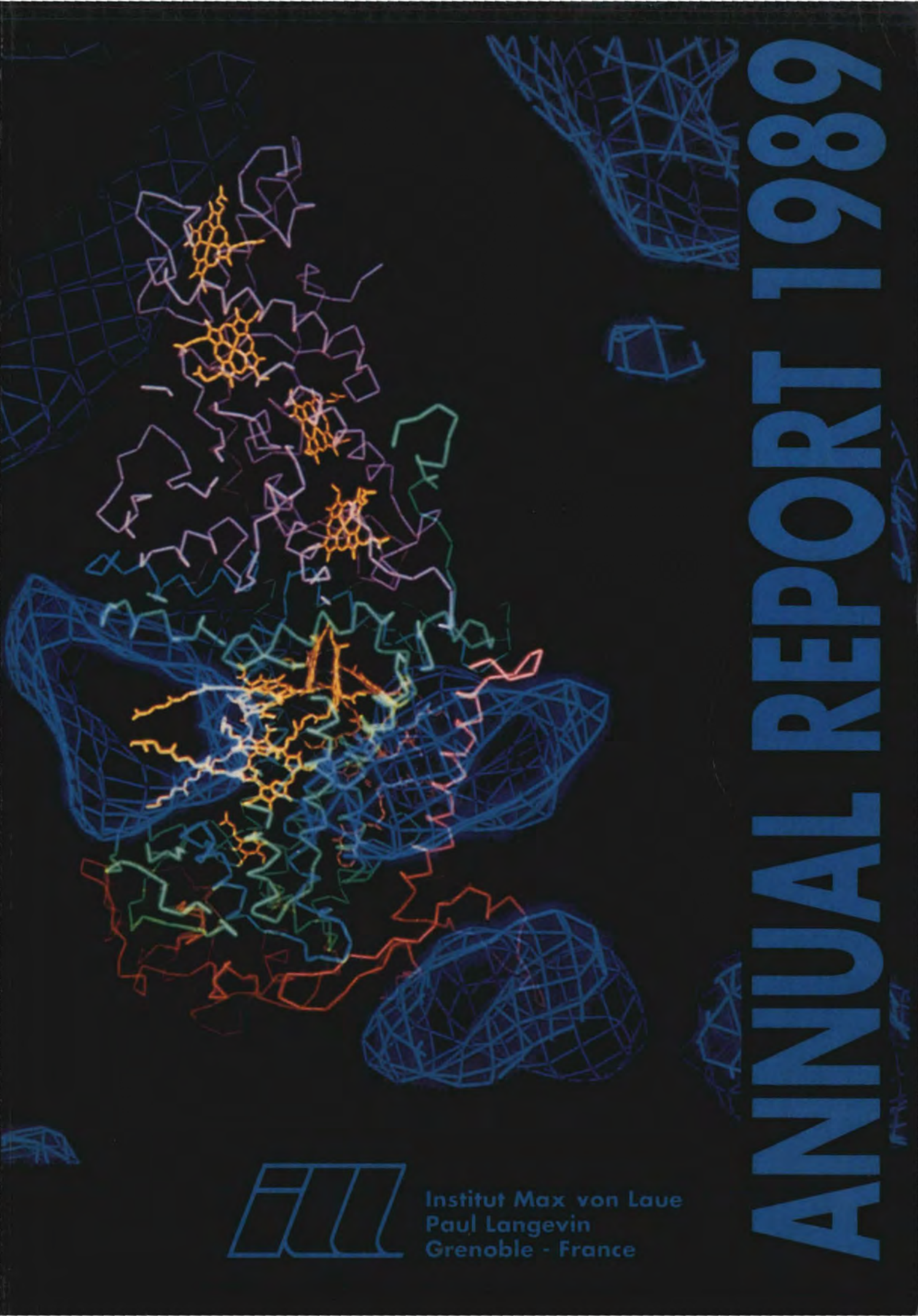

ANNUAL REPORT 1989

Institut Max von Laue
Paul Langevin
Grenoble - France

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Application for the use of ILL facilities

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 48 72 44 B. Maier
76 48 71 79 H. Blank
76 48 70 41 K. Mayer-Jenkins (Secretary)
76 48 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 five 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,

available from SCAPRO.

Experimental Reports and Theory College Activities 1989,

available from the ILL Library.

Front Cover

Section through the photosynthetic reaction centre in the cell membrane of the bacterium Rhodo-pseudomonas viridis (results from DB21, see College 8 report). Subunits are indicated by colours red, green and mauve. The prosthetic groups are orange. The detergent mimicking the membrane is seen in blue.

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The Institut Max von Laue - Paul Langevin

The Institut Max von Laue - Paul Langevin

The Institut Max von Laue-Paul 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. The pertinent agreement between the ILL and the Swiss Bundesrat für Bildung und Wissenschaft was signed in May 1988.*)

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 and Swiss 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 and Swiss scientist in the ILL Scientific Council as well as membership in two of our sub-committees. The participation of Spain and Switzerland to the ILL Budget is limited to 1.5% each.

External Organization of the ILL

Associates of the ILL

UNITED KINGDOM

Science and Engineering Research Council (SERC)

FRANCE

Commissariat à l'Energie Atomique (CEA)
Centre National de la Recherche Scientifique (CNRS)

FRG

Kernforschungszentrum Karlsruhe (KFK)

Countries with scientific membership

SPAIN

Comisión Interministerial de Cienca y Tecnología (CICT)

SWITZERLAND

Bundesamt für Bildung und Wissenschaft (BBW)

Steering Committee (at its last meeting)		
■ Hansen (BMFT) ■ Klose (KFK) ■ Steiner (Univ. Mainz) ■ Schunck (BMFT)	■ Comes (CNRS) ■ Cribier (CEA) ■ Sevin (CNRS) ■ Winter (CEA)	■ Clark (SERC) ■ Enderby (Bristol) ■ Newport (SERC) ■ Ritzema (DES)

Scientific Council	
Plenary Session 30 members	**Subcommittees** 68 members

General Organigram

Directorate

Director:
P. Day

Co-Directors:
J. Charvolin
P. Armbruster

Departments

Reactor Department
Head: E. Bauer
- Reactor Operation
- Operation of Sub-assemblies
- Site Security

Instrument Operation Department
Head: A. Heidemann
- Instrument Groups
- Central Group
- Sample Environment Group
- Cryogenics Service
- Site Maintenance

Instrument and Methods Department
Head: J.C. Faudou
- Instruments and Methods
- Construction & Mechanical Maintenance
- Electronics
- Monochromators
- Multi-detectors
- Special Instruments
- Multilayer Laboratory

Computing Department
Head: D. Rimmer
- Automation, Data Acquisition and Treatment
- Scientific Computing (DEC-1091)
- Telephone

Administration Department
Head: H.M. Spilker
- Personnel
- Finance & Purchasing
- Welfare & Staff Training
- Translation Office
- Secretariat of the Steering Committee

Directorate Services

Scientific Coordination & Public Relations Office
Head: B. Maier
- Co-ordination of the Experimental Programme
- Organisation of Workshops & Conferences
- Public Relations

Délégué for Safety, Medical and Health Physics Group
Bureau du Colombier

Library
Head: C. Castets

Physicists' Secretariat
Head: F. Parisot

Scientific Sectors

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

Physicists' Representatives
Scientific Staff
- 66 Experimentalists
- 12 Theoreticians
- 30 Thesis students

Instrument Groups
Head: Senior Scientists
- Fundamental and Nuclear Physics Instruments
  Head: D. Dubbers
- Three-axis Spectrometers
  Head: B. Dorner
- TOF, High Resolution, SAS, Diffuse Scattering Instruments
  Head: C. Janot, J. Suck
- Diffraction Instruments
  Head: J. Brown

31/12 1989

Visits and Events in 1989

◀ *Dr. Heinz Riesenhuber (centre), the Federal German Minister for Research and Technology, visited ILL on 2 February 1989. He was accompanied by Mme Edwige Avice (right), a minister at the French Foreign Office and D. Thoulouze (left), Director MPB, CNRS. Professor W. Gläser, the then Director of ILL, is turning towards Dr. Riesenhuber. Second from left is A. Michaudon, French Assistant Director of the ILL.*

▶ *The German Ambassador in France, Dr. Franz Pfeffer (second from left) visited ILL on 11 May 1989. He and his wife were shown round the ILL experimental halls by Professor W. Gläser.*

▲ *Peter Day (centre), Professor of Solid State Chemistry at Oxford, took up his duties as Director of ILL on 1.10.89. At the same time Peter Armbruster (left), Professor of Physics at the Heavy Ion Research Institute at Darmstadt became the German Assistant Director. Jean Charvolin (right), Professor of Solid State Physics at Orsay had been French Assistant Director since 1 July 1989.*

▶ *Mr. Robert Jackson (centre), Parliamentary Under-Secretary of State for Higher Education and Science, visited the ILL on 26 May 1989 and was guided on his tour by the ILL Director, P. Day (left).*

Director's Report

This, my first Annual Report as Director, covers a year during most of which the ILL was under the Directorship of Wolfgang Gläser, who returned to his post at the Technical University of Munich at the end of September. My opening words, therefore, are of thanks to him for initiating me into the mysteries of the Institut's functioning, and for the careful stewardship exercised in his time as Director. During that period the annual total of experiments performed at ILL rose from 740 to 850, partly due to the ever-increasing efficiency of the instruments themselves, and partly to the possibility of running again six full reactor cycles per year. The first steps were also taken (of which more below) towards defining proposals to put to our Associates for a modernisation programme designed to keep the ILL in the forefront of the world's neutron scattering centres throughout the 1990's.

Replacing Wolfgang Gläser is Peter Armbruster, formerly Director of GSI Darmstadt and one of the first group of scientists at ILL, having been responsible for the construction of the Lohengrin fission fragment spectrometer. André Michaudon also retired as French Associate Director, having been asked to remain in his post for a further six months after the normal five year term, during which, as he told me, he had served with four successive Directors. We wish him a happy and active retirement, commuting between Grenoble and Los Alamos. In his place we welcome Prof. Jean Charvolin from the CNRS Laboratoire de Physique des Solides, Orsay, a specialist in the physics of 'soft' condensed matter such as polymers and liquid crystals.

Further changes in the senior personnel came with the retirement of F. Franzetti, for 11 years Head of the Reactor Department, and the return of D. Richter, Senior Scientist in the Vercors II (time-of-flight) Group, to Jülich and a Chair at Münster University. E. Bauer, for many years Deputy Head of the Reactor Department, succeeds M. Franzetti.

During the year the Institut received a number of distinguished visitors, including both the British and German Ministers responsible for science: Mr. Robert Jackson MP and Bundesminister H. Riesenhuber. The German Ambassador to France, Herr Franz Pfeffer, also spent a day with us, and among our scientific visitors were Monsieur F. Kourilsky, the Director General of the CNRS, and Mr. J. Fairclough, Chief Scientific Adviser in the UK Cabinet Office, Whitehall.

Reactor Operation and Experimental Programme

The first and most important remark to make about the operation of the reactor in 1989 is that, as our community of users has come to expect, it continues to be extremely reliable. That such a statement can be made so briefly is a tribute to all the staff concerned, because in some respects 1989 was not a straightforward year.

At the beginning of the year, there remained quite a bit of uncertainty about continuity in the supply of fuel for the reactor. However, as the year progressed the situation relaxed considerably with the granting of an export licence by the American authorities in April for the uranium ordered in 1988, which was supplemented in the autumn by a further delivery and by the first instalment of the fuel that would have been used by our former suppliers of fuel elements, NUKEM. Consequently, though fabrication and delivery of fuel elements is still taking place on quite a tight schedule, there is no reason for the time being to fear any interruption in supply.

As a legacy of the interruption at the end of 1988 and beginning of 1989, the longer shutdown for maintenance, which normally takes place in the summer, was rescheduled to the winter period. Nevertheless, despite the postponement of the reactor startup till February, it was still possible to run six full cycles in the year, albeit at the cost of several abnormally short intervals for fuel element exchange.

With the increase from five to six cycles from 1988 to 1989 came a corresponding rise in the number of experiments scheduled, from 807 to 858. At the same time, though, the number of proposals received also increased, from 1069 to 1129, and of the 12,148 days of instrument time requested during 1989 only 7,829 could be accommodated in the schedule. It is also important to note the high proportion of publications arising from the beamtime allocated: the numbers noted by the library for 1987 and 1988 were respectively 407 and 501. A particular statistic may be of general interest: over the last five years no fewer than 62 articles on work emanating from ILL have appeared in Physical Review Letters, i.e. on average a quarter of all the issues of that journal have carried a paper containing new results from our Institut.

Instruments on the Horizontal Cold Source

The major part of the instrument development programme at the Institut remains centred on the construction of instruments for the horizontal cold source. The first of these, the triple-axis spectrometer IN14 in the reactor hall, was placed in the schedule for outside users from the beginning of the year, though the polarizing option remains to be installed in January-February 1990. In the second guide hall itself, the guides with their shielding and shutters are installed and will be functioning normally from the end of 1989. As to the instruments to be installed in the guide hall, construction of the chopper and Doppler machine for the backscattering spectrometer IN10C continues on schedule in collaboration with Jülich. A call for tenders for building the rest of the instrument has gone out, with the aim that the instrument will be mounted in the guide hall during 1990. Construction of the major components for the basic version of the high resolution neutron spin echo spectrometer IN15 is virtually complete and assembly of the main structural elements has begun on site.

Finally, just before Christmas, the 20m long detector tube for the small-angle scattering spectrometer D22 was delivered and assembly is about to begin. The tube is designed to house a large area (75 x 75 cm) detector similar to one just completed by ILL for delivery to HMI Berlin. However, initial tests can be made with the spare detector from D11.

Scientific Highlights

A notable scientific highlight of 1989, and a source of great pleasure to their many friends at ILL, was the award of the Nobel Prize for Physics to two longstanding colleagues and collaborators of the Institut, Wolfgang Paul and Norman Ramsey. Both have been users of the very cold and ultra cold neutron source called the TGV-turbine on level D of the reactor. Wolfgang Paul, Professor at the University of Bonn, was the inventor of a ring for storing neutrons in a toroidal

magnetic field, which was used in the earlier determinations of the lifetime of the neutron, now rendered even more precise by the use of 'bottled' neutrons (see College "Fundamental & Nuclear Physics"). Norman Ramsey, from Harvard University, has been associated with one of the other major experiments at ILL on fundamental properties of the neutron, namely the search for a possible electric dipole moment. In this experiment, the technique called 'Ramsey separated oscillating fields magnetic resonance' is applied to polarized ultra cold 'bottled' neutrons. In fact, such a procedure constitutes the most sensitive test yet proposed that might provide evidence for the possible violation of time reversal symmetry.

Among the new results of particular interest arising from the 1989 experimental programme, mention has already been made of the increasing precision in the estimate of the neutron lifetime: the latest value now stands at 887 ± 3 seconds, and the 'bottled' neutron technique gives every hope of even greater precision in the future. In the field of nuclear physics, attention should be drawn to the first observation (on PN1, the fission product separator Lohengrin) of three new very neutron-rich nuclei (^{69}Co, ^{68}Co and ^{68}Fe). Knowledge of the properties of such nuclei is important in astrophysics, in order to understand the processes governing formation of the stable chemical elements on whose relative abundance the whole of chemistry and biology is founded.

Our understanding of the existing high T_c copper oxide superconductors has already been greatly advanced by neutron scattering experiments, a significant fraction of which were performed at ILL. Notable new results continue to emerge. For example, a direct correlation was found between T_c and the apical Cu-O bond length in the square-pyramidal CuO_5 units that form layers in $YBa_2Cu_4O_8$, by determining both the crystal structure and T_c as a function of pressure. In the original prototype '2:1:4' family, spin waves were measured in La_2CuO_4 and $La_{1.95}Ba_{0.05}CuO_4$ on the hot source triple-axis spectrometer IN1 up to higher energies (0.1 eV) than would have been possible anywhere else in the world at this time. The crystal and magnetic structure of the closely related analogue La_2NiO_4 has also been determined by single crystal diffraction, and of the parent compound Nd_2CuO_4 to the series of electron superconductors by powder diffraction.

The so-called quasi-crystalline state of matter with pseudo-five-fold symmetry continues to fascinate crystallographers. Diffraction data have now been obtained on powders and single quasi-crystalline grains of the AlLiCu system with double isotopic substitution on both Li and Cu. Thus, the phases of the partial structure factors could be evaluated corresponding to the 6-dimensional periodic structure that relates to the actual 3-dimensional quasi-periodic arrangement of atoms.

Turning to a completely different field of science, that of polymers, it has been clear for many years that in a molten polymer the dynamical behaviour of the long molecular chains must be controlled by their entanglement, which hinders motion over a large distance scale. In de Gennes celebrated theory of 'reptation', it is assumed that each chain is trapped in a tube formed by the other chains, but although this theory accounts for the macroscopic properties of polymer melts, there has been no direct microscopic evidence for this intermediate length scale. Such evidence has, indeed, been obtained now in the form of a splitting of the curve relating $s(q,t)$ to $q^2t^{1/2}$, measured at different q, which provides the signature of the narrow tube diameter.

Finally, two significant contributions to molecular biology should be mentioned. One is the first determination of the binding arrangement of a protein repressor to a gene. The experiment, using SANS (D11), throws light on the mechanism that leads to build-up of resistance to the antibiotic tetracycline in bacteria, causing the infection in hospital patients called 'hospitalism'. The other is the determination by low resolution neutron diffraction of the arrangement of lipid-like detergent molecules around the membrane protein constituting the photosynthetic reaction centre.

Modernisation Programme

The final section of my report looks towards the future. A little over ten years ago the ILL Associates approved a programme of modernisation at the Institut (the so-called 'Deuxième Souffle'), to keep the ILL at the forefront of neutron scattering centres throughout the 1980's. A strong belief has developed that the time is once again ripe to begin designing a programme of renewal and improvement of our equipment and infrastructure to carry us forward into the 1990's. The reflection and debate required to delineate the outline and set the priorities for such a programme occupied many scientists and technical experts at the Institut during 1989. This intense in-house activity has been accompanied by a widespread effort of consultation with specialists in national neutron scattering centres and, most important of all, with our community of users. The latter are represented by the eight subject committees of our Scientific Council, each of which has had the opportunity to discuss the suggestions being made and, through the Chairmen, to contribute to the two extensive discussions held so far at the Scientific Council itself. The representative group most closely concerned with the technical proposals is the Instrument Sub-committee, which held two extended workshop-type meetings during the year to hear presentations of the many proposals in the presence of experts from the national centres.

This report is not the place to go into detail about the proposals themselves, because they are still being discussed by a series of study groups. Suffice it to say that they fall into four categories: new sources (an enhanced hot source and a novel, intense positron source), new techniques (polarisers and guides), new instruments (among others Laue diffractometry and further development of neutron spin-echo), and finally enhancement of the Institut's infrastructure of user support such as sample environment, computing and sample characterisation. Discussion of the latter is taking place in full consultation with our sister Institute the ESRF.

It is right to end my report by looking forward, because a lesson I have quickly learnt about our Institut is that after 22 years the intellectual atmosphere is as vibrant as it ever was and the ideas flow as fast as ever. This is a suitably public opportunity to commend all my colleagues and members of staff whose continued strenuous efforts make ILL such an exciting place, and the writing of the Director's Report such a pleasure.

P. Day

Bericht des Direktors

Dies ist mein erster Jahresbericht als Direktor. Er bezieht sich auf ein Jahr, in dem das ILL noch 9 Monate unter der Leitung von Herrn W. Gläser stand. Dieser kehrte Ende September an seinen Lehrstuhl an der Technischen Universität München zurück. Während seiner Amtszeit stieg die Zahl der durchgeführten Experimente von 740 auf etwa 850 dank der erhöhten Leistungsfähigkeit der Instrumente und der wiedererreichten maximalen Betriebslast von 6 jährlichen Reaktorzyklen. Mit meinen einleitenden Worten möchte ich ihm für seine Einführung in die Besonderheiten des Institutsbetriebs sowie für die sorgfältige Ausübung seines Amtes als Direktor danken. Während seiner Amtszeit wurden erste Schritte zur Ausarbeitung von Vorschlägen für ein Modernisierungsprogramm unternommen, welche den ILL Gesellschaftern vorgelegt werden sollen und den Ausbau der Spitzenstellung unseres Instituts unter den Neutronenforschungszentren in den 90er Jahren zum Ziel haben.

Die Nachfolge von Herrn Gläser trat P. Armbruster an, ehemaliger Direktor der GSI-Darmstadt und einer der Wissenschaftler, die für die Konzeption des Lohengrin-Spaltproduktspektrometers verantwortlich waren. Auch die Amtszeit von Herrn A. Michaudon als stellvertretender französischer Direktor ist 1989 ausgelaufen, nachdem er mit vier aufeinanderfolgenden Direktoren zusammengearbeitet hatte.

Wir wünschen ihm einen glücklichen und aktiven Ruhestand, den er wechselweise in Grenoble und Los Alamos verbringt. An seine Stelle trat Jean Charvolin vom CNRS (Labor für Festkörperphysik) in Orsay, Spezialist in der Physik der "weichen" kondensierten Materie, beispielsweise von Polymeren und flüssigen Kristallen.

Weitere Änderungen in Leitungsfunktionen erfolgten durch die Pensionierung von F. Franzetti, 11 Jahre lang Leiter der Reaktorabteilung sowie durch die Rückkehr von D. Richter, Senior Scientist in der Vercors II Gruppe (Flugzeit), nach Jülich und auf einen Lehrstuhl an der Uni Münster. E. Bauer, seit vielen Jahren stellvertretender Leiter der Reaktorabteilung, wurde Nachfolger von F. Franzetti.

Während des vergangenen Jahres besuchten eine Reihe von bedeutenden Gästen einschliesslich des britischen und deutschen Wissenschaftsministers, das ILL: Mr. Robert Jackson MP und Bundesminister H. Riesenhuber. Der deutsche Botschafter in Frankreich, F. Pfeffer, war ebenso einen Tag bei uns. Unter den wichtigen wissenschaftlichen Besuchern waren K. Kourilsky, Generaldirektor des CNRS und Mr. J. Fairclough, oberster Wissenschaftsberater im britischen Kabinett in Whitehall.

Reaktorbetrieb und Experimentierprogramm

Als wichtigster Punkt ist zu bemerken, dass der Reaktorbetrieb, wie es unsere Benutzergemeinde erwartet, äusserst zuverlässig verlief. Dass diese Feststellung so lakonisch getroffen werden kann ist als Anerkennung der Leistung des gesamten Reaktorpersonals zu werten, denn in mancher Hinsicht war 1989 kein einfaches Jahr.

Zu Jahresbeginn herrschte beträchtliche Unsicherheit über die Lieferung der Reaktorbrennelemente. Im Laufe des Jahres jedoch entspannte sich die Lage erheblich durch die im April von der amerikanischen Regierung gewährte Exportlizenz für das im Jahr 1988 bestellte Uran. Diese wurde im Herbst durch eine weitere Lieferung sowie durch eine erste Teillieferung desjenigen Urans ergänzt, das von unserem ehemaligen Lieferanten von Brennelementen, NUKEM, zur Aufarbeitung übernommen worden wäre. Demzufolge gibt es im Augenblick keinen Grund zur Sorge über eine Unterbrechung der Versorgung, obwohl Herstellung und Lieferung von Brennelementen nach einem ziemlich dichten Terminplan erfolgen.

Als Folge der Unterbrechung gegen Ende 1988 und Anfang 1989, wurde der lange, normalerweise im Sommer stattfindende Reaktorhalt in die Winterperiode vorgezogen. Dennoch war es, trotz der Verzögerung der Wiederaufnahme des Reaktorbetriebs bis Februar möglich, 6 volle Zyklen im Jahr zu fahren, was allerdings nur auf Kosten von verkürzten Intervallen für den Brennelementwechsel möglich war.

Mit der Erhöhung der Anzahl der Zyklen ging ein entsprechender Anstieg der Zahl der geplanten Experimente von 807 auf 858 einher. Gleichzeitig jedoch stieg auch die Anzahl der eingereichten Versuchsvorschläge von 1069 auf 1129 und von den 12148 für 1989 beantragten Instrumenttagen konnten nur 7829 in den Zeitplan aufgenommen werden. Erwähnenswert ist ebenfalls die grosse Anzahl von Veröffentlichungen, eine direkte Folge der zugeteilten Strahlzeit: Die von der Bibliothek registrierten Zahlen lagen bei 407 im Jahre 1987 und bei 501 im Jahre 1988. Eine speziell ausgearbeitete Statistik zeigte, dass in den letzten 5 Jahren nicht weniger als 62 Artikel über am ILL durchgeführte Arbeiten in den Physical Review letters erschienen, was bedeutet, dass im Durchschnitt ein Viertel aller Ausgaben dieses Journals eine Veröffentlichung über neue Resultate vom ILL enthielt.

Instrumente an der Horizontalen Kalten Quelle

Der Schwerpunkt des Programms zur Entwicklung von Instrumenten liegt weiterhin beim Bau von Geräten für die horizontale Kalte Quelle. Als erstes dieser Instrumente wurde das Dreiachsenspektrometer IN14 in der Reaktorhalle für den Benutzerbetrieb zu Beginn des Jahres freigegeben, obwohl der Einbau der Polarisierungsvorrichtung noch aussteht (voraussichtlicher Termin: Januar/Februar 1990). In der zweiten Neutronenleiterhalle sind alle Leiter einschliesslich ihrer Abschirmung und Strahlverschlüsse aufgebaut und werden ab Ende 1989 routinemässig in Betrieb gehen. Von den im Bau befindlichen Instrumenten in der Leiterhalle ist zu berichten, dass die Erstellung des Choppers sowie der Doppler-Maschine für das Rückstreuspektrometer IN10C (in Zusammenarbeit mit Jülich) weiterhin planmässig verläuft. Die vorgenommene Kostenausschreibung für den Rest des Geräts hat den Aufbau des Spektrometers im Laufe des Jahres 1990 zum Ziel. Der Bau der wesentlichen Teile der Grundausstattung des hochauflösenden Spin-Echo-Spektrometers IN15 ist praktisch abgeschlossen und der Aufbau der wichtigsten Elemente hat vor Ort begonnen.

