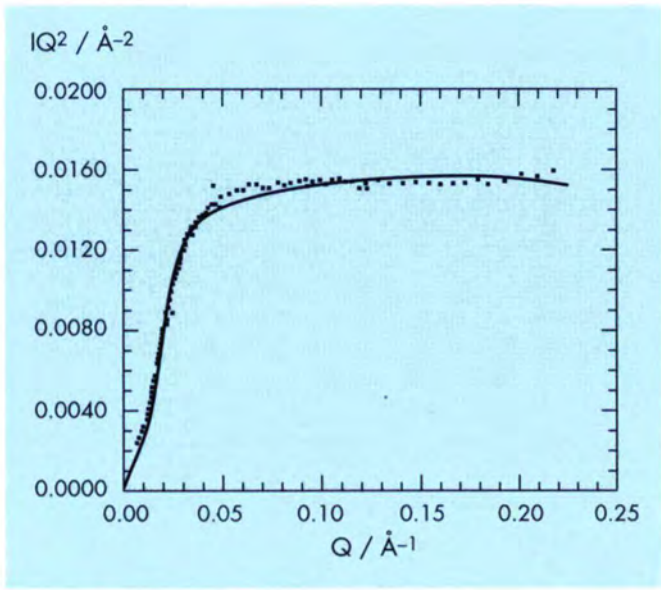


Fig. 5 Dots: Kratky - Plot of PEKEKK. Continuous line: Scattering function of Yamakawa fitted to the data. $I=N_W$ x $P(Q)$ with N_W = degree of polymerization and $P(Q)$ = form factor.

Steady state - SANS experiments under external constraints
P. Lindner

Non-equilibrium sample environment

In a standard small angle neutron scattering (SANS) experiment the (liquid) sample is usually confined in a container of quartz (or another material transparent to neutrons) with defined path length and in thermodynamic equilibrium with its environment, at given chemical composition (concentration), pressure and temperature. *Without* external constraints, the scattered intensity (e.g. from a dissolved macromolecule) is under these equilibrium conditions a result of the space and time average of all molecular conformations and orientations and an (azimuthally) isotropic scattering pattern is observed on a two dimensional multidetector.

In a non-equilibrium experiment [1], an external field is applied to the sample. External constraints can be imposed for instance by applying either a *magnetic*, an *electric*, or a *hydrodynamic field*. Furthermore, different modes of operation are possible. (i) Thus, in a *kinetic or relaxation* experiment, the sample is allowed to relax back to equilibrium after an externally imposed perturbation of its equilibrium configuration. (ii) In a *cyclic* experiment the sample is periodically distorted around its equilibrium state. (iii) A third type of non-equilibrium experiment is the *steady-state* experiment with keeping the external constraints constant.

A particularly interesting combination is *steady-state flow* where the liquid sample is exposed to a hydrodynamic field *during* the scattering experiment [2]. The solute particles experience forces due to viscous drag in the streaming fluid which tend to orient and to deform them. The intensity distribution on the two-dimensional multidetector might become anisotropic with respect to the direction of flow. In the field of *colloid and polymer science* this relatively new class of experiments has attracted considerable attention in recent years because, using a classical scattering technique in combination with an externally applied field, important information is obtained, for instance, about structural changes of deformable or anisotropic particles (e.g. shape and size) and on dynamic properties (e.g. flexibility) as well as on thermodynamic behaviour (e.g. spinodal decomposition) when the system is in a non-equilibrium state. A further aspect is the possibility of investigating the structure factor of colloidal dispersions under applied shear. Although the macroscopic features (e.g. viscoelasticity) are well known from rheological measurements, the underlying mechanisms on the *molecular scale* have not so far been completely understood [3] and are a matter of increasing experimental interest in polymer and colloid physics. It is obvious that an "on-line" scattering study of *flowing systems* gives insight into a very realistic state of matter since many natural phenomena (e.g. human blood circulation) or industrial processes (e.g. polymer fibre and foil extrusion, flocculation, covering techniques) involve such *non-equilibrium* rather than equilibrium conditions.

Experimentally relevant velocity gradients

When a liquid is exposed to a hydrodynamic field, different types of flow can be distinguished which are of experimental relevance either in pure form or in combination with each other:

(i) *elongational* flow with a *longitudinal* gradient $\dot{\varepsilon}$ is best illustrated by a fluid flowing from an orifice in the bottom of a vessel due to the action of a gravitational field. (ii) pure *shear* flow with a *transverse* velocity gradient is realized when a fluid streams through a tube at constant flow rate. The velocity at the tube wall is zero and increases towards the centre of the tube. The parabolic velocity profile, called *Poiseuille flow*, causes a non constant transverse flow gradient which linearly decreases from its maximum value at the tube wall to zero in the central tube axis. (iii) *Couette flow*, another experimentally important shear flow with a *transverse* velocity gradient, is given between two parallel plates, one at rest and the other plate moving with constant velocity v_z due to the action of a constant external force. In the case of the *plane* Couette flow the gradient $\dot{\gamma}$ can be written as:

$$\dot{\gamma} = \frac{V_z}{d} = \text{const}$$

where d is the distance between the two plates.

Flow apparatus for SANS

From theoretical aspects as well as for experimental reasons, the linear, laminar Couette flow is of great importance because of its simplicity. A Couette-type shear apparatus was constructed for neutron scattering experiments with liquid systems in a constant shear gradient at the SANS instruments D11 and D17 [4]. The sample container consists of an inner fixed piston and a concentric outer rotating beaker, both made of quartz glass, which is highly transparent for thermal and cold neutrons and shows a very low small angle scattering background. The sample is confined in the annular gap between rotor and stator. The gap width is sufficiently small ($d \propto 0.5$ mm) in comparison to the cylinder diameter ($d \propto 48$ mm) so that to a good approximation a plane Couette flow with a constant transverse (or shear)

gradient is realized in the annulus (sample volume ≈ 4.5 ml). The ILL shear apparatus, an example of a specific development carried out at the Institute, has become extensively and routinely used equipment for small angle scattering experiments with sheared polymeric and colloidal systems in the course of the last few years. Moreover, similar shear flow equipment (which fulfils special requirements, like a variation of the shear gradient direction with respect to the direction of the primary neutron beam or an airtight flow cell for investigation of volatile liquid systems) had been constructed also by several outside user groups and was successfully used at the ILL SANS instruments [5-7].

SANS experiments under laminar and turbulent tube flow can be performed with an *Poiseuille type apparatus* which was constructed in collaboration with the University of Dortmund for use on D11. The turbulent flow experiment revealed structural evidence for the orientation of rod-like micellar additives under drag reduced, turbulent flow conditions [8].

Polymer conformation in sheared, dilute solution

In particular, the shear-induced deformation of a single, flexible chain molecule has been systematically studied by SANS experiments in laminar shear flow at the ILL [9]. Under such conditions, information about the morphological changes on the molecular level are of fundamental interest for an understanding of the macroscopic properties of the flowing system: to what extent is the conformation of a single, more or less flexible polymer chain altered by the velocity gradient in the streaming liquid? A distortion of the polymer coil conformation in flow has long been predicted by theories. In a longitudinal gradient $\dot{\varepsilon}$ a sharp coil-stretch transition should occur for $\dot{\varepsilon}\tau \geq 1$, where τ is the largest relaxation time of the intramolecular chain motion [10], whereas in a transverse (or constant shear) gradient $\dot{\gamma}$ a gradual transition towards an anisotropic intersegmental distance distribution is expected with increasing shear gradient [11]. A common feature of the different theoretical treatments of the ideal flexible chain molecule in shear flow is to consider the balance of (i) frictional forces, (ii) contractile forces and (iii) Brownian motion of the chain segments. The friction forces acting on the polymer chain segments in the shear gradient result in a combined rotation and deformation of the coil beside the translative motion in flow direction, whereas the elastic properties of the chain resist against a change of the shape to less probable chain conformations. According to the theories, the coil shape is deformed in shear flow and changes to an anisotropic conformation with the symmetry of an ellipsoid of rotation. A dynamic effect, however, limits the deformation of the single coil in shear flow: shape changes require changes in chain conformation, e.g. intramolecular bond rotations which are hindered by local energy barriers.

With *scattering* techniques it is possible in principle to observe the overall molecular dimensions *directly* and to prove the chain extension of a macromolecule under flow conditions without dependence upon theoretical assumptions. SANS, resolving the range of momentum transfer Q in the polymer scattering curve from length scales of the order of the overall coil size to the scattering of the flexible segment, is a particularly suitable method for obtaining information on the statistical conformation of the coil molecule in flowing solution.

The normalized scattering curve of a sheared polystyrene chain (dissolved in a thermodynamically "good" solvent) as measured in a D11 SANS experiment with the Couette type shear apparatus at a gradient of $\dot{\gamma} = 6\,000\ s^{-1}$ is plotted in Fig. 1. The (anisotropic) two-dimensional multidetector data have been evaluated in the preferential directions parallel ($||$) and perpendicular ($\perp$) with respect to the flow direction in the gap of the flow cell.

A distinct anisotropy is observed in the region of small values of the momentum transfer Q, where the length scale of the radius of gyration (a measure of the overall molecular size of the polymer chain) is examined. The anisotropy of the form factor is decreasing with increasing momentum transfer Q. The cross-over to

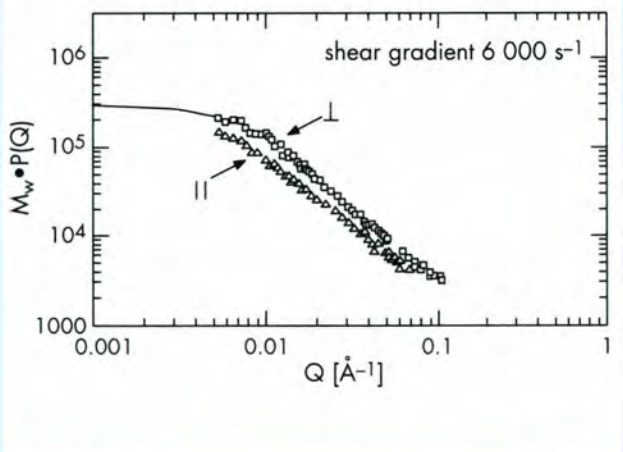


Figure 1. Normalized scattering curve $M_w \cdot P(Q) = f(Q)$ of polystyrene (M_w = 280 000 g/mole, good solvent) in a shear gradient of $\dot{\gamma} = 6\,000\ s^{-1}$, evaluated in the directions perpendicular ($\perp$) and parallel ($||$) with respect to the flow direction. The drawn line corresponds to the (isotropic) scattering curve of the polystyrene in solution at rest.

isotropic scattering (with respect to the directions parallel and perpendicular) observed at large Q-values, shows that the short range distribution of chain segments, on the length scale of the statistical chain element, is not affected by the flow field.

Figure 2 shows the experimental radii of gyration, resulting from the low Q region, as a function of the various shear gradients $\dot{\gamma}$ applied to polystyrene solution. The value $<R||>$ increases significantly with increasing shear gradient $\dot{\gamma}$, whereas the value $<R_{\perp}>$ within experimental error is identical to the radius of gyration of the unsheared polystyrene <Riso> and independent of $\dot{\gamma}$ (see Fig. 2).

Based on the experimental radii of gyration, the deformation ratio of the polystyrene chain can be calculated as a function of the applied gradient and allows quantitative comparison with theoretical predictions, including the effect of limited dynamic rigidity. An ideal flexible behaviour is only found at low gradients whereas with increasing shear, the deformation of the polymer chain is proved to be smaller than for a dynamically infinitely flexible molecule, in accordance with theory [9].

Shear induced aggregation in colloidal dispersions

Colloidal particles can be bridged together by adsorbed macromolecules. If a macromolecule is long enough, it can collect many particles in a single necklace. In dispersions of silica spheres which have been bridged by PEO macromolecules, at low ionic strength all particles are collected in necklaces, and there are 5 to 10 particles per necklace. Shear thickening occurs in concentrated dispersions of such necklaces at volume fractions $\phi > 0.01$. At low shear the dispersion is a good liquid with a viscosity comparable to that of pure dispersion. There is a threshold at a shear rate of $\dot{\gamma} \approx 600\ s^{-1}$, where the viscosity rises suddenly, and the dispersion turns into a gel. If the shear is increased beyond the peak, the dispersion begins to phase separate into flocs and solvent, and the overall viscosity falls (Fig. 3).

In a recent SANS experiment at D11 [12] the structures of these dispersions were examined under shear. At rest the scattering pattern shows a circular ring which matches the average distance between particles in the dispersion (Fig. 4a). Just below the threshold, the dispersion aligns along the flow direction; the degree of order must be quite high, since all the intensity is collected in 2 spots on the vertical axis (Fig. 4b). If the dispersion is sheared beyond this point, a vertical stripe appears in the middle of the pattern, indicating anisotropic aggregation (Fig. 4c). With further shear, the pattern is swamped by an isotropic rise in intensity near the beam, indicating that the aggregation process becomes isotropic. At this point, visual observation shows that the dispersion has separated into lumps (flocs) and water. These findings can be analyzed as a shear-induced phase separation. In this respect the important observation is that the phase separation is preceded by full alignment of the necklaces.

Outlook

Only two examples have been given to illustrate the many possibilities for investigations with the flow apparatus. Thus, neutron scattering is a very convenient technique for performing non-equilibrium experiments:

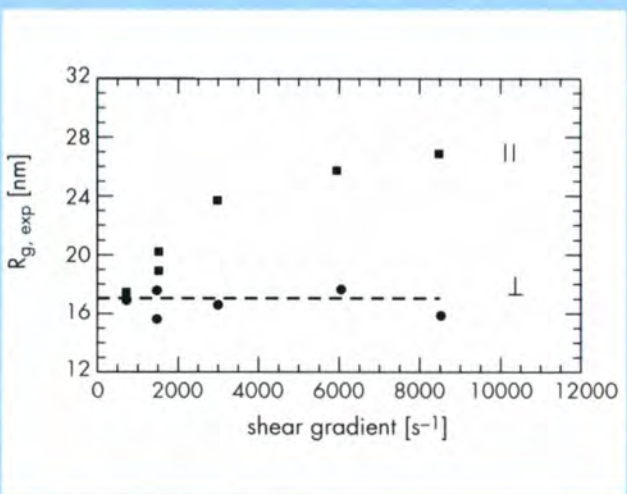


Figure 2. Experimental radii of gyration from a polymer solution at rest (dashed line) and from sheared solutions ($<R_{\perp}>$: filled circles, $<R||>$: filled squares) as a function of shear gradient .

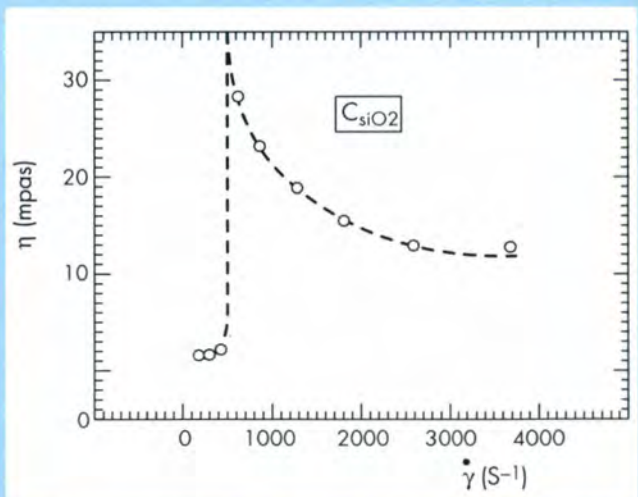


Figure 3. Shear viscosity of a concentrated colloidal dispersion of silica spheres bridged by PEO

SANS in conjunction with steady state shear flow provides a unique method for relating changes of the microscopic structure to macroscopic bulk behaviour. The Couette type shear apparatus has been modified by installation of a torque transducer. First on-line shear-viscosity measurements with a rod-like micellar solution during a SANS experiment in laminar shear flow have been performed recently. This modification provides an interesting extension of shear experiments for interfacing structural properties with rheological behaviour of flowing colloidal or polymeric fluids in the sense that viscosity *(rheology)* and scattering intensity *(structure)* are measured simultanously and with the same apparatus.

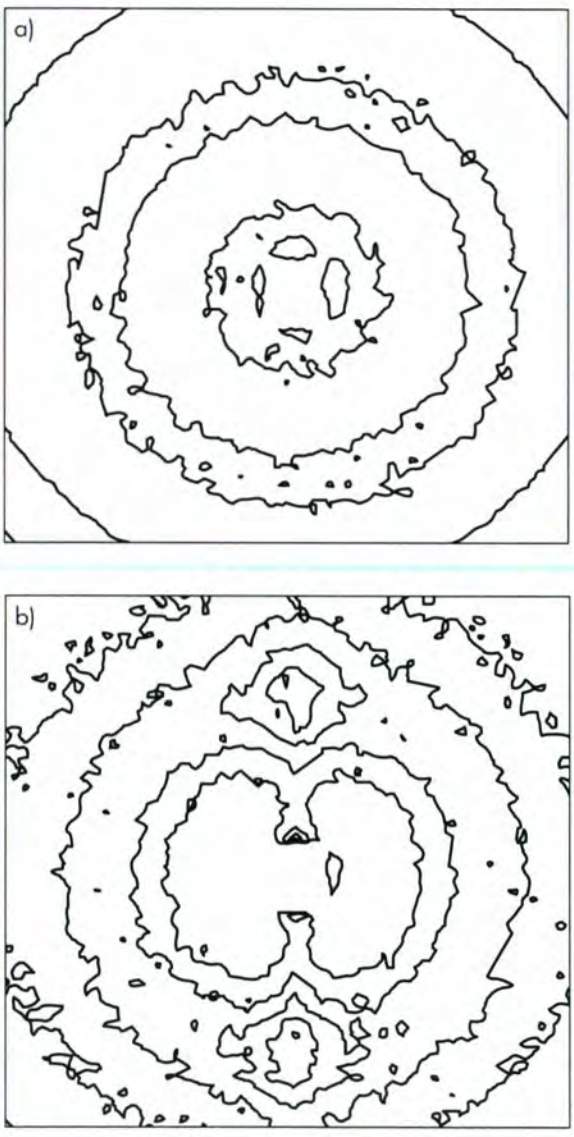


Figure 4. D11 contour plots of silica/ PEO dispersions a. at rest, b. scattering pattern just below the threshold shear rate of $\dot{\gamma} \approx 600\ s^{-1}$, c. scattering pattern above a shear rate of $\dot{\gamma} \approx 600\ s^{-1}$.

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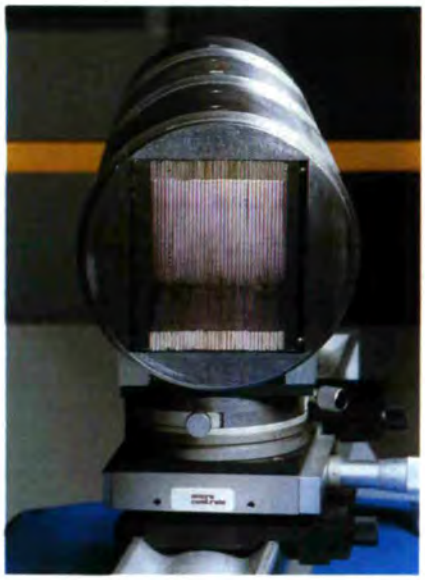
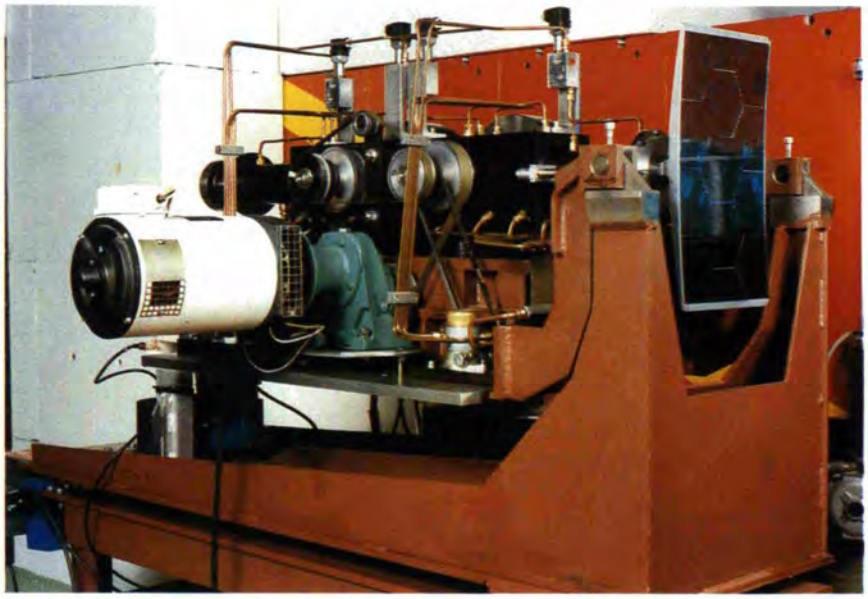


New 600 mm long IN11 analyzer with cobalt-titanium supermirror coating.

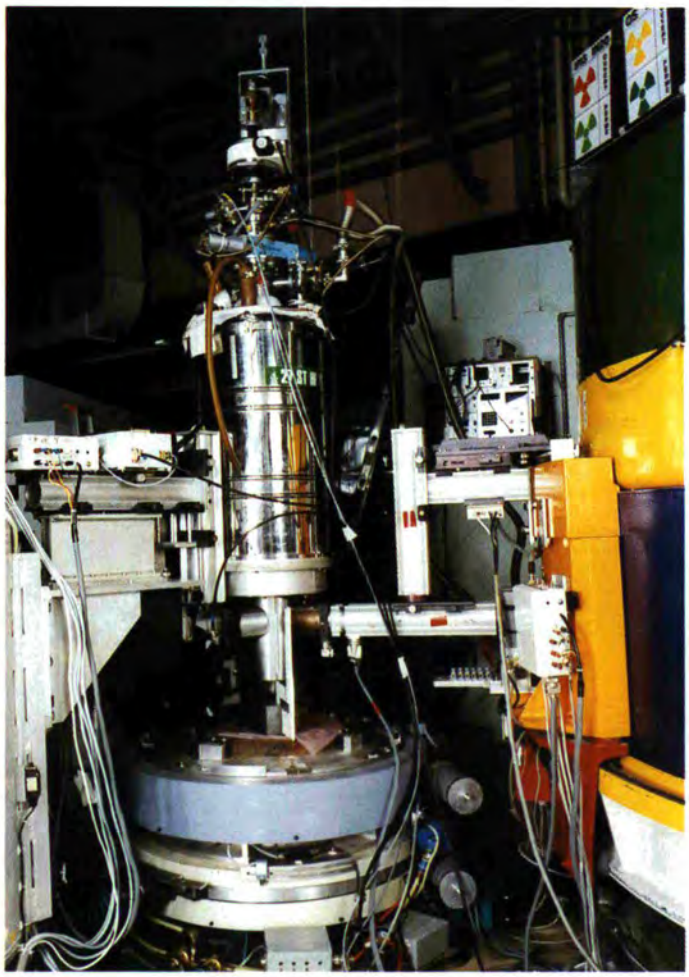
Set-up of the new D20 multidetector in the test hall.

View of the central part of the new Neutron Spin Echo Spectrometer IN15 in the second Guide Hall. In the centre is the sample table with the coils of the guide fields on both sides.



The Doppler machine of the new Backscattering Spectrometer IN10C at the Horizontal Cold Source.

The analyzer of the new Backscattering Spectrometer IN10C.

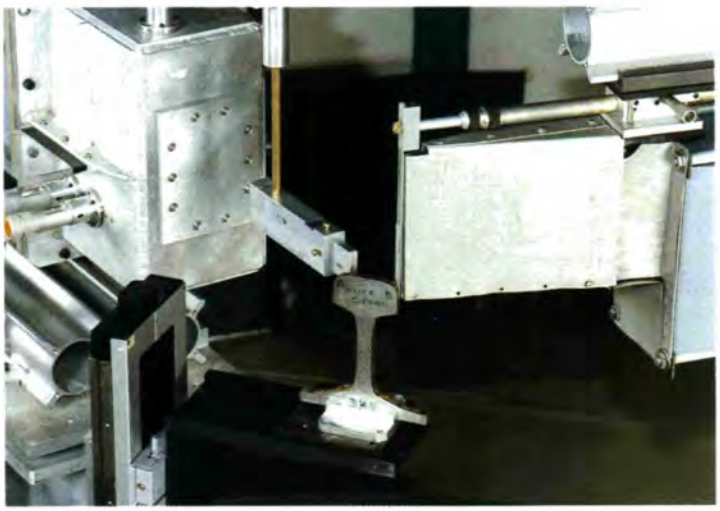


The Cryogenic Polarization Analysis Device (CRYOPAD) in operation on the IN20 sample table. This novel Zero Field Polarimeter makes use of neutron transparent Meissner shields to achieve the full control of the neutron polarization vector before and after the scattering process. Therefore, General Polarization Analysis (GPA) is becoming routinely applicable in thermal neutron scattering. This technique is adding a new dimension to the area, the potential of which has been shown recently in the study of complicated antiferromagnetic structures.

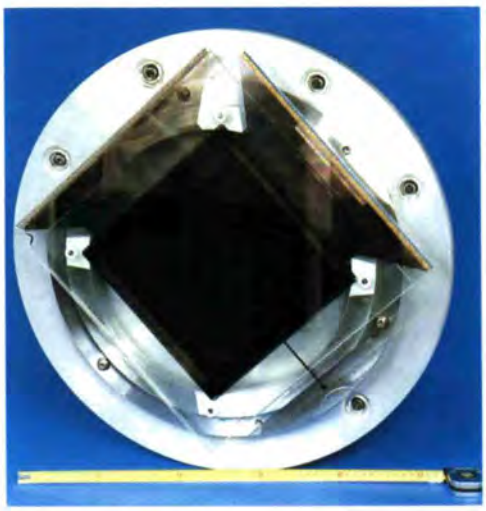
Advanced polarization tools for the CRYOPAD. Vertically mounted perpendicular to the beam in the sample axis these large test tubes are made of thin Niobium walls transparent to neutrons. Once cooled at liquid Helium temperature they surround the sample chamber with concentric superconducting shields. These magnetic Meissner shields are essential elements for the control of the three components of the neutron polarization.

View of the upper platform installed on "niveau D" for the upgraded EDM apparatus. The storage chamber with its surrounding magnetic shield can be seen in the centre of the new platform; on the left is the cabin housing the high voltage supply.
In the centre of the intermediate floor is the facility which guides the ultra-cold neutrons in the upward direction through a polarizing foil. By this way space has been made available on this floor for other UCN experiments.
The long wavelengths (100 Å) interferometer is housed in a cabin which can be seen on the right of the same floor.

P. Webster (Salford University) (left) and P. Convert at the D20 diffractometer used as neutron strain scanner.



A railway rail head is mounted on D20 and ready for neutron strain scanning.



Top view of the 128 x 128 cells multidetector (1,5 mm wire spacing) with delay-line readout.

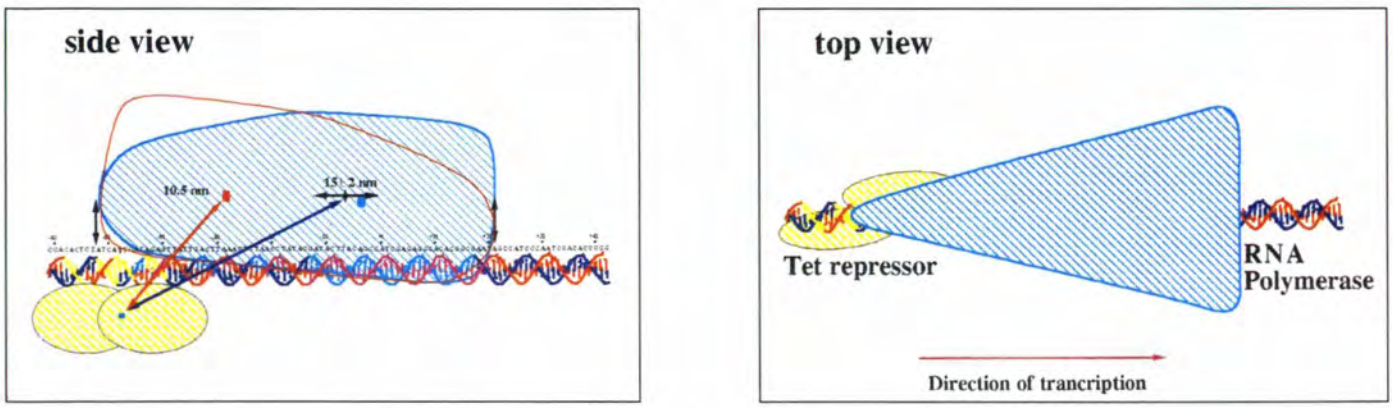


Figure 2 (College 8). The orientation of RNA polymerase (RNAP) with respect to the direction of transcription was determined by measuring its centre-of-gravity distance from a Tet repressor bound to a site artificially placed opposite of the promotor site binding RNAP. The value of 150 Å found by small-angle neutron scattering is compatible only with the large side of the asymmetric RNAP facing downstream.

Advanced Cryogenic Service

This service is responsible

i) for sample environment below 1 K and for high magnetic fields,

ii) for thermometry and temperature control.

The last batch of five ILL precision temperature controllers have been delivered and installed on the instruments. The design and development of a new temperature controller called ILLSEC (ILL Sample Environment Controller) has started. A number of small development projects have been pursued: a new monitor for transurania experiments and improved level gauges for helium and nitrogen vessels. Thermometry at very low temperatures has been significantly improved by a calibration campaign of thermometers down to 20 mK.

The dilution insert for the 6 Tesla TAS cryomagnet has been successfully used for two scheduled experiments reaching its designed base temperature of 30 mK. Interest in the use of magnetic fields as a sample environment seems to be growing (more than 180 days between the two pool magnets).

Very low temperature experiments (20 mK < T < 1 K) have been performed on 25 samples. The dilution insert for IN5 and IN6 (orange cryostat with 70 mm bore) has been completely rebuilt. In collaboration with the Institut LAPP (Annecy) and the Walther-Meissner Institut (Garching) a dilution insert in an orange cryostat was tested and commissioned. The development of a dilution refrigerator insensitive to gravity was continued in collaboration with the CRTB [A. Benoit, S. Pujol, LT 19, (1990)]. The results are now sufficient to start the construction of the dilution 4-circle cryostat. Some progress has been made in the construction of the project 'Godfrin', i.e. the 5 mK dilution refrigerator.

Central Service

The Central Service is responsible for the general organisation and maintenance of the experimental halls, assistance for the running instruments and provision of sample environment for temperatures above 1.2 K. In collaboration with the Reactor Division and the Instrument and Methods Department, the work connected with the beam tube exchange of H8 and H10, i.e. the dismantling and reinstallation of the instruments IN1, D4, IN8 and D15, was carried out successfully. New instrument cabins were installed for IN20, PN8 and IN4. An extensive campaign of control and verification of beam shutters was started. New illuminated trefoils to indicate the state of beam shutters were developed in collaboration with the Reactor Division.

Sample Environment

Two new top loading closed cycle refrigerators, a cryofurnace, improved manual cold valves, a pneumatically driven automatic cold valve and an automatic liquid helium filling device are among the developments which have been completed during 1990. The construction of cryofurnaces for IN13 and IN10C is in progress. Approximately 70 000 litres of liquid helium were used with a recovery of 90 % of the gas. The manpower of the high temperature-high pressure group has been increased by one new member. However C. VETTIER has stopped his activity as the high pressure animator and local contact. K. GOBRECHT took over part of this difficult role. We would like to take the opportunity to thank C. VETTIER for the tremendous effort he made to develop, to run and to improve the ILL high pressure cells.

40 experiments on 16 different instruments were performed in 1990 at pressures above 1 kbar. Two high pressure generators using He up to 5 kbar are now available. The CuBe (amagnetic) and the TiZr (zero-matrix) cells are more and more frequently used. New materials for clamp cells and pressures above 20 kbar are under study (SiN).

'Non-magnetic' furnaces have been developed for IN11 (1 600°C) and D7 (1 000°C). Existing furnaces have been improved (better vacuum, temperatures up to 1 800°C). Development work was carried out for the very successful test experiment on IN10, where the Doppler drive was replaced by a temperature scanning device (see section 'Instrument Groups').

The vacuum laboratory group continued to improve and replace existing vacuum material. Three turbo-molecular pump sets and one hydrocarbon-free pump set became available. The new evaporator for the Nuclear Physics Group has been ordered and will replace the old one in 1991. The responsibility for noise reduction in the experimental halls (noise created by pumps) was transferred to the vacuum group. Important improvements have already been achieved. The vacuum group also participated in the preparation and carrying out of leak tests of the transuranium sample containers.

Chemistry and Biology Laboratories

The biochemistry laboratory has been completely reconstructed and its size increased to accept in addition to the short term ILL users a team of long term visitors from the CNRS working on the structure and the biochemistry of proteins of the Adeno-virus. Improvements have been made in the equipment of the chemistry laboratory (new balances, ice machine, vacuum furnace).

Building Maintenance and Modifications Service

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

The principal work carried out in 1990 included the repainting of ILL1, the installation of a gas supply for the chemistry laboratory, the removal of the 'special water' drain, the construction of two storage buildings and the renovation of the roof of ILL15. Offices have been modified in ILL4, ILL6 and ILL20. The shielding and electrical equipment of the new instruments IN10C, IN15, D22 and EVA was completed. Handling devices, air conditioning systems, instrument computer cabins and working platforms have been installed on several experimental sites. The Service also took part in the beam tube exchange of H8 and H10. The maintenance of the building and technical installations of the EMBL outstation and participation in the common ILL/ESRF site preparation and studies for the Common Building were other tasks of the Service.

Nuclear and Fundamental Physics

PN1 Fission product separator (Lohengrin) on beam-tube H9 (H.R. Faust, I. Gartshore).

PN2 Beta spectrometer (BILL) on the vertical beam-tube V3 (S. Judge, B. Krusche/U. Mayerhofer, H. Just)

PN3 Three curved crystal spectrometers (GAMS 1,2,3) and one flat crystal spectrometer (GAMS4) on the throughgoing beam-tube H6-H7 (H. Börner, S. Robinson, P. Schillebeeckx/A. Williams, R. Oliver).

PN4 Ge(Li) pair spectrometer on beam-tube H7 (S. Robinson, R. Oliver).

SN5 Ultra-cold (UCN) and very cold (VCN) neutron source with 2 beam positions on the inclined beam-tube IH3 (P. Ageron, W. Mampe, R. Bender).

SN7/PN7 Cold polarized neutron beam at end position of guide H14 (K. Schreckenbach, J. Last).

PN8/SN8 Fission product coincidence spectrometer (Cosi Fan Tutte) (P. Geltenbort).

H17 Cold neutron guide with liquid helium UCN source (P. Ageron, R. Golub).

H18 Cold neutron guide (W. Mampe).

H22 Thermal neutron guide: neutron induced particle emission (H22D) (P. Geltenbort); prompt gamma activation analysis (H22E), (S. Robinson, R. Oliver); γ,γ angular correlation (H22F), (S. Robinson, K. Schreckenbach).

TGV Vertical VCN guide in cold source connected to Steyerl turbine producing UCN (Niveau D), (P. Ageron, W. Drexel, W. Mampe, M. Pendlebury, R. Bender, H. Just, A. Steyerl).

$n\bar{n}$ Neutron-antineutron oscillation experiment at the cold neutron beam H5 (D. Dubbers, K. Gobrecht, J. Last).

Fission Research

PN1

The instrument control via a PC (PC-bus and IEEE-interface system) proved reliable during the year. Electric fields, magnetic field and the tape facility to collect fission products at the exit slit of LOHENGRIN are now fully controlled by the personal computer. Work is in progress to monitor all relevant instrument parameters (vacuum, high tension formation current, diaphragm position etc) using the PC. The optimisation of the high tension regulation proceeded successfully with the implantation of an improved version of the slow regulation loop. The project for the implementation of a third field on the LOHENGRIN spectrometer (magnetic dipole) is in progress.

Spectroscopy

PN2

During 1990, a number of improvements have been initiated for PN2. A microVAX has been installed which, in the long term, will replace the instruments' PDP11. Apart from the day to day advantages of easier file transfers, programming etc. that the new computer gives, it will be possible to offer visiting scientists a 'user-friendly' software for data acquisition and analysis.

Two projects have been set up to improve the capabilities of PN2 for measuring subshell ratios of conversion electrons: firstly, software has been written to take into account the effect of natural linewidth on the shape of the spectra, and secondly, a 64-wire proportional counter is under development to improve counting statistics at high resolution.

Finally, a new vacuum evaporator for producing targets has been purchased.

PN3/4

Experiments at the in-pile (n,γ) facility were shared between the bent crystal spectrometers GAMS 1,2,3, the double flat crystal spectrometer GAMS4 and the pair/anticompton spectrometer PN4, leading to a heavy demand for this beam position. Various improvements were implemented at the instruments.

The interferometers of the two-axis flat crystal spectrometer GAMS4 were upgraded. The determination of the rotation of the spectrometer arms attached to the two diffracting crystals is now carried out by using a stabilised He-Ne-laser in a two-frequency mode.

Simultaneously, both GAMS2/3 and GAMS4 were connected to a new μVAX, which is better suited to handle the control of these instruments.

A new Compton γ-polarimeter for the use at GAMS4 was constructed and a preliminary calibration of this polarimeter was carried out. By increasing the cross sectional area of the collimator slit inside the magnet core by a factor of 4 an appreciable improvement in counting statistics will be achieved.

By adapting the associated analogue electronics and adding a further ADC to the system, it is now possible to configure the pair spectrometer PN4 in a Compton suppression mode. The sensitivity of this set-up is approximately equivalent to a normal, unsuppressed, Ge detector. Therefore, by running the pair and Compton modes in parallel, the problem of changing detectors is eliminated and more statistics can be gathered than previously possible.

S51/S34

These beam positions at the thermal neutron guide H22 were used for nuclear spectroscopy research and prompt γ-ray activation analysis of geological samples. A new, microcomputer based, multiparameter aquisition system has been bought. This will enable much simpler data aquisition set-ups for coincidence experiments and also multidetector counting for simple single spectra. Short sections of neutron guides have been bought, which will be used to extend the current neutron guide by an extra few metres (with gaps for intervening instruments) thus improving the flux to both the S51 and S34 instruments.

Fundamental Physics

A variety of fundamental physics experiments were performed in 1990 on different neutron beams: VCN beam and UCN beams from the neutron turbine (TGV on Niveau D), the original UCN source SN5, the cold neutron beams H17, H18 and PN7, the cold beam for $n\bar{n}$ and several dedicated experiments at various instruments or other beam positions. The results of the experiments are summarized in the scientific section for College 3. Some comments are given here as to technical developments and use of the beams.

VCN beam and UCN beams at level D

The technical development at this very cold and ultra-cold neutron facility on level D of the reactor is described in the section Special Instruments and Experiments. In fundamental physics the search for an EDM of the neutron was continued (Harvard-ILL-Rutherford-Sussex-Washington collaboration). After completing the recent measurement of the neutron EDM published in 1990 the instrument used on level D has been rebuilt with the innermost magnetic shield removed to make room for a larger neutron storage chamber, see photograph page... It is intended that the instrument will run again in 1991 with a fivefold increase in neutron counting rate and with a new atomic magnetometer which will simultaneously occupy the same storage volume as the neutrons.

The neutron life-time was precisely determined in a UCN storage experiment (Kurchatov Institute, Moscow-ILL). Storage time and neutron leakage were measured for various temperatures and surface areas. Thermal neutrons created by the upscattering of stored UCN were counted. The time distribution of these counts was an important feature of the data (see the College 3 part of the annual report).

The work at the long base line neutron interferometer for 100 Å neutrons was continued and the installation has been improved by adding a cabin to control the air temperature and keep out sound and by modifying the levelling system for the table (Vienna-Munich) (see also Instrument Group "Special Instruments").

H18

Polarized 15 Å neutrons were used to search for a diffraction pattern which could be interpreted as neutrons with mean spin component larger than 1/2 (Heidelberg/ILL).

SN5

Various surfaces of neutron guides were investigated by multiple reflection of 60 Å neutrons, providing data on total reflection angle and loss per reflection.

PN7

The former special beam position SN7 was converted into a PN instrument. During the year the polarized beam was used for a beta asymmetry measurement in the free neutron decay (LAPP-Chambéry-ILL), a calibration of a γ-polarimeter by almost 100 % longitudinally polarized γ-rays from the $(\vec{n},\gamma)$ reaction (ILL) and experiments on parity violation in $(\vec{n},f)$ and $(\vec{n},\gamma)$ (Leningrad, Moscow, Tübingen). An improved method for the determination of the degree of polarisation was developed. The polarizer and analyser were cyclically permuted using three different supermirror polarisers. Together with two spin flippers the method yielded the spin flip efficiency (99 %) and polarising power (98,5 %) for each spin-flipper/polarizer with a precision of 0,2 %.

$n\bar{n}$

The experiment searching for $n\bar{n}$ oscillations was running continously over the year. The magnetic compensation of influences from nearby instruments was improved.

S50

The long baseline experiment for a precise determination of h/m_n, operational at the monochromatic thermal beam S50 (PTB Braunschweig), was continued. The meander coil system operating at 750 kHz, used for modulating the neutron spin direction, will soon be replaced by a single coil with a ferrite core running at the same frequency. For the more distant future a chopper is being developed to modulate the beam intensity at 5 MHz.

Coordinator: K. Schreckenbach

Three-Axis Spectrometers

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

IN8 3-axis spectrometer on the thermal beam-tube H10 (J.L. Martinez, B. Fak, J. Bossy, R. Arthaud).

IN12 3-axis spectrometer on the cold guide H142 (S.M. Hayden, B. Fak, H. Godfrin and D. Puschner).

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

IN20 3-axis spectrometer for neutron polarisation analysis on the thermal beam-tube H13 (A. Severing, C. Vettier, A. Dorn).

Instruments

IN1 Hot source three-axis spectrometer (H8).

The instrument operated reliably over the scheduled period, which was slightly extended at the expense of the Be-filter spectrometer time. A new cabin will be installed shortly. This cabin will be shared between IN1, INFB and D4. It will provide the users with a more quiet environment for on-line data treatment during experiments. Finally, starting in January 1991, a technician will be available for the three instruments on the H8 beam-tube.

INFB Be-filter (H8).

The Be-filter is used in combination with the Cu(200) and Cu(220) monochromator crystals. With varying incident wavelength, the automated interchange between the two crystals is required in order to match the 5 meV resolution of the filter itself. The Be-graphite combination filter, with a resolution of less than 2 meV, usually requires the Cu(331) monochromator crystal. Both instruments have operated without any problem during the last cycles.

IN8 Three-axis spectrometer on the thermal beam-tube H10

During the winter shut-down, the H10 beam-tube was replaced. The exchange operation, performed by the Reactor Department in collaboration with Edex, was entirely successful, and the spectrometer could be rapidly re-assembled. The instrument became fully operational again in May 1990. Apart from a general 10 % loss in flux due to the reactor power reduction, the performances and reliability of the machine have not been affected.

The two "in-pile" collimators (15' and 30'), located between the monochromator and the reactor face, have been replaced as well. New 30' collimators are available in the monochromator-to-sample and analyser-to-detector positions. In order to minimize the IN8 users' exposure to radiations, the control teletype of the instrument has been relocated at a position further removed from the irradiated area. The spectrometer movements may still be visualized on a video camera monitor. Finally, an additional secondary beam-shutter has been installed, which completely isolates the monochromator section from the experimental area. This new safety feature is particularly useful during collimator interchange operations.

IN12 Three-axis spectrometer on the cold guide H142.

The instrument has operated satisfactorily throughout the year. Although there have been no major changes to the spectrometer, a number of improvements are planned in the near future. The polarized beam version of the instrument will be updated to allow for an easier and more flexible mode of operation. The monochromator protection will be modified in order to accommodate shorter collimators. As a result, the collimator interchange procedure will also be simplified.

IN14 Three-axis spectrometer on the horizontal cold source (H53 guide).

The instrument has been available for scheduled experiments during most of the year. The remaining beam-time was set aside for instrument tests and developments.

A new vertically-focussing composite Si (311) monochromator was installed and calibrated in the Spring. It was found to offer interesting possibilities for high resolution experiments in the 8-to-15 meV incident energy range. Much of the test time has been devoted to implementing the polarized beam option, using a polarizing supermirror bender and a Heusler (111) analyzer. The bender transmission was found to vary from 50 to 25 % across the available incident energy range (2 to 14 meV), with a polarization efficiency of the order of 90-95 %.

The polarization and reflectivity characteristics of the Heusler analyzer were also tested and proved very satisfactory, particularly for low energy, high resolution work. A complete description of the instrument performance, in both polarized and unpolarized versions, is available on request. Further developments will involve a second bender, optimized for long-wavelength neutrons and a variable-wavelength higher-order filter.

IN20 Three-axis spectrometer with polarization analysis on the thermal beam H13

The experimental zone of the instrument has been extended to accommodate the precession coils for the spin-echo option. This was achieved without any interruption in the experimental program. However, some disturbances have occurred due to breakdowns of the TAS cryomagnet which is heavily used on IN20 for polarized neutron work over all reactor cycles. This difficult situation could be eased with the acquisition of another vertical field cryomagnet.

New encoders for the sample goniometers have been installed. Because they are insensitive to fringe fields from magnets, accidental tilts of magnets should be prevented.

Coordinator: R. Currat

Time-of-Flight, High Resolution and Diffuse Scattering

IN4 Time-of-flight spectrometer on the thermal tube H12 (A. Murani, H. Mutka, A. Dorn (technician)).

IN4C New TOF spectrometer with a Brillouin option (project) (H. Mutka).

IN5 Multichopper TOF spectrometer on the cold guide H16 (G. Kearley, F. Rieutord, H. Blank, S. Jenkins (technician)).

IN6 Focussing TOF spectrometer on the cold guide H15 (A.J. Dianoux, R. White, S. Jenkins (technician), Y. Blanc (technician)).

IN10 Upgraded backscattering spectrometer on the cold guide H15 (B. Frick, J. Cook, P. Joubert (technician)).

IN10C New backscattering spectrometer at the horizontal cold source (project) (B. Frick, J.L. Coquin, Y. Blanc (technician)).

IN11 Spin-echo spectrometer on the cold guide H15 (B. Farago, J.F. Legrand, J. Bauchat (technician)).

IN13 Backscattering spectrometer for short wavelengths on the thermal guide H24 (W. Petry, J. Williams, J.F. Barthélémy (technician)).

IN15 High-resolution spin-echo spectrometer for long wavelengths (project) (A. Kollmar, F. Mezei, D. Richter, F. Douchin, J.F. Barthélémy (technician)).

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

IN4 TOF spectrometer on the thermal tube H12

Following the major modifications carried out at the beginning of 1989 we have now installed a motor driven translating monochromator table with a graphite plus two copper (1,1,1) and (2,2,0) monochromators. This now permits a remote monochromator change providing great flexibility for energy selection (E_i = 17, 45, 68, 115 and 155 meV) as well as saving beam time necessarily lost (cooling down period for reactivity plus intervention time) during the earlier manual exchange. When suitable monochromator elements become available it is hoped to incorporate curvable monochromators within the translating table.

The problem of noisy working conditions within the reactor hall has been partially solved by installation of a cabin housing the computer terminal are providing limited working space for experimentalists. The suite of software for instrument control as well as data inspection and analysis has also been improved.

IN4C New TOF spectrometer with a Brillouin option

Since the approval of the instrument concept in March the project on the high efficiency thermal TOF spectrometer has now entered the phase of technical study. At present the work concentrates on the technical optimization of the background choppers, which is a critical point in determining the geometry. The beam size, by consequence the area of the monochromator with variable curvature and the exact focussing conditions will depend on the final results of this chopper optimization. According to the actual budget plans the main part of the financing will be available in the period 1992 to 1993 and the instrument will be operational by 1994. We can recall that this instrument is designed for a (Q,ω)-range from 0.1 to 10 $Å^{-1}$, 1 to 100 meV, with a resolution adjustable in the range from 2 to 5 %.

The Brillouin option proposed to operate in parallel on the same beam hole aims at inelastic experiments at low angle and good resolution with incident energies (10 to 50 meV), in the range 0.01 $Å^{-1} < Q < 0.2$ $Å^{-1}$, 0.1 meV $< \omega <$ 5 meV where no standard instrumentation exists at present. During the coming year real scale tests are to be carried out in order to gain experience under real conditions, necessary for extrapolating towards the proposed instrument parameters concerning the stringent wavelength and angular resolution requirements.

IN5 Multichopper TOF spectrometer on the cold guide H16

IN5 is now controlled by a microVax. A completely new software package which IN5 has in common with IN4 and IN6 has been developed. Data inspection using GENIE (RAL) is available on all three instruments and is appreciated by British users.

After 5 years fairly continuous running of the chopper system a mechanical overhaul became urgent. All vacuum seals were replaced and readjusted. Two damaged chopper disks were found which account for the high level of wavelength impurities encountered before the overhaul. One disk was replaced by the only spare and an appropriate means of repairing the damaged gadolinium coating is being investigated.

We are presently testing a system of in-guide collimation for low-q experiments using a D11 spare detector. The q-resolution should be improved by more than a factor of 2 at λ = 10 Å. Another major improvement for these experiments will be next year installation of an evacuated flight path presently under construction.

IN6 Focussing TOF spectrometer on the cold guide H15

This year again the instrument has worked satisfactorily and despite the long reactor shutdown at the beginning of the year, 46 experiments have been performed. Only one experiment had to be rescheduled due to the breakdown of the furnace, which had no replacement at that time.

In the second half of the year, the data were also accumulated with the new VME electronics, working in parallel with the old CAMAC system. This has permitted the carrying out of extensive hardware and software tests of the new system. During the November shutdown, the new data acquisition software has been implemented on the instrument. At the reactor start the data acquisition was definitively switched over to the VME electronics and the experimental programme was continued subsequently with practically no disruption. The new system will permit the use of a variable channel width across the spectrum. This will lead to a better definition of the spectrum in the quasi-elastic region.

IN10 Upgraded backscattering spectrometer on the cold guide H15

Of the 180 scheduled measuring days on IN10, effectively no losses were incurred after allocations of buffer time (apart from those caused by unscheduled reactor shutdowns).

During 1990 complete revisions have been made of the furnace, cryofurnace and sample goniometer. The furnace is now mounted with an Alcatel 5150 turbo-molecular pump, in compliance with the evolving ILL standard. The VAX-station has recently acquired VMS version 5.3 and a replacement D.C. motor and associated control electronics has been bought for the Doppler drive. Two new large area, unpolished Si(111) analysers (4 plates) are also foreseen for 1991.

A completely new mode of operation of IN10 is currently under development [1] in order to greatly extend the dynamic range afforded by the Doppler drive. The principle is similar to that of IN13, whereby a cryofurnace arrangement is used to change the monochromator d-spacing and therefore the incident energy. Recent test measurements have been performed for a KCl monochromator using the backup continuous-flow nitrogen cryofurnace of IN13, mounted on a specially-designed goniometer. In the available temperature range (77 - 770 K), an energy transfer range of $+83 < \omega\ (\mu eV) < -16$ (for Si(111) analysers) was possible with little loss in intensity at the higher temperatures (see Fig. 1). (The theoretical maximum energy transfer for KCl being about 150 μeV close to the melting point). The energy resolution (FWHM) was measured to be around 0.9 μeV and the intensity is estimated to be greater than one half of that for the current Si(111) unpolished monochromator. By using a selection of similar monochromator crystals it is hoped to cover a continuous range of energy transfers from ~+160 μeV to around -300 μeV. During 1991, it is planned to build a dedicated cryofurnace permitting a very homogeneous monochromator temperature. IN10 will thus be able to offer an energy transfer range similar to that of IN13 but with an energy resolution between 0.6 and 1.0 μeV.

[1] J.C. Cook, W. Petry, B. Frick, A. Heidemann, ILL Internal Report, in preparation.

IN10C New backscattering spectrometer on the cold guide H15

The construction of IN10C showed considerable progress in 1990. Two major components of the instrument were finished this year: the monochromator and the graphite deflector-chopper.

The system for guiding the monochromator (about 6 kg) was changed. This way the monochromator is fixed now directly onto the piston of the Doppler drive, thus eliminating a major part of the vibrations. The monochromator itself was manufactured at the ILL and the Si(111) single crystals (4x4 mm^2 each) were glued onto the spherically curved support. The tests with neutrons revealed: i) good optical quality, i.e. a sharp image of the exit window of the supermirror guide, ii) a flux increase of a factor of 5 compared to IN10, when the incoming beam was deflected by graphite cassettes to the monochromator using a wavelength of 6.27 Å and backscattering to the focal point.