Schliesslich wurde, kurz vor Weihnachten, das 20 m lange Detektorrohr für die Kleinwinkelstreuanlage D22 geliefert und die Montage steht unmittelbar bevor. In diesem Rohr soll ein grosser Multidetektor (75 x 75 cm) eingebaut werden, ähnlich dem, den das ILL gerade zur Lieferung an das HMI Berlin fertiggestellt hat. Zunächst jedoch können die ersten Tests mit dem Ersatzdetektor von D11 erfolgen.

Wissenschaftliche Höhepunkte

Ein bemerkenswerter Höhepunkt 1989 und Grund zur Freude ihrer vielen Freunde am ILL war die Verleihung des Physik-Nobelpreises an zwei langjährige Kollegen und Gäste des Instituts, Wolfgang Paul und Norman Ramsey. Beide sind Benutzer der Sehr Kalten und Ultrakalten Neutronenquelle, der sogenannten Neutronen-Turbine auf dem Reaktorniveau D. W. Paul, Professor an der Universität Bonn, ist der Erfinder

eines Neutronenspeicherrings unter Benutzung eines toroidalen Magnetfeldes, welcher zu einer Bestimmung der Neutronenlebenszeit benutzt worden war. Diese konnte jetzt sogar noch genauer mit Hilfe einer "Neutronenflasche" gemessen werden (siehe College "Nuclear and Fundamental Physics"). N. Ramsey, von der Universität Harvard, hat an einem der anderen grossen Experimente zur Bestimmung grundlegender Eigenschaften des Neutrons mitgearbeitet: Die Suche nach einem möglichen elektrischen Dipolmoment. In diesem Experiment wird die sogenannte "Ramsey separated oscillating fields magnetic resonance" Methode auf polarisierte, in einer "Flasche" eingeschlossene ultrakalte Neutronen angewandt. Dieses Verfahren stellt in der Tat den zur Zeit empfindlichsten Test für die mögliche Verletzung der Zeitumkehr-Symmetrie dar.

Unter den neuen interessanten Ergebnissen des Experimentierprogramms wurde bereits die Erhöhung der Messgenauigkeit in der Abschätzung der Neutronenlebensdauer erwähnt: Der neueste Wert liegt jetzt bei (887 ± 3) Sekunden. Die Technik der "Neutronenflasche" gibt für die Zukunft Anlass zur Hoffnung auf eine sogar noch grössere Genauigkeit. Auf dem Gebiet der Kernphysik, sei auf die erste Beobachtung von 3, sehr neutronenreichen Kernen (^{68}Co, ^{69}Co und ^{68}Fe) bei der Spaltung von ^{239}Pu hingewiesen (Messungen am Lohengrin-Spaltproduktseparator). Die Eigenschaften dieser Kerne sind für die Astrophysik wichtig, um den Entstehungsprozess der stabilen chemischen Elemente zu verstehen, deren relativ häufiges Vorkommen Grundlage von Chemie und Biologie sind.

Neutronenstreuexperimente, die zu einem beträchtlichen Teil am ILL durchgeführt wurden, haben unser Verständnis der Hochtemperatur-Supraleiter auf der Basis von Kupferoxid bereits erheblich erweitert. Bemerkenswerte, neue Ergebnisse kommen ständig hinzu. Es wurde z.B. eine direkte Beziehung zwischen der Temperatur T_c und der apikalen Cu-O Bindungslänge in quadratisch-pyramidalen CuO_5 Einheiten gefunden, welche Schichten in der Verbindung $YBa_2Cu_4O_8$ bilden. Dies wurde durch Bestimmung der Druckabhängigkeit der Kristallstruktur und der kritischen Temperatur T_c erreicht. In der Prototyp-Familie "2:1:4" wurden Spinwellen in La_2CuO_4 und $La_{1,95}Ba_{0,05}CuO_4$ mit dem Dreiachsen-Spektrometer IN1 an der heissen Quelle bis zu Energien von 0,1 eV untersucht. Dieser Energiebereich ist gegenwärtig nirgendwo anders auf der Welt erreichbar. Kristall- und Magnetstruktur der eng verwandten, analogen Verbindung La_2NiO_4 ist durch Einkristallmessungen untersucht worden, ebenso die verwandte Substanz Nd_2CuO_4 mittels Pulverdiffraktion.

Der sog. quasikristalline Zustand der Materie mit pseudo-fünffacher Symmetrie fasziniert weiterhin die Kristallographen. Kürzlich wurden Diffraktionsergebnisse an Pulvern und einzelnen quasikristallinen Körnern des AlLiCu Systems unter Anwendung zweifacher Isotopensubstitution sowohl an Li als auch an Cu erzielt. Hieraus konnten die Phasen des partiellen Strukturfaktors entsprechend der sechsdimensionalen periodischen Struktur ermittelt werden, die sich aus der dreidimensionalen quasi-periodischen Anordnung der Atome ergibt.

Auf dem Gebiet der Polymerforschung war seit Jahren bekannt, dass das dynamische Verhalten der langen Molekülketten in einem geschmolzenen Polymer von seiner Verknäuelung beeinflusst ist, welche Bewegungen über einen grossen Entfernungsbereich behindert. In der berühmten "Kriech-Theorie" von de Gennes wird angenommen, dass jede Kette in einer Röhre gefangen ist, die von anderen Ketten gebildet wird. Obwohl diese Theorie die makroskopischen Eigenschaften von geschmolzenen Polymeren berücksichtigt, hatte es bisher keinen direkten mikroskopischen Nachweis dieses Ordnungsphänomens gegeben. Dieser Beweis wurde jetzt durch die Aufspaltung der Kurve s (q,t) in Abhängigkeit von $q^2t^{1/2}$ bei verschiedenen q-Werten erbracht und somit der enge Röhrendurchmesser ermittelt.

Schliesslich seien zwei bedeutende Beiträge auf dem Gebiet der Molekularbiologie erwähnt. Der eine betrifft die erstmalige Bestimmung der Ankoppelung eines Proteinrepressors an ein Gen. Unter Anwendung der Kleinwinkelstreuung (D11) klärt dieses Experiment den Vorgang auf, der zur Ausbildung der Resistenz gegen das Antbiotikum Tetracycline bei Bakterien führt, welche Infektionen bei Krankenhauspatienten, den sog. "Hospitalismus", verursacht. Ein weiterer Beitrag ist die Bestimmung der Anordnung fettähnlicher Detergentien um das Membranprotein, dem Reaktionszentrum der Photosynthese.

Modernisierungsprogramm

Der letzte Abschnitt meines Berichts befasst sich mit der Zukunft. Vor etwas mehr als 10 Jahren hatten die Gesellschafter des ILL ein Modernisierungsprogramm gebilligt (den sog. "Deuxième Souffle"), welches die Führungsrolle des ILL unter den Neutronenforschungsinstituten für die 80er Jahre sicherstellen sollte. Es ist unsere feste Überzeugung, dass die Zeit wieder reif ist, die Ideen für eine Erneuerung und Verbesserung der Einrichtungen und Infrastruktur des ILL zu Papier zu bringen, um uns in die 90er Jahre zu führen. Viele Wissenschaftler und technische Fachkräfte des ILL waren im vergangenen Jahr mit Nachdenken und Diskussionen beschäftigt, um die Konturen dieses Programmes zu entwerfen. Diese intensive Aktivität unserer Experten wurde von gross angelegten Bemühungen begleitet, Spezialisten in anderen Neutronenforschungszentren und vor allem unsere Benutzergemeinde zu konsultieren. Diese wird durch die 8 Unterausschüsse des Wissenschaftlichen Rats vertreten. Jeder dieser Ausschüsse hatte die Gelegenheit, die Vorschläge zu diskutieren und, vertreten durch seinen Vorsitzenden, an den beiden Diskussionen über dieses Programm im Wissenschaftlichen Rat teilzunehmen. Der Instrumenten-Unterausschuss ist am stärksten von den technischen Vorschlägen betroffen. In seinem Rahmen wurden zwei ausgiebige "workshops" abgehalten, wo in Gegenwart von Experten anderer nationaler Forschungszentren die vielen Vorschläge erörtert wurden.

Dies ist nicht der Platz, um auf Einzelheiten der Vorschläge einzugehen, zumal diese noch von einer Reihe von Arbeitsgruppen diskutiert werden. Es soll hier lediglich erwähnt werden, dass diese in 4 Kategorien fallen: Neue Quellen (eine verbesserte Heisse Quelle und eine neuartige, intensive Positronen-Quelle), neue Verfahren (Polarisatoren und Leiter), neue Instrumente (u.a. Laue-Diffraktometrie, Weiterentwicklung der Neutronen-Spinecho-Technik) und schliesslich die Erweiterung der ILL Infrastruktur im Bereich des Benutzerbetriebs, z.B. auf dem Gebiet der Probenumgebung, Informatik und Probencharakterisierung. Diskussionen über das letztere Arbeitsgebiet finden in enger Zusammenarbeit mit unserem Nachbarinstitut, der ESRF, statt.

Zu Recht schliesse ich meinen Bericht mit dieser Vorausschau, denn ich habe schnell erkannt, dass nach 20 Jahren die intellektuelle Atmosphäre des ILL nach wie vor so prickelnd ist wie früher und die Ideen sprudeln wie eh und je. Dies ist eine passende Gelegenheit, an öffentlicher Stelle all meinen Kollegen und Institutsmitgliedern mein Lob auszusprechen, welche durch ihr beständiges Bemühen das ILL zu einem solch stimulierenden Ort und mir das Verfassen dieses Berichtes zu einer solchen Freude machen.

P. Day

Rapport du Directeur

Ce Rapport Annuel est le premier que je rédige en tant que Directeur. Il recouvre une année dont la plus grande partie a vu l'ILL placé sous la direction de Wolfgang Gläser. Ce dernier a repris son poste à l'Université Technique de Munich fin septembre. Mes premiers mots s'adresseront donc à lui, pour le remercier de m'avoir initié aux mystères du fonctionnement de l'Institut, et du soin qu'il a apporté à la gestion de l'Institut pendant son mandat de Directeur. Pendant cette période, le nombre annuel des expériences effectuées à l'ILL est passé de 740 à 850, grâce d'une part à l'amélioration constante des instruments et d'autre part à la décision de faire fonctionner le réacteur pendant six cycles complets. Les premiers aspects d'un programme de modernisation (explicités ci-dessous) ont également été ébauchés à l'intention de nos Associés, dans la perspective de maintenir l'ILL en tête des autres centres de diffusion des neutrons au cours de la prochaine décennie.

Wolfgang Gläser a été remplacé par Peter Armbruster, précédemment Directeur de la GSI (Darmstadt), mais aussi un des premiers scientifiques de l'ILL à sa fondation, en tant que responsable de la construction du spectromètre à produits de fission Lohengrin. André Michaudon a quitté son poste de Directeur Français Associé, après avoir accepté de prolonger de six mois son mandat normal de cinq ans. Au cours de cette période, m'a-t-il dit, il a travaillé en collaboration avec quatre Directeurs successifs. Nous lui souhaitons une retraite heureuse et active à Grenoble et Los Alamos. Pour le remplacer nous avons accueilli Jean Charvolin, du Laboratoire de Physique des Solides du CNRS d'Orsay, spécialiste de la physique de la matière condensée dite "molle" concernant les cristaux liquides, les polymères et les colloïdes.

D'autres changements se sont produits au niveau du personnel d'encadrement, avec le départ à la retraite de F. Franzetti, Chef du Département Réacteur pendant 11 ans, et le retour à Jülich de D. Richter, "Senior Scientist" dans le Groupe Vercors II (temps de vol), qui a également obtenu une chaire à l'Université de Münster. E. Bauer, Adjoint au Chef du Département Réacteur pendant de nombreuses années, succède à M. Franzetti.

Au cours de l'année écoulée, l'Institut a reçu un certain nombre de visiteurs de marque, notamment les Ministres Britannique et Allemand chargés de la recherche scientifique: M. Robert Jackson et H. Riesenhuber. L'Ambassadeur d'Allemagne en France, M. Franz Pfeffer, a également passé une journée avec nous, et parmi les personnalités scientifiques, M. F. Kourilsky, Directeur Général du CNRS et M. J. Fairclough, Conseiller Scientifique en Chef au Gouvernement Britannique, nous ont honorés de leur visite.

Fonctionnement du réacteur et programme expérimental

La première remarque, et la plus importante, à faire au sujet du fonctionnement du réacteur en 1989 est que, comme notre communauté d'utilisateurs s'y est maintenant habituée, notre installation continue à être extrêmement fiable. Qu'un tel constat puisse être fait si brièvement est un hommage à tout le personnel concerné, car à certains égards, 1989 n'a pas été une année si facile.

Au début de l'année, une assez grande incertitude planait encore sur la continuité de la fourniture de combustible pour le réacteur. Toutefois, le temps passant, la situation s'est considérablement améliorée; en effet, les autorités américaines autorisaient en avril l'exportation de l'uranium commandé en 1988 et une seconde livraison fut faite à l'automne. Enfin, nous reçûmes le dernier lot de ce qui aurait été utilisé par notre ancien fournisseur d'éléments combustibles, NUKEM. Par conséquent, en dépit d'une programmation de fabrication et de livraison des éléments combustibles encore très difficile, il n'y a pour le moment aucune raison de craindre une interruption des approvisionnements.

A cause de l'interruption qui eut lieu de fin 1988 à début 1989, la période de maintenance prolongée qui a normalement lieu en été, fut repoussée en hiver. Le redémarrage tardif du réacteur, en février, n'a pas empêché l'exécution de six cycles complets en un an, bien qu'au prix de réduction anormale de la durée des arrêts entre les cycles du réacteur, destinés au changement des éléments combustibles.

L'augmentation de cinq à six cycles de 1988 à 1989 a été accompagnée d'un accroissement correspondant du nombre d'expériences programmées, qui sont passées de 807 à 858. Pendant cette même période, le nombre de propositions reçues s'est également accru de 1069 à 1129. Sur les 12 148 jours de temps de mesure demandés en 1989, 7 829 jours seulement ont pu être accepté dans le programme. Il est également important de noter la proportion élevée de publications par rapport au temps de faisceaux alloué: les chiffres enregistrés par la bibliothèque pour 1987 et 1988 ont été respectivement de 407 et 501. Il est intéressant de noter un élément statistique particulier: au cours des cinq dernières années pas moins de 62 articles sur des travaux émanant de l'ILL ont paru dans la revue Physical Review Letters, ce qui veut dire qu'en moyenne, un numéro sur 4 de cette revue contenait un article présentant de nouveaux résultats obtenus dans notre Institut.

Instruments de la source froide horizontale

A l'Institut, la majeure partie du programme de développement des instruments reste ciblée sur la construction d'appareils pour la source froide horizontale. Le premier de ces instruments, le spectromètre trois axes IN14 dans le hall réacteur, a été inclus dans la planification d'expériences pour les utilisateurs extérieurs depuis le début de l'année, bien que l'option neutrons polarisés ne soit pas encore installée (ce qui sera fait en janvier-février 1990). Dans le second hall de guides, les guides ainsi que leurs protections et leurs obturateurs sont maintenant installés et ils fonctionneront normalement dès la fin de 1989. En ce qui concerne les instruments à installer, la construction du chopper et de la machine Doppler pour le spectromètre à rétro-diffusion IN10C continue selon le calendrier prévu, en collaboration avec Jülich. Un appel d'offres pour la construction du reste de l'appareil a été lancé, dans le but de monter l'appareil à l'intérieur du hall de guides au cours de 1990. La fabrication des composants principaux de la version de base du spectromètre à haute résolution à écho de spin IN15 est pratiquement terminée, et le montage des principaux éléments de construction a commencé sur le site.

Enfin, le tube de détection de 20 m de long pour l'appareil de diffusion aux petits angles D22 a été livré juste avant Noël, et le montage va commencer incessamment. Le tube a été conçu pour recevoir un détecteur de grande surface (75 x 75 cm) semblable à celui qui vient d'être terminé par l'ILL et qui doit être livré au HMI de Berlin. Toutefois, il est possible d'effectuer les essais préliminaires avec le détecteur qui existe en réserve pour D11.

Evénements scientifiques majeurs

Un des événements scientifiques importants de l'année 1989 a été l'attribution du Prix Nobel de Physique à deux collègues et collaborateurs de longue date de l'Institut, Wolfgang Paul et Norman Ramsey, ce qui a réjoui leurs nombreux amis de l'ILL. Tous deux ont utilisé la source de neutrons très froids et ultra-froids appelée turbine

TGV au niveau D du réacteur. Wolfgang Paul, professeur à l'Université de Bonn, est l'inventeur d'un anneau de stockage pour neutrons dans un champ magnétique de forme toroïdale qui a servi aux premières déterminations de la durée de vie des neutrons, rendues maintenant encore plus précises grâce à l'utilisation de neutrons "mis en bouteille" (voir College "Fundamental & Nuclear Physics"). Norman Ramsey, de l'Université d'Harvard, a été associé à l'une des expériences majeures menées à l'ILL sur les propriétés fondamentales des neutrons: la recherche d'un éventuel moment électrique dipolaire. Dans cette expérience, la technique baptisée "Résonance magnétique des champs oscillants séparés de Ramsey" est appliquée pour polariser les neutrons ultra-froids "mis en bouteille". En fait, cette procédure constitue le test le plus sensible actuellement proposé qui puisse mettre en évidence la violation éventuelle de la symétrie de l'inversion du temps.

Parmi les nouveaux résultats présentant un intérêt particulier obtenus au cours du programme expérimental de 1989, il a déjà été fait mention de l'augmentation de précision de l'estimation de la durée de vie des neutrons: la valeur la plus récente s'établit maintenant à 887 ± 3 secondes, et la technique des neutrons "mis en bouteille" laisse espérer une précision encore supérieure dans l'avenir. Dans le domaine de la physique nucléaire, il faut noter que pour la première fois on a pu observer (sur le spectromètre à produits de fission Lohengrin, PN1) trois nouveaux noyaux très riches en neutrons (^{69}Co, ^{68}Co et ^{68}Fe). En astrophysique, il est important de connaître les propriétés de ces noyaux, pour pouvoir comprendre les processus intervenant dans la formation d'éléments chimiques stables sur lesquels toute la chimie et la biologie sont fondées, en raison de leur relative abondance.

Nous avons déjà grandement amélioré notre compréhension des supraconducteurs d'oxyde de cuivre à T_c élevée grâce aux expériences de diffusion des neutrons, dont beaucoup ont été faites à l'ILL. De nouveaux résultats importants ne cessent d'être obtenus. On a constaté, par exemple, une corrélation directe entre T_c et la longueur de la liaison Cu-O dans les unités CuO_5 pyramidales à bases carrées qui forment des couches dans $YBa_2Cu_4O_8$, en déterminant la structure cristalline et T_c en fonction de la pression. Dans la famille '2:1:4' prototype d'origine, on a mesuré des ondes de spin dans La_2CuO_4 et dans $La_{1,95}Ba_{0,05}CuO_4$ jusqu'à des énergies très élevées (0,1 eV) grâce au spectromètre trois axes IN1 placé sur la source chaude. Ceci, à cette époque, n'avait été possible nulle part ailleurs au monde. La structure cristallographique et magnétique de l'analogue La_2NiO_4, qui lui est très proche, a également été déterminée par diffraction sur monocristal, ainsi que celle du composé voisin Nd_2CuO_4 par diffraction de poudre.

L'état de la matière dit "quasi-cristallin" à symétrie icosaédrique continue à fasciner les cristallographes. Des données de diffraction ont maintenant été obtenues sur les poudres et des monodomaines quasi-cristallins du système AlLiCu, avec double substitution isotopique sur Li et Cu. On a pu ainsi évaluer les phases des facteurs de structure partiels correspondant à une structure périodique à 6 dimensions qui détermine la disposition tridimensionelle quasi-périodique des atomes.

Dans un domaine totalement différent, celui des polymères, on pensait depuis de nombreuses années, que dans un polymère fondu, le comportement dynamique des longues chaînes moléculaires doit être contrôlé par leur enchevêtrement, qui empêche leur mouvement sur une grande échelle de distance. Dans la célèbre théorie de De Gennes sur la "reptation", on supposait que chaque chaîne était emprisonnée dans un tube formé par les autres chaînes. Bien que cette théorie rende bien compte des propriétés macroscopiques des polymères fondus, il n'y avait pas de preuve microscopique directe à cette échelle intermédiaire. Cette preuve a maintenant été obtenue dans la courbe reliant $s(q,t)$ à $q^2t^{1/2}$, mesurée à différentes valeurs q, et qui est significative du faible diamètre du tube.

Enfin, deux contributions importantes en biologie moléculaire doivent être mentionnées. L'une concerne la première détermination de la disposition de la liaison d'une protéine répressive sur un gène. L'expérience, utilisant la diffusion à petits angles (D11), donne des indications sur le mécanisme de constitution d'une résistance à l'antibiotique tétracycline dans les bactéries entraînant l'infection que l'on peut constater chez certains patients hospitalisés, appelée "hospitalisme". L'autre concerne la détermination par diffusion neutronique à faible résolution de la disposition des molécules de détergent semblables à des lipides autour de la protéine membranaire constituant le centre de réaction de la photosynthèse.

Programme de modernisation

La dernière partie de mon rapport concerne les perspectives d'avenir. Il y a un peu plus de dix ans, les Associés de l'ILL approuvaient un programme de modernisation de l'Institut (appelé le "Deuxième Souffle") pour que l'ILL reste le "meilleur" des centres de diffusion de neutrons, tout au long des années 1980. Il apparaît maintenant, qu'à nouveau l'heure soit arrivée de concevoir un programme de renouvellement et d'amélioration de nos équipements et de notre infrastructure, en vue des années 1990. Les réflexions et les débats nécessaires pour esquisser le profil d'un tel programme et en définir les priorités ont mobilisé de nombreux scientifiques et experts techniques à l'Institut en 1989. Cette intense activité interne a été accompagnée d'un effort de consultation très étendue auprès de spécialistes des centres de diffusion de neutrons dans différents pays, et, ce qui est très important auprès de notre communauté d'utilisateurs. Ces derniers sont représentés par les huit sous-comités de notre Conseil Scientifique, chacun d'eux ayant eu la possibilité de discuter des suggestions faites et, par l'intermédiaire de leurs Présidents, de contribuer aux deux discussions approfondies qui ont déjà eu lieu au sein du Conseil Scientifique. Le groupe de représentants concerné le plus directement par les propositions techniques est le Sous-comité Instruments qui a tenu, au cours de l'année, deux réunions étendues du type "workshop" pour écouter les présentations des nombreuses propositions en présence d'experts des centres nationaux.

Ce rapport ne saurait être l'occasion de donner des détails sur ces propositions, dans la mesure où elles font encore l'objet de discussions dans un certain nombre de groupes d'études. Il suffit d'indiquer qu'elles sont classées en quatre catégories: les sources nouvelles (une source chaude améliorée et une source intense de positrons de conception nouvelle), les techniques à développer (polariseurs et guides), les nouveaux instruments (entre autres, la diffractométrie Laue et de nouveaux développements de l'écho de spin des neutrons), et enfin, l'amélioration de l'infrastructure de soutien aux utilisateurs de l'Institut, comme par exemple l'environnement des échantillons, l'informatique et la caractérisation des échantillons. Ce dernier point fait actuellement l'objet de discussions en concertation avec notre Institut frère, l'ESRF.

Je pense qu'il convient de conclure mon rapport en tournant le regard vers l'avenir, car s'il est une leçon que j'ai vite apprise sur notre Institut, c'est que 22 années après sa fondation, l'atmosphère intellectuelle y est toujours aussi dynamique, et les idées y circulent toujours aussi vite. Je profite de cette occasion publique de m'exprimer pour faire l'éloge de tous mes collègues et membres du personnel dont les efforts soutenus font de l'ILL un endroit si stimulant et la rédaction du Rapport du Directeur une tâche si agréable.

P. Day

ILL/ESRF cooperation

The year 1989 finished with two points for ESRF: the text of the European Convention signed by the member countries was ratified by the French Parliament on 24.11.89, and the contract between ESRF and its multinational building consortium was signed on 1.12.89. The preparation of these documents, establishing the legal and physical existence of the ESRF, also encouraged the joint reflexions of ESRF and ILL with a view to developing their cooperation in a way favourable to the establishment of a powerful, high-quality scientific centre. There has however been a slight disappointment, when it was found that the ESRF's financial difficulties, due to the increase in the estimated costs of the construction work under contract B, would delay that covered by contracts C and D, and in particular that of the ILL/ESRF Joint Building. The two institutes were concerned by this delay to the extent that the early construction of this Joint Building, which will incorporate meeting places for scientists at all levels, was intended to permit the start of real collaboration even before the ESRF is operational.

To return to the cooperation itself, the two institutes follow a pragmatic approach: the scientific and administrative Directors meet every month in a Joint Management Committee to identify points which could be the subject of cooperation, submit these points for consideration to Joint Working Groups, analyse the proposals of these groups and implement them.

The first points dealt with in this way were administrative and technical; ESRF had to call on certain ILL services to provide the necessary basis for its operation as quickly and economically as possible. To this end, two general working groups meet regularly, the Working Group on Joint Services, set up by the Joint Management Committee to examine the possibilities of joint services and to prepare the necessary legal documents, and the Thursday Group, responsible for dealing with practical and technical questions of cooperation, where the technical experts reach agreement to facilitate everyday cooperation. The work of these groups during the year resulted in the signature of a site security contract on 24 May 1989, the preparation of a contract on the Joint Building, which is currently being studied, the preparation of a "Memorandum of Understanding" on the telephones and networks, and an initial consideration of the management of books and journals in common. It should also be noted that the ILL Collective Agreement, signed on 29 June 1989, is at present being studied by ESRF, who may use it as a starting point for their own Collective Agreement. Finally the two institutes decided to continue their joint financial support for the International Schools this year, as the local education authorities have not yet taken over this responsibility on behalf of the French Ministry of Education, as provided for in the ESRF Convention.

The really new and important point this year is, in our view, the first identification of possible scientific collaboration, or Joint Scientific Activities, at the Joint Management Committee meeting on 15.9.89. This meeting was not concerned with the search for subjects of joint experimental studies, but rather with that for common needs for experimental equipment and common skills for the development of experimental facilities.

The following activities were considered as susceptible to collaborative efforts: optics (development and construction of mirrors and monochromators), chemistry and biology (to provide members of the institutes and their users with equipment for preparing and characterising fragile samples before examination in the beams, which could also involve EMBL), sample environment (equipment permitting the definition of the experimental conditions in the beams), computing (acquisition, analysis and transfer of experiment data), and a beam line at ESRF common to the two institutes (for testing equipment, particularly monochromators). Working Groups, including staff from both institutes, are being set up to consider each of these activities. The coordinators will be B. Jacrot (ILL) and A. Miller (ESRF).

It should be noted that this is a very favourable time for such reflexions, as ILL has to prepare its modernisation programme, while ESRF is preparing its experiment programme. The two programmes cannot be developed separately from each other if it is desired to take the best account of the complementary aspects of neutrons and X-rays in the design of the instruments. With this in view, ILL staff members attended the ESRF users' meeting and ESRF staff have joined the ILL working groups on modernisation programme projects.

The two institutes also wished to demonstrate their collaboration to the outside world by organising events in common such as "Joint Colloquia", monthly seminars at which subjects of general scientific interest are presented, and "Joint Workshops", conferences centred on the complementarity of X-rays and neutrons in the study of materials. They have also constructed joint stands for scientific or technological exhibitions.

In conclusion, despite the delay on the construction of the Joint Building, we are convinced that the two institutes can take advantage of a favourable period to give their scientific cooperation a good start: the preparation of the ILL modernisation programme and the ESRF experimental programme should compensate for the effects of this delay by providing opportunities for exchanges between scientists.

J. Charvolin

The contract between the ESRF and the multinational building consortium was signed on 1 December 1989. (From right to left: Prof. R. Haensel, Director General of the ESRF, M. Dersy (Bouygues), Prof. J. Charvolin, Assistant Director of the ILL, M. Costa (ANSALDO), Herr Schlösser (STRABAG), Herr Küpper (STRABAG)).

College 2

Theory

Members of the College

H. Capellmann
F. Dalfovo
I. Jolie
P. C.W. Holdsworth
A. Hüller
M. Lavagna
P. Nozières
J. P. Rodriguez
N. Schopohl
R. Tahir-Kheli
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 the topics studied include superconductivity and quantum liquids, magnetism, liquid crystals, rheology of suspensions, protein dynamics and rotational tunnelling. The activities in nuclear physics include parity violation, 3-body forces, nuclear structure and the analysis of Gamma-Ray Induced Doppler broadening measurements and conversion electron measurements carried out at the ILL.

Scientific Trends and Highlights in 1989

Condensed matter physics

H. Capellmann continued his experimental neutron scattering collaboration together with O. Schärpf and K. Ziebeck to investigate aspects of the mutual influence of magnetic and lattice degrees of freedom.

F. Dulfovo calculated in collaboration with S. Stringari the surface tension of pure liquid ^{3}He using a local approximation for the entropy. Fair agreement between theory and experiment was reported. They also studied bound states of ^{3}He impurities on ^{4}He-clusters and derived a new sum rule to study multipair excitations in liquid ^{3}He.

P.C.W. Holdsworth collaborated with D. Loss to calculate the d.c. conductivity of a system of localized electrons subject to phonon assisted hopping. Also he continued his investigations of two-dimensional liquid crystals assuming non-separable pair potentials in the molecular orientation and intermolecular vector. These potentials cause a strong coupling between translational and rotational degrees of freedom. Numerical evidence was found that this coupling may lead to spin-glass-like behaviour in systems with quenched positional degrees of freedom. In a different investigation together with M.J.P. Gingras and B. Bergesen he carried out a stability analysis of an infinite-range Ising spin glass taking into account the effect of a (Gaussian) random field. At large field strengths, the transition temperature $T_c(h)$ was found to deviate quantitatively from the Almeida-Thouless line.

Alfred Hüller has worked on the temperature dependence of rotational tunnelling. The tunnelling lines as observed by high-resolution inelastic neutron scattering are due to transitions between states of different symmetry of a highly symmetric molecule in the orientational potential in a crystal. The level scheme for the different symmetry species differs only little and there are no transitions between the species when no neutron is present. It is therefore possible to replace the tunnelling molecules by harmonic oscillators of different frequencies such that the lowest two energy levels of each symmetry are reproduced exactly. Then the whole system consisting of the molecule and the lattice phonons can, in principle, be diagonalized exactly and the relevant correlation functions can be calculated. For practical reasons, a cumulant expansion is performed which yields a simple expression for the temperature-dependent shift and breadth of the inelastic tunnelling line. The results are in agreement with the experimental findings.

Alois Würger and Alfred Hüller have extended the calculations to the quasielastic line which stems from transitions between the partners of a degenerate Kramers doublet. There the oscillators replacing the two different symmetry species have identical frequencies. The broadening is due to the coupling of the molecule to resonant lattice phonons with different phase factors for the two species. This mechanism has been detected by AloisWürger in his Ph.D. thesis. For the harmonically replaced molecules the corresponding phase factor is introduced via a coupling to the momentum of the oscillator. Again the correlation functions can be calculated exactly. The quasielastic line turns out to be much narrower than the inelastic ones in agreement with experiment.

M. Lavagna continued to work on the problem of strongly-correlated Fermi systems using the "slave boson" representation. She extended the results of Kottliar-Rückenstein (which are equivalent to the Gutzwiller ansatz) by taking into account the Gaussian fluctuations around the saddle point. In this way she derived new results for the effective quasi-particle interaction in the density and spin channel of the Hubbard model. M. Lavagna and N. Schopohl collaborated in constructing a new "fractional" slave representation between bosons and fermions to gain insight into the microscopic origin of the flux phases. These phases are believed by some to contain the essence of the physics of the much discussed t-J model in the context of high T_c superconductivity.

P. Nozières worked on the melting of surfaces and crystallization. He continued his studies of interfacial instabilities and structure formation, with main emphasis on a descriptive theory of the morphology of the growth behaviour and of the geometry of two-dimensional structures. Also he investigated the rheology of suspensions and elucidated several

paradoxa originating from imprecise definitions of averaged quantities using an analogy to electrostatics.

J.P. Rodriguez worked in this past year on correlations in two-dimensional antiferromagnets with the main emphasis on the quantum aspect of the problem. He studied the topological excitations about the 2d-Néel state which are point-like defects and can be thought of as domain wall loops. An anomalous spin-wave damping rate near the antiferromagnetic Bragg point caused by low lying collective sound modes propagating in the liquid of these point defects (so called skyrmions-antiskyrmions) should be observable with inelastic neutron scattering methods. He also worked on doped electronic systems with 2d-antiferromagnetic correlations. Together with B. Doucot he investigated the t-J model in the large U limit of the Hubbard model employing a slave-boson large-N formulation. It is found that flux phases are stable for small hopping parameters carrying a number of dynamically generated flux quanta per plaquette given by the electronic filling fraction.

N. Schopohl and D. Waxman continued their studies of the phase boundary between superfluid ^{3}He-A and ^{3}He-B. It was predicted that the moving A-B phase boundary should push polarization ahead of and deplete polarization behind the interfacial region due to polarization dependent Andreev reflection and transmission of quasi-particles. This theoretical prediction was confirmed recently by S.T.P. Boyd and G.W. Swift from the Los Alamos National Laboratory. N. Schopohl and A. Baratoff continued their collaboration on the magnetic properties of anisotropic high-T_c superconductors. By replacing the cut-off procedure of the standard London approach by a variational ansatz for the amplitude of the order parameter inside the vortex core they derived a more accurate theory. The phase diagram of the vortex lattice for uniaxial and biaxial anisotropy and for arbitrary orientation of the external magnetic field was calculated. It turns out that as a function of the orientation and the strength of the external field relative to the crystalline axes there exist new types of vortex arrays different from the Abrikosov triangular vortex lattice.

R. Tahir-Kheli studied low frequency protein dynamics and ligand migration. Assuming that the diffusion of excitations is predominantly one-dimensional he analysed successfully $1/T_1$ relaxation data of NMR experiments over a wide range of frequencies in the interval between 10^4-10^9 Hz. In between the high and low temperature regimes he predicts a cross-over of the exponent of the frequency dependence of $1/T_1$ depending on the concentration of excitations and the hopping rate.

A. Würger continued his studies of rotational tunnelling due to the exchange symmetry of the protons of small molecules.

In the last year the emphasis of his work lay on the effects of thermal motion and rotor-rotor-coupling. The prefactor of the inelastic tunnelling width was estimated as an upper bound, which turns out to be independent of details of the phonon system. Together with A. Heidemann he also measured the tunnelling spectrum of $Sn(CH_3)_2Cl_2$ as a function of temperature between 5 and 232 K, and a fair qualitative agreement between the experiment and theory was found.

Nuclear Physics

I. Jolie worked part of his time on the analysis of the Gamma-Ray-Induced Doppler broadening measurements carried out at ILL. Also, he continued his theoretical work on the problem of odd-odd nuclei. Using the method of extended supersymmetry he and I.V. Isacker calculated the electromagnetic decay of excited levels in ^{76}As.

Secretary: N. Schopohl

Nuclear and Fundamental Physics

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General Summary

The year 1989 was again very fruitful for College III. The activities included experiments in fundamental physics, nuclear fission, nuclear spectroscopy, solid state physics, positron physics and geology.

The study of the thermal neutron induced fission process with the fission product spectrometer Lohengrin (PN1) has now been extended to both the minimum (^{229}Th) and maximum (^{249}Cf) target masses available until now at the spectrometer. Also, three more very neutron rich exotic nuclei (^{69}Co, ^{68}Co, ^{68}Fe) have been observed in the fission of ^{239}Pu.

The nuclear spectroscopy instruments, the electron spectrometer BILL (PN2), the crystal gamma-ray spectrometers GAMS (PN3) and the pair spectrometer (PN4) were in very high demand. Besides many interesting nuclear structure studies, these instruments demonstrated again their potential in attacking problems they were not originally designed for.

The investigation of Bhabha scattering with the BILL spectrometer has set the most stringent lower limit on the lifetime of hypothetical neutral particles which were proposed to explain the still-not-understood coincident electron-positron events in heavy-ion experiments at the GSI, Darmstadt.

The ultra-high resolution twin flat crystal spectrometer GAMS4 was used for the first measurement of the electronic structure factor in a Germanium crystal. The study of the slowing down process of recoiling atoms has been pushed to recoil energies as low as 3 eV which allows the study of not only gamma ray, but also neutrino induced Doppler broadening with GAMS4.

In the field of fundamental physics, five independent measurements of the neutron lifetime were completed and/or published in 1989. Two of them used ultra-cold neutrons which were either stored in a fluid-walled bottle (W. Mampe et al.) or in a magnetic storage ring (W. Paul et al.). The others were in-beam experiments carried out at the cold neutron beam SN7 with a helium filled time projection drift chamber (K. Schreckenbach et al.) or superconducting solenoids (D. Dubbers et al., J. Byrne et al.).

Also at the SN7 beam, several experiments studied parity violating processes, among them the first observation of parity violation in γ-resonant scattering.

The EDM collaboration improved the limit on the electric dipole moment of the neutron by one order of magnitude and is now preparing the next generation of the experiment.

The neutron-antineutron oscillation experiment was continuously taking data throughout 1989 and has pushed up the lower limit for the $n\bar{n}$-oscillation period by one and a half orders of magnitude.

Scientific Trends and Highlights in 1989

Nuclear Fission

The year 1989 brought, in a certain way, the accomplishment of one of the main scientific domains on the Lohengrin (PN1) spectrometer since this instrument went into operation : the publication of nuclear mass, charge and energy distributions of the reactions ^{229}Th(n,f) and ^{249}Cf(n,f) including mass chains down to 1 % of chain yield. These two fissile systems, being separated by almost 20 mass units, can be regarded as the corner stones for which fission characteristics can be measured with Lohengrin. It turns out that observables characterising fissile systems in between, which have been measured at the spectrometer for many years, follow some sort of smooth interpolation between the extreme cases. The dependence of the observables in low energy fission on parameters of the compound system is shown in Figure 1.

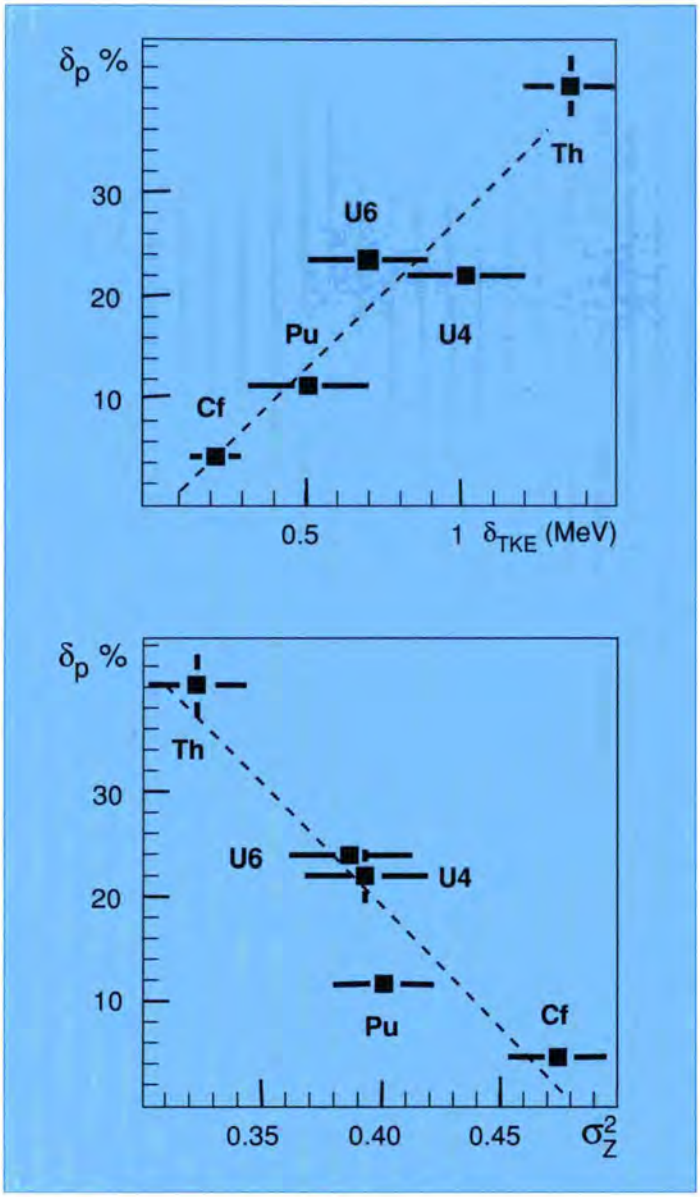


Fig.1 *Some observables in low energy fission showing the role of ^{230}Th and ^{250}Cf as corner stones in the process on parameters of the compound system:*

(a) the proton odd-even effect as a function of the odd-even effect on the total kinetic energy.

(b) the amplitude of the proton odd-even effect correlates with the average isobaric nuclear charge variance.

The second domain of fission, where a big effort to measure and establish empirical trends was undertaken at PN1, is the far asymmetric fission process. The measurements for the systems ^{236}U and ^{240}Pu including A = 86 to A = 70 mass chains, have been completed. A strong neutron odd-even effect in the yields, never observed previously, was established for the far asymmetric mass splits. A first measurement was made to determine nuclear mass, charge and kinetic energy distributions for asymmetric events in the ^{249}Cf(n,f) reaction (Fig.2).

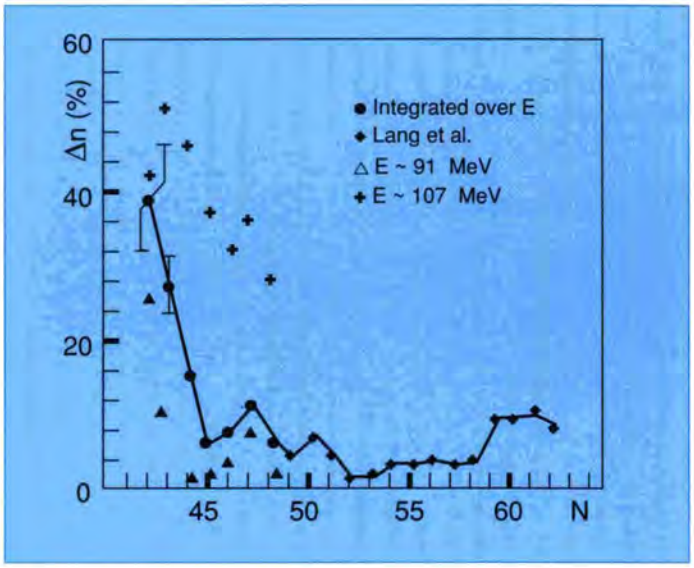


Fig.2 *Neutron odd-even effect in the isotonic yields of ^{236}U summed over the kinetic energies (line) and for two selected energies as a function of N. For N higher than 49 the values are taken from earlier measurements on ^{236}U.*

Further effort was undertaken to understand the aspects of symmetric fission, which represents the third main field of activity around Lohengrin. The scarce database including until now only the systems ^{236}U and ^{243}Am was extended to ^{250}Cf.

The measurements of the emission of light charged particles in neutron induced fission continued with the systems ^{236}U and ^{243}Am. An almost complete data set is now available for the isotopes of Beryllium, Carbon and Oxygen from the ^{236}U(n,f) reaction.

The determination of lifetimes along the r-process was extended. The yield of rare Ni and Cu isotopes was optimized using different fissile systems. Half lifes of $^{74, 75}$Cu and $^{71, 72, 73, 74}$Ni were obtained.

Most of the beam time available at the coincidence fission spectrometer COSI FAN TUTTE (PN8) was devoted to the first ever measurement of correlated fragment mass, kinetic energy and nuclear charge distributions in thermal neutron induced fission of ^{232}U. The analysis of the event-by-event data is still in progress.

At COSI FAN TUTTE the analysis of the ^{229}Th(n,f) reaction was finished and published, while the data evaluation of the ^{239}Pu(n,f) reaction is almost complete. The global light mass distribution after neutron evaporation with a mass resolution of SM ≈ 0.7 amu is shown in Figure 3a. As already known for other fissile systems, the mass distribution becomes more and more structured for increasing kinetic energy E_L of the light fragment. For cold fission most of the mass yield is concentrated around M_L = 106 amu (see Figure 3b). This enhanced mass yield can be accounted for by the influence of the Z = 50, N = 82 shell closure which stabilizes the complementary heavy fragment. The associated light

fragments coincide with a mass region where large groundstate deformations have been predicted and measured. The small structure around M_L = 85 amu might result from the N = 50 neutron shell closure.

Nuclear Structure

The use of the thermal neutron capture reaction for the spectroscopy of low spin states has yielded a vast amount of nuclear structure data throughout the years. The unique feature of this reaction lies in the possibility to get almost complete level schemes in a certain spin window and up to a certain excitation energy. In this way, many states with increasing excitation energy can be identified in a small range of accessible spins. This information is somewhat complementary to the results from heavy ion physics. The latter is usually restricted to states in a small band above the yrast line, which means that even though the range of accessible spins is much larger than for the (n,γ)-reaction, only the few lowest lying states can be identified for a given spin. The complete level schemes obtained from (n,γ)-spectroscopy play an important role in two different aspects of testing nuclear models. First it is evident that such tests, e.g. of the IBM model are much more significant, if not only the states just above the yrast line, but also higher states are included which involve additional degrees of freedom of the nucleus. Furthermore crucial tests may involve not only finding predicted states but also confirming the absence of states which are not predicted by theory.

Second, the extensive level schemes form the basis for the identification of the often very weak γ-ray transitions which turn out to be crucial for the discrimination between different model approaches.

The ability to study, in much detail, the (n,γ)-reaction at the ILL is mainly based on the high resolution electron spectrometer PN2 (BILL), the crystal gamma ray spectrometers PN3 (GAMS 1, 2, 3, 4) and the triple coincidence spectrometer PN4.

The testing of different derivatives of the Interacting Boson Model (IBM) has again prompted a lot of the nuclear spectroscopy work. The interest has shifted more and more to odd-A and odd-odd nuclei, reflecting the developments of theory which now allows the treatment of these complicated nuclei.

Four separate experiments have been carried out this year at the BILL and GAMS spectrometers which aim to test the supersymmetry approach of the IBFM.

First the conversion electron spectra from the ^{196}Hg (n,e$^-$) ^{197}Hg reaction have been studied in the energy range from 20 keV to 2.5 MeV. No previous conversion electron data were available for this nucleus. This is partly due to the rareness of the ^{196}Hg isotope (only 0.15 % of natural mercury), but also reflects the problems in preparing a suitable and safe in-pile target. Even the most stable mercury compounds like red mercury sulfide (HgS) tend not to survive the radiation heating under vacuum at the BILL target site. This problem was finally overcome by coating the active target area with a thin carbon layer which increases the emissivity. The γ-ray spectra from this reaction will be measured in 1990. A low spin level scheme of ^{197}Hg up to 1 MeV excitation energy will be determined and compared to the U(6/12) supersymmetry scheme.

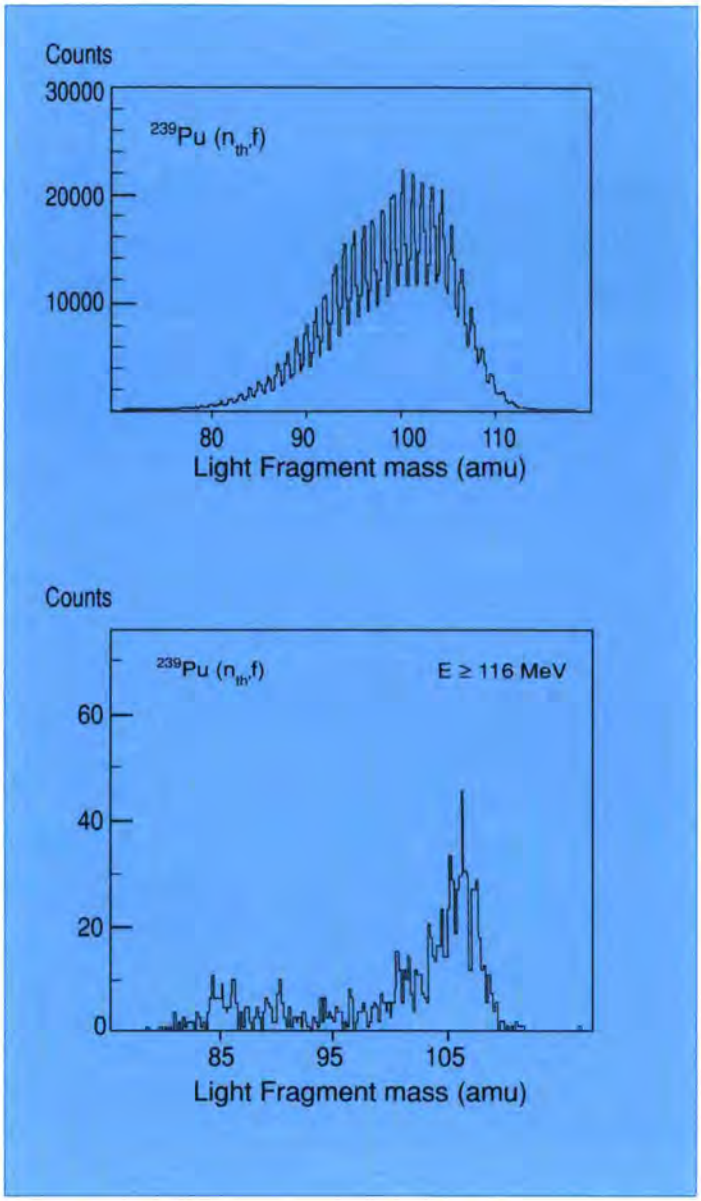


Fig. 3 *(a) Global light mass distribution of thermal neutron induced fission of ^{239}Pu*

(b) Mass distribution for light fragments with $E_L \geq$ 116MeV in the ^{239}Pu (n_{th},f) reaction.

In a longstanding effort the study of levels and transitions in ^{198}Au has finally been completed by measuring the gamma ray and electron spectra from the ^{197}Au(n,γ) and ^{197}Au(n,e$^-$) reactions (collaboration with TU Munich). The resulting level scheme is expected to provide a testing ground for several nuclear models which claim to be able to describe such nuclei, e.g. the ^{196}Pt- ^{197}Pt - ^{197}Au - ^{198}Au supersymmetry quartet.