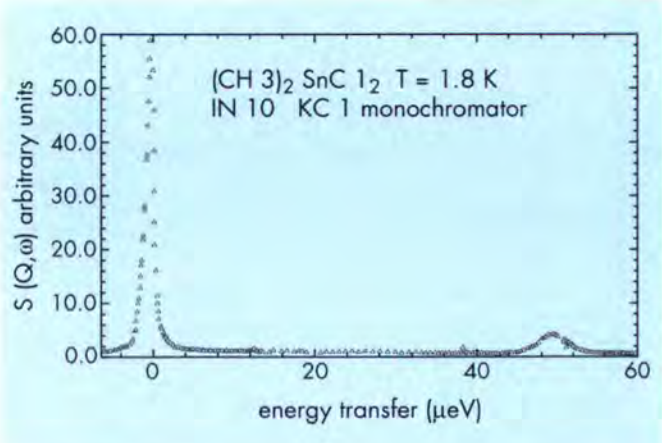


Fig 1. Elastic peak and rotational tunnelling peak ($\hbar\omega$ ~ 50 μeV) of methyl groups in $(CH_3)_2 S_nCl_2$ measured with the prototype KCl monochromator in the temperature range 80K < T < 700K.

The capture flux, measured by gold foil activation at the end of the focussing supermirror guide, was determined to 1.4 x 10^7 n/cm^{2}s.

The graphite deflector-chopper, a delicate and novel element realized on this instrument, is now mounted and is turning without problems at a speed which is 15 % higher than the designed value (2600 rpm). Tests with neutrons are under way.

Furthermore all six wide angle analyser plates (manufactured at the KFA-Jülich) have been delivered. One of them is completely covered with Si(111) single crystals (about 60000 crystals per plate with 4x4 mm^2 each). Optical as well as neutron tests were carried out and gave satisfactory results. The half-rings (Debye-Scherrer analyser rings) and the small angle analyser rings will be finished at the beginning of 1991. The initial aim, the complete mounting of the main components during 1990 was not achieved due to financial problems. The contract for the mobile platform and the secondary shielding was placed in the second half of the year. The general study of these components was then started as well as the construction of the mobile platform. This platform has just arrived and will immediately be mounted. The rest of the shielding is expected to be ready in February 1991.

All major parts of IN10C are expected to be completed in summer 1991.

IN11 Spin-Echo spectrometer on the cold guide H15

The NSE spectrometer worked without major problems in the last 12 months. In November 1990 the new Ni-Ti analyser was installed. The gain factor in flux compared to the old Fe-Ag supermirrors is substantial, although slightly less than expected (about 2.2 at 4.5 Å instead of 3). One half of the mirrors in the Soller arrangement have only 70 % reflectivity on average compared to the other half. This might be due to the imperfections of the preparation or the curvature which is less well defined because of the large size of the analyser. At 8 Å the gain is about 10 %.

The new Gobert type selector was delivered, it will be installed next year after adjustment of the rotor. It is expected to permit the extension of the wavelength range up to 4-12 Å with the same resolution of 18 % FWHM.

The IN11C project was started this year by placing the order for the wide angle magnet. The definitive installation will start after having tested the magnetic inhomogeneities in detail.

IN13 Backscattering spectrometer for short wavelengths on the thermal guide H24

There have been no major changes of the instrument over the last 12 months and with the exception of a starting period after the long shut down in Spring 1990 the instrument showed an exceptionally good performance.

To prevent unforeseen failures of the instrument, major renewals are foreseen for 1991: The PDP11 instrument computer will be replaced by a microVax and the complete electronics including coders of 2/3 of the 17 motors will be exchanged.

IN15 High resolution Spin-Echo spectrometer for long wavelengths

The assembly work is now finished as regards the classical mode of NSE (static), referred to as IN15 standard. It includes some major improvements: high speed velocity selector, high quality precession coils, new flippers, 32 x 32 multidetector. Characteristics of the different components have been controlled, including the stability of the 25 DC power-supplies.

VME electronics is running for all main functions except selector tilting. Informatic control has been implemented at different levels (local control by MacIntosh or instrument program installed at the VME under OS9). Certain technical developments aim at a better transparence of the Fresnels coils (Aluminium or Silicium) and a reduction of neutron losses along the flight path of the neutrons.

Neutron tests are being made since September 1990, with a polarization which is limited by the existing prepolarizing FeCo guide and polarization analysis by a provisional cassette system. A reflection analyser (supermirrors provided by O. Schärpf, ILL) was dispatched to the KFA-IFF Jülich for tests and will be used while awaiting the transmission analyser from HMI Berlin in 1991.

Neutron flux measurements confirm the preliminary results (gold foils). Spin echos obtained up to the limit of 18 Å and with a maximum precession field (1500 G) shows a very good behaviour of the whole magnetic lay-out of the instrument. The delivery of a transmission polariser (HMI) will make the IN15 standard fully operational for test measurements at the beginning of 1991. (The picture on page 78 shows the precession coils, without the flippers and other components).

Tests of the "Time-of-Flight" version referred to as - IN15 TOF - will become possible after the delivery by KFA-Jülich of the control electronics, under test at KFA-ZEL with the ILL-built triple chopper array.

A prototype of a toroïdal mirror (microroughness 3 Å) has been ordered at CARL ZEISS (RFA) for testing in real conditions the third version of IN15 with neutron focussing of the longest wavelengths, referred to as IN15 focussing. These tests will take place in the second half of 1991.

D7 Diffuse-scattering instrument with polarization analysis on cold guide H15

D7 has had a normal experiment program, and has not undergone any major modifications or improvements, contrary to what is planned for 1991.

D11 Small-angle scattering diffractometer on the cold guide H15

As in previous years, the experimental programme on D11 was carried out without any major difficulties. In addition to a total number of 99 normally scheduled experiments (corresponding to 144 days) in 1990, 7 days were used as industrial beam time.

The D11 chemistry laboratory which was completely renovated at the end of last year has proved to be a very useful installation for sample preparation immediately before and during experiments. It was not only used by D11-users but also by visitors from D17 and various other instruments.

Systematic time-of-flight measurements were carried out with both velocity selectors (Brunhilde, Dl/l = 9 % and Adele, Dl/l = 40 %) and served as a wavelength recalibration. The delivery of the new, lightweight 10 % velocity selector which was foreseen for 1990 is delayed due to technical problems encountered by the manufacturers during high speed tests.

In April 1990 the VAX 11-730 computing system, which had been in operation since 1985, was replaced by a MicroVAX II computer. Furthermore, a VAX 3100 workstation has been installed for graphical data treatment. The LA 100 Letterwriter has been replaced by a small LA 75 Companion Printer for output of the experimental protocol.

A user-friendly optical alignment system has been installed in the casemate near the sample zone. A silicon wafer is placed at a tilting angle of 45° in the primary beam and acts as a mirror for a light beam shining through a quartz window from either a halogen-lamp or a laser, both fixed outside the evacuated neutron guide. The sample position can thus easily be adjusted to the neutron beam by operating a button on the wall next to the "black nose", without breaking the vacuum and without opening the guide section in the casemate.

Due to the advanced age of the CAMAC electronics, intermittent faults have appeared, and several components had to be replaced. A new digital-to-analogue converter module has been installed which provides 8 channels in a range of 0 to 10 Volts DC for interfacing with users' equipment.

All the collimating guide-sections were realigned and worn mechanical parts were exchanged. Preparatory work for installation of the new, antimagnetic collimation system has started. The computer control of the 7 guide sections is currently under test and the whole sytem will finally be installed during a shutdown in February-March 1991. In view of the replacement of the collimation, systematic flux measurements have been performed by gold-foil irradiation at l = 0.6 nm and l = 1.0 nm and by direct measurements with a calibrated monitor with a known efficiency as a function of wavelength ($0.45 \leq \lambda$ (nm) ≤ 2.0) and position of the collimation guides.

In order to reduce the acoustic background noise around the instrument, noise-absorbing shieldings around the instrument's pumps will soon be installed. A modification of the D11 cabin is foreseen for early 1991: since the new computing system needs much less space, the air-conditioned part of the cabin will be made smaller and the working area for visitors will hence be increased.

D17 Low-Q, low-resolution diffractometer on the cold guide H17

In general, D17 has been running smoothly during 1990, but an incident in August caused a temporary shutdown of the instrument. The beam shutters and the beam control and supervision systems have been modified on D11 and D17.

Since about a third of all scheduled instrument days now are used for reflection measurements, the equipment for this kind of experiment has been further improved. An antivibration table has been purchased and used for the first time, and a computer-controlled step motor drive is now available for changing the height of the sample position, e. g. as a function of the angle of incidence of the impinging neutrons. The bearings of the sample-height adjustment table were exchanged and ensure a smooth movement again. Two Microcontrôle slides with step motors have been bought for replacing the manual mechanism defining the entrance slit for reflection measurements.

In a continuing effort to simplify the use of D11 and D17 for visitors, a new digital-to-analogue converter module identical to the one on D11 has been installed.

On the computer side, a MicroVax II for the data acquisition together with a Vax-3100 workstation for data treatment have replaced the ageing Vax-730. The workstation is under test with the PV-WAVE software for graphical manipulation of diffraction data. The instrument software group has taken over the maintenance and improvement of all the data acquisition and instrument control programs. A simplified data acquisition system for the small-angle scattering instruments is expected during the next year.

D22 New low-Q diffractometer on the cold guide H512

D22 is slowly approaching the state of a working instrument. Due to the budgetary constraints encountered, D22 cannot, however, be made available for users before the beginning of 1992. Instrument tests will be possible in the course of the next year.

The lower parts of the protection "casemate" (in concrete) have been built. A marble floor (about 1.5 m^2) has been laid for the air cushions of the lead casemate-entrance door. Subsequently, the entrance module of 1.5 m length (which can be replaced by a polarizing unit in the future) and the rotating collimation unit have been installed and successfully tested for vacuum tightness and function.

The neutron guides, which were delivered in April and May 1990, will be installed soon. The upper parts of the casemate have to be poured in lead and will be inserted later this year.

Offers for the programmable automate controlling the non-encoded movements of the instrument and the selector-security and vacuum systems were received. The system will be chosen before the end of the year. Working prototypes of the data-acquisition and shaft-control electronics for D22, which are being developed by ILL's electronics service have been promised for the end of 1990.

The 1 m x 1m detector with 128 x 128 resolution elements of 0.75 x 0.75 cm^2 was ordered from CERCA in December. The ^3He counting gas for the detector was bought earlier in the year.

The price for the 10% resolution Dornier velocity selector has considerably increased since our first estimations, mainly due to the risk involved for guaranteeing speeds up to 28 000 rpm. Nevertheless, we have decided to purchase this high-tech equipment since it meets the specifications for D22. A delivery delay of 6 to 9 months is quoted by the manufacturer.

The installation of electrical cables and of air and water supply pipes has begun. A working group for defining the details of the vacuum system has been established; valves and additional pumps were bought within the budget allocation for 1990, and the installation of the common pipe along the instrument was started; all parts of D22, with the exception of the velocity selector, will be evacuated by one group of pumps under control of the automat mentioned before. The last mechanical assemblies to be studied are the sample zone and the beam-stop mechanism.

As usual, the instrument computer will be purchased at a relatively late stage, in order to take advantage of favourable price and technology developments. It will be ensured that the hardware and software will be compatible with the other low-Q instruments at the ILL.

Coordinators: A.J. Dianoux

R. May

25th Anniversary of neutron backscattering

This year the Neutron Backscattering Spectrometry celebrates its 25th anniversary. This powerful high resolution method has been proposed by H. Maier-Leibnitz. The first backscattering experiments were carried out at the Munich research reactor by B. Alefeld [1]. The basis for the development of this method may have been 'thinking in phase space' as promoted by H. Maier-Leibnitz at that time [2]. The improvement of the energy resolution of conventional neutron spectrometers from meV to μeV was a daring step. Many scientists doubted wether the small intensity expected for such a resolution would be enough to perform spectroscopy. The prototype backscattering spectrometer was built in Munich by B. Alefeld, M. Birr and A. Heidemann [3]. With an energy resolution of 0.3 μeV (HWHM) measurements of hyperfine splittings (see fig. 1) and very narrow quasielastic scattering were performed for the first time. These experiments were on the limit of feasibility because of the low cold neutron flux of the Munich reactor with 4 MW and no cold source. Nevertheless, the results were exciting and created many discussions. The way of backscattering then led to the KFA Jülich in 1971 with its reactor FRJ-2 with about ten times higher flux and a cold source. For the first time high resolution backscattering spectroscopy was applied to the study of rotational diffusion, tunneling in molecular crystals [5] and to hydrogen diffusion in metals. The commissioning of the backscattering spectrometer IN10 in 1974 at the ILL, led to the international break through of this method. This instrument can be considered as the work horse in μeV resolution spectroscopy in ω-space (see fig. 2).

In 1978 the thermal neutron backscattering spectrometer IN13 started operation opening a new field in Q-ω space, i.e. high energy resolution at large momentum transfers up to 5.5 A^{-1}. We hope that the next generation cold neutron backscattering spectrometer IN10C will start its test experiment in 1991. The new instrument should supply a significantly higher flux than the old IN10 with even slightly improved resolution.

A great variety of physical problems are being studied with backscattering spectroscopy, ranging from hyperfine interactions to fractals and from rotational tunnelling to diffusion mechanisms in metals. More than 200 original papers have been published on results obtained with this method.

Future trends are μeV resolution at near meV energy transfers and neV resolution measurements in ω-space at momentum transfers up to 2 A^{-1}.

[1] B. Alefeld, Bayer. Akademie der Wissenschaften, Math. Naturwiss. Klasse 11, 109 (1966).

[2] H. Maier-Leibnitz, Nukleonik 8, 61 (1966)

[3] B. Alefeld, M. Birr, A. Heidemann, Naturwissenschaften 56, 410 (1969)

[4] A. Heidemann, Z. Phys. 238, 208 (1970)

[5] B. Alefeld, A. Kollmar, Phys. Letters 57A, 289 (1976)

[6] A. Heidemann, Z. Phys. B20, 385 (1975)

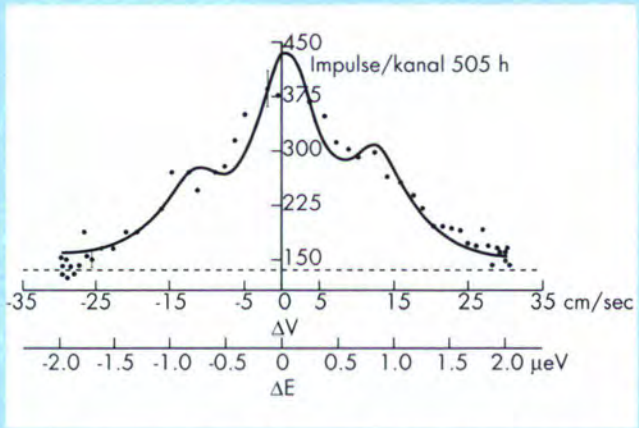


Fig. 1. Inelastic spin-flip spectrum of V_2O_3 at 105 K measured with the prototype backscattering spectrometer in Garching. Measuring time: 21 days! The hyperfine splitting is 0.8 μeV corresponding to an internal magnetic field at the vanadium nucleus of 175 kOe [4].

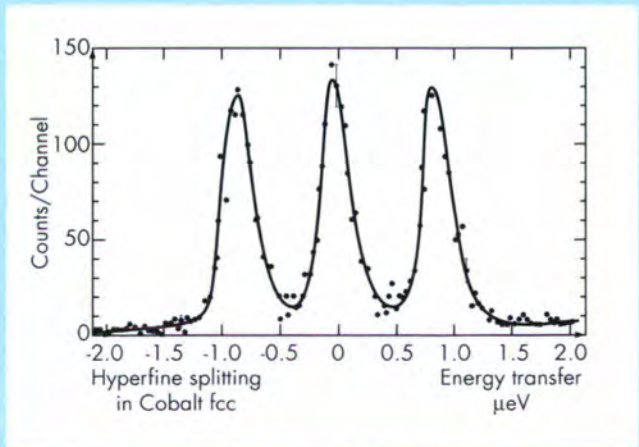


Fig. 2. Inelastic spin-flip spectrum of cobalt at 300 K measured on IN10. Beam time: 0.5 days. Note that the absorption cross section of cobalt is about 5 times higher than that of vanadium [6].

Diffraction Instruments

D1A: High resolution powder diffractometer on thermal guide H22 (A.W. Hewat, J-K. Cockcroft, J. Davies).

D1B: Two-axis diffractometer with multidetector on thermal guide H22 (C. Ritter, J.L. Soubeyroux, K. Ben Saidane).

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

D3B: Two-axis polarized neutron diffractometer with lifting counter on thermal beam H5 (F. Tasset, M. Vrtis (in part), A. Steinhof (in part), P. Feder).

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

D9: Four-circle diffractometer on the hot beam H3 (G. McIntyre (in part), M.S. Lehmann, J. Archer).

D10: Four-circle triple-axis spectrometer on thermal guide H24 (C.M.E. Zeyen (in part), G. McIntyre (in part), T. Brückel, R. Chagnon).

T12: Neutron camera on thermal guide H23.

D15: Four-circle MK6 diffractometer on the inclined thermal beam IH4 (J. Brown, M. Reehuis, G. Schmid).

D16: Four-circle MK6 diffractometer on cold guide H16 (G. Zaccai, E. Pebay-Peyroula (in part), V. Rodriguez (in part), J.M. Reynal (in part) R. Gay (in part)).

D19B: Multidetector diffractometer for protein crystallography on the thermal beam H11 (S.A. Mason, S. Bramwell, J. Archer, D. Robinson).

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 (E. Pebay-Peyroula (in part), C. Wilkinson (EMBL), P. Agnes). CRYOPAD Cryogenic Polarization Analysis (F. Tasset, A. Steinhof (in part), P. Feder)

D1A High resolution powder diffractometer on the Guide H22

Two features of D1A ensure that it continues to be in great demand - high resolution with long wavelength neutrons from the guide tube with a high take-off angle, and D1A's unique suitability for stress measurements. D1A can reach much larger d-spacings than current time-of-flight machines, essential for magnetic structures and for large structures in general, and does not suffer from higher order wavelength contamination as do reactor-face machines.

As well as a large number of scientific proposals, D1A is used more than any other ILL machine for paid industrial work, essentially stress experiments. Money earned from paid experiments was used in 1990 for example, to buy large numbers of vanadium sample cans for all ILL powder instruments, and to extend the detector bank of D1A from 10 to 25 detectors. The expensive Soller collimators will be contributed by the Gatchina (Leningrad) laboratory under an exchange agreement also financed by paid experiments.

D1B Two-axis diffractometer with multidetector on the thermal guide H22

No major changes took place on D1B in 1990. Some 60 experiments were carried out successfully, problems with the banana-detector appearing at the end of the year were provisionally fixed and will be definitely solved in early 1991 with the change of parts of the data acquisition electronics. The detector is now equipped with a 2θ- coder facilitating its reproducible positioning. The mounting of a small furnace inside a Eulerian cradle was completed to allow for texture experiments at elevated temperatures. A careful realignment of monochromator-filter-evacuated tube-sample table resulted in a gain of nearly 10 % in flux, compensating the loss due to the lower reactor power.

D2B High resolution powder diffractometer on the thermal beam H11

A new mirror furnace has been tested with promising results.We hope to reach 3000 K during 1991. More and more users take advantage of the short wavelength option (1.05Å and shorter). Unfortunately the monochromator problem is still pending. It is hoped that problems with squashing the crystals can be solved to enable users to exploit the full capabilities of D2B as a high-resolution diffractometer.

D3B Two-axis polarized neutron diffractometer with lifting counter on the hot beam H4

Owing to the pugnacity of S. Pujol and P. Feder during the unforeseen reactor shutdown, the old 4.62 Tesla cryomagnet was restored to its normal performance early this year. D3B therefore coped successfully with most of its programme which relies on this cryostat for moderately high applied magnetic field (1.5 Tesla - 4.6 Tesla).

A useful modification for experiments on electron densities (Schwinger effect) consisted in a new set of pole-pieces for the electromagnet. The "thin tail" variable temperature cryostat now in the pool (inherited from D5) can now be used on D3B extending the temperature range from 1.5K to 300K for experiments at low applied field (0.01 Tesla- 0.5 Tesla).

Three weeks of polarized beam-time were invested in an exciting test for the idea of a gaseous ^{3}He neutron polarizer.

D4B Disordered-materials diffractometer on the hot beam H8

The H8 beam tube was replaced in the early months of 1990. At the same time the mechanics controlling the monochromator curvature was upgraded. As a result of these modifications the flux at the sample level is now slightly increased, especially at 0.7 Å wavelength where the gain is about 10 %.

D9 Four-circle diffractometer on the hot beam H3

As usual D9 has covered a wide range of investigations from diffraction studies of chemical and physical problems - including structure analysis of high T_c compounds- through measurements using external conditions with laser activation of the sample or attempts at sample polarization by electric fields, to basic studies of the relationship between resonant scattering and atomic thermal motion. Further pressure work has also been carried out, in collaboration with groups from the University of Karlsruhe, and this culminated at the end of the year in a first test of single crystal neutron measurements at 30 Kbar.

In parallel to this, some improvements have been made to the instrument, notably on the level of the monitor environment. This has reduced the general background, which is essential for the correct operation of the small position-sensitive detector, and at the same time automatic location of the second-order filters has been installed.

During most of the year the position-sensitive detector with its 32 x 32 pixels has continued to be an invaluable part of many studies. A good example of this was a calibration of the new high-temperature, high-stability furnace employing the α-(INC)-β phase transition of quartz at 845K.The growth and movement of the satellite reflections of the INC phase across the transition was clearly demonstrated (see Fig. 1 a,b,c,d).

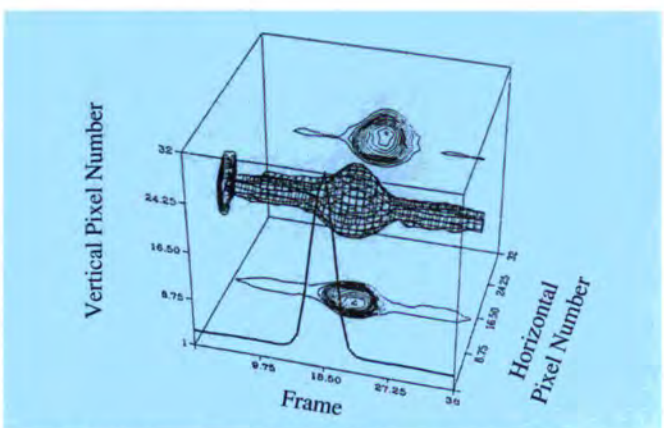


Fig 1a. 220-type reflection in the β-phase at 846K. Note the diffuse tails in the scan direction.

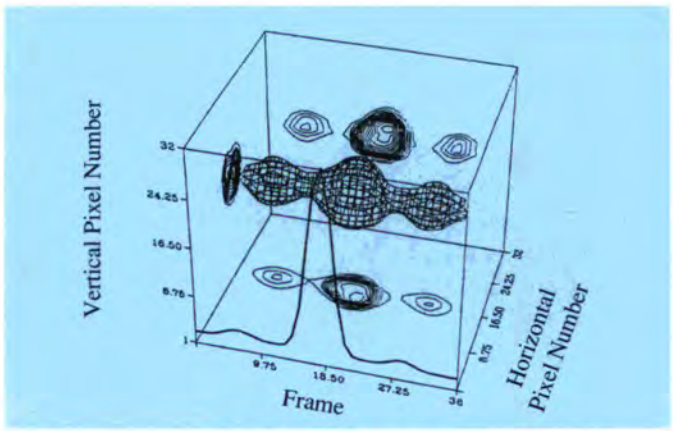


Fig 1b. 220-type reflection in the INC phase at 845K. Only 2 of the 6 satellites are seen due to the limited instrumental resolution.

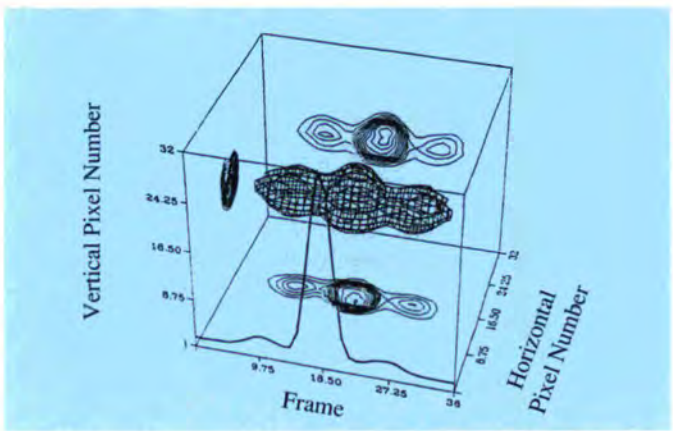


Fig 1c. 220-type reflection in the INC phase at 844.6K. The satellite reflections have moved closer to the fundamental peak.

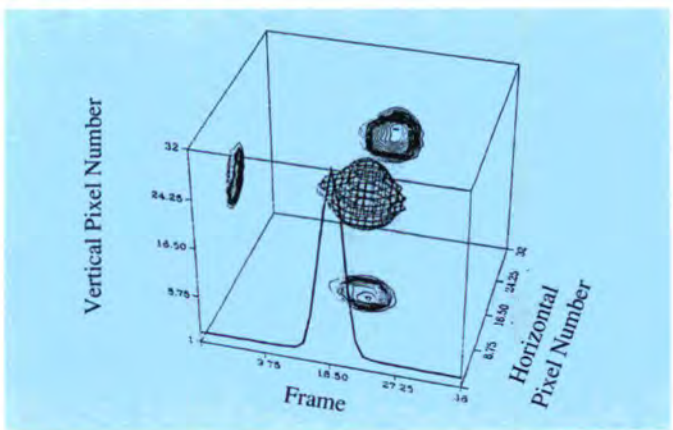


Fig 1d. 220-type reflection in the a-phase at 844.4K. A single reflection without diffuse tails.