The third nucleus studied in this context was the doubly odd ^{194}Ir. (collaboration with Institut of Physics, Riga). Measurements of the low energy (15 to 300 keV) electron spectrum were carried out at the BILL spectrometer. They will be combined with the high energy electron spectrum and the γ-ray spectrum measured previously. This nucleus can be described as being close to the U(6/4) supersymmetries (odd-A iridium isotopes) or to the O(6) limit of the IBM (even-even Os/Pt nuclei).

A considerable effort has been made recently to study the odd-odd nucleus ^{76}As in the framework of the ^{75}As - ^{76}As - ^{76}Se - ^{77}Se supersymmetry quartet. Based on this theoretical work and the extensive level scheme already set up from (n,γ) and (n,e$^-$) spectroscopy, certain regions of the electron spectrum were selected for more extensive measurements. In this way, previously unknown branching ratios and multipolarities of weak transitions between positive parity states were measured. These transitions are crucial because the supersymmetry model predicts selection rules for them (collaboration with University Tübingen).

A detailed study of the conversion electron spectrum of the heavy odd-A nucleus ^{243}Pu was mainly prompted by the interest in mixed single particle - vibrational excitations. Evidence for the presence of 0^+ phonon mixing can be obtained by determining the E0 admixtures to the M1/E2 de-exciting transitions of the states under observation (collaboration with LLNL).

It was already mentioned in the last annual report that the experimental determination of the decay modes of the so called "scissor-mode" collective 1^+ excitations in deformed nuclei is a very exciting topic. In 1989, two experiments made initial attempts to study such transitions. These were the measurements of the ^{155}Gd(n,e$^-$) (collaboration with TU Munich) and ^{157}Gd (n,e$^-$) reactions (collaboration with the University of Sussex) at the BILL spectrometer. Both experiments aimed at constructing extensive level schemes of the nuclei in question. These schemes are certainly of great value on their own, given the many interesting nuclear structure aspects involved, such as transitions between excited 0^+ states, testing of IBM, collective and unified models for highly deformed nuclei and so on. Furthermore this extensive spectroscopy is the only chance to identify finally the collective 1^+ states in the (n,γ) reaction. This justifies the big effort involved in studying the extremely complex high-energy spectra. The experiments were further complicated by the ultra high capture cross sections of 61000 b and 254000 b respectively, which meant that the targets were used up very quickly and had to be renewed often (daily in the case of ^{158}Gd).

Almost all the nuclear structure studies carried out with the BILL spectrometer make use of published tabulations of internal conversion coefficients or, in the case of E0 transitions, conversion probability electronic factors in order to determine the multipolarities of the transitions. The assumptions involved in the calculation of the tables have to be checked experimentally. The relative intensities of conversion electrons from different shells have been measured at BILL this year for the 1305 keV E0 transition in ^{114}Cd and the 362 and 1405 keV E0 transitions in ^{172}Yb for comparison with the calculations.

The ultra high resolution obtained with the twin flat crystal spectrometer GAMS4 has provided the basis for a number of studies in different domains of physics. A preliminary study of photon scattering amplitudes in Ge crystals for energies of 342 keV and 1381 keV has been carried out. The results suggest that crystal structure factors can be measured accurately enough to test the lowest order radiative corrections to the standard electron-photon interactions (collaboration with NIST and ESRF).

Continued systematic studies using GRID (**G**amma-**R**ay **I**nduced **D**oppler broadening) have extended the understanding of the slowing down process of recoiling atoms in matter at low recoil velocities (see box Annual Report 1988). Following the earlier studies of monoatomic targets the slowing down in diatomic systems has been studied experimentally, by a comparison between Ti and TiC, and self-consistent results were obtained.

This study of slowing down processes has also been extended to much lower recoil energies and in particular to that induced by neutrino emission following the electron capture decay of ^{152}Eu to ^{152}Sm. In this case the recoil energy is as low as 3 eV, corresponding to a recoil velocity of only 2000 m/s. This energy is insufficient to break the bonds with neighbouring atoms and the recoiling atom must then give up its energy to the bulk of the material by phonon creation. In order to understand this process the slowing down in $EuCl_3$, EuF_2, EuF_3 and Eu_2O_3 has been measured using NID (**N**eutrino **I**nduced **D**oppler broadening). The resulting dependence of this continuous slowing down process on the chemical species involved is shown in Fig.4.

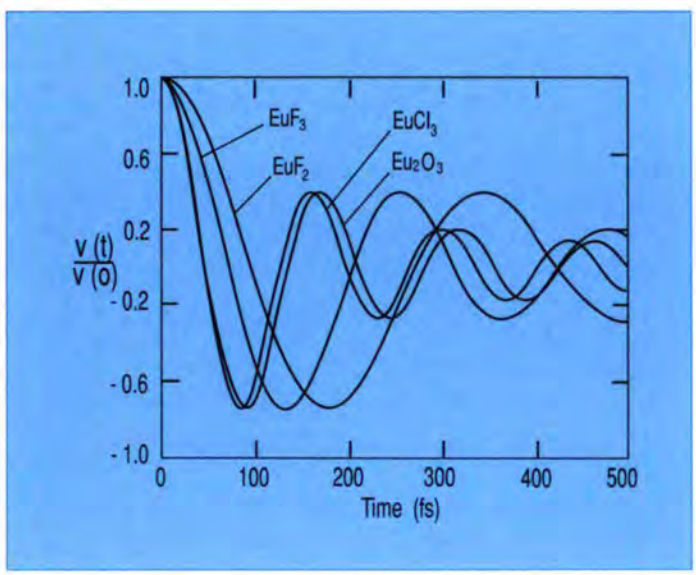


Fig.4 Slowing down of Sm atoms in different Eu compounds.

The initial applications of the GRID technique were to determine lifetimes of excited nuclear levels in light nuclei and for cases where direct feeding mechanisms were predominant. Such a study of levels in ^{57}Fe (mentioned in last years report) has contributed to a rather complete survey of this nucleus and its interpretation in terms of the nuclear shell model (collaboration with Univ. of Göttingen). The same group has, this year, also performed GRID measurements on transitions in ^{59}Ni. With a reasonable number of such measurements now completed we are in a position to compare the GRID technique with the more standard methods such as DSAM (**D**oppler **S**hift **A**ttenuation **M**ethod). From Fig. 5 which shows such a comparison for three of the nuclei studied so far, it can be seen that especially for very short lifetimes GRID yields the more precise values.

As well as the simple case of direct feeding, systems involving cascade and statistical feeding have now also been measured. It is known that in lifetime measurements which involve Doppler broadening one ususally tries to avoid cascade feeding effects as they produce delays for which it is difficult to correct. If, on the other hand, such cascade feeding occurs via a statistical process the feeding time depends on the gamma-ray strength from, and the level density of, the feeder states. Using the ^{143}Nd(n,γ)^{144}Nd reaction the GRID technique has been used to directly test predictions of such statistical feeding by determining the lifetimes of 11 levels in ^{144}Nd below an excitation energy of 2.4 MeV.

A consequence of this latter study is that very precise absolute energies have been obtained for the strongest transitions in ^{144}Nd. It is expected that these will complement the results of a more conventional measurement of the complete spectrum using the bent crystal spectrometers GAMS 1/2/3 and the BILL spectrometer and so aid in the construction, using the Ritz combination, of a very complete level scheme for this nucleus up to high excitation energy. The interest in this nucleus comes from the fact that it lies only two neutrons away from the N = 82 closed shell and so is expected to show many different aspects of nuclear excitations such as collective vibrations of the complete nucleus, excitation of single particles and so-called intruder configurations which may have a more deformed structure.

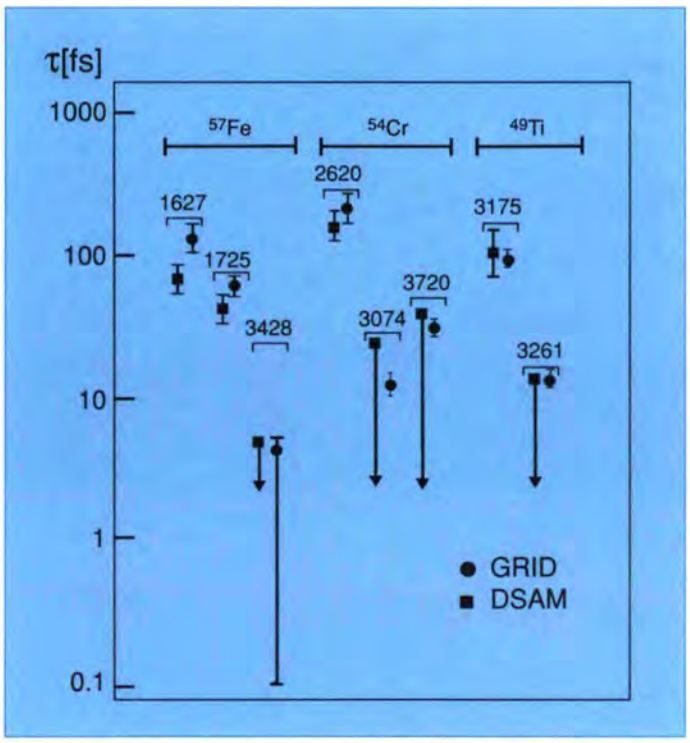


Fig.5 Comparison of lifetime results obtained with GRID and DSAM.

The double escape 'pair' spectrometer PN4 is often used in conjunction with such experiments to provide information on the high energy gamma transitions in a nucleus and especially those from the neutron capture state itself (so-called primary transitions).

This was again the case with the studies of ^{59}Ni, ^{144}Nd and ^{198}Au mentioned above. However, in light nuclei the gamma spectrum is often simple enough that studies with PN4 alone are sufficient. In particular a systematic study of level densities and gamma strengths in such nuclei has been continued this year by a study of the ^{50}V(n,γ)^{51}V reaction (collaboration with Univ. of Göttingen). In addition the search for double-neutron capture in ^{74}Ge leading to a possible determination of the neutron binding energy of ^{76}Ge (see Annual Report 1988) has continued (collaboration with CEN Bordeaux).

Beside the nuclear structure experiments the BILL spectrometer PN2 was again used for fundamental physics, namely the search for neutral resonances in Bhabha scattering (collaboration with GSI, Darmstadt). The existence of such resonances has been postulated to explain the observation of the coincident electron positron pairs created in heavy ion collisions. Previous experiments at BILL (see Annual Report 1988) had set the most stringent lower limit on the half life of such particles as 3.5 x 10^{-12} s. This limit already surpassed the sensitivity of the constraints deduced from a contribution of a hypothetic point like scalar particle to the precisely known (g-2) factor of the electron. More important, the limit is independent of assumptions about the internal structure of the hypothetical particles. In 1989 the search concentrated on lifetimes longer than 10^{-13} s. The set-up of the new experiment is shown in Figure 6. The positrons were again focussed onto a 4.6 mg/cm beryllium foil (20 x 100 mm^2) which was tilted at an angle of 30° to the positron beam. The idea was that neutral particles with lifetimes longer than 10^{-13} s would decay outside the foil because they are produced with a velocity of 0.8 c. The high background due to electron positron pairs from prompt Bhabha scattering could therefore be eliminated by interposing a plastic scintillator between the foil and one of the detector arrays. The energy of the incident positrons was scanned from 2.1 to 2.4 Mev, but no evidence for the hypothetical particle was found. A limit for the cross-section for the formation of the particle was calculated as a function of half life, and the result is shown in Figure 7. The experiment ruled out the existence of particles with a half life from 7 x 10^{-13} to 7 x 10^{-12} s.

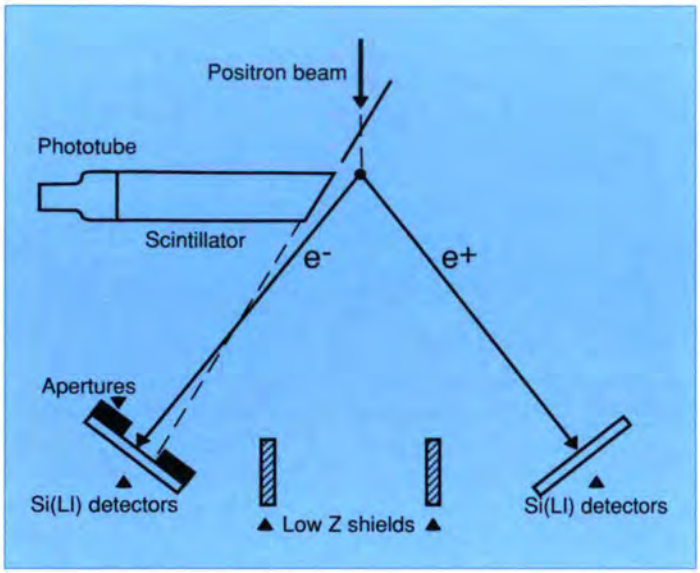


Fig.6 *A schematic diagram of the apparatus used in the search for the decay of a hypothetical neutral particle created in positron-electron collisions. The BILL spectrometer was used to focus a beam of positrons (with a kinetic energy in the 2.3MeV region) onto a Beryllium foil. Any neutral particles created in the foil recoil out, and then decay by emitting an electron-positron pair which could be detected in the two Si(Li) detector arrays. The plastic scintillator was positioned in order to block electron-positron pairs from elastic (Bhabha) scattering events in the foil itself, and hence to improve the sensitivity of the experiment.*

The BILL spectrometer has also been used to study, in more detail, the positron production from absorption of neutron capture γ-rays. This was not so much in view of a further improvement of the 'high energy' titanum-platinum source used for the Bhabha scattering experiments, but it was part of a feasibility study for a high intensity reactor based source of moderated positrons. A source favoured by numerical simulations of the process consists of a cadmium-tungsten combination. Intensities, spectral shapes and angular distributions of such sources were measured to check the calculations.

Fundamental Physics

The activities of the college in fundamental physics center around the very-cold and ultra cold (VCN, UCN) neutron beams provided by the neutron turbine on level D (TGV) and the cold neutron beam SN7, which can provide continuous or chopped beams of unpolarized or polarized neutrons. A remarkable activity was devoted to the study of the properties of the neutron itself (see also blue box).

The EDM collaboration (Sussex, RAL, Seattle, Harvard, ILL) has continued data taking and development of the apparatus installed at the neutron turbine until May 1989. Parallel to this work, all data have been analysed by using three different and independently written algorithms which produced results in good agreement which each other. The result obtained for the neutron's EDM from all runs on the turbine is $d_n = -(3 \pm 5) \times 10^{-26}$ ecm which can be interpreted as a limit: $|d_n| < 12 \times 10^{-26}$ ecm with 95% confidence. The uncertainty was reduced by one order of magnitude compared to the result from the last generation which was published in 1985. Since the total error is 2.6 times larger than the uncertainty given by statistics alone , it has been decided to upgrade the experiment by reducing systematic errors. The main modifications consist of an elevated, larger storage volume and the integration of a mercury vapour magnetometer. More details can be found in the technical report.

Later in the year the EDM beam has been used for measurements helping to define the geometry of the new EDM experiment. It was further used for a detailed study of the energy and temperature dependence of the UCN reflection properties of Fomblin oil, grease and other materials. The energy resolution achieved by using D. Richardson's gravity monochromator was better than 7 neV. The neutron lifetime experiment using ultra-cold neutrons from the turbine test beam stored in Fomblin oil coated bottes of variable size, gave a lifetime of $\tau_n = (887.6 \pm 3)$s. Detailed calculations have been performed by the participants of the experiment and F. Faure for a better understanding of a correction (<1%) due to the action of gravity on the UCN during storage. The test beam is at present being used for investigations of neutron guide transmission under various conditions.

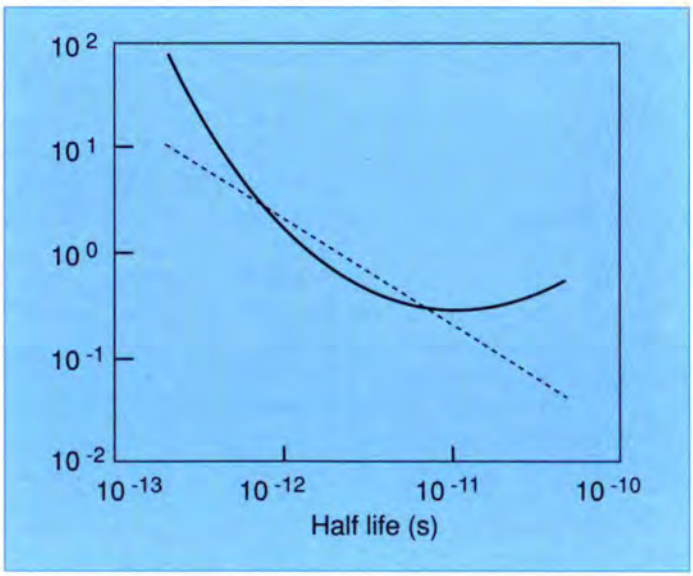


Fig.7 *This figure shows the limit on the (energy integrated) cross-section for the formation of a neutral particle obtained from the experiment (solid line), and also the theoretical minimum possible cross section (dotted line). The experiment therefore ruled out the existence of such neutral particles with a half life between 7×10^{-12} and 7×10^{-11}s.*

The very cold beam section of the TGV is occupied by the long baseline interferometer of a Vienna-Munich-ILL collaboration. The wavelength is tuned to 100 Å. A 6 m long optical table with vibration isolation carries the optical elements for the neutrons as well as a Laser interferometer which serves for adjustment and stabilisation purposes. The neutron optical elements are three high-precision diffraction phase gratings with a lattice constant of 2 μm, which are used in transmission mode. A prototype interferometer with an overall length of 50 cm has been set up and successfully tested. This prototype is the first demonstration of a neutron interferometer using very long wavelength neutrons over a large distance. It allowed the investigation of the compatibiliy of the extreme stability requirements with the in this sense hostile environment on the top level of the reactor.

The experiments at the cold neutron beam SN7 were devoted to the study of some neutron decay properties and to parity-violating effects in polarized neutron induced fission.

In two different experiments the neutron lifetime was determined. With the superconducting solenoid "PERKEO" the neutron decay electrons from a pulsed neutron beam were magnetically guided to plastic scintillator detectors. The number of neutrons per pulse were measured by activation analysis of nuclei in the neutron beam absorber. The ratio of the decay electrons to the number of the radioactive nuclei produced measures the neutron lifetime. Based on the experience from a previous experiment using this method several technical improvements were realized. The data evaluation is underway (University of Heidelberg, Argonne, ILL).

In the second neutron lifetime experiment at SN7, a continuous neutron beam was passed through an electromagnetic trap for the decay protons (energy < 800 eV). The proton trap consisted of a superconducting solenoid and an electrostatic potential along the neutron beam for a radial and axial proton confinement, respectively. The decay volume was variable and defined by the length of the distance of the electrostatic potential barriers (high voltage ring electrodes). The trap was periodically emptied by changing the electrostatic field and the protons were detected in surface barrier detectors. The measurement of the neutron density, necessary to derive the neutron lifetime in this method, was performed by means of the (n,α) reaction in thin boron layers. As preliminary result a value of τ_n = 894(6) was derived (SUSSEX-NIST collaboration).

Starting with the last reactor cycle 1989, the SN7 beam is being used for a measurement of the parity-violating beta asymmetry in the free neutron decay (coefficient A). In this experiment, a polarized neutron beam passes through a helium-filled time projection chamber (TPC). The emission angle of the decay electrons relative to the neutron spin is determined for each event by the ionisation track in the TPC. The beta energy is measured in plastic scintillators placed outside the TPC (LAPP, Annecy-ILL collaboration).

The polarized SN7 beam was simultaneously used for two reactor cycles by two experimental groups studying parity violation in neutron induced fission. Some years ago, Danilyan et al. observed an asymmetry in the emission probability of light and heavy fission fragment relative to the spin of the fission inducing neutron. The effect was of the order of a few times 10^{-4}. Obviously, this effect is parity non-conserving (PNC) and the experiments carried out at SN7 should give more insight into the nature of this PNC effect.

In the experiment by the Kurchatov Institut-ITEP collaboration (Moscow) the PNC effect in ternary and binary fission was compared. A difference in the PNC effect would indicate a difference in the entrance channel for the two fission modes. For this investigation the fission products of ^{239}Pu were detected following polarized neutron capture. Mass resolution was obtained by time-of-flight measurements of the fission products towards multiwire proportional counters. For ternary fission the particles were detected in a ring counter perpendicular to the neutron spin. No difference in the PNC coefficient was found between binary and tenary fission. The experimental ratio was 1.06 ± 0.07 (1 σ error).

In the same polarized beam an ionisation chamber from the University of Tübingen was placed. With this high-resolution twin-ionisation chamber the PNC effect was studied for individual fission fragments and especially for cold fission events. The data were recorded in list mode and are presently under evaluation.

At the test beam T1b (at H14) parity violating spin rotation was studied for several nuclei (University of Washington, Seattle). In particular, sizeable effects were searched for in nuclei which could be polarized by optical pumping and thus used for tests on time reversal violating spin rotation (polarized target in absence of a large magnetic field). A RbC_8 monochromator was used to create a beam of 8 Å neutrons. The second order reflection at 4 Å was suppressed by a filter made of graphite monochromators. The experimental set-up was similar to earlier studies of PNC spin rotation by this group. Samples of La, Br, Cs, Na and Hg were investigated (evaluation underway).

The neutron-antineutron oscillation experiment is in continuous operation. In this experiment one searches for a process which violates baryon number conservation, but which is allowed in left-right symmetric grand unified theories. By the end of 1989 the lower limit for the n-$\bar{n}$ oscillation period was pushed by one and a half orders of magnitude to $\tau_n > 4 \times 10^7$ s. The experiment will take data for two more years.

Special Beam Experiments

The nuclear physics group has three positions at the end of the H22 thermal neutron guide. The H22E position is used mainly by a group of geologists from the University of Grenoble/CNRS for prompt activation analysis of geological samples; with special emphasis on the dosing of trace elements with large neutron capture cross sections. Although this intallation is already the most sensitive in the world,

continuing efforts have been made to further improve background conditions. In addition this position has been used by a group from the University of Rouen to irradiate biological samples for later study.

The H22F position is used for coincidence studies of nuclear level schemes and this year an ILL/Sofia collaboration has used the delayed coincidence technique to study excited state lifetimes in the nuclei ^{144}Nd and ^{198}Au - thus tying in with the extensive studies mentioned in the nuclear structure section.

At the S50 position a group from the PTB, Braunschweig is continuously improving the precise determination of the $\hbar/m_n$ constant. In 1989, possible sources of systematic errors were studied in detail. The experimental uncertainty was lowered this way by a factor of two to 4×10^{-7}. A new value of $\hbar/m_n = (3.9560344 \pm 0.0000016) \times 10^{-7}$ m^2 s^{-1} was determined and further improvements are expected. A precise value is important for the determination of other fundamental constants. In particular the fine structure constant α can be deduced with a relative uncertainty of 2×10^{-7}.

At the curved neutron guide H22D, the systematic investigation of the (n_{th}, π)-(n_{th}, α) and ternary fission process has been continued.

The thermal neutron induced ternary fission of ^{229}Th and ^{243}Am has been studied. Also the ^{36}Cl (n_{th}, π)-reaction, which is important for astrophysics, has been investigated. The present reaction cross-section is one order of magnitude lower than previously obtained.

At the H17 position a group from U. Munich constructed a correlation chopper to study the interaction of ultra-cold neutrons with superfluid ^{4}He. First observations of the temperature dependent time of flight spectrum of the upscattered UCN were made. Although the signal to noise ratio has to be further improved, the results seem to indicate deviations from earlier calculations.

Seminars, etc.

In spring 1989 a workshop was held at the ILL on Fundamental Physics with Slow Neutrons. It covered the fields: Searches for New Phenomena beyond the Standard Model, Weak Neutron-Nucleus Interactions, Free Neutron Decay, Electromagnetic Interactions of the Neutron, Neutron Optics and Quantum Mechanics, and Neutron Sources and Detectors. It was the third ILL-workshop on this topic (the first two were held in 1978 and 1983). The workshop was attended by more than one hundred physicists, half of them from outside the ILL member countries. The proceedings were published as a regular issue of Nuclear Instruments and Methods A, 284 (1989)1.

In June 1989, a meeting was organised to discuss the perspectives of a suggested reactor based high flux source of moderated positrons. Members from outside groups which are active in the field of positron physics presented their projects for the use of such a source. The view graphs presented at the meeting are available as an ILL Internal Technical Report.

Finally, two members (J.P. Bocquet and P. Schillebeeckx) left the College in 1989.

Secretary: B. Krusche

The Decay of the Neutron

D. Dubbers, W. Mampe, J. Döhner

The weak force and the electromagnetic force are twins. At high energies (> 100 GeV) both forces are found to be identical - they form one single electroweak force of remarkable symmetry. On the way down to terrestrial temperatures, however, nature suffers a phase transition accompanied by a spontaneous symmetry breaking (a phenomenon which has parallels in other fields of physics). After that, the weak force and the electromagnetic force no longer resemble each other very much, but each has found a role of its own: the electromagnetic force gives rise to the stability of atoms, molecules and matter, while the weak force determines the primordial element distribution and makes the sun shine in order to give life to these building blocks.

The main manifestation of (charged current) weak interactions is the ß-decay of nuclei and particles. It turns out that the weak interaction of the quarks in the nucleons is most precisely studied in free neutron decay. In this process, the neutron (u d d) changes into a proton (u u d) by the transformation of a down quark d into an up quark u, with the emission of a fast electron (ß-particle) and an antineutrino.

The interest in precise neutron decay data is twofold: firstly, these data are relevant for a number of central issues in elementary particle theory; secondly, all (semileptonic) weak interaction cross-sections, in use in widely differing fields, must be calculated from measured neutron decay data. The present article lists some implications of recent neutron decay results.

We recall that the strength of the electromagnetic interaction is determined by the size of the elementary **electric charge** e. Similarly, the strength of the weak interaction is determined by the sizes of some elementary **weak charges** g_V and g_A. (Two different weak charges, plus a phase angle φ, are needed because weak currents can have both polar vector (V) or axial vector (A) character. Electromagnetic currents always have polar vector (V) character.)

The overall strength of the weak quark interaction is measured by the neutron decay rate

$$\tau^{-1} = \text{const.}\ (g_V^2 + 3g_A^2), \qquad (1)$$

with the **neutron lifetime** τ, and a well known constant. (The electromagnetic analogue to τ^{-1} is the fine structure constant $\alpha = (4\pi\varepsilon_0\hbar c)^{-1} e^2$).

The relative strengths of the vector and axial vector contributions, or, in other words, the **structure of the weak quark interaction** is given by the quantity $\lambda = e^{i\phi} \left| g_A/g_V \right|$. For a time reversal (T-) invariant left-handed weak interaction we expect λ to be real with a phase angle $\phi = 180°$. Indeed, a high precision search for T-violation in neutron decay conducted at ILL gave

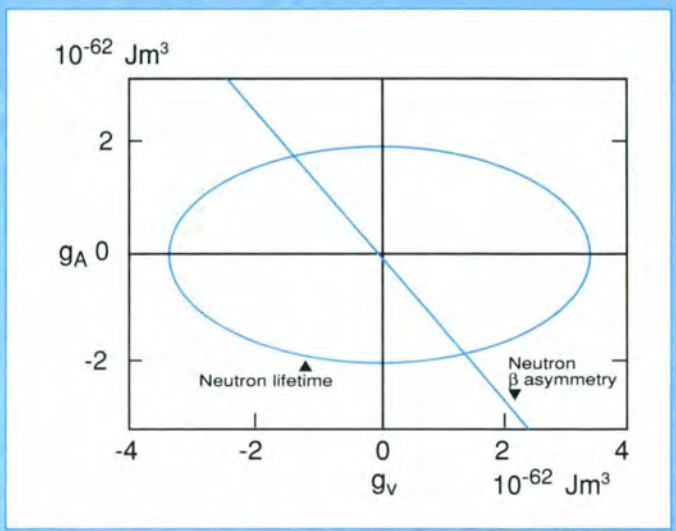
$$\phi = (180.14 \pm 0.22)°$$

and we can simply write

$$\lambda = g_A/g_V. \qquad (2)$$

This ratio is most sensitively determined from a measurement of the (parity violating) left-right ß-asymmetry in polarized neutron decay

$$A = -2\lambda(\lambda + 1)/(1 + 3\lambda^2)$$



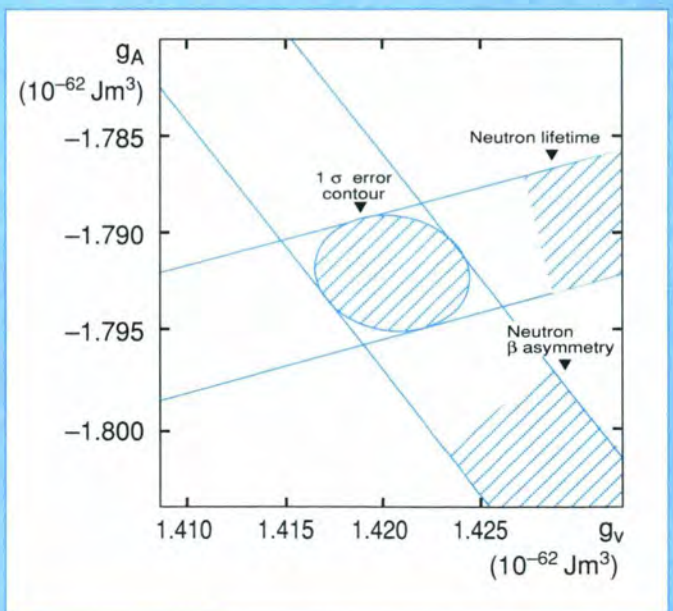


Fig. 8: Derivation of weak coupling constants g_A and g_V from measurements of the neutron lifetime, eq. (1), and of the neutron ß-asymmetry, eq. (2). Fig. 8b) is a 300 x 300 enlargement of part of Fig. 8a)

In the past few years there has been considerable activity in neutron decay experiments: in all there were seven new experiments on the neutron lifetime (five of them at ILL) and one on the neutron ß-asymmetry. Each of the lifetime experiments used a completely different approach: ultracold neutron storage by magnetic, by liquid wall or by gravity confinement; (cold) neutron beams used with a proton trap, with electron-proton coincidence, or with neutron "storage in flight" both in an electron drift chamber and in "PERKEO". The results of two of these experiments had an accuracy considerably higher than the previous world averages.

In the "liquid wall" experiment the neutron lifetime was measured to τ= 887.6(3.0) s. Together with the other lifetime measurements this leads to a world average:

$$\tau = 888.6(2.6)\ \text{s}.$$

The neutron ß-asymmetry was measured with the instrument PERKEO on a beam of polarized cold neutrons to A = - 0.1146(19), which gives λ = -1.262(5). Together with all earlier neutron decay correlation measurements this leads to a world average:

With these new data we can for the first time consistently derive both weak coupling constants from neutron decay alone to:

$$g_V = 1.4205(42).10^{-62}\ \text{Jm}^3,$$

$$g_A = -1.7921(29).10^{-62}\ \text{Jm}^3.$$

Fig. 8 shows that the lifetime and the asymmetry experiments give roughly orthogonal information of about equal quality.

Neutron decay today is the only source for a precise value of the axial coupling constant g_A ; in nuclear decays g_A is quenched by 30% and more. The vector coupling constant g_V, on the other hand, can also be derived from nuclear decays, if conservation of the weak vector current (CVC) is assumed. CVC is essential in electroweak unification, as it is the weak interaction analogue to the conservation of the electromagnetic vector current. By comparison of the neutron derived value of g_V with the value derived from nuclear ß-decay data we come to our **first conclusion**:

*The weak vector coupling g_V is of equal strength for neutrons and for atomic nuclei on the 3.10^{-3} level, in confirmation of the **conserved vector current** hypothesis.*

With some more theoretical input we can also relate our g_V and g_A values to the measured decay data of higher generation particles and come to the **second conclusion**:

*The weak vector couplings g_V of first and higher generation particles are consistent with each other on the 3.10^{-3} level, within the theoretical framework of **three generation unitary quark mixing and universality** ; on the other hand the weak axial vector coupling g_A, when compared to the (less well known) corresponding quantities in higher generation particle decays, shows a discrepancy of 6%, or more than three standard deviations, which may be due a small SU(3) **flavour-symmetry breaking** in the axial vector sector.*

Modern left-right symmetric grand unified theories also predict the existence of right handed weak currents. When the validity of CVC is assumed, then a consistency check of nuclear and neutron decay data leads us to the **third conclusion** :

***Right-handed contributions** to the (basically left-handed) weak interaction are excluded up to energy ranges of 1000 GeV (the exact value depending on the left-right mixing angle which is simultaneously constrained by the analysis).*

It had further been speculated that the long-standing solar neutrino problem (too few solar neutrinos arrive on earth) may be solved trivially if the adopted neutron lifetime from which the solar energy balance is calculated changes again as much as it did in the past six years (by 1/2 minute). Our **fourth conclusion** is :

*The **solar neutrino problem** can no longer be due to an error in the neutron decay data.*

But the field which called most for better neutron decay data is cosmology. In the standard big bang model light element abundance in the universe depends both on the number of existing neutrino generations and on the neutron lifetime. This brings us to our **fifth conclusion** :

*From the observed helium primordial mass fraction cosmologists find, using the new neutron decay data, that the **number of particle generations** is $N = 2.6 \pm 0.3$, making a fourth generation of particles very unlikely. This coincides with the latest findings from the new LEP accelerator at CERN.*

Neutron decay data find **further uses** in the calculation of :

- *astrophysical neutrino processes*
- *neutrino detection efficiencies of large detectors (examples: neutrino oscillations, proton decay, and others)*
- *weak processes in elementary particle experiments in general.*

Finally, g_V can be related to the electric charge e via the **W-boson mass** and the **Weinberg angle**, and g_A/g_V can be (though not very precisely) calculated from quark theory.

From the foregoing list we conclude that it is worthwhile to continue the search for better neutron decay data.

The present article is a summary of a paper by D. Dubbers, W. Mampe, and J. Döhner, Europhysics Letters 11, 195 (1990).

Structural and Magnetic Excitations

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General Summary

The activities of College IV covered a broad spectrum of interest this year. As in recent years, the majority of experiments were in the field of magnetic rather than structural excitations. We continued to have a substantial number of proposals on the oxide superconductors and related systems as single crystals have become available and new systems are discovered. However, other fields such as, heavy fermions, mixed valence and low dimensional systems were well represented.

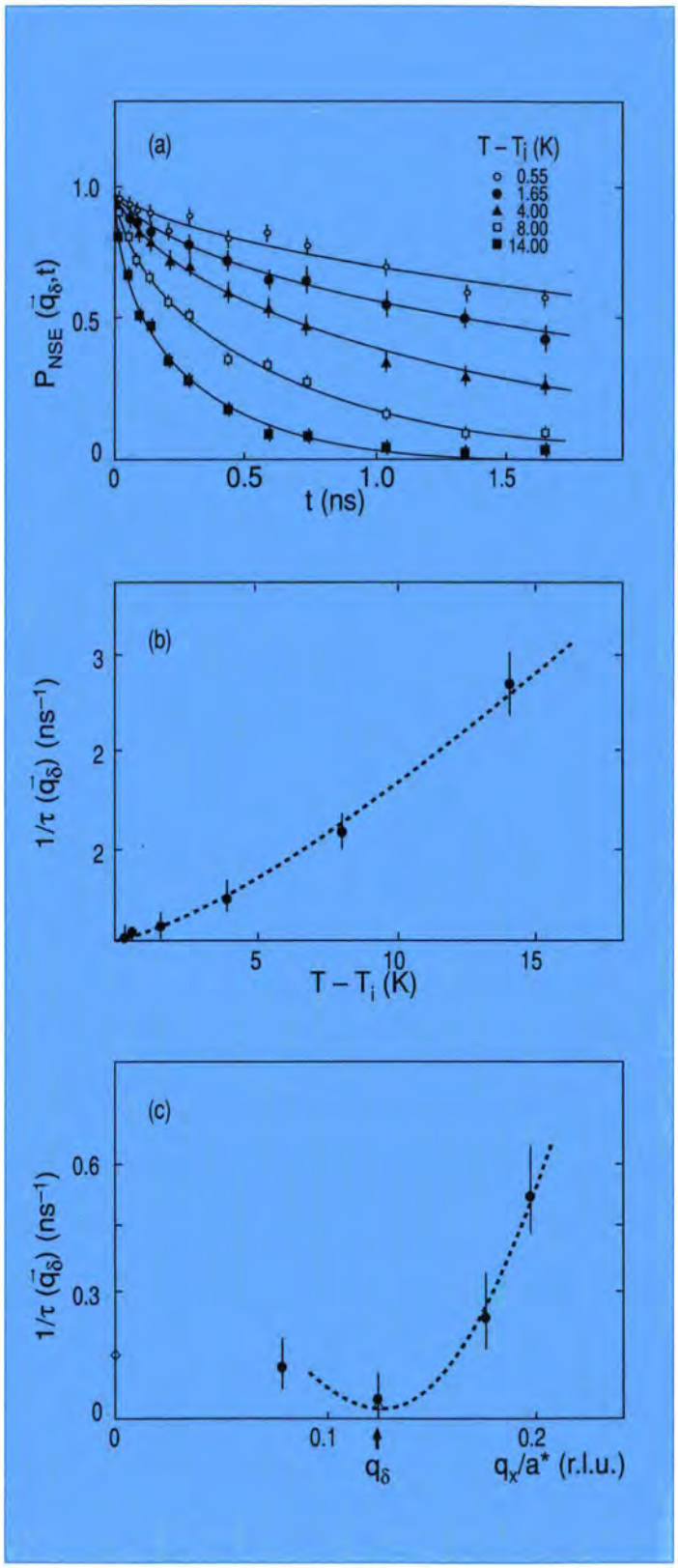

Fig . 9: Critical slowing-down of NO_2^- reorientations in $NaNO_2$: NSE spectra for several temperatures above T_i at the critical wavevector q_δ (a) and corresponding relaxation rates $\tau^{-1}(q_\delta)$. (b): q-dependence of the relaxation rate for q along a and $T = T_i + 0.3K$. (c): ultrasonic and dielectric data are shown as open triangles and squares, respectively.*

Scientific Trends and Highlights in 1989

Lattice Dynamics and Structural Phase Transitions

Orientational Ordering in $NaNO_2$

The dynamics of structurally modulated crystals continues to be actively investigated. Of particular interest is the characterization of the excitation spectrum associated with fluctuations in the local phase of the static modulation. Previous experiments on the IN12 cold-source 3-axis spectrometer have provided evidence for gapless (i.e. acoustic-like) "phason" branches in displacively-modulated insulators.

The concepts of phase and amplitude fluctuations can be generalized to order-disorder and compositional modulations. Sodium nitrite ($NaNO_2$) is a particularly simple example of such a system, where the Ising-like ordering variable is the orientation of the NO_2^- groups, parallel or antiparallel to the crystallographic b-axis. Between the disordered and the ferroelectrically ordered phases, a modulated phase is observed over a narrow temperature range ($T_f = 162.5°C < T < T_i = 164.0°C$), with wavevector along a ($0.1a^* < q_\delta < 0.12a^*$). The neutron spin-echo technique has been used [1] to investigate the collective dynamical behaviour of the groups in the disordered phase ($T>T_i$), when the order-parameter susceptibility is described by a single Debye relaxation:

$$\chi(q,\omega) = \chi(q,0) / (1 - i\omega t(q))$$

As shown in Fig. 9, the relaxation time $\tau(q)$ displays critical slowing-down behaviour on approaching T_i, for the critical wavevector q_δ :

$$\tau(q)^{-1} = \alpha (T-T_i) + \lambda (q-q_\delta)^2$$

Below T_i, the analysis of the NSE data is performed in terms of two relaxation modes, corresponding to the decoupling of the phase and amplitude degrees of freedom :

$$\tau_A^{-1}(q) = 2\alpha (T_i-T) + \lambda (q-q_\delta)^2$$

$$\tau_\phi^{-1}(q) = \lambda (q-q_\delta)^2$$

In practice, however, the NSE response is dominated by the (slow) phase-relaxation mode, and the observed spectra appear temperature-independent.

Phonon Density of States of High Temperature Superconductors

Since the discovery of high temperature superconductivity, the field of oxide superconductors has become one of intense activity. With the discovery of new systems, the subject shows no sign of quietening down. We review some of the work on the magnetic excitations in a separate section (see box).

The lattice dynamics of a number of these systems have been investigated at the ILL. Figure 10 shows the generalized phonon density of states for one such compound $Pb_2Sr_2Ca_{0.5}Y_{0.5}Cu_3O_8$ as measured by the time of flight technique [2]. Comparison with the undoped non-superconducting compound $Pb_2Sr_2YCu_3O_8$ reveals that some of the modes show considerable differences between the two compositions. Phonon anomalies have been observed in other superconducting systems giving evidence for a large electron-phonon coupling strength localized on the oxygen "breathing modes". The mechanism for superconductivity and its relationship to this strong electron-phonon coupling remains controversial.

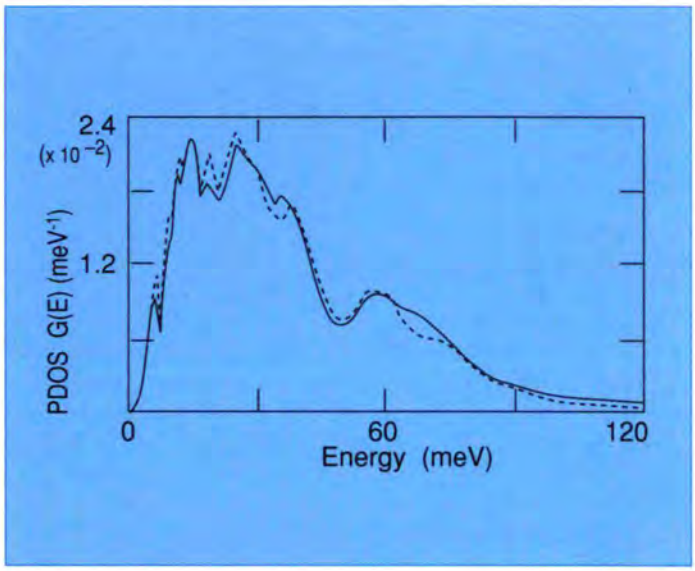

Fig. 10: Generalized phonon density of states for $Pb_2Sr_2Y_{1-x}Ca_xCu_3O_8$ at 300K: x = 0.5 (solid line); x = 0.0 (dashed line).

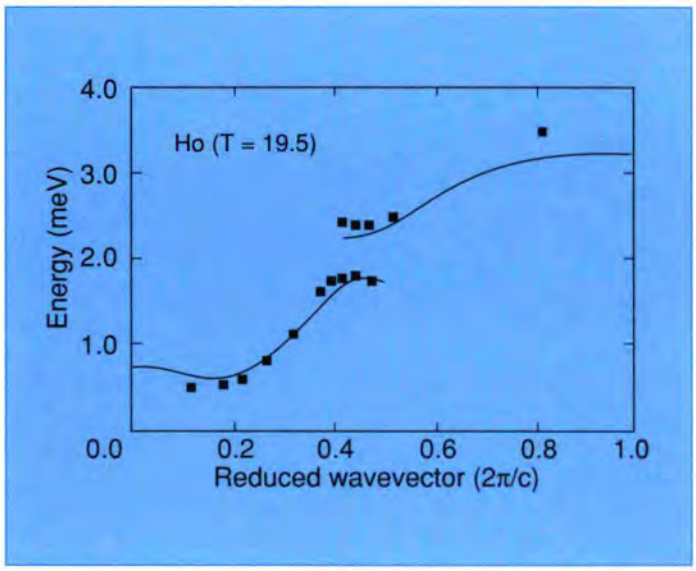

Fig. 11: The spin-wave dispersion relation along (00l) in holmium. The solid line is a model calculation [4].

Magnetism

Magnetic Excitations of Holmium in its Spin-Slip Phase

It has recently been established that, in its helimagnetic phase, the magnetic structure of holmium can be described in terms of a spin-slip model [3]. Below 90 K, the magnetic spiral is composed of commensurate blocks of an integer number, *b*, unit cells of the low temperature cone structure separated by a regular array of discommensurations or spin-slips. As a consequence of this structure, energy gaps are expected to occur in the spin-wave dispersion relation [4]. Figure 11 shows measurements of the dispersion relation made on IN12 [5] for the single spin-slip (b = 11) case where a gap of about 0.5 meV is expected and indeed observed for q = 5/11. The spin-wave dispersion relation can be seen to be in good agreement with a model calculation by Jensen [4].

Valence Transition in $YbInCu_4$

$YbInCu_4$ shows an unusual temperature driven valence transition analogous to the γ–α transition in cerium. Bulk measurements [6] show that, in this system, ytterbium is trivalent at high temperatures. On cooling the compound undergoes a first order transition at 45 K to a mixed valence state where the ytterbium moment is almost completely compensated. This change in valence state has a dramatic effect on the magnetic excitation spectrum as the measurements from IN4 in Fig. 12 show [7]. The lower frames of the figure show that above the valence transition, T = 75 K, the magnetic response is concentrated at low energies: it can be interpreted using a conventional crystal field analysis. Below the transition, T = 5 K, a very broad response in energy is observed, characteristic of many mixed valence systems.

Magnetic Excitations in $U(Pd_{1-x}Pt_x)_3$

Although inelastic neutron scattering experiments have been performed on a number of uranium metallic compounds, well-defined magnetic excitations have rarely been observed. Usually the magnetic scattering shows a broad response in energy. UPd_3 is a striking exception to this pattern of behaviour: so far it is the only actinide system in which sharp excitations have been found [8]. A systematic study of the spin dynamics of the system $U(Pd_{1-x}Pt_x)_3$ has recently been made using the spectrometers IN3, IN8 and IN14 [9], the idea being to examine the transition from the localized 5f magnetism in UPd_3 to the heavy fermion behaviour in UPt_3.

Measurements on the compositions UPd_3 and $U(Pd_{0.75}Pt_{0.25})_3$ are shown in Fig 13. UPd_3 shows a branch of excitations around 1.5 meV: with an overall dispersion of 0.5 meV (measured along the GM and GK directions). With increasing

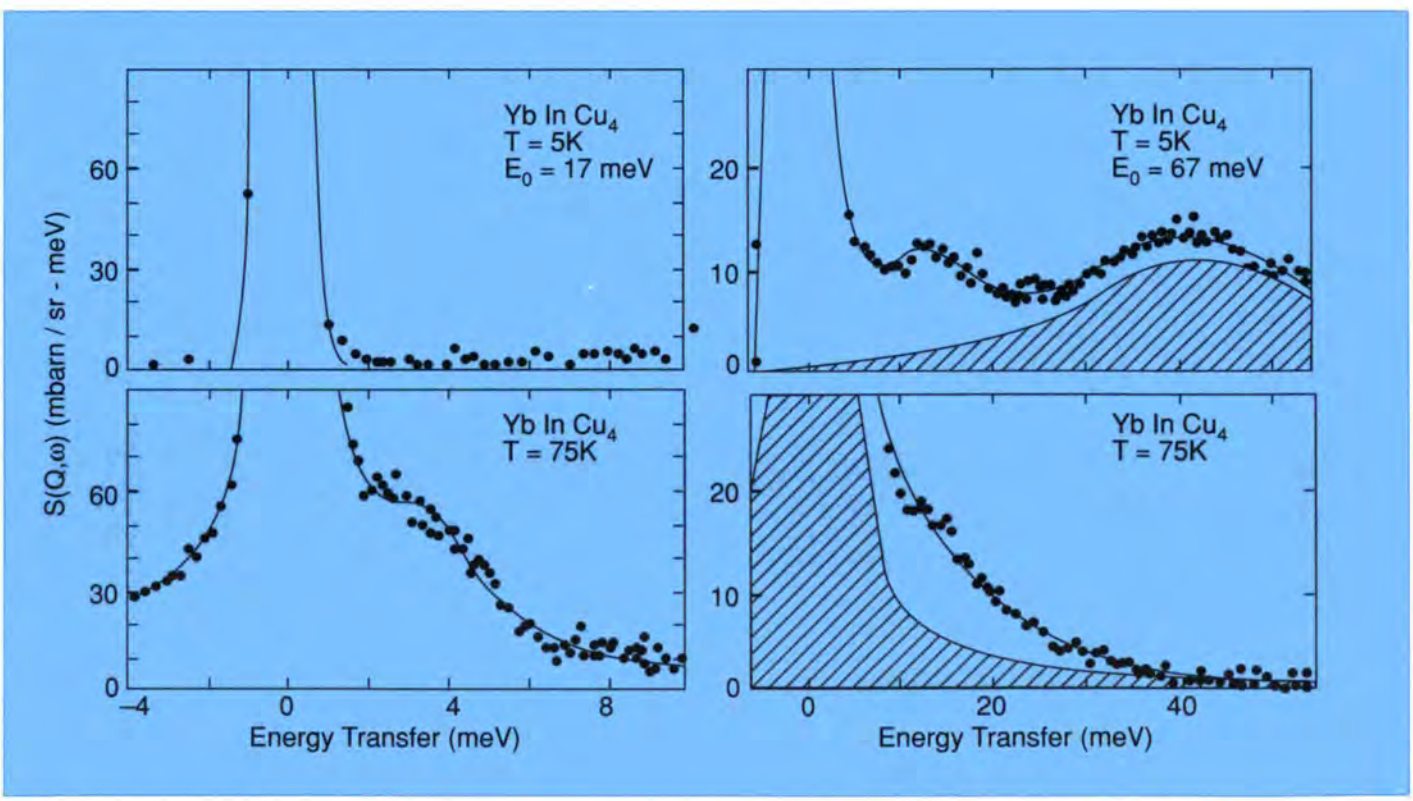

Fig. 12: Inelastic neutron spectra from $YbInCu_4$ measured on the time-of-flight machines IN4. Shaded areas represent the magnetic contribution to the scattering. The contribution from phonons has been determined by comparison with a non-magnetic reference compound $LuInCu_4$.