The β—> incommensurate (INC) —> α phase transitions in quartz

D10 Four-circle triple-axis spectrometer on the thermal guide H24

The heavy user demand for special sample environment and the wearing out of the old D10 cradle and double tilt goniometer made a complete redesign of the sample support necessary. We purchased a HUBER turntable and asymmetric open Eulerian cradle (non-bisecting geometries!) combination. The ω-axis has direct encoding with an absolute error of less than 4/1000 degree. This precision is required for the excellent resolution available on D10. All axes are equipped with BERGER-LAHR five-phase stepping motors. These are virtually resonance-free and thus allow much faster and more accurate positioning. The asymmetric cradle leaves more space for the new D10 four-circle dilution cryostat built by S. Pujol (0.1K) but also facilitates the mounting of other sample environment devices such as furnaces.

D15 Four-circle diffractometer on the inclined thermal beam IH4

D15 continues to be used for studies of single crystals under a wide range of external constraints. Unfortunately during most of the year the 32 x 32 cell multidetector has not been available because of problems with its stability. It is to be re-installed early in 1991. During the long shutdown in the spring the instrument was completely dismantled to allow the replacement of the H10 beam tube. The reinstallation was carried out successfully and the programme of scheduled experiments was restarted in early June. The realignment of the supporting structure for the monochromator on the inclined beam is not easy, and each reinstallation seems to involve a small flux loss in the monochromatic beam.

To facilitate experiments in the Thor vertical field cryomagnet an omega module which rotates the sample stick inside the cryostat has been constructed and shown to work quite satisfactorily.

D16 Diffractometer on the cold guide H16

D16 remains a unique instrument for experiments requiring good Q-resolution at low Q (~ 0.05 to 2.0 $Å^{-1}$). Experiments performed on D16 in 1990 included studies of natural and model biological membranes, collagen, polymer solutions, protein interactions, surface lattices and intercalated compounds, ordering in alloys, liquids, magnetic frustration, liquid crystals, micro-emulsions, etc. Sample environment facilities have continued to be improved with the purchase of a Time & Precision x-y-z table for the mounting of cryostats or other large equipment. Software for single crystal experiments is now fully implemented.

D19 Multidetector single crystal diffractometer on the thermal beam H11

During 1990 D19 was used for a wide variety of experiments which made use of the 4° x 64° position-sensitive detector : studies of polymeric fibres, inorganic complexes, phase transitions at very high temperature, etc. Feasibility studies of porin and parvalbumin demonstrated, again, the need for the new 20° x 64° detector, for high-resolution studies of macromolecules where only small crystals can be grown. Colour graphics programs were developed and tested on the Vax-station 3100 shared with D2B and D20. Programs for planning measurement strategy are under investigation.

D20 High-flux multidetector diffractometer on the thermal beam H11

D20 has continued to operate smoothly in 1990 in its current small detector version. There have been no major changes on the instrument during this year and the instrument has been heavily scheduled with a mix of standard powder diffraction experiments under various environmental conditions and less conventional ones such as texture measurements, H-T phase diagrams and stress measurements. Owing to the limited size of the current detector, only a few time-resolved experiments have been performed. As in the previous years, the beam-time has been equally shared between colleges 5 and 6 with in addition a few experiments from college 9.

DB21 Four-circle diffractometer with PSD for biological macromolecules on the cold guide H15

A computer upgrade to a GPX workstation for better on-line multidetector data treatment and display is scheduled to be operational by 1991.

Coordinator: C.M.E. Zeyen

Special instruments and experiments

Most of our special activities were in routine operation in 1990. Major changes, improvements or progress may be summarized as follows:

SN7 Reverted to the status of a scheduled instrument and in compensation PN8 became a special instrument, SN8 (see also Instrument Group "Fundamental and Nuclear Physics").

S18 The thermal neutron interferometer modified its double crystal set-up by using three high resolution goniometers working as a "Lenkerfeder" system and using spiral springs giving best resolutions of 2 x 10^{-6} seconds of arc per motor step. New crystals provided a beam separation of 1 cm and increased the Pendelloesung length by about a factor of 4 in comparison with the former version. Weak indications of interference effects were observed.

S20 The diffractometer S20, mainly devoted to topography, is an ILL-CNRS collaboration. It has been used by about ten European groups to perform extinction and domain investigations, mostly on magnetic crystals. The instrument improvements (enhancement of flux, automation) have considerably reduced the time necessary for a given experiment. It is thus possible to investigate new topics on single crystal magnetic materials, e.g. to follow the behaviour of a set of Bragg peaks while varying the temperature and/or the magnetic field. Motorisation and encoding permit the detector to be moved by about ± 20°, and the sample environment will be either a) a fine tail cryostat and an electromagnet or b) a 6 Tesla and 1.5 K cryomagnet. These extensions have been started and will, hopefully, be finished in 1991.

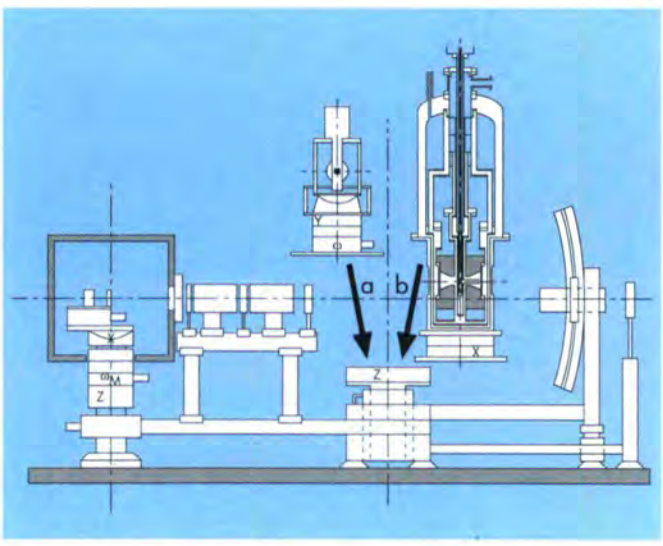


Fig. 1. Schematic drawing of S20

S21 was operated with several user groups for almost routine Ultra Small Angle Scattering (USANS) experiments. The Q-range is 5 x 10^{-6} to 5 x 10^{-5} Å^{-1} depending on the scattering power of the material under study. It is intended to extend this range to larger values by the use of less perfect crystals to achieve an overlap with the other ILL SANS cameras D11 and D22. The present set of Silicon (331) crystals will have to be replaced by thinner crystals to reduce thermal diffuse background scattering. Stability problems were also encountered with the present set of tilt goniometers which will have to be replaced by more accurate ones in the near future. It is planned to effect tilting and rocking movements with piezo-drives for improved accuracy.

S50 The experiment for the precision determination of h/m_n. Efforts are continued to improve its instrumentation. In order to replace the Meander coil, a ferrite modulator will be installed early next year and an intensity modulator is under construction; it consists of a mechanical choppper of 30 cm diameter, a rotational speed of 15.000 rpm with 20 µm wide slits and 20 µm wide Gd-absorbers resulting in a pulse frequency of 5 MHz (see also Instrument Group "Fundamental and Nuclear Physics").

With the **EVA**nescent wave diffractometer surface sensitive Bragg scattering was observed from various samples (Si, CaF_2, InP). Surface scattering was separated from bulk scattering (see fig. EVA for scattering geometry) by pushing the exit angle resolution to 1.5 mrad with typical countrates from near surface Bragg scattering (≤ 200 Å) of 1 neutron/sec. After improving the shielding the signal to noise ratio is now 10^3 for surface scattering and an additional PSD is expected to further improve noise and resolution. Observation of the temperature dependence of these Bragg reflections should be possible. Several reflectivity measurements were performed for studies of surface roughness and mean scattering length densities, reflectivity being measured down to 10^{-6}. Recently, a new monochromator (two slightly misaligned PG crystals) doubled the flux to 1.8 x 10^5 neutrons/cm^2/sec with 1 mrad vertical divergence. Gradient crystals may improve this further. For glancing angle studies an accurate cryostat has been developed (15 mdeg) and the vacuum chamber will soon be usable over a wide range of temperatures. For sample preparation a cold room has been installed near the EVA-site.

The activities in the field of ultra-cold and very cold neutron research **(VCN/UCN)** can be summarized as follows:

The EDM apparatus has been modified and will resume measurements in 1991. - The construction of a new neutron lifetime bottle for use with monochromatic UCN has started. - NESSIE, the neutron gravity spectrometer was equipped with an improved interior shielding resulting in lower and flat background. - The VCN optics facility acquired a cabin reducing simultaneously sound and temperature fluctuations.

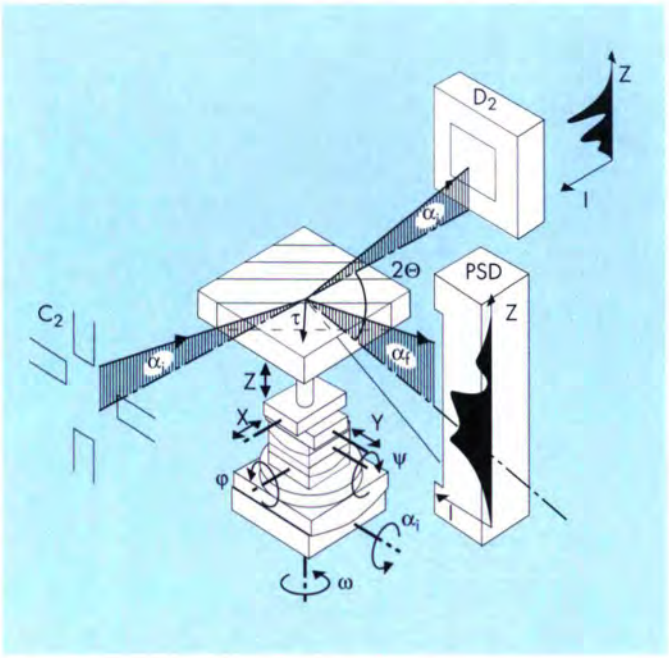


Fig. 2. Scattering geometry of the EVAnescent wave diffractometer
D2: Specular beam detector with a radial intensity spectrum represented behind
PSD: Position sensitive detector for surface Bragg scattering.

The levelling system of the optical bench has been equipped with new high precision valves so that variations in supply pressure no longer interfere with the levelling performance. The level stability of the top surface is now better than 4 arcsec in 3 days. The alignment procedure for the optical elements is servocontrolled by a personal computer. A new series of transmission phase gratings with a grating constant d = 1 μm has been tested successfully. It should now be possible to measure the phase shift of the neutron due to the Earth's gravitational field as well as Berry's phase shift (see also Instrument Group "Fundamental and Nuclear Physics").

Coordinator: W. Drexel

Scientific Coordination and Public Relations

Statistics of the Scientific Programme

Due to the unforeseen reactor shutdown at the beginning of the year the scientific programme was shortened. Beam-time allocated in April 1990 included half a cycle (cycles are now 46 days), which will actually be run in January 1991. 1268 proposals (S-instruments included) were submitted. The total beam-time requested was 10205 days (S-instruments excluded); 4935 days were allocated. For the Scientific Council in October 1990 (beam-time allocation in 1991) the ILL recorded a top number of proposals: 657. We take this opportunity to thank the Subcommittee members for achieving their difficult task of adjudication. Fig. A shows the number of proposals covered by each College - the record is held by College 6.

The instrument PN8 became an S-instrument, SN8, at the beginning of September 1990 and SN7 was reappointed a scheduled instrument, PN7. This change is due to SN8 now being used by one group, whereas the demand from different groups on PN7 has increased over the last Subcommittee meetings. The instrument statistics (Fig. B) display the beam time for the two instruments in their PN mode only.

Fig. B shows the beam-time statistics on the scheduled instruments. The overload factor is 2.1 which is partly due to the reduced beam-time available (228 days of reactor operation) in comparison to 1989 (262 days). On D4, D15, IN1 and IN8 less beam-time was available than usual, since their beam tubes had to be replaced.

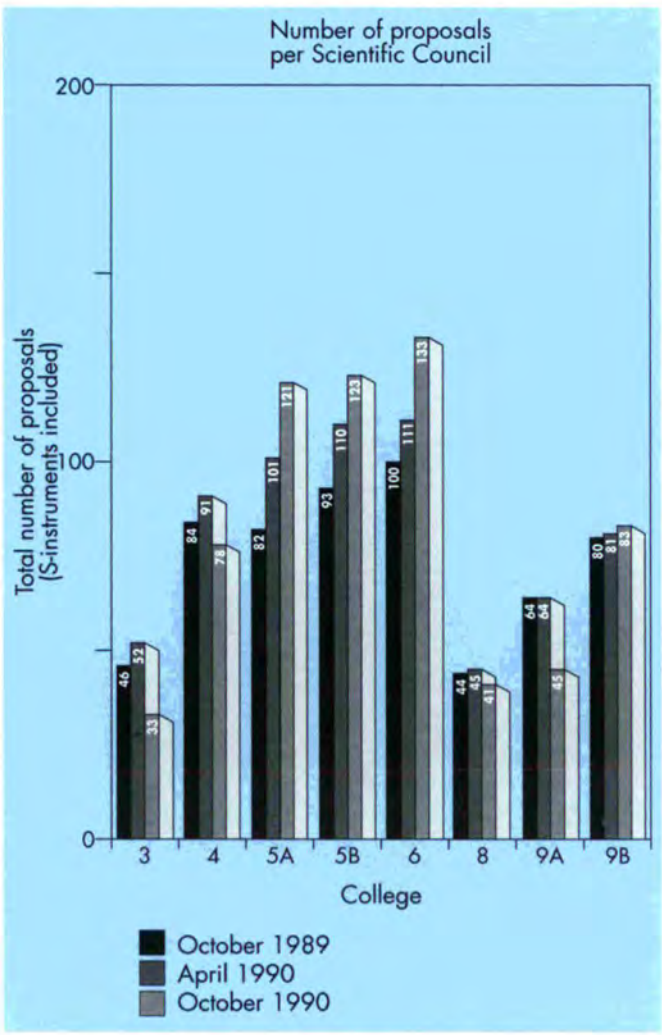


Figure A: Number of proposals per College

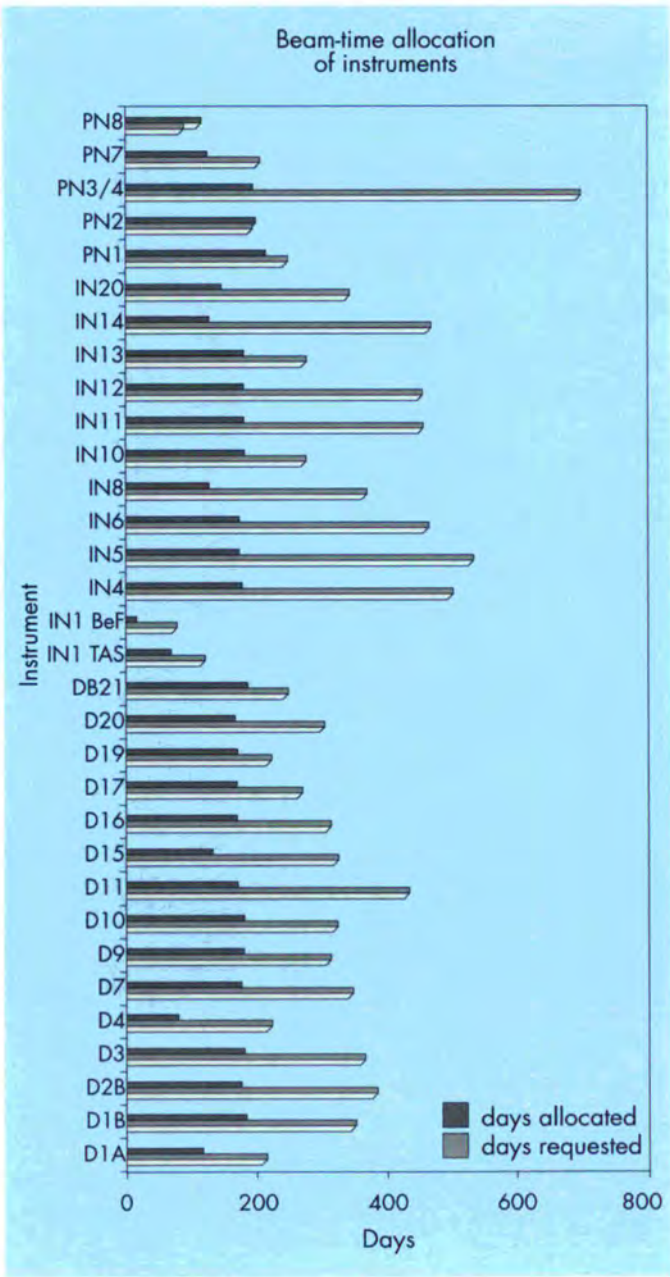


Figure B: Instrument statistics in 1990

Austria joined the ILL as a third scientific member in 1990. Fig. C shows the distribution of beam time amongst the 6 member countries (S-instruments are excluded).

The distribution of the experiments amongst the different Colleges is shown in Fig. D.

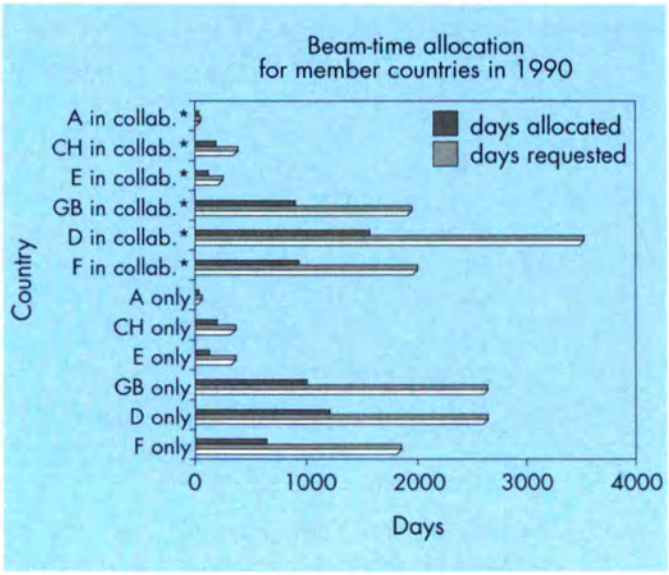


Figure C: Beam-time allocation for the six member countries
** may be counted several times*

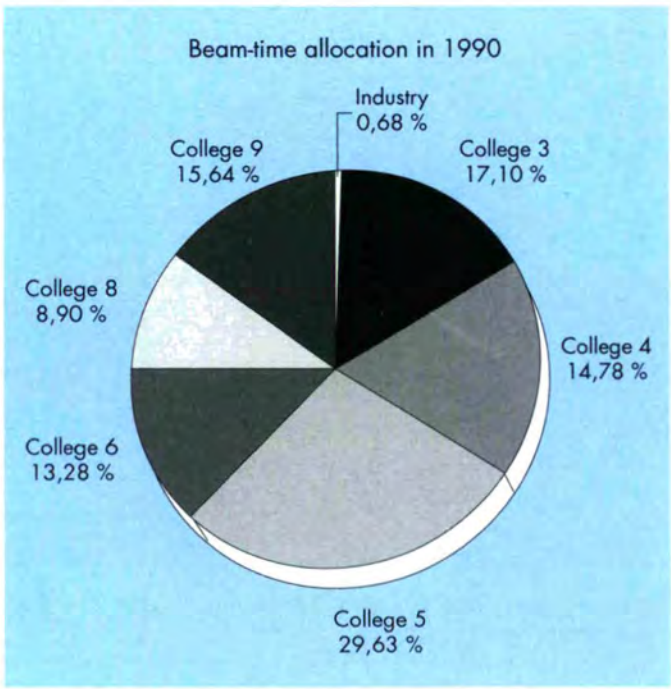


Figure D: Instrument days allocated per College in 1990 (total of 4935 days)

Safety, Medical and Health Physics Group (SPS)

Health Physics and General Safety Units

As part of their support function for the various departments at ILL and the guest scientists, the Health Physics and General Safety units participated in the following activities this year:

- provision of neutrons for the new experimental instruments IN10C and IN15 in the second Guide Hall ILL22 for tests for their provisional and final acceptance
- removal of the last section of drains for "eaux spéciales";
- replacement of beam tube liners H8 and H10;
- continuation of the programme of renewal of the remote detection fire alarm system;
- organisation at ILL of overhead crane driving courses for scientists;
- updating by CAD of safety intervention plans for the ILL buildings.

Works Medical Service

The Works Medical Service monitors the technical and scientific staff as a function of the risks to which they may be exposed in their work. The Service carries out medical examinations and biological, radiological and toxicological tests. These examinations also permit pathological conditions to be identified and advice given to staff.

The Service also studies workstations and conditions of work to determine the medical surveillance criteria, and to evaluate the risks in connection with work, in collaboration with the Safety and Health Physics units, and is represented at meetings of the CHSCT (Committee on Health, Safety and Working Conditions).

These activities make it possible to evaluate the actual or potential effect of work on health and to propose modifications to working conditions as necessary.

The medical team comprises a part-time doctor, a full-time nurse, and a part-time nurse and secretary.

Joint ILL-ESRF Library

The "Agreement on the Operation and Maintenance of a Joint ILL-ESRF Library" was signed by the Directors of the ILL and ESRF and the ILL Library became the "Joint ILL-ESRF Library".

Following this agreement, the ESRF contributed 20 % for 1990 to all library costs and literature acquisition was increased by 10 %. Despite this, increases in subscription prices necessitated an adjustment of 45 F in literature costs.

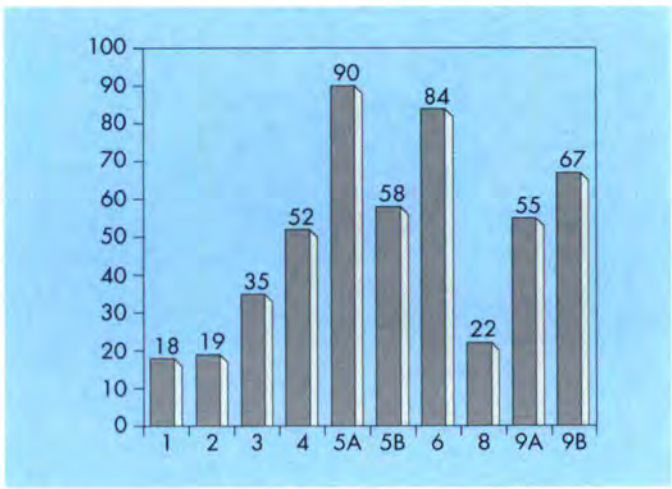
The overall budget was 925 KF (ILL: 740 KF, ESRF: 185 KF)

In 1990 :

- 780 books were processed:
  - 430 for the Joint Library
  - 100 deposited with the ILL Departments
  - 150 deposited with ESRF.
- 350 purchase orders were typed:
  - 90 for the Joint Library
  - 130 for the ILL
  - 130 for the ESRF.
- 660 volumes of journals were bound.
- 60 online searches were performed on computerized databases.

In close connection with the scientific life of the ILL,

- 500 publications
  - 400 with ILL authors and coauthors
  - 100 without ILL authors and coauthors but related with ILL experiments.
- 500 experimental reports were received.



Publications received in 1990 by subject
From classification in use at ILL:
1 – Instruments and Methods; 2 – Theory; 3 – Nuclear Physics
4 – Excitations; 5a – Crystal Structure; 5b – Magnetic Structure
6 – Liquids, Disorder, Metal physics; 8 – Biology;
9a – Molecular spectroscopy, Surfaces; 9b – Large molecules

Physicists' Secretariat

Organisation of Visits to the Institute

Each year, ILL receives many requests from foreign or French universities and laboratories for visits to its installations.

In 1990, there were 60 visits with a total of 1080 visitors who were shown around the neutron guide hall and the experimental hall of the reactor. These visitors (scientists, students, and non-scientific visitors) were guided by scientists, engineers or technicians representing as closely as possible the fields of research, the various ILL departments and the experimental facilities.

The following table shows the number of visitors per country:

France	750
Germany	115
Italy	50
Switzerland	35
Spain	27
U.K.	20
USA	15
Sweden	15
Others	53

Mechanical Engineering

As in previous years, the work of the mechanical engineering group in 1990 comprised three main parts:

1) Continuation of the construction of major new instruments to use the neutrons from the horizontal cold source (IN10C, IN15, D22).

2) Intervention work on existing instruments for improvements, additional equipment, maintenance or repair work.

3) In connection with the two points above, the systematic search for all new products or techniques developed by industry, which can contribute to providing better solutions (more efficient, more reliable or less expensive) to the technical problems raised by the scientists (use of composite materials or non-magnetic components, or of their low weight associated with the anisotropy of their resistance to mechanical stresses to improve the performance of choppers, etc.)

The continuation of construction of major instruments includes:

the mechanical assembly of the flight tube of the small-angle instrument D22 with the help of the supplier, alignment of guides, design and construction of the new "casemate" for the velocity selector.

Assembly on site of the new spin-echo spectrometer IN15, with composite material beams supporting solenoids (weight of the order of 2 tons).

As regards IN10C:

Choice of supplier and ordering of large mechanical assemblies for this new backscattering spectrometer (sample support and shielding for analyzers, installation to be completed in 1991).

Construction and long-term testing of the chopper supporting the graphite deflectors

Assembly of the new selector (80% composite materials) supporting a solenoid for guide field

Construction for this same spectrometer of a system for time-of-flight analysis, based on 3 concentric axes mechanical choppers. This system, of which the mechanical part was entirely designed and built by the Group, was produced as part of a collaboration with KFA Jülich on motorization and electronic control.

Among the many interventions on existing instruments may be mentioned:

the complete production of ILL-type selectors for D11 and IN11. They are due to start up early in 1991.

Complete responsibility for the construction and assembly of new non-magnetic collimator for D11. This 40 m long assembly incorporates internal guides for which removal from or insertion in the beam access can be controlled from a distance. We hope that the particularly careful examination of the assembly and test conditions will make it possible to install this in record time at the beginning of 1991, so as to minimize the instrument closure period.

Intervention work on IN5 for a Brillouin scattering on T13A, D3B, IN14, IN20, etc.

The drawing office, workshop and test workshop team have contributed to these major projects, partly with the aid of the following additional equipment:

- a second CAD work station
- replacement of a lathe
- a complete mechanical overhaul of the Gambin milling machine.

Finally, with the help of an extension of the test workshop assembly area, assembly has started of the largest banana-type detector ever built, due to be installed on D20 early in 1992.

Electronics Group

1990 was the year of the VME, the new standard in electronics.