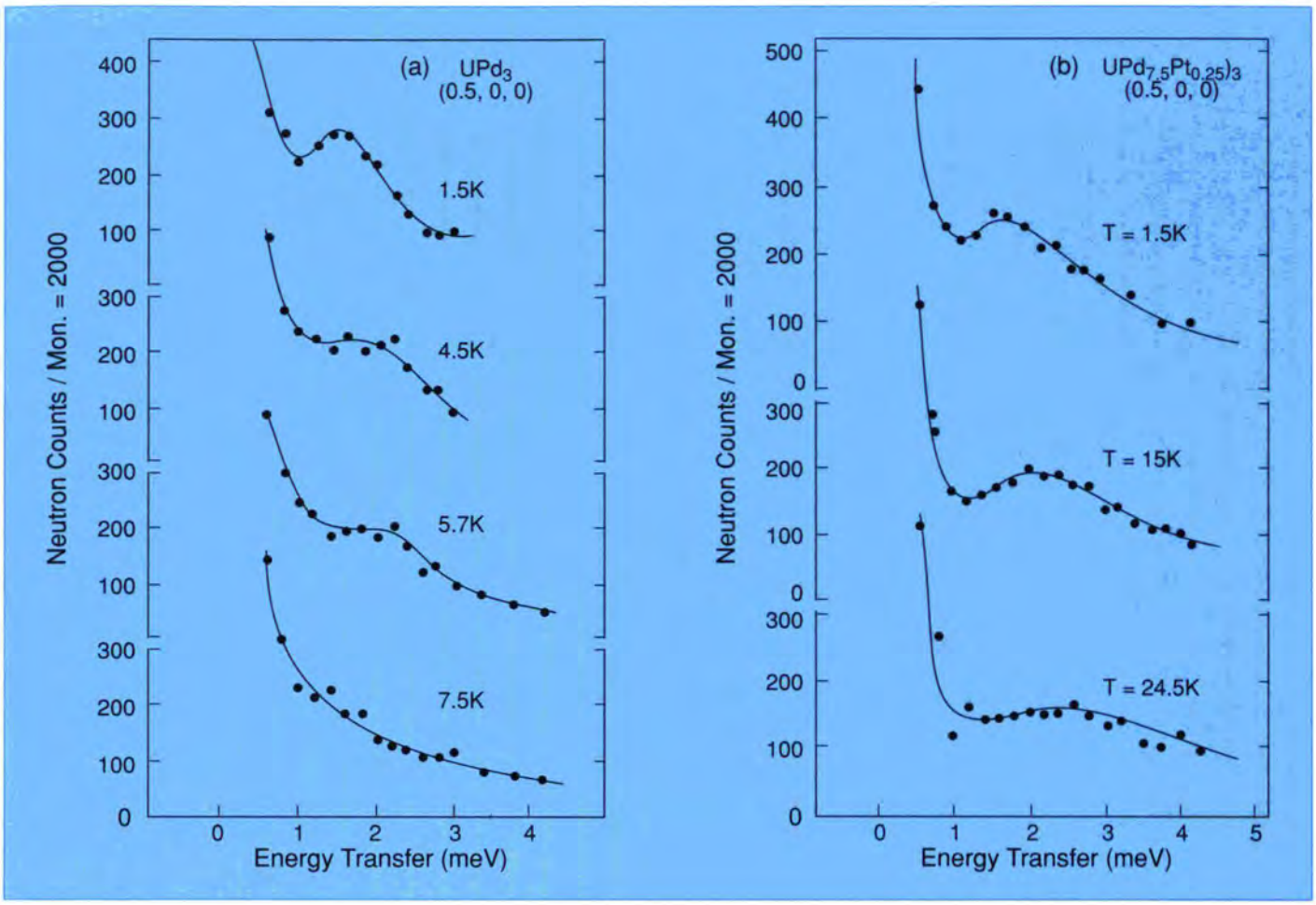

Fig. 13: The temperature dependence of the magnetic excitation at Q = (0.5,0,0) in (a) UPd_3 and (b) $U(Pd_{0.75}Pt_{0.25})_3$.

temperature, the energy of the excitations increases slightly, whilst the intensity decreases rapidly. In comparison with UPd_3, the low energy excitations in $U(Pd_{0.75}Pt_{0.25})_3$ show a much more pronounced dispersion, with the energy varying between 1.8 and 3.8 meV. Though clearly defined, the excitations are considerably broader than in UPd_3. In $U(Pd_{0.75}Pt_{0.25})_3$, the excitations can be seen to exist over a much larger temperature range than in UPd_3. From this study it was concluded that progressive substitution of Pd by Pt leads to an enhanced damping of the magnetic excitations, presumably resulting from an increasing 5f-4d electron hybridization.

Longitudinal Fluctuations in Nickel

Despite a great deal of theoretical and experimental investigation into the spin dynamics of isotropic ferromagnets, the nature of the longitudinal fluctuations below T_c has remained unclear. Inelastic neutron scattering performed with polarization analysis allows the separation of the longitudinal and transverse components of the dynamical susceptibility in a ferromagnet. In a recent experiment [10] on the polarized beam triple-axis spectrometer IN20, the magnetic excitations were measured just below T_c on a single crystal of ^{60}Ni. Figure 14 shows the non-spin flip scattering which measures the longitudinal fluctuations. The data have been corrected for non-magnetic scattering from phonons and elastic scattering from the sample and furnace. We can see that the longitudinal excitations are quasielastic in nature in the range $0.06 < q < 0.18$ Å^{-1}: in fact the longitudinal fluctuations are found to be very similar to the paramagnetic scattering above T_c. The width of the scattering is found to vary as $\Gamma \approx Aq^{2.5}$ where A = 300 meVÅ$^{2.5}$ and the integrated intensity varies as $(\kappa^2+q^2)^{-1}$ as would be expected from spin diffusion. In contrast, the transverse excitations, which correspond in a simple picture to precessions of the spins, are propagative in nature as can be seen from the insert to the central frame.

College Secretary: S. M. Hayden

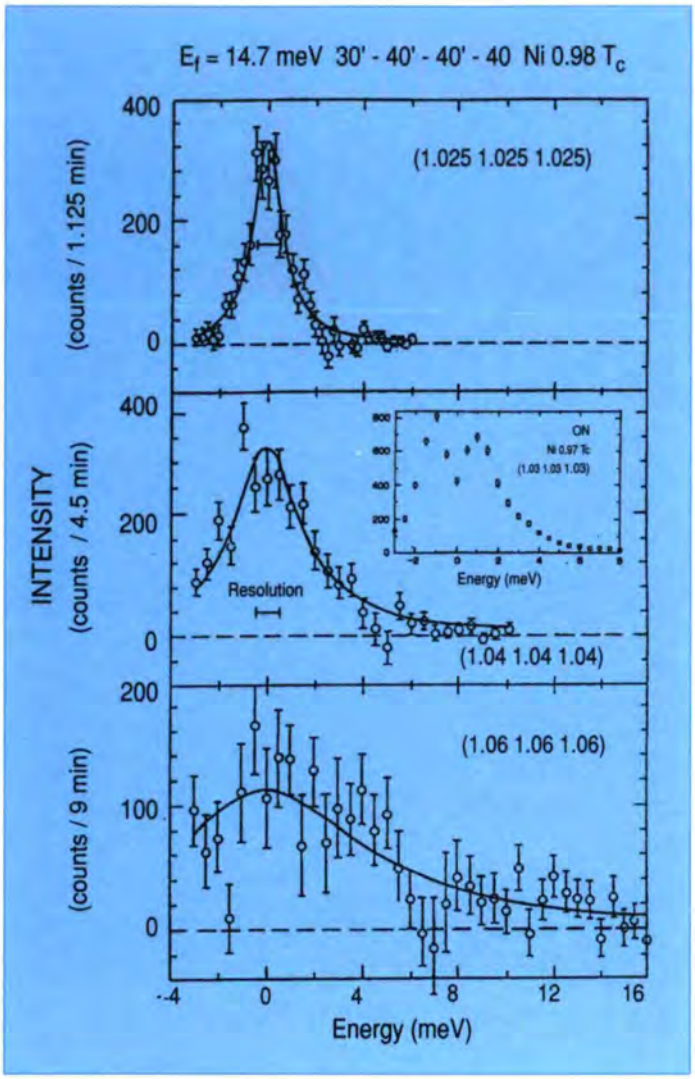

Fig. 14: The q dependence of the longitudinal fluctuations in Ni. The solid line represents a fit of a Lorentzian convoluted with the resolution function of the spectrometer. The spectra have been corrected for the finite flipping ratio of the polarized beam. Non-magnetic contributions have been subtracted from the data. The inset to the central frame shows the spin-flip scattering.

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ERRATA

A type-attribute error in the computerized typesetting of the Annual Report has caused certain formulae on pages 35 and 36 to be incorrectly printed. The correct presentations are:

- $H = \sum_{<i,j>} J_{ij}^{//} S_i^z . S_j^z + J_{ij}^{\perp} (S_i^x . S_j^x + S_i^y . S_j^y)$

- $\frac{d^2\sigma}{d\Omega d\omega} = \frac{k_1}{k_f} A(\omega) \{\delta(\omega - cq) + \delta(\omega + cq)\}$

- in the text, for Ì read ħ.

Neutron Scattering From $La_{2-x}Ba_xCuO_4$ and $YBa_2Cu_3O_{6+x}$

S. M. Hayden, C. Vettier

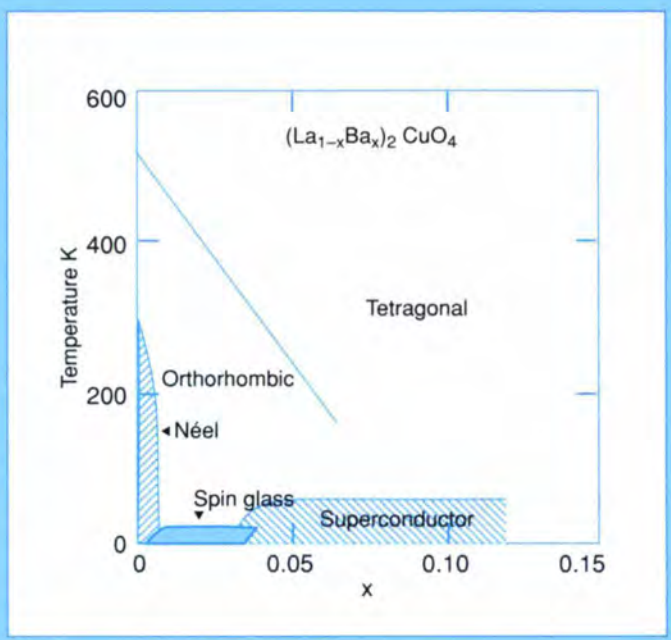
Soon after the discovery of high temperature superconductivity in the $La_{2-x}(Ba,Sr)_xCuO_4$ and $YBa_2Cu_3O_{6+x}$ systems, it was found that for some compositions the copper spins exhibit strong antiferromagnetic correlations and antiferromagnetic order [1]. These magnetic properties are very sensitive to doping: electron holes may be introduced into the CuO_2 planes either by substituting Ba or Sr for the La or by varying the oxygen concentration. Figure 15 shows the phase diagrams [2,3] of the two systems. The insulating parent compounds La_2CuO_4 and $YBa_2Cu_3O_6$ are both antiferromagnetic insulators with Néel temperatures of 300K and 415K respectively. Both systems have a layered structure with an extremely spatially anisotropic magnetic coupling between the copper spins. La_2CuO_4 consists of CuO_2 planes in which Cu^{2+} spins have a strong (intra-planar) superexchange interaction, the (inter-planar) coupling between spins in neighbouring planes is about 10^{-5} times smaller. The $YBa_2Cu_3O_{6+x}$ system has a structure which consists of CuO_2 bilayers separated by CuO planes. The Cu atoms within the bilayers are labelled Cu(2) and the non-magnetic atoms in the CuO planes Cu(1). As in La_2CuO_4, there is a strong coupling between spins in the same plane and a weaker (again about 10^{-5} times less) coupling between spins in different bilayers.

Initial investigations of the magnetic excitations concentrated on the insulating parent compounds. Thermal neutron scattering [1] showed that the coupling between the copper spins within the CuO_2 planes in both systems was extremely large (see below), however, only a lower bound could be put on its value. At ILL, a study of the magnetic excitation spectrum over a large energy range has been performed on pure La_2CuO_4 using a wide range of incident energies [4]. This study yielded a value for the spinwave velocity, $\grave{I}c = 850 \pm 30$ meVÅ at T=5K. It was found that the spin dynamics can be well described by conventional spin wave theory for energies, $\grave{I}\omega > \grave{I}c\xi^{-1}$ (ξ, the correlation length is a lengthscale characterizing the disorder in the antiferromagnetism). This description is based on the Heisenberg Hamiltonian (for the ordered state)

$$H = \sum_{<i,j>} J_{ij}^{//} S_i^z . S_j^z + \hat{J}_{ij} (S_i^x . S_j^x + S_i^y . S_j^y)$$

where $\Delta J = J^{\perp} - J^{||}$ is the anisotropy in the exchange coupling between in-plane and out-of-plane spin components. From the spin wave velocity corresponding to propagation within the CuO_2 planes, a value for the in-plane coupling constant, $J \approx J^{||} \approx J^{\perp} = 0.160(5)$eV is obtained. For high energy transfers, when we can neglect the anisotropy in the coupling between the in-plane and out-of-plane spin components, we may use the cross-section for a simple antiferromagnet

$$\frac{d^2s}{dWdw} = \frac{k_I}{k_f} A(w)\{d(w-\omega) + d(w+\omega)\}$$



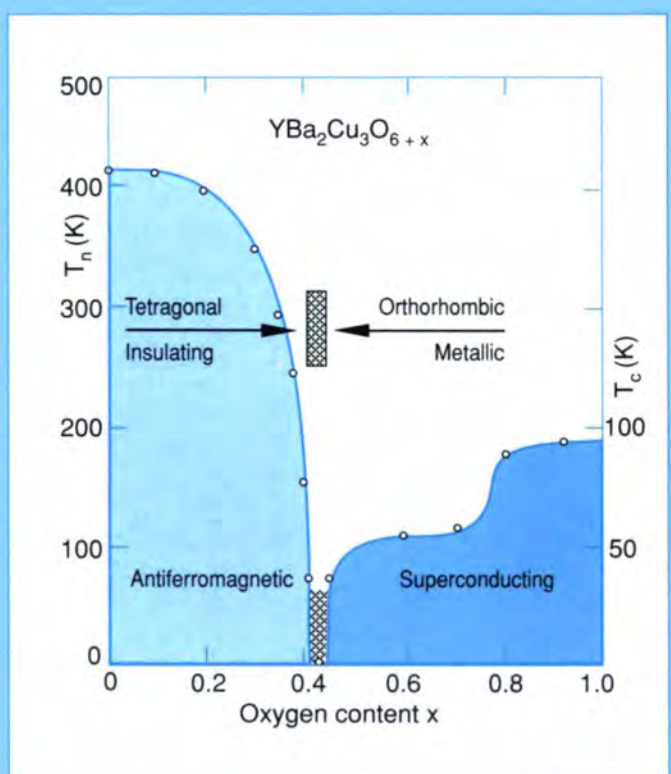


Fig. 15: Phase diagrams of the $(La_{1-x}Ba_x)_2CuO_4$ and $YBa_2Cu_3O_{6+x}$ systems [2,3]

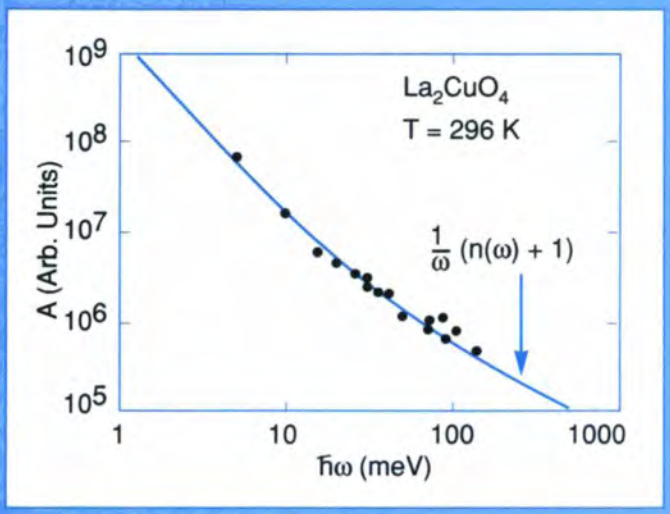


Fig. 16: Measurements of the spin wave intensity for La_2CuO_4 for a wide range of energy transfers. The solid line is the calculated intensity derived from classical spin wave theory.

Where k_I and k_F are the initial and final wavevectors respectively and $A(\omega) \sim 1/\omega \times \{1\text{-}\exp(-\grave{\imath}\omega\beta)\}^{-1}$ contains the matrix element connecting the Néel state and a one magnon state and a thermal population factor. It can be seen from Fig. 16 that spin wave theory provides a good description for the variation of the intensity for energy range investigated. For wavevectors less than the inverse correlation length, we expect spin wave interactions to cause the response to be overdamped and this is indeed observed experimentally [5]. It should be pointed out that La_2CuO_4 in its paramagnetic phase is an extremely good realisation of a two-dimensional quantum Heisenberg antiferromagnet, a system of fundamental importance in statistical mechanics.

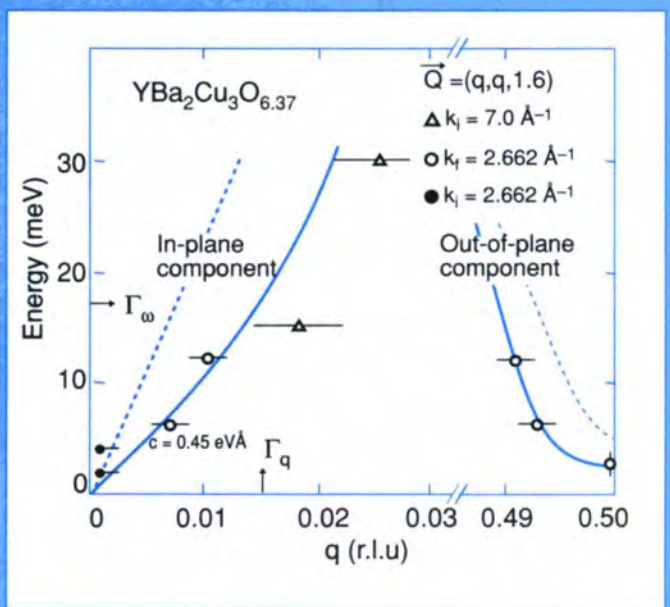


Fig. 17: Excitation energies of in-plane and out-of-plane spin components in $YBa_2Cu_3O_{6.37}$. For comparison the excitations in the undoped material (x=0.15) are shown by the dotted lines.

The spin dynamics of undoped $YBa_2Cu_3O_{6+x}$ in the ordered state has also been found to be well described by spin wave theory. In this system the in-plane spinwave velocity is somewhat larger, of order 1.0 eVÅ [3], The corresponding in-plane coupling constant, J ≈ 0.17 eV.

Of particular interest is the effect of doping on the magnetism in these systems. A systematic study has recently been performed on the $YBa_2Cu_3O_{6+x}$ system by varying the oxygen concentration [3]. For small x, x<0.2, the oxygen enters the Cu(1) planes and induces electron transfers only within the Cu(1) plane with little effect on the CuO_2 planes. The magnetic properties are close to those of the parent compound. With x in the range, $0.2 < x < 0.4$, a small number of holes are created in the Cu(2) planes. These holes induce static magnetic disorder within CuO_2 planes and in the magnetic coupling of the Cu(2) bilayers by creating magnetic defects (polarons). The Néel temperature and the long range ordered moment of the Cu^{2+} ions on the Cu(2) site are strongly reduced and abruptly vanish at x = 0.4. The disorder is evidenced by the appearance of finite correlation lengths, and a reentrant behaviour at low temperature. The reentrant behaviour corresponds to the transfer, at low temperatures $T<T_c$, of scattered intensity from the magnetic Bragg peaks to rods of diffuse scattering. The correlation length or distance between magnetic defects or polarons in the planes is related to the hole concentration ($n_h \propto 1/\xi^2$). Three dimensional magnetic ordering disappears when $n_h \geq 2\%$. The magnetic defects disturb strongly the propagation of in-plane spin excitations (see Fig. 17). This may be interpreted as a reduction of the magnetic stiffness. For $0.4 < x < 0.5$ larger numbers of holes are transferred into the Cu(2) planes giving rise to a metallic state and the onset of superconductivity.

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Crystal and Magnetic Structures

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Introduction

In 1989, visitors and ILL scientists again collaborated in a larger number of increasingly difficult experiments. Attempts to routinely reach higher pressures and temperatures were not always successful. As the time per experiment decreases, the need for more reliable furnaces, pressure cells and cryostats places much strain on limited resources. Position sensitive detectors have become standard equipment on many instruments and a new generation of data-treatment programs has emerged. The Cryopad for analysis of polarization is under intensive development and is in regular use (see Diffraction Group report). D20 is fully scheduled and is finding increasing use for many experiments broadly classified as engineering science, as are D1A and D1B. However, a purpose-designed materials diffractometer is seen as the only way to satisfy demand.

At the Allevard get-together of scientists, many College members were involved in proposing new diffraction instruments for the ILL in the context of a possible "Troisième Souffle". These included a quasi-Laue diffractometer for medium-sized unit cells ; materials-science diffractometers for studies of stress and preferred orientation ; a thermal neutron flat-cone diffractometer with polarization analysis ; use of a high-resolution position-sensitive detector for quantitative neutron topography; and the Steichele very high resolution time-of-flight powder diffractometer. Other topics discussed included stroboscopic measurements, improvements in monochromators, and a substantial increase in investment in position-sensitive detectors.

There is much interest in the development of a ^{3}He filter: the aim is to build high-efficiency polarising transmission filters adaptable to a variety of instruments.

Pressure to study high T_c materials has not abated: good proposals were rejected on both single-crystal and powder diffractometers in a fast-moving field.

Members of the College are actively involved in preparing Microsymposia and Satellite Meetings in conjunction with the 15th I.U.Cr. Meeting to be held in Bordeaux in July 1990.

Scientific Highlights in 1989

Crystallography of Non-Magnetic Systems

Complementary synchrotron/neutron studies

Following the development of very high-resolution powder diffraction machines on synchrotron sources, much attention has focussed on the possibilities offered by complementary synchrotron radiation/neutron studies. One typical application has been the ab-initio structure determination of sodium methyl ($NaCD_3$) from powder diffraction data collected on 9.1 at the synchrotron source at Daresbury (UK) and on D1A and D2B at the ILL. The Na and C positions of this interesting structure were determined by direct methods from the synchrotron data followed by location of the D atoms from the neutron data sets.

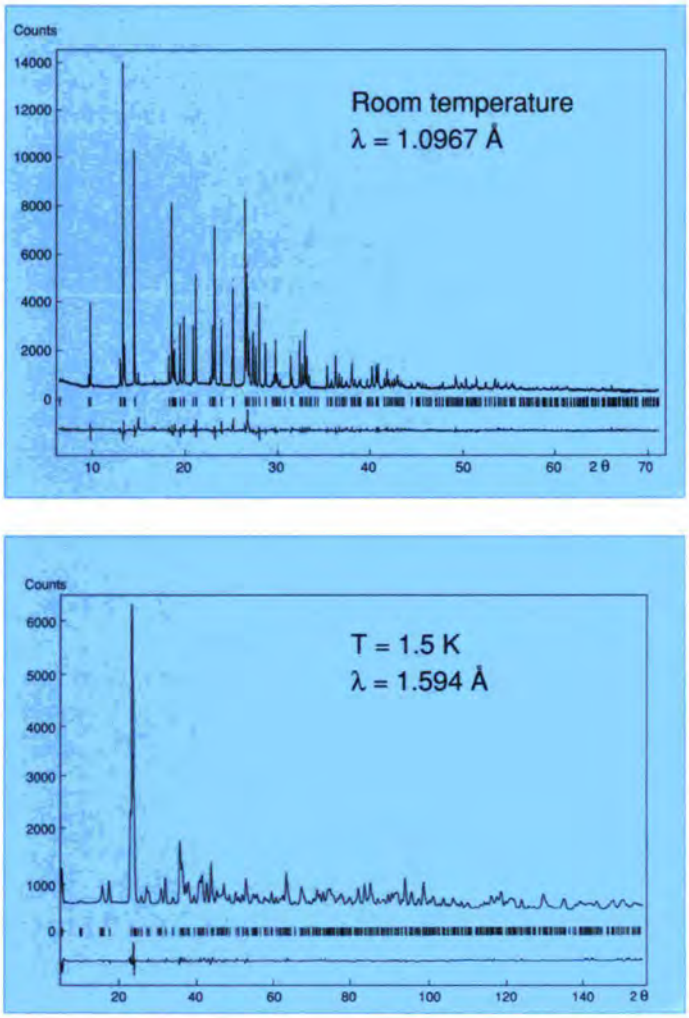

Fig. 18: Synchrotron (top) and neutron diffraction (bottom) patterns of $NaCD_3$.

The advantage of using the two techniques in combination are clear: the much higher resolution available (see Fig. 18) from the synchrotron data set enabled the unit cell, space group, and heavy atom positions to be determined unambiguously with the neutron data producing the best atomic coordinates for all of the atoms. (Collaboration with the Universities of Hamburg and Keele).

Agostic interactions

The first example of a main group intermolecular agostic interaction has been fully characterized by single crystal neutron diffraction using D19. The very air sensitive complex $[MgR_2]$ where R = $\{CH(SiMe_3)_2\}$ forms a polymeric type of structure in the solid state in which these weak interactions run from the Mg atom of one molecule through the methyl group hydrogen and carbon atoms of an adjacent molecule. Short Mg...H intermolecular separations of 2.333 and 2.414 Å are observed with concomitant distortions in the geometry of the agostic methyl group. The angles Si-C...Mg, 172° and C-Mg-C, 140° from preliminary X-ray work, suggested a possible molecular association in the solid state, rather than such distortions arising simply from packing effects. However accurate location of all hydrogen atoms was required to quantify the hypothesis. (Collaboration with Universities of Brighton and Bristol).

Dyotropic rearrangement

The thermal dyotropic (intramolecular group transfer) rearrangement process is of fundamental interest and yet hitherto there are no reports of the ground state structures of either isomer, A or B, (Fig. 19). Model calculations give short separations (2.92 Å) between the 'double' bonds and suggest a very small hydrogen nuclear displacement accompanying the transfer. The X-ray data for A show a separation of greater than 3 Å which is thought to be a consequence of the Woodward-Hoffmann symmetry rules by which the close approach of two parallel double bonds is part of a process, which in the electronic ground state is symmetry forbidden and therefore associated with extra non-bonding repulsions. To alleviate this, a shift of π-electron density from the exo to the endo-side of the norbornene moiety is expected and also a substantial pyramidalisation of the sp^2 C atoms. The single crystal study of A, where R^{1-4} = Cl, and R^{5-6} = H, (Fig. 20) (using neutron diffraction data measured on D19) shows distinctly different C... H(C) separations of 2.440 and 2.362 Å, with C...C greater than 3 Å (3.079 and 3.105 Å respectively.) There is an out of plane shift, i.e. a pyramidalisation at C(13) and C(14), of 0.04 Å, corresponding to an interplanar angle of 1.8 degrees. Accurate knowledge of the hydrogen atom positions will allow correlation between the kinetic, structural and theoretical data on these molecules, of which we now have several examples, with varying R, R' groups, since the rate of the π-switching process seems highly dependent on these substituent R groups. (Collaboration with University of Bristol).