IN6 Conversion from CAMAC to VME carried out without any major hold-up of experiments. This means that a large time-of-flight spectrometer is now operational using the VME standard.

IN10C The instrument is built completely in VME: there is a VAX as host computer

- data acquisition
- Doppler control
- access control
- chopper control with phase adjustment.

T13A The instrument is built completely in VME: there is no host computer. The data are automatically stored on DIVA. There is only a MACINTOSH as front end computer; programming in Basic.

- data acquisition
- axis control (11 axes)
- control of shielding
- position indication on additional TTY

IN15 The instrument is built completely in VME: there is a VAX as host computer.

- data acquisition operates via multidetector
- static coil current power supply control by VME and IEEE488 operational
- velocity selector control: currently under test
- dynamic part to be supplied from Jülich in 1991 (chopper control, ramp control, etc.)

D22 The instrument is to be completely built in VME.

- data acquisition in course of development

- collimation:
  – to be controlled by a programmable controller.
  – Design study for programmable controller completed; invitation to tender in progress

D20

- 1600 addresses
- definition phase for data acquisition and prototype phase completed
- invitation to tender for series in progress
- 3D-graph data presentation on MACINTOSH completed.

S3 Rebuilt in CAMAC-standard with MACAMAC (after destruction by fire) and commissioned.

Monochromators

The group has continued to give advice and provide assistance in the construction of monochromators, e.g. for IN10C, IN4, D2B and EVA. In parallel, development work on projects such as Si-Ge based gradient crystals and wafer based monochromators with extreme anisotropy are being pursued actively. An extension for three years of a collaboration with the MPI für Metallforschung in Stuttgart for growing Be single crystals was signed in the spring. All other long term partners of the ILL in this project are favourably considering this continued commitment or have already signed the relevant contracts. Part of the work of the ILL consists in checking the quality of the as-grown crystals, and a particularly interesting structural defect is shown in Fig. 1.

There is a continuing high level of demand for beam time on the diffractometers of the group for both genuine workload of the group and test time requested by users preparing experiments. It is expected that this situation will ease when T13A is commissioned by the end of 1990. In close collaboration with the Computing Department, the installation of software which closely follows the systems on other single detector diffractometers at the ILL has been extended.

Numerous requests from external laboratories are addressed to the group for help in the construction of neutron monochromators. In view of the means available, these requests cannot be considered favourably. Exceptions can only be made when the entire manpower is provided by the home institute, as was the case this year, when Dr. M. NISHI from the University of Tokyo joined us for six months to prepare the crystals for one Heusler monochromator.

Finally it should be mentioned that present studies for the new improved hot source of the ILL have been largely supported by the group.

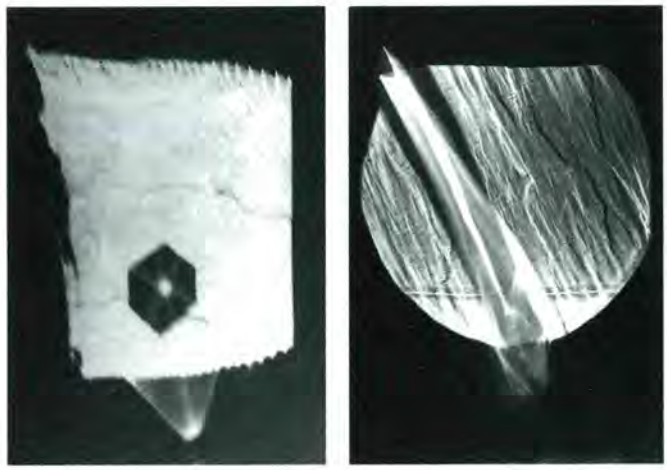


Fig 1: X-ray topography taken at LURE on a structural defect in an as-grown Be-crystal. The geometrically well defined white beam (10 μm) intersects the crystal parallel and perpendicular to its growth axis on the left and right side of the figure, respectively (support from J. BARUCHEL is acknowledged).

Multilayer Laboratory

The Electrotech evaporator has operated without major break-downs. The adsorption pumps of the Riber evaporator, needing long cooling times with liquid nitrogen, were replaced by a turbomolecular pump, giving a considerable gain factor in pumping time. New software for the Camac control of the evaporation process was written.

The main supermirror production time was spent on the new 600 mm long IN11 analyser. Due to the unscheduled reactor shutdown, part of the supermirror production could not be checked. Production faults were therefore not corrected immediately and many supermirrors had not the required quality. A first version was assembled and tested on the IN11 spectrometer (see photograph page 78).

Special developments were the 140 layer Titanium-Cobalt bandfilter for a special beam experiment on the H18 neutron guide and a prototype for the focussing mirror device [5].

Results of the IN14 polariser designed for λ=2.5 Å measured on the IN14 spectrometer and of the provisional supermirror analyser on the IN15 spectrometer are now available. The small polariser with a channel width of 0.4 mm for the Zero Field Spin-echo experiment shows a transmission of 40 % at 2 Å and 20 % at 1.4 Å with flipping ratios of 40 and 20 respectively. It was also used to measure the magnetic field in the long shielded flight tube of

the neutron-antineutron experiment [1]. Tests of Heusler single crystals were performed by M. Nishi and A. Magerl using 2 Å neutrons polarised by a supermirror bender.

Some time was devoted to work for external laboratories and industry in the framework of the Supermirror Collaboration. A supermirror coating on Borkron glass substrates polished using a new method developed by Cilas for the KFA convergent neutron guide gives reflectivity results comparable with float glass. In collaboration with PSI, diamond-like carbon layers with deuterium were tested and show encouraging results [6]. The test facility was used by PSI Würenlingen, HMI Berlin and Cilas Marcoussis.

Visitors from external laboratories are interested in the fabrication of polarising supermirrors. A.F. Schebetov from the Leningrad Nuclear Physics Institute and M. Nishi from the Institute for Solid State Physics of the University of Tokyo spent some time at ILL to learn about the equipment .

Publications and conference contributions:

[1] U. Schmidt, "Weiterentwicklung eines Prototyps eines Neutronresonanzspinechospektrometers" Diplomarbeit Heidelberg 1990

[2] O. Schärpf, "Die Zukunft von Experimenten mit polarisierten Neutronen" GKSS-Experimentiereinrichtungen am Forschungsreaktor FRG-1, Geesthacht März 1990

[3] O. Schärpf, "Flugzeitspektroskopie mit polarisierten Neutronen" DPG 54.Physikertagung, München März 1990

[4] O. Schärpf, "Status and performance of multilayers and supermirror polarizers" Workshop on Neutron Optics, Grenoble Sept. 1990

[5] D. Dubbers, "High intensity neutron spots" Workshop on Neutron Optics, Grenoble Sept. 1990

[6] P. Böni, I.S. Anderson, R. Hauert, P. Ruterana, K. Solt, B. Farnoux, G.J. Hertman, J. Penfold, O. Schärpf, "Investigation and growth of multilayers" paper presented at the ICANS-XI Conference, Tsukuba Oct. 1990

Multidetector Group

A major effort was made with the production of an easy-to-use **P**osition **S**ensitive **D**etector for neutrons (PSD) based on the principle of a wireless **M**icro**S**trip **P**roportional **C**ounter (MSPC) first developed at ILL (see Annual Report 1989). For position determination the charge division method was chosen. Firstly, because in a gaseous neutron detector the pulse shape on the electrodes varies due to different ionization tracks, and secondly, because only a small amount of less dedicated electronics is needed. Up to now a prototype of a one-dimensional PSD with an active

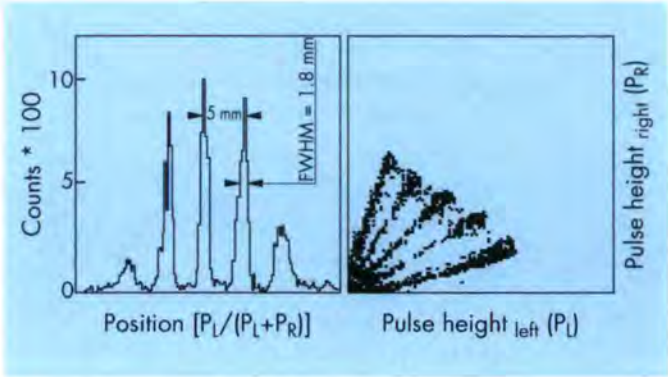


Fig. 2: Pulse height matrix of the one-dimensional MS prototype detector with 5 aequidistant beam spots for charge division read-out (right) and deduced one-dimensional position spectrum (left)

area of 80 mm x 64 mm has been constructed. Its performances are shown in the raw pulse height matrix (Fig. 2 right) from which, on-line, a position spectrum (Fig. 2 left) can be deduced. The measured spatial resolution is 1.8 mm (FWHM), in accordance with theory. It depends of course on the mean trace length of the charged particles created in the neutron reaction. Currently tests with a two-dimensional detector of this type are in progress.

In MS plate based detectors - alternating narrow and broad conducting strips in the submillimeter range on alternating electric potentials - the positive ion cloud produced in the avalanche does not screen the electrodes for a substantially long time, as the drift distances are very short. Their limiting count rate is therefore higher than for common wire detectors. To benefit from this intrinsic property a ^{3}He counting tube has been made by simply replacing the central anode wire by a small piece of an MS plate. In Fig. 3 the pulse height spectrum of a commercial ^{3}He counting tube is compared to this new MS counting tube. It should be noted that the energy resolution is comparable, whereas the applied high voltage is moderate for the MS tube. In a first test a limiting count rate more than an order of magnitude higher has been measured. However, the attainable limit was not yet reached.

Of course, the detector group continues to develop and construct **M**ulti**W**ire **P**roportional **C**ounters (MWPC) which still offer several interesting features. For an experimental installation at the Orphée Reactor in Saclay a 128 x 128 wires detector with a wire spacing of 1.5 mm has been built including analog and read-out electronics. In this multidetector a delay line read-out is used to determine the positions of the incoming neutrons. It has been in smooth operation since May (see photograph on page 81).

Within the framework of the transfer of this MWPC technology to industry and with the direct aid of ILL staff, different PSDs for neutrons have been built successfully or are under construction. Among them a PSD (32 x 32 cells with 10 mm wire spacing) with individual read-out and a huge Banana type detector with 9024 cells for the HMI Berlin may be cited.

At ILL the new IN15 multidetector has been installed at its final beam position in the new guide hall after increasing the partial pressure of the stopping gas propane to 0.5 bar. The multidetector is now in an operational stage.

As another part of the activities of the detector group two MWPC detectors have been modified. This was necessary because of instabilities and a general diminution in their performances. Various tests have been done to reveal the origin of their defects. It was found that different wires were locally damaged. This was probably caused by trace impurities in the gas provoking local precipitations on these electrodes. In the case of the D15 multidetector the electrodes have been completely replaced by a new set. In addition, the stopping gas was changed: propane, which has a tendency to polymerize under elevated neutron fluxes and to deposit on the anode wires, was replaced by CF4. In the D9 case similar but less serious symptoms have been found. After repair, both detectors have been tested extensively. They are again ready for operation and have already been set up again at their normal measuring positions.

During the year, a third fully equipped and versatile pumping and filling unit for detectors has been built up. One of the units has been equipped recently with a hygrometer, which permits measurement of traces of water vapour down to the ppm level. As water is one of the most difficult vapours to eliminate from a detector housing, such an instrument leads to a reliable measure of the cleanness inside the housing. This is a very important - but often neglected - criterion for the quality and lifetime of a detector.

Last but not least the group frequently provided assistance to inhouse staff and users for the various types of neutron detectors and monitors installed at the Institut.

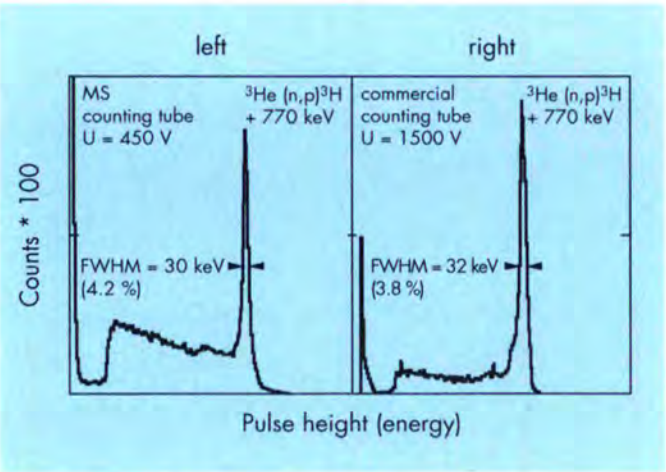


Fig. 3: Pulse height spectrum of the MS counting tube (left) compared with a commercial counting tube (right).

Other Activities

First test at ILL of a ^{3}He neutron polarization filter

^{3}He is a very efficient absorbing gas for neutrons. In fact it is only the singlet combined state of these two spin 1/2 nuclei which is absorbing [1]. If it is fully polarised ^{3}He doubles its absorption cross-section for "down" neutrons and becomes transparent for "up" neutrons. Although, the unique features of polarised ^{3}He as a broad band polarising filter for thermal and epithermal neutrons has been recognised for over two decades [2], it is only recently that decisive progress in the techniques of optical pumping made the idea of a gaseous ^{3}He neutron polariser feasible [3].

Having discussed several possibilities [4] we are now embarked at ILL in a collaboration with Harvard University and Grenoble University for the development of a polarised 3He gas filter [5].

The polarising process is based on the optical pumping of a Rb/^{3}He mixture which offers directly the appropriate high density of ^{3}He necessary for a neutron polariser. A beam of polarised light transfers angular momentum to the alkali atoms, which in turn exchange polarisation with the ^{3}He spins through hyperfine interaction.

A first feasibility test was recently conducted at D3B with neutrons of 0.84 Å wavelength [6]. The incident neutron beam was almost completely polarized (98.5 %) by the (200) Bragg reflection of the CoFe monochromator crystal of the instrument and could be totally reversed by action of the cryoflipper. The tunable Titanium: Sapphire laser was providing 2W at 795 nm of which 30 % could properly be coupled with the Rb vapour. The measured flipping ratio (ratio of up/down neutron transmission) is reported in Figure 4 as a function of the pumping time. The deduced ^{3}He polarisation is also given.

As expected, the neutron signal was very easy to measure and confirmed that the cells were filled at optimised ^{3}He thickness, and that the principle was operating properly. Unfortunately the cell was having a relatively short relaxation time (2.3 hours) and therefore did not allow us to build larger polarisation.

Very successful application would require cells with much higher polarisation (75 %). This is becoming possible if we reach relaxation times at least 10 times longer. This improvement is not unrealistic since very long times (250 h) have been quoted in literature [7] The next crucial step in developing this potentially ideal polarising tool for our neutron beams, is to understand what limits this parameter in large cells at high pressure.

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[6] F. Tasset, T. Chupp, J. P. Pique, A. Steinhof, A. Thompson,E. Wasserman, M. Ziade, ILL Report in preparation

[7] W. A. Fitzsimmons, L.L. Tankersley and G. K. Walters, Phys. Rev. 179 (1969) 156

Special products

Major projects were the coating with gadolinium charged resin of the wheels for the new IN15 chopper, the fabrication of ZnS(Ag) charged lithium converters for neutron photographs, the lithium painting of the variable wavelength pyrolitic graphite filter for the IN14 spectrometer, and the sintering of lithium-fluoride plates for diaphragms and beam stops.

This activity suffered from the loss of staff. Two technicians have left this year causing a loss of knowhow, especially in the domain of lithium converter screens for Laue photographs. In consequence the work was done partially by inexperienced staff on loan.

Neutron guides

The alignment of the IN15 guides and the first 4 m of the D22 guides is completed. The mounting of the collimation exchange mechanics of D22 was carried out in collaboration with ABT technicians, the alignment of the 16 m collimation guides is planned for beginning of 1991. The replacement of the D11 collimation section is under way.

Preliminary studies for the prolongation of the H21 guide, the replacement of the H1/H2 in pile part and supplementary guides of the vertical cold source have started.

Computer aided design

The latest versions of Autocad (10.0) and Euclid (2.1) have been installed on the 386 PC and the two Vax working stations of the Project Office and the SCM drawing office respectively.

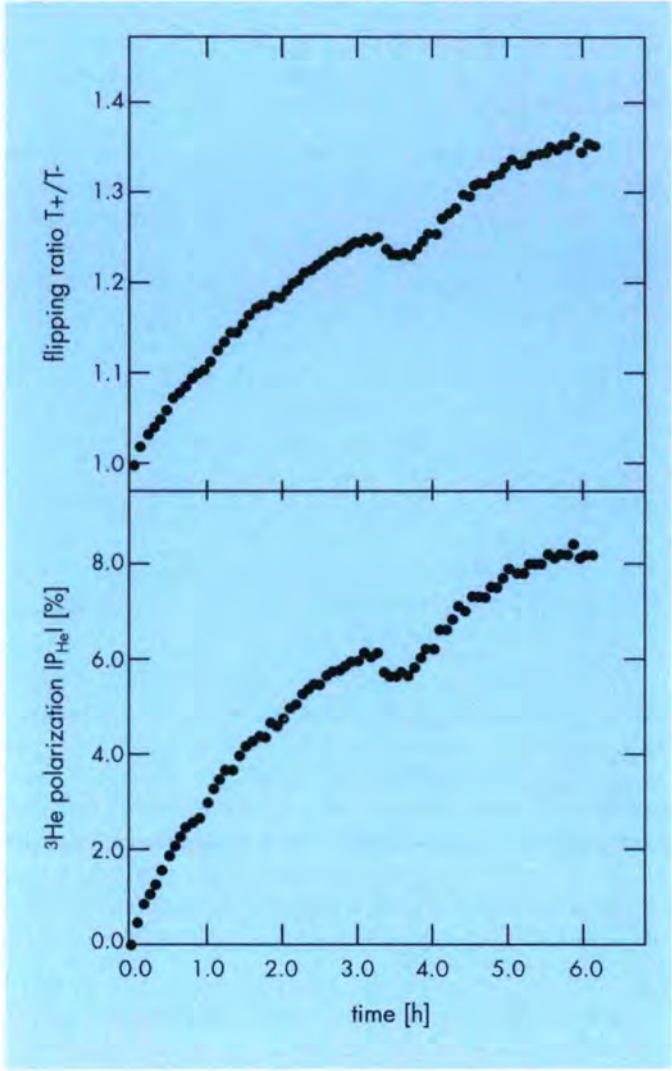

Fig.4. Gaseous ^{3}He neutron polariser: evolution with the optical pumping time of the polarised neutron flipping ratio and the corresponding ^{3}He polarisation. The kink in the curve is due to a 15 minutes disruption in laser light.

Central Facilities Service

Operations

The use of the cluster, consisting essentially of a VAX 8650 and a VAX 8700, increased slightly this year. In general on-line operations saturate the two units during working hours. To conserve the maximum of resources for on-line users we have therefore had to stop batch operation during this period of the day and only run it as background during the rest of the time. To compensate for this reduction in production of this work, part of it has been transferred and performed as a background task on VAXstation units associated with the cluster.

The level of utilisation of machines has been more than 1000 hours/month (Reference VAX 8650) with peaks up to 1200 hours/month. The ESRF share in these figures was of the order of 240 hours/month.

To improve access to experiment data, we acquired additional disks to store the current cycle and the 2 previous cycles on-line, which corresponds to approximately 3 gigabytes. All the experiment data for the previous years has been archived on optical disk.

In cooperation with the administration and office computing group, the team of operators participated in the operation of the administrative computers and the work of transferring ITOS documents to Macintosh. Following a reorganisation of the users of the ITOS wordprocessing system on a single machine, it was possible to release a microVAX II and make it available to an instrument.

As regards assistance to users, the operation group has been organised to ensure a first level maintenance for the terminals and Macintoshes: on call intervention work, diagnosis of any problems and coordination of assistance on problems with the maintenance companies.

Systems and communications

This group deals with the administration of a cluster of three VAXes (VAX 8650, VAX 8700, VAX 750) and of a local area VAXcluster (VAXstations) associated in operation with the previous VAXes, particularly for sharing of disks. A considerable effort has been diverted to the study and improvement of the performance of the machines, to permit work to continue smoothly, particularly during working hours. This study has been carried out in collaboration with Digital, and resulted in various measures, particularly as regards reorganisation of disks and the distribution of batchwork over the different central units available.

The utilisation of the external networks (EARN, TRANSPAC, JANET, HEPNET) has considerably increased. For example traffic on the EARN network amounts to some hundred outgoing messages or documents per day, and twice as many incoming.

To ensure that these communications function correctly, we have to provide continuous monitoring, particularly on the control of access and utilisation. At the request of the scientists we are looking at solutions for connection to the Internet network.

As regards network mailing we have obtained new products for development in accordance with the new standard X400.

A UNIX station, DECstation 5000, has been purchased and integrated in the ILL local network. This equipment:

- offers a UNIX environment to the CRAY users who will thus be able to prepare the work and examine the results on return,
- will be able to take over certain applications which do not operate satisfactorily on the cluster.

It will also be noted that two PC based workstations has been provided for scientists and visitors.

Mathematics

A seminar was organised with the theory and crystalllography colleges on the mathematica software, and after a test period it was decided to purchase it and support it on a Macintosh.

A contract has been signed between ILL and CEA on utilisation of the CRAY. The link with this machine has been effected with the SUN at ESRF. The service will provide the necessary assistance to future users of this new computing facility. A commission has been set up by the Central Computer Users Committee to examine proposals and allocate time on the CRAY on the basis of the budget for this purpose.

As regards the application ABFfit (maximum likelihood methods in powder diffraction refinements) the emphasis has this year been put on the publication of the results and the implementation of a new version. ABFfit-2D has been put on a transputer-based system by ESRF. The Orient Express software, version IBM PC, of the LAUE program has been commercialised by CYBER STAR under a joint CENG-ILL licence. This is a product for testing and orientation of crystals with the aid of the LAUE crystallographic technique. The VAX version has been expanded, with, in particular, simulation of Q vector satellite reflexions.

To respond to needs for data processing by image treatment techniques, we have acquired the OPTILAB software operational on Macintosh.

The persons responsible for this activity have also taken part in more general tasks in the operation of the service, such as writing the VAX user's guide, rewriting on Macintosh the message diffusion system on the video network, and subcontracting the product to assist the conversion of ITOS documents into WORD documents.

Graphics

As regards software a certain number of products have been transferred to VAXstations; these are programs for modelling and display of data (SCHAKAL, CHEMX, VIEW).

For the instruments D11 and D17 a contour program has been developed on the basis of the DISSPLA library.

As to hardware, the graphics group has a colour PC for evaluation of the graphics products available on the market or from research organisations. The demand for production of images in 256 colours and high definition is increasing; for this reason, after analysis of the market in slide generators and colour printers, we have chosen a POSTSCRIPT printer.

At the request of the biologists and chemists, it was decided to purchase a new graphics station (Evans & Sutherland or Silicon Graphics) in addition to the present Evans & Sutherland PS 300, to operate display software for polymers, proteins and electron density maps and structure analysis.

Telecommunications

Telephone:

in connection with the memorandum for a joint ILL/ESRF telephone service, a market study was carried out with the view to equipping the two institutes with the same system. The OPUS 4000 was chosen.

The two systems will be interconnected as a network to facilitate communications between ILL and ESRF and to share certain resources (control of payment units, voice messages, etc).

The responsibility for the internal paging system has been transferred from the Reactor to this group. The present system is an old design and results in maintenance problems with the receivers. A study has been carried out on new equipment which would integrate better with the new telephone system. The ILL and ESRF will acquire the same type of equipment, operated in common by the joint service.

Computing networks:

The group has participated in the development of the Ethernet and Appletalk networks. The considerable increase in the number of Macintoshes will require a reorganisation of the Appletalk network, for which a preliminary study has already been made.

Administration and office computing

Finance and purchasing:

At the beginning of the year the DEAL application was transferred to a microVAX 3300 (ATLAS), which is more powerful than the previous microVAX II. This has permitted the resolution of a number of problems due to a lack of hardware resources. We participated in the study of a CONCENTRATOR project, which should permit improvement of the handling of the implementation of the budget during the year.

Salaries and personnel:

The PACHA-T application on the SOPRA computers is running satisfactorily. The HERA package provides personnel management and training functions; this has been installed on a network of PCs in the administration, available to the sections concerned.

Office computing:

The shutdown of the MISMIS microVAX (transferred to an instrument) necessitated a reorganisation of users of the ITOS wordprocessing system on the MISVAX VAX 750. The decision to replace ITOS by the Microsoft product WORD on Macintosh was taken in November 1989, and the conversion programme should be completed as planned early in 91.

Modernisation of the MISILL applications (Scientific visitor programme):

A first application covering the handling of proposals for scheduling of experiments (SCAPRO) was implemented in March 90 on a microVAX 3000 called MISTER. The analysis by the MERISE method was carried out at ILL, and the specifications were supplied to an external company for implementation. The product was developed using an ORACLE database.

Studies of other applications such as library operation, travel office, and control of access to the site are in progress in collaboration with ESRF.

Instrument Service

In 1990 the aims of the Instrument Service were:

- maintenance of the hardware of the service and the rest of the department,
- standardisation of hardware and software on instrument computers,
- development and implementation of software for VME electronics,
- supervision of the in-house computer network,
- support for all the Macintoshes at ILL.

Maintenance

Support was provided for the service and the Nuclear Physics group; on a number of occasions work was done on various installations, particularly "S" instruments.

Standardisation of hardware and software on D and IN instruments

Two microVAXes were installed on D11 and D17, to replace VAX 11/730 machines; this was the opportunity to start rewriting programs for these two instruments, to enable the instrument service to provide full support to D11 and D17. The software for the time-of-flight instruments - IN4, IN5 and IN6 - has been standardised and a number of improvements have been made. The software for the triple axis instruments is being developed - (esp.) in collaboration with Mr Frick - to prepare for the transfer of the triple axis IN instruments to the MicroVAX standard and VMS.

The computers for the "Monochromator" group instruments are being standardised; installation of a PDP11/73 on the five gamma diffractometers (on RSX11M), installation of a PDP11/24 on T13C - these items are operational - development of the control software via a MicroVAX for T13A.

Several display programs have been developed for the "Multidetector" instruments D19, D9 and D15, on the basis of PV-Wave, and utilities are under test for IN4, IN5 and IN6.

The VIXEN unit, used for special measurements with polarisation analysis (CRYOPAD) on IN20 and D3, has been completely rebuilt.

A number of improvements have been carried out for D9, D15, D2B, D3, D10 and IN13.

Projects have been prepared for the replacement of the computers on DB21 and IN20.

Development and implementation of VME

The very considerable effort started in 1988 to develop the VME electronics has been continued and is starting to take shape; replacement of the IN10A software, installation of VME on the first "time-of-flight" instrument, IN6, complete replacement of CAMAC, software for the controls of the VME motor modules on IN10C, control software for power supply to coils on IN15 (in collaboration with Mr. Dagleish). The installation of VME on IN6 makes it possible to prepare the installation of the standard on IN4, IN5 and, as soon as the mechanical parts are available, on IN10C and IN15.

Monitoring of the network

Great efforts have been made to improve monitoring, safety, correct operation and reliability of the Ethernet computing network at ILL. Several programs and automatic procedures have been developed, and the network increased from three segments at beginning of 1990 to six in October 1990. The associated Institutes - EMBL and ESRF - and the *NN* instrument have been separated from the network by bridges in order to limit unnecessary traffic (in particular LAVC). The "administration" network comprising the MIS computers has been separated for reasons of security and confidentiality. This involved the recabling of a considerable part of the network - ILL4, ILL1 and ILL19. Efforts are now concentrated on the problems of performance and on the availability of the Ethernet network in all the buildings: reactor level C, test workshop, etc. Finally as there is a considerable increase in requests for the connection of personnel computers, a study is in progress incorporating the problems of the Appletalk networks.

Macintosh support

This support is becoming increasingly important, as the number of Macintoshes increases, both in the scientific area and the secretariats.

The year 1990 has been a very busy year for the Instrument Service, despite reduced budgets. Efficiency can be achieved essentially by increased standardisation of hardware and software. But a considerable proportion of the time is spent on support and assistance to users; this standardisation permits a simplification of the contact between the users and the various members of the Instrument Service.

Data and projects group

The Group supports current data treatment, and examines future strategies and systems for furthering this aim.

During the past few years the price of workstations has progressively fallen. The Group has recognised the high price/performance ratio for certain activities. A number of these systems, compatible with the central computer, have been acquired and placed in service. A Distributed File Service software, offering transparent access by a workstation user to remote files (typically those on the Central Cluster) has been implemented. Although this

simplifies workstation management it does entrain overheads on the file server system and network. Examples include installation of graphics workstations on D11 and D17 which, with the development of some network software, appear to be fully integrated into the individual instrument control computer environments. A further use of workstations at ILL has been demonstrated by theoreticians using the Group's own systems in a background batch mode, which have thus delivered several months equivalent central-computer time, without hindering development work.

Using two identical workstations, one running VMS and the second running under a UNIX supervisor (Digital's ULTRIX) it has been possible to start making direct comparisons of performance and operations on the two systems.

With the welcome addition of student effort the simulation using transputers for signal analysis for a multidetector has advanced. The aim is to test a number of algorithms for position location, identifying potential bottlenecks in the logical path before advancing to specifying a hardware design during the course of 1991.

Development of data-treatment was discussed more generally within the framework of a working group for the modernisation plan. The Group's general aims for developing a standard user interface were endorsed by these members.

As in the past the Group has assisted the principal services of the Computing Department from time to time. Lying across the activities of both, one function has been to emphasize the need for standardisation of the environment sensed by the experimenters who use both facilities.

Working with small groups of scientists has lead to several reports concerning data treatment, and to the preparations for a data treatment workshop in 1991.

Nuclear physics and special instruments group

This group is responsible for "Nuclear Physics" and "S" instruments.

The year 1990 was essentially one of general standardisation of instrument hardware and software, and of the use of existing networks, primarily Decnet.

1 Nuclear Physics

- PN1 regulation of magnetic fields by a VECTRA computer (HP) and acquisition by ATARI connected to a MicroVAX II GPX.
- PN2 change of computer to MicroVAX II.
- PN3 complete reorganisation on GAMS 2/3 and 4 to operate on MicroVAX II.
- PN7 study for automation of the polariser.
- "S" Instruments
- S52.B New experiment (first acquisition on exabyte).
- S21 Sample changer.
- S20 Standardisation of conventional diffractometer.
- S20-A New detection system by PM.
- MAMBO Replacement of MACAMAC by PDP11.

2 General

- $N\bar{N}$ Installation of bridge on optical fibre.
- Level D Installation and extension of the Ethernet network in level D for experiments BILL (PN2) and EDM.
- Standardisation of graphical procedures for the use of X-Window terminals.

Reactor Operation 1990

The reactor operating schedule had to be modified as a result of the reactor shutdown between the 24 January and 10 April 1990, which was required by the Safety Authorities (SCSIN) following the discovery that the reactor had been operating from the beginning at a power greater than the nominal power. During this shutdown, the consequences of the excess coolant flow and of the approximately 10 % excess power of the reactor were analyzed, and the replies given to the SCSIN led to the authorization to restart the reactor.

Because of this extended shutdown, the 1990 schedule had to be limited to 4.5 cycles of reactor operation.

Cycle 1/90

The reactor operated from 9 January to 14 May with an interruption from 24 January to 10 April for the above reasons.

Apart from this shutdown, the cycle was completed without incident.

Cycle 2/90

Operation from 29 May to 14 July. The scheduled dates were respected and the cycle was completed without incident.

Cycle 3/90

Operation from 25 July to 9 September. The start of the cycle was delayed by 1 day to complete work on the mechanism of the control rod, and the end of the cycle was also delayed by 1 day in compensation. During the cycle there were two brief shutdowns following a disturbance on the EDF power supply and a safety rod release; in addition a two day shutdown was necessary for work on one of the main pipes of the secondary cooling circuit.

Cycle 4/90

Operation 25 September to 10 November. The scheduled dates were respected and the cycle was completed without incident.

Cycle 5/90 (part 1)

Operation from 27 November to 21 December. The scheduled dates were respected and the cycle was completed without incident.

Data for 1990

Number of days originally scheduled	264
Actual number of days of operation	204
Number of equivalent days of full power	206
Actual operating time as proportion of year (%)	72
Actual operating time in relation to time scheduled (%)	77
Number of fuel elements used	5
Number of new elements received	5
Number of unscheduled shutdowns	5
including:	
brief shutdowns	3
shutdowns with Xenon poisoning	2

Apart from the usual maintenance work and the renewal of installations to ensure safe and reliable operation of the reactor, a number of important points should be mentioned.

There were no problems for the supply of new fuel elements in 1990, but the reprocessing of fuel elements has still not resumed, and the ILL storage facilities were fully occupied at the end of 1990. Continued operation of the reactor is subject to the removal and interim storage on another site of our used fuel elements. After studying several solutions, it has been decided to use the Pégase installations at CEN-CADARACHE for storage. The first elements should be despatched at the end of January 1991.

The study on the behaviour of the steel reactor shell if subjected to pressure following an explosion on the motorway has been forwarded to the Safety Authorities.

The containment of the emergency control room in the building ESRF 2 has been completed.

The reheaters before the filters in the gaseous effluent network in the reactor building have been installed and commissioned.

The analysis of the origin and consequences of the underestimate of the heavy water flow for cooling the reactor has been completed.

The study of the consequences of a complete failure of electrical energy on the cooling of the reactor (transfer to natural convection) has been continued.

Irradiated samples of zircaloy and stainless steel have been removed and despatched to the KFK laboratory for a study of their mechanical characteristics.

Operations associated with the ordering, manufacture and acceptance of major replacement parts are continuing, particularly with a view to the replacement of beam tube liners and others parts of the reactor block.

Finance

Implementation of the 1990 Budget

The Budget authorized for 1990 amounted to a total of approx. 303 MF excl. taxes. Total expenditure in 1990 is anticipated to be 286.9 MF, the difference being mainly due to the impossibility of shipping fuel elements for reprocessing to the USA, and also to the delay in the construction of the joint ILL/ESRF building, now planned for 1991/92.

More detailed information on the expenditure and income trends between 1989 and 1990 is given in the following tables:

Comparison of 1989 and 1990 Budgets (Expenditure)

Expenditure	Expenditure 1989		Estimated Expenditure 1990		Change
	MF	%	MF	%	%
1. Staff costs	160.5	55	171.4	59	+ 6.8
2. Fuel elements	34.2	12	22.3	8	-34.8
Consumables	28.8	10	27.9	10	-3.1
Long term supplies and services	7.1	2	8.6	3	+21.1
Short term supplies and services	13.3	5	12.6	4	-5.2
Travel	2.4	1	2.1	1	-12.5
Miscellaneous adm. costs	8.2	2	7.2	2	-12.2
Taxes and fees	1.4	1	1.5	1	+7.1
3. Operation	61.2	21	59.9	21	-2.1
Total Operation	**255.9**	**88**	**253.6**	**88**	**-0.9**
Buildings	0.9	–	0.3	–	-67.0
Equipment	6.1	2	7.2	3	+18.0
Instruments	16.4	6	16.7	6	+ 1.8
Other investments	11.6	4	9.1	3	-21.5
Total Investments	**35.0**	**12**	**33.3**	**12**	**-4.9**
Total Expenditure	**290.9**	**100**	**286.9**	**100**	**-1.4**

Comparison of 1989 and 1990 Budgets (Income)

Income	Income 1989		Estimated Income 1990		Change
	MF	%	MF	%	%
Collaboration with ESRF	0.8	0.3	1.2	0.4	+ 50
ILL's own income	8.7	3.0	9.000	3.1	+3.4
Reabsorption of provision	–	–	0.7	0.2	–
Spanish, Swiss, Austrian contributions	8.6	3.0	13.5	4.7	+57.0
Associates' contributions	269.5	92.6	276.7	96.5	+2.7
Carry forward 1988 to 1989	+15.4	5.3			
Carry forward 1989 to 1990	-12.1	-4.2			
Carry forward 1990 to 1991			-16.2	-5.6	
Use of Reserve account			+ 2.0	0.7	
Total Income	**290.9**	**100**	**286.9**	**100.0**	**-1.4**

A comparison of expenditure between 1989 and 1990 shows an increase in staff costs of 6.8 %, which includes general salary increases, increased social charges, the increase in the ILL allowance, new measures to improve the attractiveness of the ILL for non-French staff and an increase in the number of scientist posts as a result of Austrian membership.

The considerable reduction by 34.8 % in expenditure on fuel elements results from the postponement until 1991 of delivery of 56 kg uranium, the delay in the production of fuel elements, and the suspension of reprocessing of fuel elements in the USA.

The other operation expenditure is about 2 % lower, mainly as a result of the economies due to the omission of one and a half reactor cycles.

Although total investment decreased by about 5 %, it was possible to maintain and even slightly increase (+ 1.8 %) investments for instruments in 1990 due to additional funds made available through the scientific participation of Austria, and internal transfers following economies in operation costs as a consequence of the reactor shutdown early in the year. Scientific investments were in both years mainly used for the completion of the instruments on the horizontal cold source, maintenance and improvement of existing instruments as well as the development of methods.

Other investments - outside the scientific sector - decreased overall by 2 MF. Extension work on building ILL20 was finished in 1989; there were also less purchases of computers and reactor equipment in 1990 than in 1989.

Budget 1991

At its meeting in Grenoble on 27 November 1990 the Steering Committee adopted the 1991 budget with total expenditure of 314.9 MF, including the following main headings: staff costs 177.7 MF, fuel elements 41.2 MF, other operation expenditure 62.7 MF, investments 33.3 MF.

Forward look

The main goals for scientific investments in the multiannual financial estimates can be summarized as follows:

– completion of the instruments for the horizontal cold source with approximately 4.7 MF in 1991 and approx. 4.0 MF in 1992 (D22, IN15, IN10C);

– maintenance and smaller replacement investments for existing instruments ("group budgets";

– specific major upgrades (in particular IN4C, PN1, PN3);

– improvement of existing instruments and refurbishment of guides (in particular detectors D20 and D19, high speed selectors), overall investment in this field between 2 and 3 MF per year over the planning period (1992-1996);

– development of methods with approx. 1.6 MF per year on average; special emphasis on Be crystals, detectors and thin layers.

These investments will be coordinated with the scientific goals pursued by the new development programme presently under discussion.

Outside the scientific sector the following investments during the planning period should be mentioned:

– a new telephone system, to be used jointly with ESRF, will be installed in 1991;

– the build-up of a reserve of three fuel elements, to be completed by the end of 1991;

– the joint ILL/ESRF building (library, offices for theoreticians, canteen, cafeteria) will be completed in 1992;

– replacement of equipment necessary for the safety and reliable operation of the reactor.

Purchasing

In order to ensure Uranium supply, 32 Kg of Uranium (93% enriched) was purchased from COGEMA (F) who were also awarded a contract for the re-enrichment and transport of a further 24 Kg of reprocessed Uranium. As irradiated fuel elements can at present no longer be sent to the USA for reprocessing and the ILL's storage capacity is rather limited, it became vital to find an alternative solution for storage of spent fuel elements. After an invitation to tender, CEN CADARACHE (F) was awarded the contract for this interim storage of fuel elements; we are studying offers for the transport of these elements, at the time of writing.

Nukem (D) were awarded an important supplement to the existing contract for the manufacture of the beam tube H1/H2 which originally provided for a piece with 5 beam holes for cold neutrons. The new design will provide 2 additional cold neutron beams without affecting the cold source or the essential parts of the H1/H2 beam tube.

Also, for the Reactor, a new pair of filters for the pumping station were ordered from Perrier (F), the original supplier; an important order for Deuterium gas was placed with Airgaz (D) for the Detritiation plant.

For the new instruments on the Horizontal Cold Source, four major purchases are in progress. The shielding and central platform of the secondary spectrometer for IN10C is under construction at SEIV (F). A prototype toroidal mirror for the optical focussing system of IN15 has been ordered from C. Zeiss (D), and a further 7 mirrors will be ordered if this prototype performs satisfactorily. The neutron velocity selector for D22 will be manufactured by DORNIER (D) and the multidetector for D22 was awarded to CERCA (F). A similar order for the multidetector of D19 was also placed with CERCA. These and other detectors require Helium 3 gas which has been ordered from IC Chemikalien (D).

Other important purchases for the instruments included a vacuum evaporator for Nuclear Physics ordered from LEYBOLD (D), and a goniometer for D10 from Huber Diffraktionstechnik (D).

A new telecommunications system has been ordered from Opus Alcatel (F) for installation in April 1991, to be operated jointly by ILL and ESRF.

In the computing area 3 Vaxstations and 2 Microvax computers were bought from Digital (USA). Several Macintoshes were purchased. The Finance and Purchasing Service acquired a new Microvax 3300 which has greatly improved response time.

As usual about a quarter of expenditure was spent on service contracts such as electricity, telephone, cleaning, restaurant, and contracts with the CENG for heating, helium supply and radioprotection services, as well as the maintenance contracts for computers and other equipment.

Considerable savings were achieved by competitive tendering for major purchases, as well as by negotiations with the regular suppliers for routine orders. Whenever possible an international call for tenders was carried out for

major purchases; offers were compared on an ex-works basis so as not to disadvantage British, German, Swiss, Spanish and Austrian firms compared with local suppliers. The distribution of ILL purchases (orders exceeding 50 KF) in the first 10 months of 1990 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.

Stores

The former Head of Stores retired in 1990 and 2 other storemen moved on to new jobs. A new team has been built in stores offering fresh challenges to the newcomers, including a second ESRF storeman.

All deliveries of purchased equipment were received and checked quantitatively by the storemen who at the same time arranged the despatch of samples, returned equipment, etc, and the provision of raw materials.

This joint ESRF/ILL stores facility operates successfully and will continue, allowing economies for both partners, until the new ESRF stores is completed at the end of 1991.

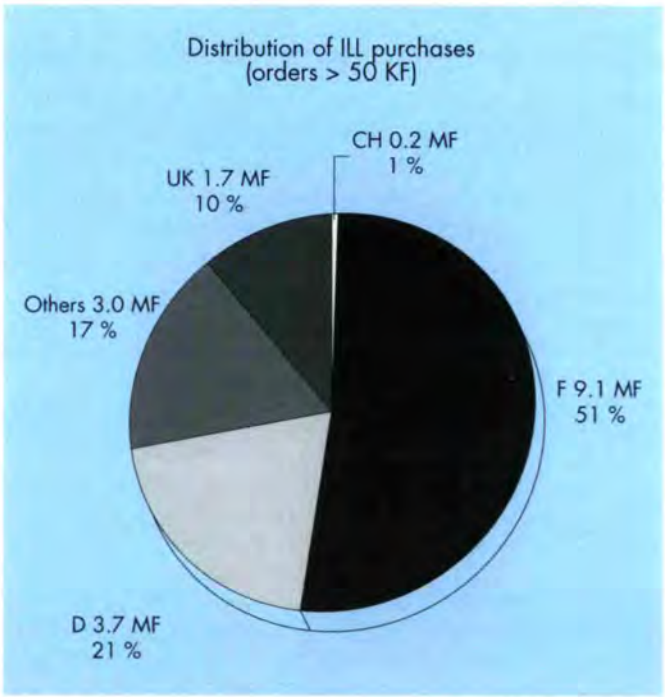

Fig.: Distribution of ILL purchases (orders > 50 KF)

Personnel

Staff

In 1990 there was a total of 483 staff on posts, practically the same figure as in 1989 (482).

However there has been a change in the breakdown by nationalities in relation to 1989 :

French	61.9 % instead of	65.2 %
German	16.6 % instead of	14.9 %
British	15.1 % instead of	13.9 %
Others	6.4 % instead of	6.0 %

The table showing the staff complement situation gives details of these changes, notably the reduction in French staff (-15) in 1990. With the change in 1989 (-11) there has been a reduction of 26 in the French staff, while over these two years the German (+13) and British (+8) staff show a significant increase.

The new staff already recruited for 1991 indicate a continuation of this trend.

Salaries

The salary increases known for 1990 amount to 2.7 %, of which 1.5 % was awarded at 1.03.90, 0.2 % at 1.07.90 and 1.0 % at 1.09.90.

In addition the ILL allowance was increased to 12 % of the basic salary (previously 10 %) with effect from 1.01.90, following an agreement signed by the ILL Management and unions.

Guest scientists

There were approximately 2200 visits by 1400 guest scientists to the ILL between January and December 1990.

Of these visitors 30 % came from laboratories in France, 28 % from Germany, 25 % from the UK and 17 % from other countries.

Staff complement situation in 1990
(by categories and nationalities)

	POSITION ON 31.12.89					CHANGES IN 1990 AND POSITION ON 31.12.90													
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)	12	5	8	6	31	+ 1		13			5		- 1	7	+ 1		7	+ 2	- 1	32
- Scientists (non permanent)	12	8	11	6	37	+ 8	- 3	17	+ 4	- 2	10	+ 3	- 3	11	+ 7	-6	7	+ 22	- 14	45
- Engineers			2		2									2						2
TOTAL	24	13	21	12	70	+ 9	- 3	30	+ 4	- 2	15	+ 3	- 4	20	+ 8	-6	14	+ 24	- 15	79
OTHER "CADRES"	15	8	39		62			15	+ 1		9	+ 1	- 2	38				+ 2	- 2	62
TOTAL CADRES	39	21	60	12	132	+ 9	- 3	45	+ 5	- 2	24	+ 4	- 6	58	+ 8	- 6	14	+ 26	- 17	141
2 - THESIS STUDENTS	9	8	9	3	29	+ 3	- 3	9	+ 1	- 1	8	+ 2	- 2	9	+ 1		4	+ 7	- 6	30
3 - NON CADRES																				
- Technicians	15	26	138	3	182	+ 1		16	+ 4	- 2	28	+ 2	- 7	133			3	+ 7	- 9	180
- Others	9	12	107	11	139	+ 1		10	+ 2	- 1	13	+ 2	- 10	99		- 1	10	+ 5	- 12	132
TOTAL NON-CADRES	24	38	245	14	321	+ 2		26	+ 6	- 3	41	+ 4	- 17	232		- 1	13	+ 12	- 21	312
TOTAL	72	67	314	29	482	+ 14	- 6	80	+ 12	- 6	73	+ 10	- 25	299	+ 9	- 7	31	+ 45	- 44	483

G: German, B: British, F: French, O: Others, T: Total

Welfare and general services

Housing

ILL has 20 furnished flats for rent by guest scientists staying for at least two weeks, or for new ILL or ESRF staff starting work in Grenoble. In 1990 seventy-four persons or families made use of these facilities, including 50 from ILL, 21 from ESRF, 2 from IRAM and 1 from EMBL. The proportion of occupation was 95 %. When the reactor is operating, more requests are received than can be satisfied.

Finding accommodation

New arrivals, in particular non-French staff, are helped to look for flats or houses. The housing market in Grenoble area has become easier over the last three or four years, which facilitates this work. Existing staff also consult us.

Employer's contribution to housing

This contribution is used either for loans for housing, in accordance with French legislation, or to reserve flats.

Fifteen loans were granted, totalling 784 300 F (minimum loan: 9 300 F over 2 years, maximum: 80 000 F, reimbursed over 10 years).

Two flats were reserved with housing associations (HLM).

Assistance for german staff

Since January 1989, Frau Hildebrandt, who is German and a psychologist, has been detached to the ILL by the German Associate, the KFK.

She helps the German community, dealing specifically with questions of integration encountered by ILL German staff and their families at Grenoble (employment for wives, recognition of qualifications, pension matters, administrative formalities, etc). In the course of her work, Frau Hildebrandt is in contact with municipal departments in Grenoble, the employment exchange, various firms in the Grenoble area, German pension funds and the German Consulate at Lyon. Her appointment has been extended for a further two years (1991-92).

Welfare Assistant

Mme Pennec, the Welfare Assistant, assists staff and their families with administrative formalities (e.g. for family allowances, unemployment benefit, and contacts with job centres), or in case of occasional serious personal difficulties. She collaborates closely with the various subcommittees of the Works Committee (e.g. those dealing with housing and holidays), the Welfare and General Services Group, the ILL staff "Mutuelle", the Personnel Group (particularly on retirement and pensions), and the Medical Service.

She provides assistance to the staff of both ILL and ESRF.

International education

All the school years from the beginning of Primary School to the Level of the "Baccalauréat" are now covered. This International Schooling is extremely popular at Grenoble, which raises the question of selection of French children, in particular in the lowest class in the Primary School (children of 6 to 7) and in the "sixième" at the L.I.S. (Lycée International Stendhal). Almost 600 children attend the English and German "sections".

Since September 1990 the French Ministry of Education has been responsible for payment of the English and German teachers. Discussions are still in progress on the extension of this to cover intensive French tuition for new foreign children at the Houille Blanche Primary School. This post is essential to enable the children to integrate rapidly in their new environment.

Training

The ILL French courses include ILL and ESRF staff, their wives, long-term guest scientists, scientists at the university, etc. The classes are attended by about 80 persons, spread over 7 levels. The teachers are Mme Cédile and Mme Gobrecht. In addition, excursions and small celebrations organised by the teachers produce a sociable atmosphere in groups comprising people of very varied nationality and culture.

Technical and professional training courses cover mainly computing techniques, use of software, automatic control devices, etc. A group of technicians was very interested by a course on quality assurance. This type of course will be continued in 1991.

Seminars

College 2

Theory

"Vortex inclinés dans les supraconducteurs quasi 2d".
A. BUZDIN, Université de Moscou.

"Structure statistique des polymères conjugués solubles".
Annie VIALLAT, Spectrométrie Physique, Grenoble.

"High resolution electron energy loss study of the surfaces and energy gaps of cleaved high temperature superconductors".
B.N.J. PERSSON, Institut für Festkörperforschung, KFA Jülich.

"Application des méthodes thermodynamiques variationnelles à la métallurgie physique".
A. Pasturel, Laboratoire d'Electrochimie de Grenoble.

"Frustrated antiferromagnetic and antiferro spin glasses".
E.F. Shender, ILL and Leningrad.

"Superfluid kinetic equation approach to the dynamics of the ^{3}He A-B phase boundary".
J. PALMERI, CEN-Saclay.

"Statistical mechanics of granular materials : statics and dynamics".
A. MEHTA, Cavendish Laboratory, Cambridge.

"Morphological surprises during epitaxial crystal growth".
A. ZANGWILL, School of Physics, Georgia Institute of Technology, Atlanta.

"Un système désordonné : le tas de sable, résultats récents et conjectures".
J. RAJCHENBACH, Université P. et M. Curie, Paris.

"Energy gaps in layered superconductors".
L. BULAEVSKI, Lebedev Institute, Moscow.

"Absence d'universalité dans la transition de phase des systèmes hélimagnétiques".
P. AZARIA, Université Paris VI.

"Slave boson approach to the theory of heavy fermions".
S. EVANS, Laboratoire Physique des Solides, Orsay.

"Magnetic properties of the ideal Fcc antiferromagnet Cu at nano Kelvin temperatures".
A. LINDGÅRD, Atomic Energy Commis. Research Establ. Risø.

"Computer simulation of incommensurate phase".
K. PARLINSKI, Institute of Nuclear Physics, Cracow.

"A theory of high T_c superconductors".
C. VARMA, Bell Laboratories, USA.

"La solidification orientée de systèmes eutectiques".
Ch. MISBAH, Groupe de Physique des Solides, Paris Jussieu.

"Scattering of electrons by kinks on the dislocation line of a metal".
S.I. MUKHIN, Institute of Steel and Alloys, Moscow.

"Charge density waves and superconductivity in $Ba_{1x}K_xBiO_3$".
WU PEI SU, Department of Physics and Texas Center for Superconductivity, University of Houston, Texas.

"Mathematica : a program of symbolic computation. Overview and physical applications".
B. AUTIN, CERN, Genève.

"X-ray, photoemission and absorption spectroscopy as a probe of electronic and structural properties of condensed matter".
C. NATOLI, Laboratory INFN Frascati and ILL Grenoble.

"Fermions sur réseau avec forte répulsion locale : quelques règles de somme pour le spectre à une particule".
K. MATHO, CRTBT-CNRS Grenoble.

"Scaling theory of interacting light and heavy fermions in one dimension".
J. SÓLYOM, Central Research Institute for Physics, Budapest.

"Formation de structures par dépot cathodique".
L. SANDER, Université de Michigan.

"Fermi liquid nesting in high temperature superconductors".
J. RUVALDS, University of Virginia.

"Non-linéarité et désordre".
J.S. KIUSHAR, Université de Kharkov.

"Une théorie des champs pour les verres de spin".
C. DE DOMINICIS, Physique Théorique, CEN-Saclay.