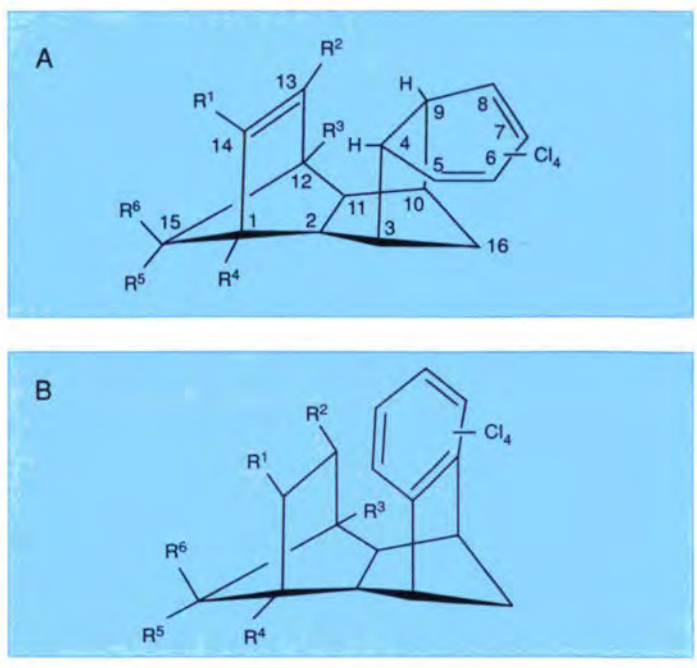

Fig. 19: Isomers of a norbornene derivative.

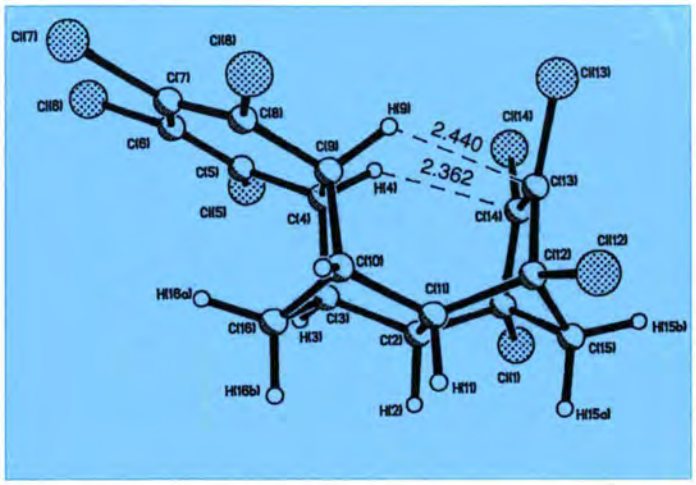

Fig. 20: Structure of isomer A.

Pressure effects on the structure and T_c of the new superconductor $YBa_2Cu_4O_8$

The 90 K superconductor $YBa_2Cu_3O_7$ has several practical disadvantages, including the ease with which it can lose oxygen and the twinned nature of the crystals. A more stable phase, $YBa_2Cu_4O_8$, with double CuO-chains can be made under oxygen pressure (Fig. 21). This material is not normally twinned (though like $YBa_2Cu_3O_7$ it is orthorhombic) and the chain oxygen cannot easily be lost because this would leave planes of copper in contact.

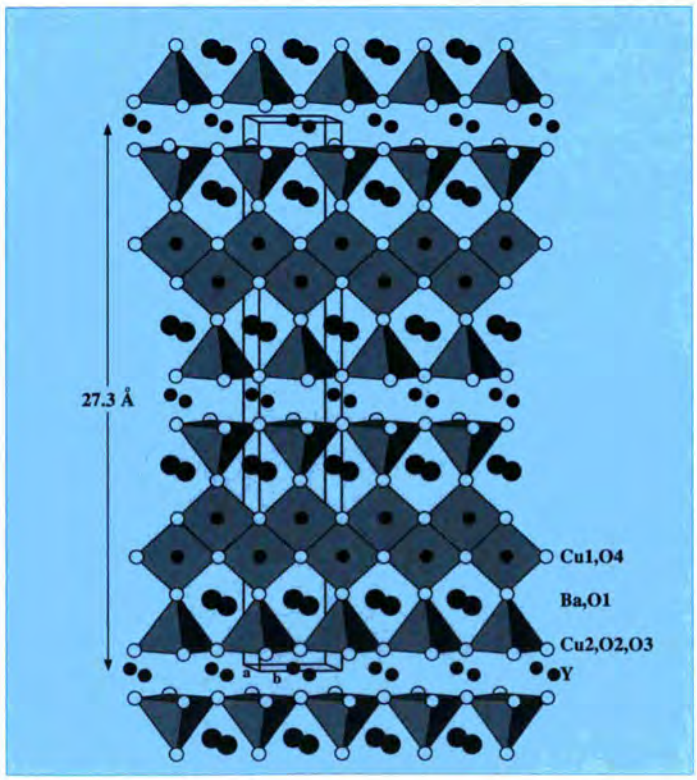

Fig. 21: Structure of $YBa_2Cu_4O_8$ showing the double CuO chains.

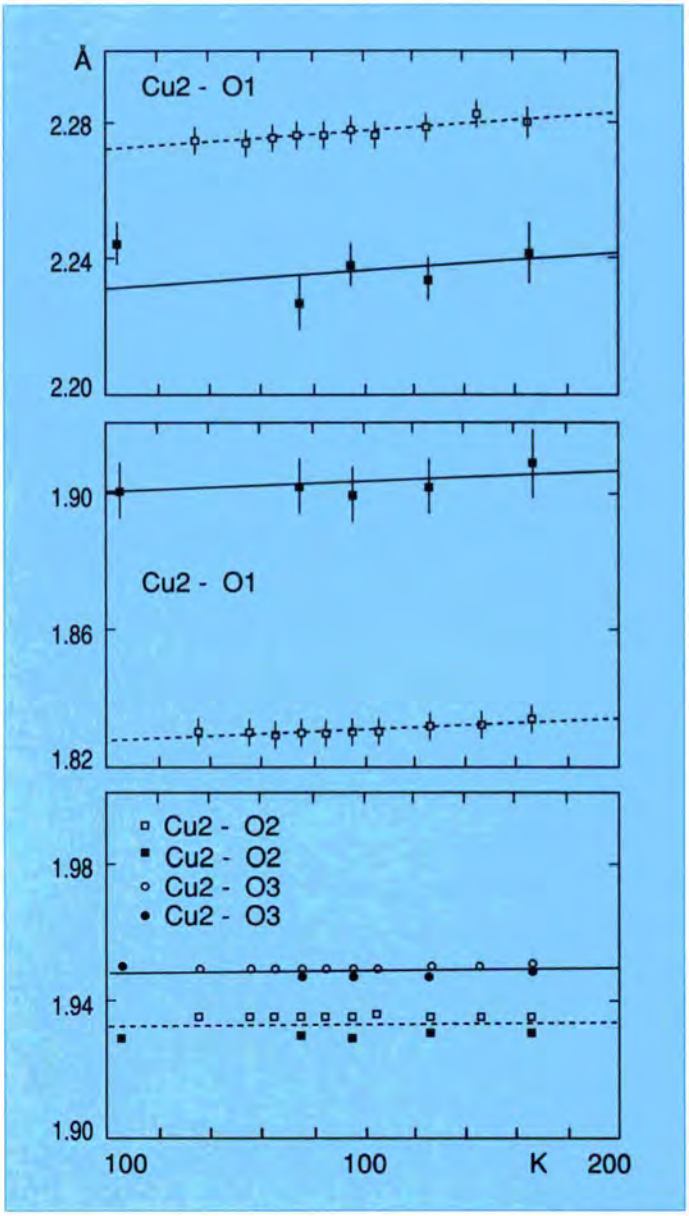

Fig. 22: Cu-O distances in $YBa_2Cu_4O_8$. The solid points are at 10 kbar, and show that the bridging oxygen O1 moves towards the Cu2-planes, and away from the Cu1-chains with pressure and increasing T_c.

T_c increases strongly with applied pressure, so that even with the relatively low pressures possible with neutron powder diffraction, T_c can be increased by 5.5 K by applying only 10 kbar. Kaldis et al. [1] have therefore been able to use neutron powder diffraction to measure the detailed changes in the Cu-O bond lengths as pressure (and T_c) increases. This is a particularly clean experiment, since no extra oxygen or other dopants are added.

It is remarkable that the only structural feature that really changes with pressure is the position of oxygen O1 bridging CuO-planes to CuO-chains. Just as oxidising $YBa_2Cu_3O_{7-x}$ to increase T_c causes O1 to move closer to the CuO-planes [2], pressurising $YBa_2Cu_4O_8$ to increase T_c produces a similar effect on the structure !

Figure 22 shows that the bond length Cu2-O1 is strongly reduced with pressure (solid points), while Cu1-O1 is correspondingly increased. This is not the result of the compressibility of the structure, which is relatively small. The Cu-O distances within the planes and chains are reduced by only very small amounts by such a low pressure.

Applying the ideas of Bednorz and Müller, pressure is seen to increase the number of electron holes (Cu^{3+}) on the CuO-planes (with a corresponding reduction on the double CuO-chains). Since this is the only obvious structural change, Kaldis et al. linked it directly to the increase in T_c.

Similar effects of pressure have also been obtained by the Zürich-Grenoble team with $YBa_2Cu_3O_{6.5}$ and the 123-124 mixed layer superconductor $Y_2Ba_4Cu_7O_{15}$, but in the original $(La,Sr)_2CuO_4$, Howard et al.[3] have not yet been able to confirm such changes in Cu-O distances with pressure.

Thus in both $YBa_2Cu_3O_7$ and $YBa_2Cu_4O_8$, the CuO planes appear to be mainly responsible for superconductivity, but the CuO chains also appear to play an essential rôle, as "charge reservoirs", controlling the electron hole concentration on the planes, and hence T_c.

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Three-dimensional display of single-crystal reflections

One of the most significant recent advances in single-crystal neutron diffractometry has been the implementation of 2-D position-sensitive detectors. The first detectors (e.g. that on D19) were relatively large, being intended primarily for measurement of a large number of Bragg reflections simultaneously. There was little interest in the local details of the reflection, partly since it was usually the integrated intensity of the reflection that was sought, but also partly because methods to display and inspect the 3-D array of counts about each reflection were not available. However, with the advent of small position-sensitive detectors (e. g. those on D9 and D15), and as development of the integration algorithms for the large detectors proceeded, the need for display programs to inspect the local details of Bragg reflections and to assess the effectiveness of the integration algorithms became apparent.

The display of a 3-D count distribution is not a straightforward task. The first programs reduced the local 3-D array around each reflection to a 1-D profile of the intensity as a function of the crystal rotation ω as would be observed with a single detector. Much information may be lost in this way, since the location of the peak within each frame, denoted here by $\Delta\gamma$ and $\Delta\nu$ is unknown (here γ corresponds to the horizontal direction in the plane of the detector and ν to the vertical direction). An improvement on the 1-D profile is display of the projection of the distribution onto the $\Delta\omega$-$\Delta\gamma$ plane as a surface or contour plot. Since the surface plot displays all visible counts of the projection it is particularly advantageous for revealing subtle features in the tails of peaks, as illustrated by the scan in Fig. 23 through three incommensurate magnetic reflections of $TlFeCl_3$. Details perpendicular to the $\Delta\omega$-$\Delta\gamma$ plane are still unresolved in this projection.

The shortcomings of these methods have led to development of an algorithm based on the DISSPLA library, which combines the 1- and 2-D projections with a representation of the 3-D distribution by wireframe contouring similar to that used to display electron-density distributions in protein model-building programs. The principal features of this display are shown in Fig. 24. The scan is represented by a 3-D box with edges along ω, γ and ν. The 3-D wire-frame contour is set typically to 10% of the maximum count. The projections onto all three planes $\Delta\omega$-$\Delta\gamma$, $\Delta\omega$-$\Delta\nu$ and $\Delta\gamma$-$\Delta\nu$ are also plotted, as well as the 1-D profile in ω, since this is usually the direction of best resolution. The following examples illustrate some of the advantages that 3-D display of single-crystal reflections can offer.

The presence and form of twinning can be more quickly determined in the 3-D display of the count distributions. Fig. 24 shows one of the first scans from an uncharacterized crystal of twinned orthorhombic $Ba_2YCu_3O_7$. From prior knowledge of the twinning pattern in this compound, the groups of

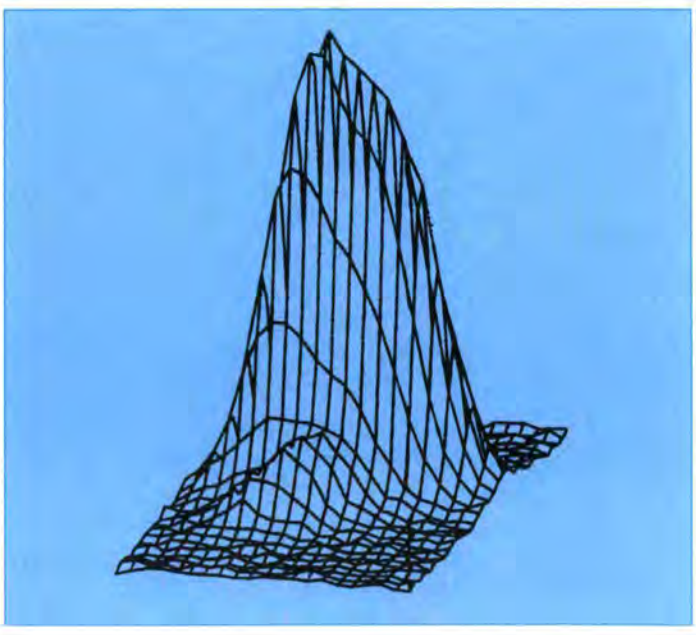

Fig. 23: Projection onto the $\Delta\omega\Delta\gamma$ plane of the three overlapping incommensurate magnetic reflections near the $^1/_3, ^4/_3, 0$ reciprocal lattice point of $TlFeCl_3$.

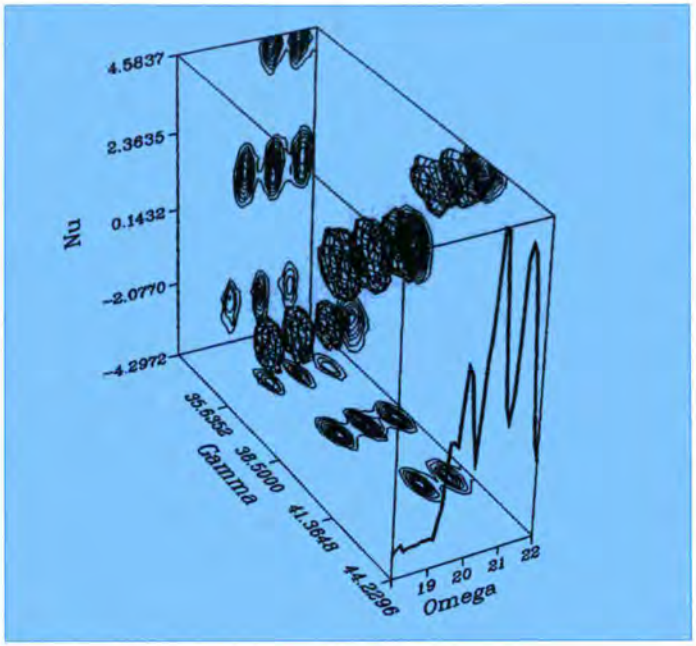

Fig. 24: 3 - D plot of a scan through a number of twinned reflections of orthorhombic $Ba_2YCu_3O_7$.

reflections could be immediately identified as being of the type hhl (only three spots are observed compared to the four expected for general hkl reflections), and the direction of the short c* axis determined. (Collaboration with CEN Grenoble).

Investigation of second-order phase transitions where a suitable order parameter is related to the cell parameters can be greatly aided by 3-D display and analysis of the reflections as a function of the external influence. This is particularly true if the direction of greatest sensitivity to the order parameter is not perpendicular to the crystal rotation axis. For example the heavy fermion compounds $ReCu_6$ (Re = Ce, Pr, La) undergo a transition from orthorhombic to monoclinic Bravais symmetry as the temperature is decreased, which leads to a two-fold splitting of reflections parallel to the a*c* plane. Unless the crystal is mounted with b* along the rotation axis the 1-D scan profile will not be so sensitive to the orthorhombic strain. The 3-D distributions (Fig. 25) however do reveal clearly the change in strain, and could be fitted to give a reasonable estimate of the transition temperature. Another advantage is that the individual intensities of the two peaks can be determined much more easily than with a single detector count array. (Collaboration with Argonne National Laboratory).

Zircon and zirconia at high temperatures

In collaboration with the Institut für Kristallographie and Mineralogie München, a mirror furnace, adapted from the kind used in a space-lab mission, was tested on the high-resolution powder diffractometer D2B and the four-circle diffractometer D19.

In both cases temperatures in the range of 2000 K were accessible.The furnace uses the geometrical properties of a rotational ellipsoid by positioning the sample at one focal point, and the halogen lamps used as heating elements at the other, thus ensuring that all the emitted light is reflected onto the sample. Two of these ellipsoidal mirrors are joined together with one common focal point as the sample position (see Fig. 26).

The furnace can be cooled by a small 10 litre closed-cycle cooling device and needs no special electrical power supply. At the moment the sample is in air but a special gas environment is foreseen. On D2B the monoclinic-tetragonal phase transformation in undoped zirconia (ZrO_2) was followed between 1100 and 1850 K.

The data obtained allowed two-phase Rietveld refinements in the coexistence region.

On D19 a natural single crystal of zircon ($ZrSiO_4$) containing alpha emitters like uranium and thorium which create fission tracks within the material leading to a highly disordered structure was annealed by heating up to 2000 K.

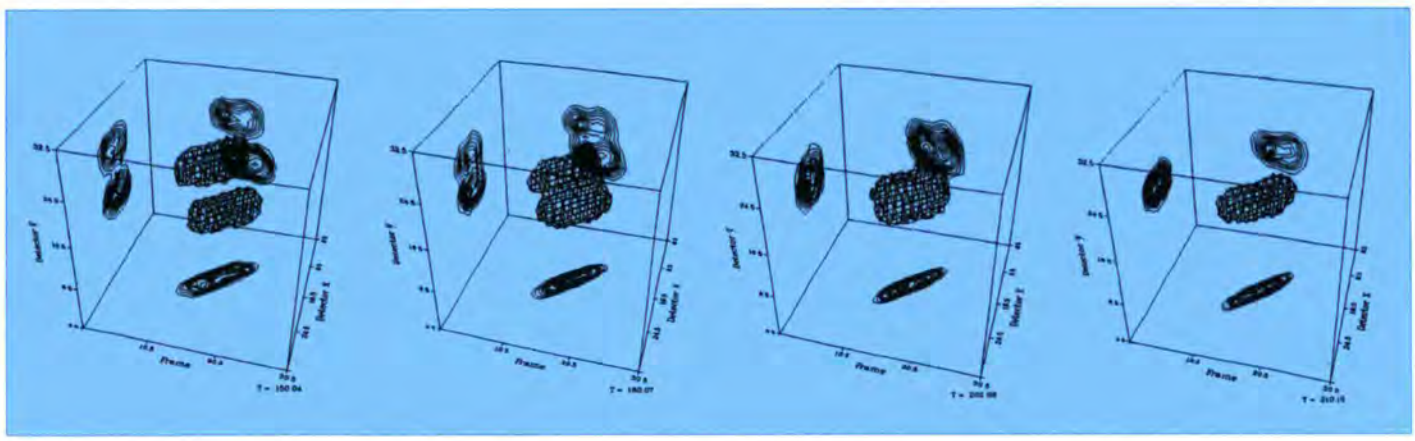

Fig. 25: Scans through the 800 reflection of $PrCu_6$ as a function of temperature. The transition between the orthorhombic and monoclinic lattices occurs at 207 K.

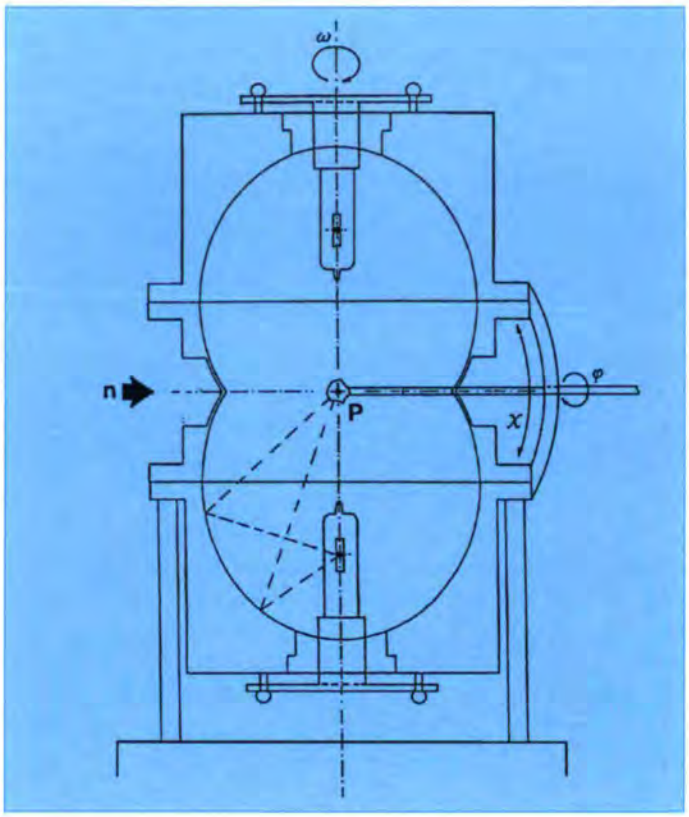

Fig. 26: Schematic drawing of the Munich mirror furnace.

On stress

The service properties of a workpiece manufactured by metal-forming processes are greatly influenced by the residual stress inherent in the material. These residual stresses are caused by local differences in strain, which due to geometrical conditions can be influenced by the tool design. X-ray scattering is commonly used to determine the residual stress state, however due to the high absorption of X-rays the method is limited to the near surface region. As a non-destructive method, neutron diffraction supplies information on the stress in the interior of the material.

Deep drawn brass cups were investigated using the so-called $\sin^2\psi$ method on D1A where the d_{hkl} spacings of the lattice plane are measured under different ψ angles. ψ is the angle between the surface normal and the scattering vector. In a d_{hkl} *vs* $\sin^2\psi$ diagram a linear curve provides the possiblity to calculate the stress directly: in contrast to other methods the exact value of the d-spacing in the stress-free state does not have to be known. A tensile stress of about 180 MPa was calculated from the appropriate plot. As the intensities of the different $\sin^2\psi$ values show about the same value a strong texture of the material can be excluded. It was found that the tangential residual stress decreases greatly from tension to compression on going from the outer to the inner surface of the cup wall. The comparison of two measured cups with different punch radii gave information about the crack corrosion behaviour. (Collaboration with Stuttgart).

Crystallography of Magnetic Systems

Structural phase transitions and three-dimensional magnetic ordering in Nd_2NiO_4 oxide

Neutron diffraction on polycrystalline samples of stoichiometric Nd_2NiO_4 shows complex structural and magnetic behaviour as a function of temperature. The room temperature (RT) phase is orthorhombic (Bmab) and Ni^{2+} ions are 3-D antiferromagnetically ordered ($T_N \approx 320$ K), with a propagation vector k = [100] and spins oriented parallel to the propagation vector i.e. along the a axis. The magnetic structure can be described as a g_x mode (Shubnikov group $B_pm'ab'$). The conditions ruling the existence of the magnetic reflections for mode g are: h = 2 n, k and l odd or h = 2 n+1, k and l even. In all other cases the magnetic intensity is zero. With this structure the first and most intense reflection is (011) as is observed (see Fig. 27). In contrast with the case of La_2CuO_4 whose magnetic structure is described by the mode g_ya_z ($a_z \approx 0$, $B_pm'a'b'$), in Nd_2NiO_4 the spin direction coincides with the tilt axis of Ni octahedra, as in La_2NiO_4. The origin of this magnetocrystalline anisotropy could be either dipolar or result from single ion anisotropy. The magnetic moment for Ni^{2+} is 1.57 μ_B at 160 K. The system undergoes a structural phase transition from orthorhombic to tetragonal ($P4_2/ncm$) at $T_1 \approx 130$ K. The tetragonal phase allows the existence of a ferromagnetic component along c axis in the Ni^{2+} spin structure, the magnetic structure can be described either as a $g_xc_yf_z$ mode (Shubnikov group Pc'c'n) or as a $g_x+c_y\ f_z$ mode (Shubnikov group $P4_2/nc'm'$). The effect of this structural transition on the magnetic structure is the appearance of a ferromagnetic component along the c axis. The spin structure changes as indicated by the decrease of I_{011} going down from 170 to 70 K. The ferromagnetic component created at 130 K is allowed for the one dimensional representations of Pccn and $P4_2/ncm$ with basis functions: $g_xc_yf_z$ and $g_x+c_y\ f_z$. The notation g_x+c_y means that x and y spin components are coupled so that $|s_{ix}| = |s_{iy}|$. Neutron powder diffraction is unable to distinguish between these two possibilities. However, taking into account the fact that the exchange integral between Ni atoms belonging to different perovskite slabs must be small, and considering the origin of the anisotropy to be single ion, it is very likely that the spin directions are along the tilt axis of the octahedra. As this axis is rotated by 90 degrees between adjacent planes along the c axis, the tetragonal symmetry ($P4_2/nc'm'$) for the magnetic structure is a good candidate to be the correct one.