"Solitons and dislocations for the current conversion in charge density wave crystals".
S. BRAZOWSKII, Landau Institute of Theoret. Physics.

"Slave boson representations of correlated fermions".
P. WÖLFLE, Universität Karlsruhe.

"Modèles de transfert de charge pour les supraconducteurs à haute T_c".
D. NUÑEZ-REGUEIRO, ILL, Grenoble.

"Triplet Cooper pairing in nuclei : a new type of superfluidity in nuclear matter, heavy nuclei, neutron stars".
I.S. SHAPIRO, Lebedev Institute, Moscow.

"Lois d'échelle pour T_c positif, nul ou négatif. Des ferromagnétiques aux fermions lourds, et des verres de spin aux verres structuraux".
J. SOULETIE, CRTBT-CNRS, Grenoble.

"Quantum corrections to soliton-induced properties in spin chains".
H.J. MIKESKA, University of Hannover, Germany.

"Relationship between lattice motion and carrier dynamics in high T_c superconductors".
W.E. PICKETT, Naval Research Laboratory, Washington.

"Un principe d'extremum pour la turbulence".
B. CASTAING, CRTBT-CNRS, Grenoble.

"Multineural interaction model for neural networks".
R. IGLESIAS, Porto-Alegre, Brésil.

"Derivation of a single-band model for the cuprate superconductors".
J.H. JEFFERSON, Royal Signals and Radar Establishment Malvern, Worcs., U.K.

"^{3}He impurity states of liquid ^{4}He : from thin films to the bulk surface".
J. TREINER IPN Orsay.

"Figures de souffle : un problème de probabilités géométriques".
C. GODRECH, Orme des Merisiers, Saclay.

"Phase separation and superconductivity in an extended Hubbard model".
M. GRILLI, Université de Rome.

"Fluctuating chains and membranes with internal degrees of freedom".
J. PALMERI, Physique Théorique, Orsay.

College 3

Fundamental and nuclear physics

"The Sudbury Neutrino Observatory".
W. DAVIDSON, Nat. Research Council, Canada.

"Energy and angular correlation of the e^+e^- pairs emitted in heavy-ion collisions using the GSI double orange spectrometer".
W. KOENIG, GSI Darmstadt.

"The BNL high flux beam of moderated positrons".
K.G. LYNN, Brookhaven National Laboratory, New York.

"Optics and interferometry with very cold neutrons".
A. ZEILINGER, Wien.

"On the microscopic interpretation of interacting bosons in nuclei".
D. JANSSEN, Rossendorf.

"Existence of two-phonon vibrational states in deformed nuclei".
R. PIEPENBRING, ISN, Grenoble.

"M1 - Resonances in spherical nuclei".
A. VDOVIN, Dubna.

"Ion beam induced transport of matter in hard coatings".
W. BOLSE, Göttingen.

"Intruder states in 120 Xe".
W. WALTERS, University of Maryland.

"Accelerator mass spectroscopy of ^{41}Ca".
A. STEINHOF, ILL, Grenoble.

"Development of a new technique to search for the neutron EDM".
R. GOLUB, ILL, Grenoble.

"Metal cluster fission : Condensed matter analogue to nuclei".
W.A. SAUNDERS, Ecole Polytechnique Fédérale de Lausanne.

"Neutron β-decay and right-handed current problem".
Yu. V. GAPONOV, Kurchatov Institute, Moscow.

"The neutron EDM experiment in Gatchina".
V. LOBASHEV, Gatchina.

"P-odd effects in neutron-nuclear interaction".
Yu.G. ABOV, Inst. Theor. and Exper. Phys., Moscow.

"Conversion electrons from highly ionized atoms".
W. STÖFFL, Lawrence Livermore Nat. Lab.

"The role of a University Reactor".
C.J. BAIER, Risley.

College 4

Structural and Magnetic Excitations

"Excitation scattering in superfluid helium".
A.F.G. WYATT, University of Exeter.

"Sum rules and elementary excitations in quantum liquids"
S. STRINGARI, Università di Trento.

"Quasi-one-dimensional antiferromagnetism in vanadiumthiophosphate with S = 1 Heisenberg chains".
H. MUTKA, ILL, Grenoble.

"High energy inelastic scattering studies on rare earths and actinides at ISIS".
K. McEWEN, University of London.

"Longitudinal spin fluctuations in nickel below T_c".
P. BÖNI, Paul Scherrer Institut, Villigen.

"New phases of solid hydrogen at megabar pressures and evidence for metallic hydrogen".
I.F. SILVERA, Lab. de Spectrométrie Hertzienne, INS, Paris.

"Do real interacting spins always freeze ?"
G. AEPPLI, Bell Laboratory

"Elementary excitations in liquid ^{3}He and ^{3}He-^{4}He mixtures".
B. FÅK, ILL, Grenoble.

"Phonon dispersion curves in high-T_c superconductors, a challenge for inelastic neutron scattering".
L. PINTSCHOVIUS, Kernforschungszentrum Kalsruhe.

"Phonons in strongly coupled electron - phonon systems".
A.S. ALEXANDROV, Moscow Physics Engineering Institute.

"Neutron scattering experiments on hexagonal ABX_3-type compounds (A = Cs, Rb ; B = Ni, V, (Mn); X = Cl, Br(I))".
K. KAKURAI, Tohoku University, Sendai.

"Dynamic of dipolar glasses".
J. PETZELT, Czechoslowak Academy of Science, Prague.

"Recent experiments with MARI - time-of-flight spectrometer".
M. ARAI, Rutherford Appleton Laboratory.

"Crystal-fields as a probe of the magnetism in high T_c superconductors".
R. OSBORN, Rutherford Appleton Laboratory.

"Magnetic properties of R_2CuO_4 single crystals" and "Electron paramagnetic resonance, a useful tool to study magnetic ordering in R_2Cu_4".
S. OSEROFF, San Diego State University.

"The reconstruction of molybdenium (0 0 1) : a structural phase transition at a solid surface".
D.M. SMILGIES, MPISF, Göttingen.

"Universality in a triangular antiferromagnet".
Th. MASON, ATT, Bell Laboratory, New Jersey.

"Inelastic magnetic neutron scattering study of the transition from amorphous to crystalline $PrNi_5$".
P. ALEKSEEV, Kurchatov Institute of Atomic Energy.

"Non linear excitations in quantum spin chain : domain walls, solitons and the transition to the classical limit".
H.J. MIKESKA, Theoretische Physik, Universität Hannover.

"Recent neutron scattering investigations on superconducting cuprates and titanates".
F. GOMPF, K.F.K, Karlsruhe.

"Dilution induced order in quasi-one-dimensional quantum antiferromagnets".
E.F. SHENDER, ILL and Leningrad.

"Magnetic fluctuations near the metal-insulator in $La_{2x}Ba_xCuO_4$".
Dr. S. HAYDEN, ILL.

"Recent developments at LANSCE".
R. PYNN, Los Alamos National Laboratory, USA.

"Density of states measurements in Se_xTe_{1-x} alloy systems".
L. NEEDHAM, ILL, Grenoble.

College 5

Crystallographic and magnetic structures

"Maximum entropy methods in crystallography"
C. GILMORE, University of Glasgow.

"Crystallography and crystal chemistry of orientationally disordered silicates"
C.R. ROSS, II, University Bayreuth.

"Crystallographic and magnetic structures of hydride alloys RE-3d-metals : $R_2Fe_{14}BH_x$, $R_2Fe_{17}Hx$, $YFe_{11}TiH_x$".
D. FRUCHART, CNRS-Grenoble.

"Charge, spin and theoretical densities in transition metal complexes".
B.N. FIGGIS, University of Western Australia.

"Neutron diffraction physics and the structure of the neutron".
Yu A. ALEXANDROV, JINR, Dubna.

"Powder neutron diffraction of xylene isomers in Y-zeolites".
Mirjam CZJZEK, CNRS-Villeurbanne & Technische Hochschule, Darmstadt.

"Lattice instability anharmonicity disorder in high-T_c superconducting compounds".
B. TOPERVERG, Leningrad Nucl.Phys. Institute, Gatchina.

"Simulated annealing: an introduction and a few applications to problems of structure determination".
J. PANNETIER, ILL, Grenoble.

"Frustrated antiferromagnets and antiferro-spin glasses".
E.F. SHENDER, ILL.and Leningrad.

"Single crystal neutron diffraction in inorganic chemistry".
J.A.K. HOWARD, School of Chemistry, University of Bristol.

"Random fields, phase transitions and metastability".
R.A. COWLEY, University of Oxford.

"New crystallographic methods applied to inorganic superconductors and conducting organic salts: modulation analysis, application of synchrotron anomalous scattering and the description of composite structures".
Ph. COPPENS, Department of Chemistry, SUNY, Buffalo.

"DITO, a new TOF powder diffractometer".
C. RITTER, ILL, Grenoble.

"Physintercalation process of alkanes in cesium graphitides".
H. PILLIERE, ILL, Grenoble.

"Towards an optimal strategy for diffraction data collection with position sensitive detectors".
I. VICKOVIC, Laboratory of Chemical Physics, University of Groningen.

"Maximum entropy reconstruction of magnetisation density maps".
R. PAPOULAR, Laboratoire Léon Brillouin, CEA, Saclay.

"Twin formation and structural modulations in orthorhombic and tetragonal $YBa_2(Cu_{1-x}Co_x)3O_{7-\delta}$".
W.W. SCHMAHL, Darmstadt.

"Time-resolved powder diffraction with synchrotron radiation".
Dr. P.U. PENNARTZ, Darmstadt.

"Single crystal studies of zeolites and chlathrates using synchrotron radiation X-ray or neutron diffraction techniques".
Å. KVICK, ESRF, Grenoble.

"The interpretation of electron diffraction-patterns using optical analogues".
B.H. PARRY, Lab. Chimie Minérale et Structurale, Limoges.

"Mössbauer spectroscopy using synchrotron radiation".J.B. HASTINGS, Nat. Synchrotron Light Source, Brookhaven Nat.Lab.

"Structural instability and lattice dynamics of incommensurate material : potassium, selenate revisited".
J.M. PEREZ-MATO, Universidad del pais vasco, Bilbao, spain.

"Crystallographic descriptions of incommensurate structures : representation analysis in 3D and N-dimensional space groups".
J.M. PEREZ-MATO, Universidad del pais vasco, Bilbao, spain.

College 6

Liquids, disordered materials

"Théorie des transitions de phase reconstructives".
"P. TOLEDANO, Lab. Transitions Phases, Univ. de Picardie.

"Total energy calculations for displacive transformations in solids".
B. HARMON, Ames Laboratory, Ames, Iowa.

"Solute site investigation of fast diffusing Co in bcc-Zr".
A. HEIMING, ILL, Grenoble.

"Structure of aqueous electrolyte solutions".
G. NEILSON, ILL, Grenoble, and H.H. WILLS, Physics Laboratory, University of Bristol.

"Backscattering versus spin echo or recent coherent and incoherent experiments on the dynamics of the glass transition".
W. PETRY, ILL, Grenoble.

"Non-uniform quantum systems : the desirable, the observable and the doable".
E. KROTSCHECK, Texas A and M University, USA.

"Collective excitations in dense molecular fluids".
F.J. BERMEJO, Instituto de Estructura de la Materia, Madrid.

"The vacancy defect state by positron annihilation and the structural models of quasicrystals".
R. CHIDAMBARAM, Bhabha Atomic Research Centre, Trombay, India.

"Two- and three-body effects from neutron diffraction on argon at low densities".
R. MAGLI, ILL Grenoble and University of Florence, Italy.

"Dislocations in quasicrystals as a probe for elasticity of phasons : perfect structure versus random tiling".
L. LEVITOV, Landau Institute, Moscow.

"Glass transition : characteristic length and multiplicity".
E. DONTH, Technische Hochschule "Carl Shorlemmer" Leuna-Merseburg.

"NMR measurements on ^{3}He-^{4}He mixture films".
R.B. HALLOCK, University of Massachusetts, Amherst, USA.

"Random bond and random field disorder in two-dimensional orientational glasses".
P.C.W. HOLDSWORTH, Ecole Normale Supérieure de Lyon.

"Soft relaxations near the ferroelectric phase transition in liquid crystals".
M. GLOGAROVA, Inst. Phys. Czechoslovak Acad. of Sciences.

"Neutron scattering studies on the glass transition in polymers".
B. FRICK, ILL, Grenoble.

College 8

Biology

"Investigations of trypanosomal GAPDH crystals using the Laue method : prospects for drug design".
F.M.D. VELLIEUX, Laboratory of Chemical Physics, State University of Groningen.

"Microassembly of integral membrane proteins".
J.L. POPOT, Institut de Biologie Physico-Chimique, Paris.

"The three-dimensional structure of ribosomal RNA and its implication for ribosomal function".
R. BRIMACOMBE, M-P-I für Molekulare Genetik, Berlin.

"Crystal morphology as a probe of molecular interactions".
Z. BERKOVITCH-YELLIN, Weizmann Institute Rehovot, Israel.

"Structural and kinetic characterization of intermediates in the folding of a multidomain oligomeric protein, the ß-2 subunit of E. coli tryptophan synthase".
M. GOLDBERG, Université Paris 7, Institut Pasteur, Paris.

"The structure of the complex $tRNA^{Asp}$/aspartyl-RNA synthetase from yeast".
D. MORAS, IBMC, Strasbourg.

"Crystal growth in gels. Application to the case of proteins".
M.C. ROBERT, Université P. et M. Curie, Paris.

"Single stranded model of fibrin polymerisation".
E.B. HUNZIKER, M.E. Müller Institut for Biomechanics, University of Berne.

"Diffraction neutronique à haute et à basse résolution : étude de la liaison hydrogène et des interactions intermoléculaires".
M.S. LEHMANN, ILL, Grenoble.

"Structure and function of E. Coli Met-repressor : a new DNA binding motive".
S.E.V. PHILLIPS, University of Leeds.

"Mechanism of protein biosynthesis : the allosteric three-site model for ribosomal elongation".
K.M. NIERHAUS, MPI für Molekulare Genetik, Berlin.

Three-dimensional structure of plant light-harvesting complex by electron crystallography".
W. KÜHLBRANDT, EMBL, Heidelberg.

College 9

Chemistry

"Percolation process induced by solubizing cytochrome c in reverse micelles".
M.P. PILENI, Université P. et M. Curie, Paris.

"Amphiphilic Systems : diluted phases of fluid membranes"
G. PORTE, G.D.P.C. - USTL - Montpellier.

"Structure of supercooled D-glycerol under shear".
H.J.M. HANLEY, National Institute of Standards and Technology (formely NBS) Boulder, Colorado, USA.

"Polymerisation transition in a monoatomic liquid : diffraction and SANS study of liquid sulfur".
R. BELLISSENT, Laboratoire Léon Brillouin, C.E.A., Saclay.

"Structure and growth of nitrogen films on graphite".
H. TAUB, University of Missouri-Columbia.

"Neutron scattering and thermodynamic properties of swollen polymer gels".
E. GEISSLER, Laboratoire de Spectrométrie Physique, Université Joseph Fourier, Grenoble.

"Viscoelasticity of dilute polymer solutions : internal viscosity, dynamic scaling, shear thinning, frequency-dependent viscosity and relaxation spectra".
Yitzhak RABIN, Weizmann Institute, Israel.

"Polymeric micelles".
Alice GAST, Stanford University.

"Tunnelling and reorientation studies by deuteron NMR".
Zdzislaw T. LALOWICZ, Institute of Nuclear Physics, Krakow.

"Centered cluster halides of group three and four transition metals. A versatile solid state chemistry".
J.D. CORBETT, Department of Chemistry, Iowa State University, Ames, Iowa.

"Solid-state NMR studies of molecular sieve catalysts"
J. KLINOWSKI, Department of Chemistry, University of Cambridge

"Synthesis, structure and spectroscopy of linear-chain complexes".
R.J.H. CLARK, Dept. of Chemistry, University College London.

"Neutron scattering studies of coordination compounds".
Roderick D. CANNON, School of Chemical Sciences, University of East Anglia, Norwich, U.K.

"Soft relaxations near the ferroelectric phase transition in liquid crystals".
M. GLOGAROVA, Inst. Phys., Czechoslovak Acad. of Sciences.

Thursday colloquium

"Quantum chaology of eigenvalues".
M. BERRY, University of Bristol.

"Structural slowing down and kinetic glass transition".
J.P. HANSEN, Ecole Normale Supérieure de Lyon.

"Nuclear order in copper : new type of antiferromagnetism in an ideal FCC system".
A.S. OJA, Helsinki University of Technology.

"Experiments with separated oscillatory fields and hydrogen masers".
N. RAMSEY, Harvard University, Cambridge, Mass.

"Flux pinning and creep in high temperature superconductors"
P.H. KES, Leiden University.

"Interlayer pairing and c-axis versus ab-plane gap anisotropy in high Tc superconductors".
R.A. KLEMM, Oak Ridge National Laboratory.

"Atomic-scale tip-induced electronic effects in scanning microscopes and field emission"
A. BARATOFF, IBM Zürich.

Miscellaneous

"Founding a high technology company; superconductivity and a desk-top synchrotron".
Sir Martin WOOD, The Oxford Instruments Group plc, Oxford, U.K. (Joint Colloquium ILL/ESRF).

Conference contributions

ALPE D'HUEZ (l'), France: Complementary Applications of Diffraction by Neutron and Synchrotron Radiation. Satellite Meeting of the XVth Congress of the International Union of Crystallography - 1990/07/30-08/2

BARUCHEL J. Topography studies using neutrons and synchrotron radiation. (Invited Talk)

BERGEVIN F. DE , BRUNEL M., GALERA R.M., BARUCHEL J., VETTIER C., ELKAIM E., BESSIERE M., LEFEBVRE S. X-ray resonant scattering in ferromagnetic CoPt. (Poster)

BROWN P.J., NUNEZ V., TASSET F. Magnetic structure determination using generalized polarization analysis of neutrons.

CHATTOPADHYAY T., BROWN P.J., GRUEBEL G., AXE J.D., GIBBS D. Neutron and X-ray resonance magnetic scattering in $EuAs_3$.

ALUSHTA, USSR: VIII International School on Neutron Physics - 1990/10

ULBIG S., LIEB K.P., BOERNER H.G., JOLIE J., ROBINSON S.J. GRID lifetime spectroscopy of medium mass nuclei.(Invited Talk)

ASILOMAR, Ca, USA: 7. International Symposium on Capture Gamma-ray Spectroscopy and Related Topics - 1990/10/14-19

HOYLER F., FOEHL K., BOERNER H.G., KRUSCHE B., ROBINSON S., SCHILLEBEECKX P. Features of the levelschemes of $^{164\text{-}166}Dy$. (Poster)

KESSLER E.G., DEWEY M.S., GREENE G.L., DESLATTES R..D., BOERNER H.G. Precise absolute gamma-ray wavelength measurements.

KLORA J., BOERNER H.G., VON EGIDY T., HILLER H., JUDGE S., KRUSCHE B., LIBMAN V.A., LINDNER H., LITVINSKY L.L., MAYERHOFER U., MURZIN A.V., ROBINSON S.J. Nuclear structure investigations and lifetime measurements in ^{156}Gd. (Poster)

ULBIG S., LIEB K.P., BOERNER H.G., ROBINSON S.J., BOOTEN J.G.L. GRID- Lifetime measurements and shell model calculations in ^{59}Ni.

WHITE D.H., HOFF R.W., BOERNER H.G., COLVIN G., HOYLER F., SCHRECKENBACH K. Nuclear structure of ^{241} Pu from (n,γ) and (n,e) reaction measurements.

BERLIN, Deutschland: VIIIth International Congress of Virology - 1990/08/26-31

BURNS N.R., SAILBIL H., PEARL L., PARDON J.F., TIMMINS P.A., RICHARDSON S.M.H., ADAMS S.E., KINGSMAN A., KINGSMAN S.M. Structural analysis of Ty virus-like particles.

BERLIN, Deutschland: Arbeitstreffen des Verbundes Forschung mit Neutronen - 1990/10/1-3

BRUECKEL T. Die Ladungsdichtewelle in α-U. (Invited talk)

GOBRECHT K.H. Versuch zur Beobachtung freier Neutron-Antineutron Oszillationen. (Poster)

LIED A. EVAnescent wake diffractometer. (Poster)

PETRY W. Phononen an martensitischer Phasenübergängen. (Talk)

STEINER T., SAENGER W., LECHNER R.E. Dynamics of water molecules enclosed in the cavity of beta-cyclodextrin. A quasielastic neutron scattering study. (Poster)

TRAMPENAU J., HEIMING A., PETRY W., HERZIG C. Eine symmetriebrechende Phononenanomalie in β-ZrNb. (Poster)

TRAMPENAU J., HEIMING A., PETRY W., GUETHOFF F., HERZIG C. Phononenkontrollierte Selbstdiffusion in Cr. (Poster)

WEIRAUCH W., KRUGER E., NISTLER W. Präzisionsmessung von h/m_n.

BIELEFELD, Germany: Workshop on Coordination Polyhedra in Solid State Matter - 1990/10/1-6

PANNETIER J., RODRIGUEZ-CARVAJAL J. Prediction of crystal structures by simulated annealing. (Poster)

BIVIERS, Grenoble, France: CARBON 90- Annual Meting of the "Groupe Français d'Etudes des Composés d'Insertion" - 1990/3/28

GONDRAD M., RODRIGUEZ-CARVAJAL J., STROBEL P., PERNET M., BONNET B. Insertion du lithium dans gamma-Fe_2O_3. (Poster)

PANNETIER J. Analyse des profils de diffraction de composés partiellement désordonnées par simulation numérique.

PILLIERE H., GOLDMANN M., BEGUIN F. Processus d'intercalation d'alcanes dans les graphitures de cesium. (Talk)

BORDEAUX, France: 15 Congress & General Assembly of the International Union of Crystallography - 1990/7/19-28
(Abstracts in Acta Cryst. Supplement C)

BARUCHEL J., CHEVRIER J., PEARCE A. Neutron topographic experiments on chirality domains in helimagnetic crystals. (Poster)

BELTRAN D., SAPINA F., SANCHIS M.J., IBANEZ R., BELTRAN A., RODRIGUEZ-CARVAJAL J. Crystal and magnetic structures of Bi_2CuO_4 and Li_2CuO_2. (Poster)

CALDES M.T., NAVARRO J.M., FUERTES A., FONTCUBERTA J., MIRAVITLLES C., OBRADORS X, RODRIGUEZ-CARVAJAL J., VALLET-REGI M., GONZALES-CALBET J.M. Structural and physical properties of $Bi_4Sr_8Cu_5O_{19+x}$. (Poster)

CARLING S.G., DAY P., VISSER D. Crystal and magnetic structures of layer phosphates. (Poster)

CHAILLOUT C., BORDET P., CHENAVAS J., CHEONG S.W., FISK Z., MCINTYRE G.J., MAREZIO M., MOROSIN B., SCHIRBER J.E. Phase separation and crystal structure of superconducting $La_2CuO_{4-\delta}$. (Poster)

GAVARRI J.R., CAREL C., MONNEREAU O., VACQUIER G., VETTIER C., HEWAT A.W. Simulations of structural evolutions at low-temperatures: High pressure compressibility coefficients, elastic constants and the Grueneisen parameters in high Tc superconductors.

HOWARD J.A.K., WILSON C., MACKENZIE K., JOHNSON R.E., MASON S.A., WILSON C.C. Structural studies of intra-molecular dyotropic isomers. Abstract P. C181. (Poster)

HOWARD J.A.K., LAPPERT M.F., MASON S.A. Low valent molecular "agostic" complexes. Abstract P. C237. (Poster)

KULDA J., BARUCHEL J., GUIGAY J.P., SCHLENKER M., TASSET F. Theory of recent extinction theories by polarized neutron diffraction on magnetic crystals. (Poster)

LEHMANN M.S., MCINTYRE G.J., KUHS W.F. Three-dimensional display and analysis of single-crystal reflections in neutron diffraction. (Poster)

LE BAS G., MASON S.A., RYSANEK N., TSOUCARIS G. Neutron diffraction study of alpha-cyclodextrin cyclopentanone clathrate at 20 K. Host guest interactive disorder. Abstract P. C-169. (Poster)

MCINTYRE G.J., STEVENSON A.W. Three-dimensional analysis of X-ray reflections from extended-face single crystals. (Poster)

MARMEGGI J.C., LANDER G.H., BRUECKEL T., ZEYEN C.M.E., VON SMAALEN S. High resolution neutron scattering study of the structural phase transitions in alpha uranium. (Poster)

OLOVSSON I., PTASIEWICZ-BAK H., MCINTYRE G.J. Superposition and polarization effects on the electron density. (Poster)

PANNETIER J. Neutron powder diffractometry.

STEINER T., MASON S.A., SAENGER W., Geometry of the hydrogen bonding network in beta-cyclodextrin-ethanol-octahydrate determined by neutron crystallography at T=295 K and T=15 K. Abstract P. C-107. (Poster)

BOSTON, USA: MRS Fall Meeting - 1990/11/26-30

PANNETIER J. Manganese dioxides: Structural model and in-situ neutron powder diffraction investigation of electrochemical reduction and thermal annealing.

BRAUNSCHWEIG, Germany: 90 PTB Seminar: Fundamental Constants and Physical Units - 1990/10/5-16

WEIRAUCH W., KRUEGER E., NISTLER W. Determination of h/mn. (Poster)

BRISTOL U.K: Neutron Scattering 1990 - 1990/9/11-12

ALLMAN J.M., RICHARDSON R.M., MCINTYRE G.J. A method for measuring the orientational distribution in liquid crystals . (Poster)

BERNOEFT N.R., ALLEN P.J., PAUL D.M., HAYDEN S., TIMMINS P.A., LONZARICH G.G. Small angle scattering at magnetic and superconducting phase transitions.

COWLEY R.A., MCFORROW D.F., JEHAN D.A., MCINTYRE G.J. Magnetic structure of holmium in an applied magnetic field. (Poster)

TIMMINS P.A., HAUK J., WELTE W. The influence of heptane-1,2,3-triol on the size and shape of LDAO micelles. Implications for the crystallization of membrane proteins.

CAEN, France: Céramiques Supraconductrices à Haute Température Critique. 2èmes Journées d' Etudes - 1990/10/6-7

GAVARRI J.R. Anisotropie élastique et coefficients de Grueneisen anormaux. (Poster)

GAVARRI J.R., CAREL C., MONNEREAU O., VACQUIER G., VETTIER C., HEWAT A.W. Evolutions structurales et effets de pression dans des céramiques supraconductrices. (Poster)

COLD SPRING HARBOR, USA: Molecular Biology of DNA Tumour Viruses Meeting 1990 - 1990/8/15-19

RIZO C., BARGE A., RUIGROK R.W., TIMMINS P., CHROBOCZEK J. Human adenovirus serotype 3 fiber protein.

COMO, ITALY: 11th IUPAC Conference on Chemical Thermodynamics - 1990/8/26-31

GAGO-PORT L., RODRIGUEZ-CARVAJAL J., GARCIA-RUIZ J.M., SANTOS A. Kinetics of polymorphic phase transitions in ammonium nitrate.

COPENHAGEN, Denmark: Scandinavian Structural Chemistry Meeting - 1990/01

OLOVSSON I., PTASIEWICZ-BAK H., MCINTYRE G.J. Superposition and polarization effects on the electron density of lone pairs. (Talk)

DEUSTO, Spain: I Jornadas Sobre Tecnicas de Neutrones - 1990/10/17-20

GARCIA-MUNOZ J.L. The metal-insulator transition in the $RNiO_3$ family studied by neutron diffraction.

SANDONIS J. Estudio mediante topografia con neutrones de la coexistencia de fases y efectos de extincion en la hematita alpha-Fe_2O_3.

DJERBA, Tunisie: Transphase-3, Colloque d'Expression Française sur les Transitions de Phase - 1990/07

PETRY W. Rôle des phonons dans les transitions martensitiques de la phase cubique centrée de Ti, Zr et Hf. (Invited talk)

GRENOBLE, France: Clips de Physique - 1990-11

BALLOU R., LACROIX C., NUNEZ REGUEIRO M.D. Instabilité de l'antiferromagnétisme de bande dans les réseaux frustrés.

GRENOBLE, France: Workshop on Synchrotron Radiation Topography: Present Achievements and Propects at the ESRF - 1990/8/2-3

SANDONIS J., BARUCHEL J., SCHLENKER M. Variation of the shape of the interface between the heli and ferromagnetic phases in MnP as a function of the applied magnetic field.

HERAKLION, Crete: International Discussion Meeting on Relaxation in Complex Systems - 1990/6

FRICK B. Neutron scattering studies of the glass transition in polymers.

JUELICH, Germany: Bunsenkolloquium über Atomare Aspekte der Diffusion in Festkörpern - 1990/10

PETRY W. Korrelation zwischen Diffusionsverhalten und Phononenerweichung. (Invited talk)

KYOTO, Japan: Ultrahigh Resolution Neutron Spectroscopy and Optics - 1990/03

DREXEL W. The new VCN-UCN source at the ILL and first experiments. (Invited talk)

LEUVEN, Belgium: 8. Meeting on Small Angle Scattering - 1990/08

WAGNER W., WIEDENMANN A., CHEN W., SUNDERARARAMAN M., PETRY W. Microstructural characterization of nimonic Pe16 after Cyclic loading- A study combining SANS and TEM. (Poster)

LEUVEN, Belgium: 1rst International Conference on f-Elements (ICFE) - 1990/9

DE ANDRES A., FERNANDEZ-DIAZ M.T., MARTINEZ J.L., RODRIGUEZ-CARVAJAL J., SAEZ-PUCHE R., FERNANDEZ F. Raman scattering study of $Ln_2NiO_{4+\delta}$ with Ln=La, Pr, Nd. (Poster)

FERNANDEZ F., SAEZ-PUCHE R., FERNANDEZ T., RODRIGUEZ-CARVAJAL J., MARTINEZ J.L., BOTTO I.L., BARAN E.J. Low-temperature phase transition of the stoichiometric Ln_2NiO_4 oxides. (Poster)

LISBOA, Portugal: 10th Conference of the Condensed Matter Division of the EPS - 1990/04/9-12

FERNANDEZ-DIAZ T., RODRIGUEZ-CARVAJAL J., MARTINEZ J.L., FERNANDEZ F., SAEZ-PUCHE R. Structural and magnetic characterization of rare earth nickelates ($R_2NiO_{4+\delta}$). (Poster)

LONDON, U.K: Localisation 90 - 1990/8

CHALKER J.T., BERNHARDT M. The transfer matrix approach to localization.

CHALKER J.T., EASTMOND J. Localization and the integer quantum Hall effect.

LONDON, U.K: 2nd Conference on Position-Sensitive Detectors - 1990/9/4-7

GELTENBORT P., OED A. Recent results of position sensitive gas counters with microstrip anode for neutron detection. (Talk)

OED A., GELTENBORT P., BUDTZ-JORGENSEN C. Substratum and layout parameters for microstrip anodes in AgS detectors.

LOS ALAMOS, USA: International Workhop on Cold Neutron Sources - 1990

GOBRECHT K.H. ILL cold sources (Invited talk)

LYON, France: European Physical Society. First Liquid Matter Conference - 1990/7/7-11

BAFILE U., VERKERK P., DE GRAAF L.A., BAROCCHI F., SUCK J.B., MUTKA H., Neutron Brillouin scattering in high density argon gas and the onset of non-hydrodynamic behaviour.

BAFILE U., VERKERK P., DE GRAAF L.A., BAROCCHI F., SUCK J.B., MUTKA H.: . Density expansion of experimental dynamic structure factor in argon: The two-body term.

EGELSTAFF P.A., SUCK J.B., MUTKA H., YOUDEN J.P.A.: Neutron Brillouin scattering in dense gases.

MAGLI R., FREDRIKZE H., CHIEUX P., BAROCCHI F. Three-body effects in the neutron structure factor of argon.

MONTPELLIER, France: Journées de la Matière Condensée. Société Française de Physique - 1990/9/4-6

NUNEZ REGUEIRO M.D., MEDINA G. Modèle de transfert de charge pour les supraconducteurs à haute Tc (Poster)

NEW ORLEANS, Louisiana, USA: 40th Anniversary Meeting of the American Crystallographic Association - 1990/4/8-13

MCINTYRE G. LEHMANN M.S. Three-dimensional display and analysis of single-crystal reflections. (Talk)

PARIS, France: CARBON 90. International Conference on Carbon - 1990

PILLIERE H., GOLDMANN M., BEGUIN Intercalation process of alkanes in cesium graphitides. P. 104 (Talk)

PARIS, CEN Saclay, France: RecA and Related Proteins - 1990/09/17-21

DiCAPUA E., CUILLEL M., SCHNARR M., TIMMINS P.A., RUIGROK R.W.H.
Induction of recA to LexA cleavage by non-DNA ligands.

RUIGROK R.W.H., TIMMINS P.A., DICAPUA E. Salt-induced changes in RecA.

PARIS, CEN Saclay, France: Short Range Order in Ill Ordered Materials. Satellite Meeting of the 15th Congress of the International Union of Crystallography - 1990/7

PETRY W. Dynamics of the glass transition.

PONDORLY: Réunion Francophone des Cristallographes des Protéines - 1990/3

PEBAY-PEROULA E. Détermination de la structure de la sous-unité 50S du ribosome de halobacterium maris-mortui par diffraction neutronique.

REGENSBURG, Germany: DPG Frühjahrstagung - 1990/03/25-30

BRUECKEL T. Bestimmung magnetischer Austauschwechselwirkungen mit Hilfe von Neutronenbeugung. (Talk)

FRICK B., RITTER C Temperaturabhängigkeit des Nahordnungs- und des Unordnungsspectrums eines schnell und langsam abgekühlten polymeren Glasses. (Poster)

FRICK B. Diffusion von Wasserstoff in YH_X bei hohen Konzentrationen (1,7<=X<=2,1). (Poster)

FRICK B., FARAGO B., RICHTER D. Temperaturabhängigkeit des Nichtergodizitätsparameters in der Nähe der Glastemperatur. (Poster)

HEIMING A., **PETRY W.**, TRAMPENAU J., HERZIG C., VOGL G. Gitterplatzuntersuchung von schnell diffundierendem Co in bcc-Zr. (Talk)

LOEWENHAUPT M., HOFFMANN P., CHATTOPADHYAY T., HARTWEG M. Untersuchung der Kristallfeldaufspaltung der niedersymmetrischen halbmetallischen Verbindungen REP5. (Poster)

MALETTA H., POERSCHKE E., CHATTOPADHYAY T., BROWN P.J. 2 und 3-dimensionale Ordnung in ErBa2Cu3Ox (6<=x<=7). (Poster)

PETRY W., BARTSCH E., FARAGO B., FUJARA F., KIEBEL M., SILLESCU H. Dynamik von ortho-terphenyl unterhalb und oberhalb des Glasübergangs.

REICHENAUER G., SOSNOWSKA I., GRAETSCH H., IBEL K., FRICK B. , BUCHENAU U. Niederfrequente Schwingungen in Edelopal. (Talk)

RICHTER D., SCHAEFER D., FARAGO B., FRICK B. Dynamik von schwach verknüpften Netzwerken. (Talk)

TRUMP R., THIERFELDT S., CHATTOPADHYAY T., LOEWENHAUPT M. Magnetische Struktur des Kondogitters $CeCu_2$. (Poster)

WOCHNER P., **PETRY W.**, PEISL J. Untersuchung des Orientierungsübergangs in $(KBR)_{1-X}(KCN)_X$ mit hochauflösender quasielastischer Neutronenstreuung. (Talk)

WAGNER W., PETRY W. Reaktionskinetik der Entmischung in verdünnter CuCo-Legierung. (Talk)

WAGNER W., HAHN H., AVERBACK R.S., WIEDENMANN A., PETRY W.. Charakterisierung der Porosität nanokristalliner Keramken mit Hilfe der Neutronen-Kleinwinkelstreuung. (Talk)

RUTHERFORD, U.K: WONDSA 90. Neutron Data Scattering. Data Analysis - 1990/3/14-16

PANNETIER J. Simulated annealing: An introductory review.

SAN DIEGO, Ca, USA: 35th Annual Conference on Magnetism and Magnetic Materials - 1990/10/29-11/1

VISSER D., MCINTYRE G.J., HARRISON A. Magnetic ordering in triangular antiferromagnets: A neutron scattering study. (Talk)

VISSER D., CARLING S.G., DAY P. Magnetic structure of $KMnPO_4.H_2O$. (Talk)

TRUMP R., THIERFELDT S., LOEWENHAUPT M., CHATTOPADYAY T. Magnetic structure of the Kondo lattice compound $CeCu_2$. (Poster)

STRASBOURG, France: Journées de Chimie, Alsace-Suisse - 1990/3

HELM L., COSSY C., POWELL D.H., MERBACH A.E. The hydration of lanthanide (III) ions in aqueous solution: A neutron scattering first order difference study.(Poster)

TOULOUSE, France: Powder Diffraction. Satellite Meeting of the XVth Congress of the International Union of Crystallography - 1990/7/16-19

ALCOBE X., ESTOP E., RODRIGUEZ-CARVAJAL J., ALVAREZ A., LABRADOR M., CALVET T. A neutron powder diffraction study of the structure of deuterated p-diiodobenzene ($C_2D_4I_2$). (Poster)

MEDARDE M., RODRIGUEZ-CARVAJAL J. The effect of systematic errors and structural complexity in Rietvelt refinements: A simulation study.

PANNETIER J. Recent developments in time-resolved powder diffraction.

RODRIGUEZ-CARVAJAL J. Fullprof: A program for Rietveld refinement and pattern matching analysis. (Poster)

TUTZING, Germany: 50 Years after Kramers - 1990/9/10-13

WUERGER A. Nuclear spin conversion of methyl groups.

VANCOUVER, Canada: International Biophysics Congress - 1990/07/27-08/8

CHOBROCZEK J., CHATELLARD C., RIZO C., BARGE A., TIMMINS P.A., JACROT B. Adenovirus fiber expressed in E. Coli.

ZUERICH, Switzerland: Société Suisse de Cristallographie - Chemistry and Structure. A Symposium in Honour of Professor J.D. DUNITZ - 1990/3/14-15

HOWARD J.A.K., WILSON C., MACKENZIE K., JOHNSON R.E., MASON S.A., WILSON C.C. Structural studies of intramolecular dyotropic isomers. (Poster)

Workshops organized by the ILL in 1990

ILL, Grenoble, France, September 17-18, 1990.
Workshop on Neutron Optics.
FAUDOU J.C., MAGERL A., RICHTER D.

ILL, Grenoble, France, October 23, 1990.
Industrial User's Meeting on the Development of Industrial Use of Neutrons at the ILL.
WRIGHT A.F.

Workshops sponsored by the ILL in 1990

Alpe d'Huez/Grenoble, France, July 30-August 1, 1990.
Complementary Applications of Diffraction by Neutrons and X-Ray Synchrotron Radiation. International Satellite Conference of the IUCr XVth Congress and General Assembly. (Abstracts, 90LE24T).
LEHMANN M.S., VETTIER C., HODEAU J.L.

Aussois, France, September 17-21, 1990.
International Workshop on Geometry and Interfaces.
DUBOIS-VIOLETTE E., PANSU B.

Bombannes, France, May 27-June 2, 1990.
European Workshop on Neutron-, X-Ray- and Light Scattering as an Investigative Tool for Colloidal and Polymeric Systems.
LINDNER P., RIEKEL C., WILLIAMS C., COTTON J.P., ZEMB T.

Exeter, U.K., August 10-14, 1990.
Workshop on the Excitations in 2-Dimensional and 3-Dimensional Quantum Fluids.
WYATT A.F.G., LAUTER H.J.

Krems/Donau, Austria, September 24-26, 1990.
Symposium on the Future Scientific Use of European Neutron and Photon Sources.
LAGGNER P., NETZER F., RAUCH H., REITER W., SKALICKI P., VOGL G., WEINZIERL P., ZEILINGER A.

Lyon, France, July 7-11, 1990.
European Physical Society First Liquid Matter Conference.
BRATOS S., HANSEN J.P.
(Papers published in Special Issue of Journal of Physics C Supplement A, December 1990)

Books or conferences published in 1990

Trends in Colloid and Interface Science IV. Proceedings of the Third ECIS Conference and ILL Workshop, Basel, Switzerland, September 19-22, 1989.
ZULAUF M., LINDNER P., TERECH P. Eds.
PROGRESS IN COLLOID AND POLYMER SCIENCE 81 (Steinkopff Verlag, 1990) (ISSSN 0340-255 X).

The Theory of Quantum Liquids, Vol. 2 : Superfluid Bose Liquids
NOZIERES P., PINES D.
(Addison-Wesley Publ. Co., 1990), (ISBN 0-201-50063-9).

Theses

CHENEVIER B.
Etude des transitions de phases cristallines et magnétiques dans les systèmes Fe_2P - Mn_2P, MnRuAs, MnRhAs et FeRhP.
THESE, UNIVERSITE JOSEPH FOURIER DE GRENOBLE, NOVEMBRE 1990.

CHIBANE Y.
A new magnetometer for the neutron EDM experiment.
THESIS, UNIVERSITY OF SUSSEX, SEPTEMBER 1990

COOK J.C.
Quasi-elastic neutron scattering studies of hydrogen and deuterium diffusion in the systems α'-NbH_x and α'-NbD_x.
THESIS, UNIVERSITY OF BIRMINGHAM, FEBRUARY 1990.

DEBUS O.
Untersuchung der mikroskopischen Dynamik eines niedermolekularen Glassbildners mittels inkohärenter inelastischer Neutronenstreuung.
DIPLOMARBEIT, JOHANNES GUTENBERG-UNIVERSITÄT MAINZ, 1990.

FAK B.
Elementary excitations in liquid ^3He and $^3He/^4He$ mixtures.
DOCTORAL DISSERTATION, UPPSALA UNIVERSITY, 1990.
(ACTA UNIVERSITATIS UPSALIENSIS. COMPREHENSIVE SUMMARIES OF UPPSALA DISSERTATIONS FROM THE FACULTY OF SCIENCE 239).

FANJAT N.
Etude des propriétés magnétiques statiques et dynamiques de $M_2Na_3(PO_4)_3$, M = Fe, Cr par diffusion de neutrons.
THESE, INSTITUT NATIONAL POLYTECHNIQUE DE GRENOBLE, NOVEMBRE 1990.

GIESEN U.
Zur Struktur superhelikaler und ringoffener DNA in verdünnter Lösung und im Flüssigkristall.
DISSERTATION, UNIVERSITAET KONSTANZ, AUGUST 1990.

HEIMING A.
Anomalous diffusion in bcc-Zr and bcc-ZrCo. A contribution to its understanding from neutron scattering.
INAUGURAL DISSERTATION, FREIE UNIVERSITAET BERLIN, DECEMBER 1989.

KELLERSOHN T.
Zur Strukturchemie von festen Hydraten und Hydroxiden. Neutronenbeugung, Röntgenographische und Schwingungsspektroskopische Untersuchungen an Halogenaten, Hydroxiden, Hydroxidhalogeniden und Halogeniden des Strontiums, Bariums und Bleis.
DISSERTATION, UNIVERSITÄT-GESAMTHOCHSCHULE-SIEGEN, 1990.

LEHMANN M.S.
Habilitation à diriger les recherches.
HABILITATION, UNIVERSITE JOSEPH FOURIER, GRENOBLE, JUILLET 1990.

LEMEE-CAILLEAU M.H.
Etude, sous pression, de transitions de phase dans des cristaux moléculaires. Résultats par diffusion Raman en association avec la diffusion neutronique.
THESE, UNIVERSITE DE RENNES I, AVRIL 1989.

LISS K.D.
Untersuchungen zur Verbesserung der Energieauflösung für Neutronenrückstreuspektrometer unter Verwendung von Idealkristallen mit geringer dynamischer Breite der Reflexionskurve.
DIPLOMARBEIT, TECHNISCHE UNIVERSITAET MUENCHEN, JULI 1990.

NEUMANN K.U.
Untersuchung schwerer Fermion Systeme mit Hilfe der spinpolarisierten Neutronenstreuung.
DISSERTATION, TECHNISCHE HOCHSCHULE AACHEN, 1990.

PRIEM T.
Etude de l'ordre à courte distance dans les carbures et nitrures non stoechiométriques de métaux de transition par diffusion diffuse de neutrons.
THESE, UNIVERSITE PARIS-SUD, OCTOBRE 1988.

RAZAFITIANAMAHARAVO A.
Etude structurale du film pur de cyclohexane physisorbé sur graphite. Etude thermodynamique et structurale du film mixte (krypton-cyclohexane) physisorbé sur graphite.
THESE, UNIVERSITE DE NANCY I, JUIN 1989.

REY M.J.
Supraconducteurs à haute température critique : étude de nouveaux oxydes de structure dérivée de la pérovskite.
THESE, INSTITUT NATIONAL POLYTECHNIQUE DE GRENOBLE, 1990. (Partly at ILL)

STEINBINDER D.
Neutronenstreuuntersuchungen zur Tunnel- und Diffusionsbewegung von Wasserstoff in den Metallen Niob und Vanadium.
DISSERTATION, TECHNISCHE HOCHSCHULE DARMSTADT, 1990.

Publications - Internal reports

This list groups all publications resulting from the research at the ILL during 1990.
ILL Reports are listed first. They are followed by the list of publications in the scientific literature (journals, conference proceedings, books) with ILL authors and coauthors and by publications related to experimental work performed by visiting scientists at the ILL but without ILL author or coauthor.

Internal Reports

(Code number 1 to 99) (G = General Reports, T = Technical Reports)

90BR01T
BROWN P.J., MATTHEWMAN J.C.
The Cambridge crystallographic subroutine library. Appendix A to the Mark 3 User's manual : Specifications of subroutines.
TECHNICAL REPORT.

90GR02G
THREE-AXIS GROUP
TAS (V5) User guide.
GENERAL REPORT.

90CA03G
CASTETS C.
1989 ILL experimental reports and theory college activities.
GENERAL REPORT.

90JA04T
JANOT C., BOERNER H.G., DAY P., DIANOUX A.J., FAUDOU J.C., VETTIER C., ZEYEN C.M.E.
Second modernization programme. Working group 'Instruments'. Progress report (January 1990).
TECHNICAL REPORT.

90LA05T
LAUGIER J., ROLLAND G., FILHOL A.
User's manual for OrientExpress (version 1) for IBM personal computer or compatibles.
TECHNICAL REPORT.

90GR06T
GREEN K., KILVINGTON A.I., SMITH K.F., PENDLEBURY J.M., THOMPSON D.
Some measurements on an ultra-cold neutron gas.
TECHNICAL REPORT.

90EB07T
EBELING H.
Das Neutronenschwerkraftspektrometer NESSIE am ILL, Grenoble.
TECHNICAL REPORT.

90AN08T
ANTONIADIS A., BERRUYER J., FILHOL A.
Maximum likelihood refinement of powder diffraction patterns.
TECHNICAL REPORT.

90BR09T
BROCKER C.
Studie zum Graphitprojekt am ILL.
TECHNICAL REPORT.

90RE10T
RENNIE A.R., GHOSH R.E.
DIS-ARRAY. A distributed computing solution for SANS spectrum colour display and analysis.
TECHNICAL REPORT.

90MO11G
MORELL B.
Collaboration scientifique à l'Institut Laue-Langevin de 1981 à 1990.
GENERAL REPORT

90LI12T
LINDNER P., FOUBERT J.
Power_check. A program for graphical display and printout of HFR power record.
TECHNICAL REPORT.

90CA13T
CABAU E., ANTONIADIS A., FILHOL A.
Algorithme d'affinement de profils avec séparation des paramètres à comportements linéaires et non-linéaires.
TECHNICAL REPORT. (Suite de 89DR14T)

90RO14T
ROBINSON S.J., JOLIE J.
The computer code Griddle.
TECHNICAL REPORT.

90OL15T
OLIVER R., ROBINSON S.J., VITTOZ P, VIVIER G.
Methods of instrumental activation analysis at the ILL.
TECHNICAL REPORT.

90TA16T
TASSET F.
A report on polarised neutron techniques and the need for medium and short wavelength ^{3}He-polarisers. Contribution to the 3ème Souffle Working Group 'Techniques'.
TECHNICAL REPORT.

90RI17T
RIEUTORD F.
INX - Program for time-of-flight data reduction. User's guide.
TECHNICAL REPORT.

90CA18T
CACELLES A.
Evaluation d'un détecteur de localisation courbe pour diffraction de poudres des rayons X.
TECHNICAL REPORT.

90AG19T
AGERON P., ESCOFFIER A., HAMELIN B., ROBERT A.
A hot neutron source at very high temperature.
TECHNICAL REPORT.

90IC20T
ICHE G.
Model independent deconvolution of resolution using maximum entropy and alternative methods.
TECHNICAL REPORT.

90IL21T
INSTITUT LAUE-LANGEVIN
Five-year development programme (1992-1996). Troisième souffle.
TECHNICAL REPORT.

90TH22T
THOMPSON D.
The electric dipole moment of the neutron experiment. A user's guide.
TECHNICAL REPORT.

90LI23T
LINDNER P.
Neutron flux measurements at D11.
TECHNICAL REPORT.

90LE24T
LEHMANN M.S., VETTIER C., HODEAU J.L.
Complementary applications of diffraction by neutrons and by x-ray synchrotron radiation. (Abstracts)
TECHNICAL REPORT.

90CH25T
CHATTOPADHYAY T.
X-ray resonance exchange scattering in $EuAs_3$: A research report.
TECHNICAL REPORT.

90SC26T
SCHAERPF O., GABRYS B., PFEIFFER D.G.
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90CH27T
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90LE28T
LEJEUNE G., FILHOL A.
Interfacing Pascal and C with fortran.
TECHNICAL REPORT.

90GO29T
GOMEZ M.
Projet d'informatisation du fonds documentaire et de la gestion interne d'une bibliothèque scientifique.
TECHNICAL REPORT.

Papers published in scientific periodicals, books and conference proceedings

1 - with ILL authors and coauthors (From code number 101)

90HA101
HANSEN F.Y., FRANK V.L.P., TAUB H., BRUCH L.W., LAUTER H.J., DENNISON J.R.
Corrugation in the nitrogen-graphite potential probed by inelastic neutron scattering.
PHYSICAL REVIEW LETTERS **64**, 764-767 (1990).

90LA102
LANTMAN C.W., MCKNIGHT W.J., RENNIE A.R., TASSIN J.F., MONNERIE L., FETTERS L.J.
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90BA103
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A new experimental limit on neutron-antineutron transitions.
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90RI104
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PROGRESS IN COLLOID AND POLYMER SCIENCE **80**, 53-62 (1989).

90BE105
BERMEJO F.J., BATALLAN F., ENCISO E., WHITE R.P., DIANOUX A.J., HOWELLS W.S.
Diffusional dynamics of hydrogen-bonded liquids: methanol.
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90ST106
STRAUCH D., DORNER B.
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90HO107
HOFF R.W., DRISSI S., KERN J., STRASSMANN W., BOERNER H.G., SCHRECKENBACH K., BARREAU G., RUHTER W.D., MANN L.G., WHITE D.H., LANDRUM J.H., DUPZYK R.J., CASTEN R.F., KANE W.R., WARNER D.D.
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PHYSICAL REVIEW C **41**, 484-512 (1990).

90BO108
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Characteristics of mass and nuclear charge distributions of $^{229}Th(n_{th}, f)$. Implications for fission dynamics.
ZEITSCHRIFT FUER PHYSIK A **335**, 41-48 (1990).

90GO109
GOLDMANN M., PILLIERE H., BEGUIN F.
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SYNTHETIC METALS **34**, 59-65 (1989).

90RO110
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Magnetism of $CoCl_2$ intercalated in graphite studies by elastic and inelastic neutron scattering.
SYNTHETIC METALS **34**, 513-518 (1989).

90SC111
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Amplitude, wavevector and frequency dependence of magnetic fluctuations in $YBa_2Cu_3O_{6+\delta}$.
ZEITSCHRIFT FUER PHYSIK B **78**, 345-359 (1990).

90ST112
STRAUCH D., MAYER A.P., DORNER B.
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ZEITSCHRIFT FUER PHYSIK B **78**, 405-410 (1990).

90JA113
JANOT C.
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90FO114
FORGAN E.M., PAUL D. MCK., MOOK H.A., TIMMINS P.A., KELLER H., SUTTON S., ABELL J.S.
Observation by neutron diffraction of the magnetic flux lattice in single-crystal $YBa_2Cu_3O_{7-\delta}$.
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90WU115
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