Ni^{2+} cations polarize the Nd sublattice by a local exchange field ($J_{Ni\text{-}Nd} > J_{Nd\text{-}Nd}$). Below 70 K the intensity of magnetic reflections rapidly increases due to the Nd^{3+} contribution. At low temperature, the Nd sublattice becomes fully ordered ($T_N \approx 8$ K). The onset of the Nd magnetic order is induced by two superimposed effects. In the first stages, when $J_{Ni\text{-}Nd}$ dominates, the Nd^{3+} behave as paramagnetic cations under a strong local field. The increase of the magnetic reflections is

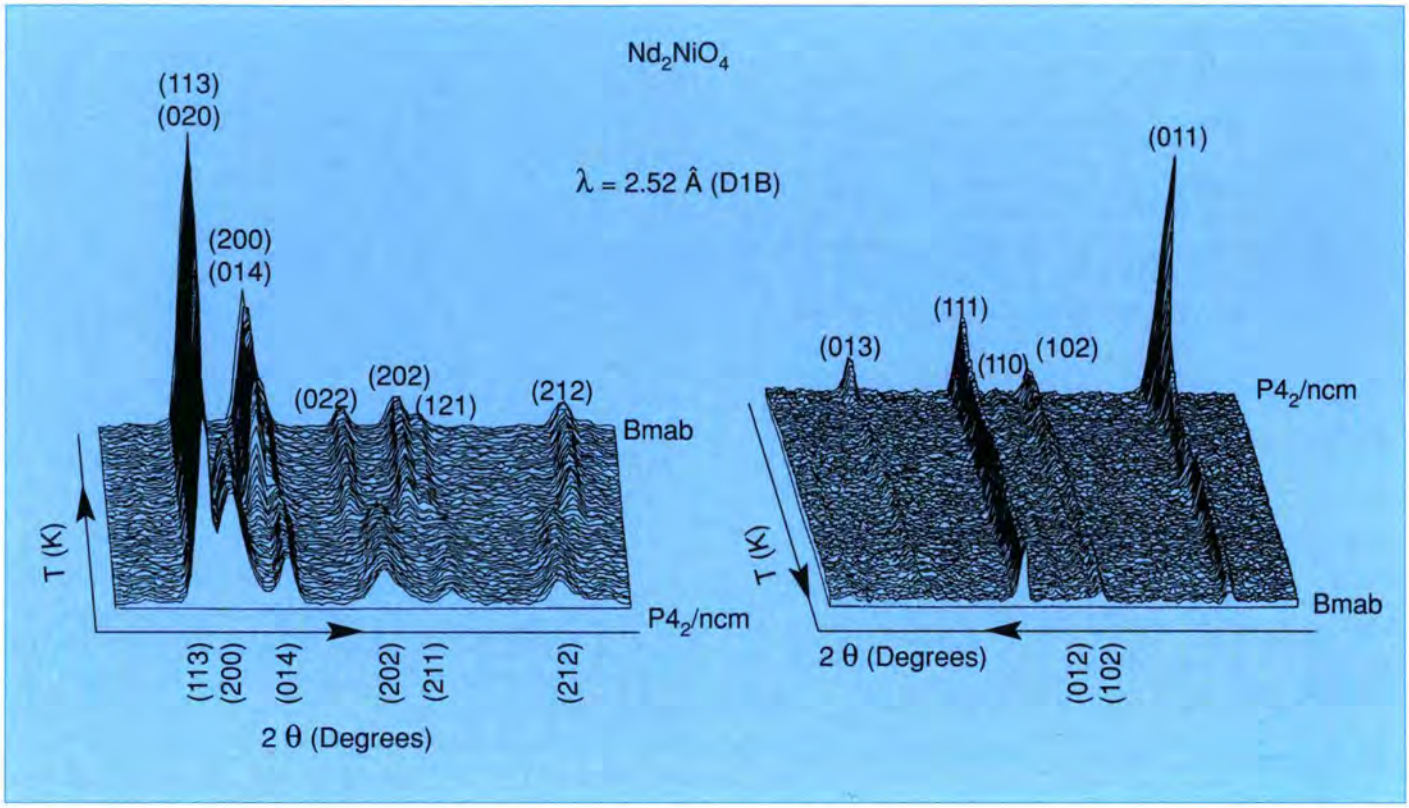

Fig. 27: 3-D plots (Intensity vs. 2θ and temperature) in stoichiometric Nd_2NiO_4. (a) Bragg peaks showing the structural phase transition at T_1 = 130 K (50 < 2θ < 70 degrees; 1.5 < T < 300 K); (b) Magnetic reflections showing the progressive ordering of Nd sublattice (20 < 2θ < 45 degrees; 1.5 < T < 300 K).

due to the Nd magnetic moment component polarized along the local field. At lower temperatures $J_{Nd\text{-}Nd}$ becomes significant and cooperative ordering is clearly observed in the temperature dependence of the integrated intensity of the (013) magnetic reflection. This reflection arises mainly from the ordering of the Nd sublattice. Another indication of Nd ordering is given by the sudden decrease of the paramagnetic scattering contribution to the background near the (011) reflection in the same temperature range. When the magnetic moment of Nd is not completely ordered, it contributes to the paramagnetic background of the diffraction pattern. As the magnetic moment becomes three dimensionally ordered, this contribution disappears and below T_N the background decreases.

The details of the thermal evolution of I_{011} are perfectly reproducible with different stoichiometric samples, but their meaning with respect to spin arrangements of Nd and Ni has not yet been analyzed in the full temperature range.

The refined magnetic moment for Nd^{3+} is 3.2 μ_B at 1.5 K, which is close to the free ion value ($\mu = g^J$, for a ground state $^4I_{9/2}$) of 3.27 μ_B. The projection of the Nd moment along the c axis implies an angle of 19.2 degrees. The low temperature magnetic structure of the Nd sublattice belongs to the same Shubnikov group (either Pc'c'n or $P4_2/nc'm'$) as the Ni one. (Collaboration with Univ. Complutense, Madrid).

Unusual magnetism of copper-chromium spinels

The unusual high Curie Temperature (370 K - 430 K) of the copper-chromium spinels of type $CuCr_2X_4$ (X = S, Se, Te) and their low total net spin of ≈ 5μ_B per mol stimulated neutron diffraction studies using D2B and D1B in its polarized neutron mode. Surprisingly it was found that copper stays monovalent (no magnetic moment), that chromium is in its trivalent state, and that two different species of anions exist (X^{2-} and X^-). The free electron of the anion aligns antiparallel to the chromium spin explaining the net spin of 5 μ_B per mole $CuCr_2X_4$. The unusual high Curie temperatures in these compounds can now be explained by strong superexchange interactions via holes in the anion valence band. The position of the additional intercalated copper in $Cu_{1+x}Cr_2Te_4$ was determined from high resolution data. Polarized neutron data no longer indicated the presence of an antiparallel aligned moment, the anion holes were effectively quenched by the intercalation reaction. Quenching these holes by replacing a chalcogen by a halogen atom should prevent further intercalation of copper. The surprising existence of a compound $Cu_{1.5}Cr_2BrSe_3$ was explainable after a structure determination using D2B revealed the formation of copper clusters, formally described as $(Cu_3)^{2+}$. (Collaboration with TU-Berlin).

2-D and 3-D magnetic ordering of Er in $ErBa_2Cu_3O_x$ ($6 \leq x \leq 7$)

Following the discovery of high temperature superconductivity in $YBa_2Cu_3O_{7-\delta}$ it has been found that substitution of Y by almost all the rare-earth elements, except for Ce, Pr and Tb, does not affect the superconducting transition T_c significantly. Many of these rare-earth substituted compounds show magnetic ordering at low temperatures and the ordered antiferromagnetic state coexists with the superconducting state. Systematic investigations on the system $ErBa_2Cu_3O_x$ have revealed interesting results (Fig. 28). Magnetization, X-ray and neutron diffraction experiments showed that the suppression of superconductivity upon oxygen removal (near $x = 6.4$) does not coincide with the orthorhombic-to-tetragonal phase transition (at $x = 6.25$), but with the changes in some bonding lengths along the c direction which elucidates the role of Cu1-O chains and their coupling to the Cu2-O planes. Neutron diffraction investigations of the magnetic ordering of Er moments in $ErBa_2Cu_3O_x$ as a function of the oxygen content x in the range $6 \leq x \leq 7$ have shown that upon oxygen removal the Er moments order three dimensionally (3-D) only in the composition range in which superconductivity is observed (i.e. in coexistence), but for composition $x \leq 6.4$, superconductivity is suppressed and the Er moments order only within the (001) plane (2-D). (Collaboration with KFA Jülich and CEN Grenoble).

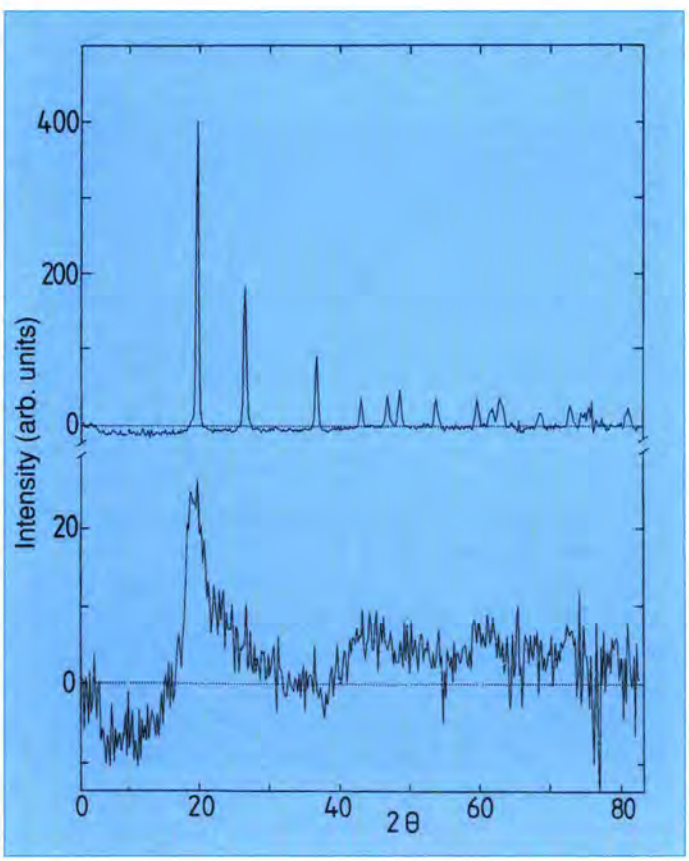

Fig. 28: Magnetic neutron diffraction diagrams of $ErBa_2Cu_3O_{6.87}$ at $T = 40$ mK (top) and at $T = 600$ mK (bottom), obtained after subtracting the nuclear scattering contribution (measured at 3 K). At 40 mK a clear three-dimensional magnetic ordering is observed whereas at 600 mK which is above T_N only two-dimensional correlation is seen.

The magnetic structures of neodymium

In a recent series of experiments we have used the high-flux powder diffractometer D20 to study the array of magnetic structures exhibited in pure neodymium as a function of magnetic field and temperature. The experiments were unusual in that they involved the use of large single crystals. By recording the multidetector diffraction patterns as a function of sample rotation, an extensive area of reciprocal space could be examined in detail.

The light rare-earth metal neodymium crystallizes into the double hexagonal close packed structure with the conventional unit cell containing four Nd atoms on two inequivalent sites of hexagonal and pseudo-cubic symmetry. In broad terms, the magnetic structures of Nd have been found to result from a subtle interplay between the RKKY interactions within and between the layers of hexagonal and cubic sites. Below $T_N = 19.9$ K, the hexagonal sites order in an incommensurate antiferromagnetic structure in which the moments are modulated by two q-vectors and at 8.3K the cubic sites order and add a further q of different length. At lower temperatures yet another series of hysteretic transitions result in changes in the lengths, directions and number of modulation vectors. In zero field, and at the lowest temperatures attained in these experiments, a general reciprocal lattice point can be surrounded by as many as 36 'fundamental' magnetic satellites, with many additional weak harmonics due to the 'squaring-up' of the moment modulation.

An early problem in the analysis of neutron scattering data concerned the unknown domain structure of the samples; for example, a hexagonal pattern of six satellites might be the result from three domains each with a single q-vector (single-q) or a single domain containing three wavevectors separated by 120° (triple-q). The solution lies in the application of a suitably oriented magnetic field (in the basal plane in the case of Nd), offset from any symmetry axis, which results in the preferential growth of one domain orientation. This technique was used in the experiments which first demonstrated the 2-q structure of the hexagonal satellites for $T > 8$K. A further motivation in the use of applied fields came from the availability of specific heat, thermal expansion and magnetostriction data as a function of magnetic field and temperature.

In the early experiments, the main area of interest concerned the structures present at low temperatures and fields. Here it was found that the structure is best described by a model in which the modulation vectors are coupled together to form a quadruple-q system, with different lengths and directions for each modulation (see Fig. 29).

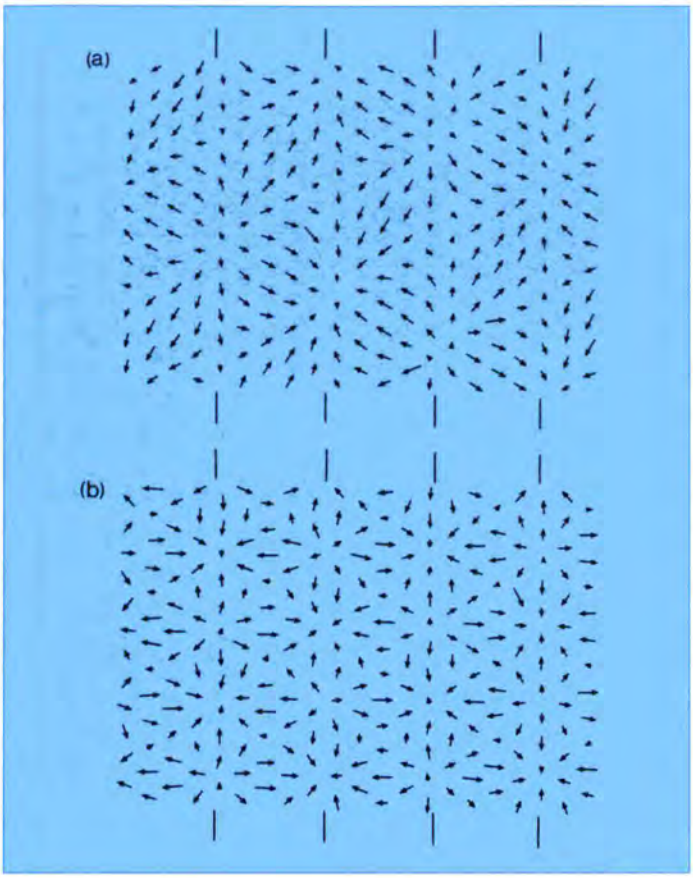

Fig. 29: A single layer of double-$\vec{q}$ structure formed: a) from $\vec{q}_1$ and $\vec{q}_2$, b) from $\vec{q}_3$ and $\vec{q}_4$. In each case the extra lines represent a repeat distance corresponding to $2\vec{q}_1$.

A companion experiment using the four-circle diffractometer D10 showed, by a rather different technique, that this is the true zero-field structure. To a good approximation, we can assign q_1, q_2 to the layers of hexagonal sites and q_3, q_4 to the cubic layers.

Why this 4-q phase exists is still not clear, but a strong clue may lie in the observation that, to within experimental error

$$\vec{q}_3 + \vec{q}_4 - 2\vec{q}_1 = 0$$

which may be attributed to a term in the free-energy expansion of the form $\mu_3\mu_4\mu_1^2$ (μ_i = the moment associated with the i^{th} q-vector), so providing the coupling energy necessary to lock together three of the four components of the quadruple-q structure.

Later experiments using D20 have investigated the magnetic structures at fields of up to 4.7 Tesla in a, b and c-directions, the latter requiring the use of the vertical field cryomagnet. As a result, we have now examined much of the neodymium B-T phase diagram, with good agreement between the positions of the various structures and the phase boundaries seen by bulk measurements.

Certainly the most surprising and spectacular finding at low temperatures was that, as the field is reduced through 4 Tesla, the structure undergoes a remarkable period doubling and redoubling (see Fig. 30). At fields of about 5 Tesla, q and its third harmonic are the only ordering wavevectors seen. At such high fields the structure is no longer quadruple-q and only a single-q structure mainly from the moments on the hexagonal sites is seen. As the field is reduced a series of subharmonics develop, until at 3.5 Tesla there are at least nine different wavevectors visible, forming a chain - an "archipelago" - stretching away from the (100) Bragg reflection. These are at q/4 and some (but not all) of its harmonics.

Qualitatively, the effect is reminiscent of the period doubling which is seen in non-linear systems approaching the onset of chaos. The underlying reason for this behaviour is not clear, but loss of order on the cubic sites with increasing fields and the single to double-q transition on the hexagonal sites with decreasing fields have both been seen to destroy the effect. It is hoped that more information about the role of interactions between the hexagonal and cubic sites will be obtained in a forthcoming D10 experiment. (Collaboration with Birkbeck College, London and University of Manchester).

The magnetic structure of erbium

The magnetic structure of erbium arises as a result of the competition between the long-range, two-ion interaction, which favours a periodic structure, and the magnetic anisotropy, which tends to align the moments along one of the crystalline directions, either in the basal plane or along the c axis. In the

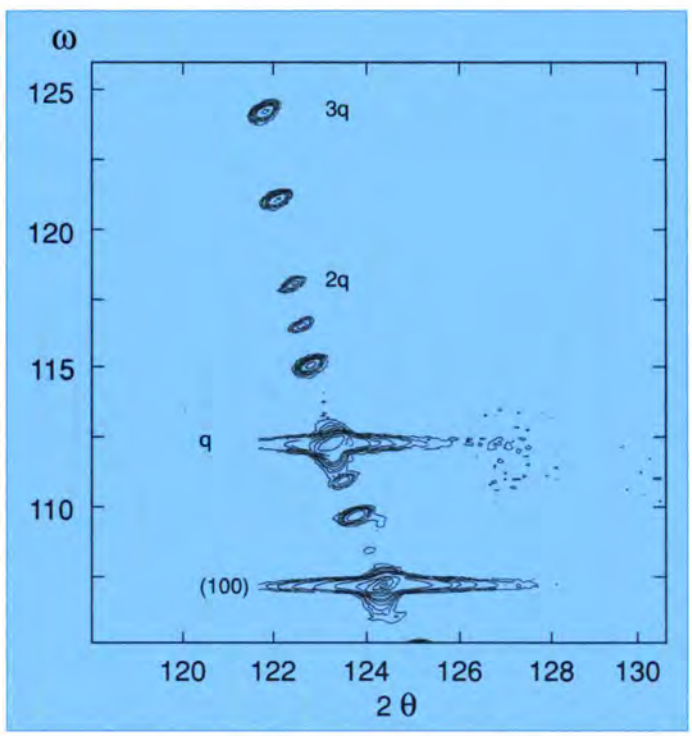

Fig. 30: Magnetic satellites near (100) in Nd at T = 1.8 K with B = 3.5 T, applied 5° from a {100} direction.

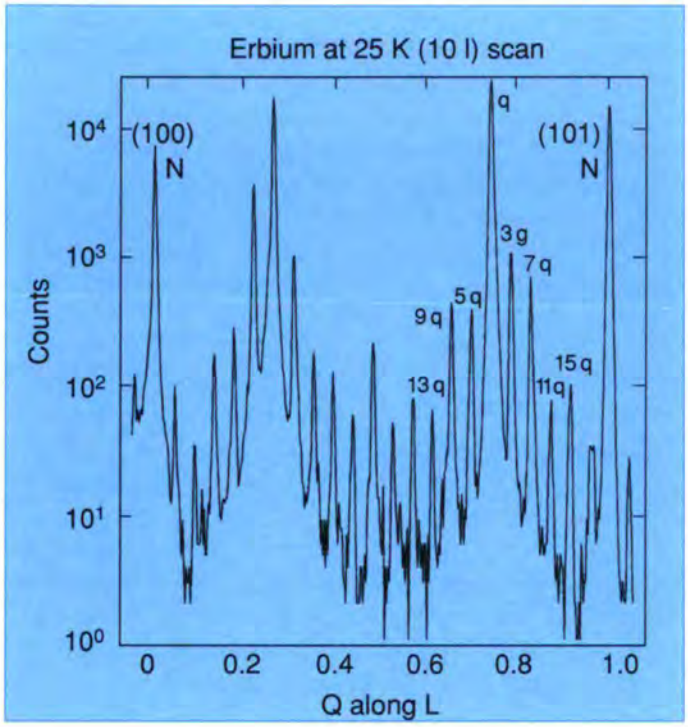

Fig. 31: A semilogarithmic plot of the intensity measured on D10 with a [10l] scan, showing the main Bragg peaks (100) and (101) as well as the associated magnetic satellites.

most complicated phase, there is a modulated moment both within the basal plane and along the c axis. This structure becomes more complex as the temperature decreases and the perturbation of the modulation by the magnetic anisotropy increases. The neutron diffraction pattern produced by such a structure exhibits a proliferation of higher order peaks (Fig. 31) caused by both magnetic scattering and magnetostrictive deformations of the lattice.

Previous investigations of the magnetic structure of erbium have been hampered by difficulties in separating all these peaks, particularly in the 00l scan which is important in this case, since it allows the magnetic structure of the basal plane to be studied in isolation. By making full use of the high resolution available on D10 we were able to identify the majority of the higher order peaks and monitor their thermal evolution, thus allowing us to refine the "spin-slip" model of the structure. However, the most interesting information can be gained from the variation of the intensities of the higher order peaks close to the transition from a modulated antiferromagnetic to a conical ferromagnetic phase (T_N = 18 K). Our measurements shed new light on the magnetic behaviour as the transition is approached. Initial evaluation of the data indicates that the modulation of the c axis and basal plane moments become decoupled as the successive commensurate spiral structures are reached (collaboration with University of Warwick).

Structural and magnetic properties of model ferromagnets

In recent years several neutron diffraction and quasielastic scattering experiments have been performed on a closely related series of ionic ferromagnets of general formula $Rb_2CrCl_{4-y}X_y$ (X = Br, I; y = 1, 2). The parent compound, Rb_2CrCl_4, is among the best characterised of all magnetic 'model' systems for the study of critical properties. The magnetic Cr^{2+} ions lie on a square lattice in well separated layers, and interact almost exclusively by near-neighbour Heisenberg superexchange. Strong single-ion crystal-field anisotropy confines the atomic magnetic moments (spins) to the basal plane. These effects cause the predominant critical properties to be those of the 2-dimensional XY model. In theory, the latter demonstrates a single phase transition caused by the unbinding of pairs of a certain type of defect in the spin structure, called 'spin vortices'. However in a system weakly perturbed by 3-dimensional coupling a conventional phase transition to a state of long range order may take place, with vortices only occurring in regions of short range order above T_c. Rb_2CrCl_4 and its derivatives, with very weak interlayer exchange coupling, may be regarded as such systems, ordering magnetically between 50 and 60 K.

Single-crystal neutron diffraction experiments on D15 have established the crystal structures of the 'mixed halides' Rb_2CrCl_3Br and $Rb_2CrCl_2Br_2$. The Br atoms occupy sites in between the magnetic $CrCl_2$ layers, and therefore barely disturb the dominant magnetic interactions. The critical properties of Rb_2CrCl_4 and $Rb_2CrCl_2Br_2$ have been studied by quasi-elastic scattering on D10, in experiments which could be closely compared. Magnetic critical scattering in these quasi-2-dimensional compounds takes the form of 'rods' perpendicular to the layers. Near T_c, the rod width and intensity was found to vary periodically with wavevector. A mean-field analysis showed this to be a result of the weak 3-dimensional coupling and led to accurate estimates of the 3-D superexchange, which was found to be a factor of 4 higher in $Rb_2CrCl_2Br_2$. Crossover to a region of 2-D critical scattering occurred above T_c, but with the 3-D critical regime being predictably larger for $Rb_2CrCl_2Br_2$. However the ratio of T_c to near-neighbour exchange was found to be insensitive to the magnitude of the 3-D coupling. This confirms theoretical predictions that the transition temperature is mainly determined by the presence of planar symmetry.

A diffraction study of magnetic interactions

A traditional method to investigate interatomic interactions or spin-spin interactions in ideally long range ordered crystals is based on an inelastic neutron scattering study of elementary excitations (phonons or magnons). The interaction parameters (interatomic force constants or exchange constants) of a model Hamiltonian can be extracted from the measured dispersion relations. In these cases diffraction measurements provide just the structural information necessary to define the ground state. For dynamically disordered systems, however, this approach

fails if sharp collective excitations no longer exist and the dynamics are governed by diffusive processes. Then, the system components (atoms, spins) will probe their local environment and remain in a certain section of their configuration space with a probability determined by temperature and the averaged local interaction. These probabilities are accessible by diffraction measurements, since diffraction provides information about the time averaged structure.

Therefore, for strongly dynamically disordered systems, diffraction is a unique tool to determine the microscopic interactions in solids. A typical example is given by the determination of rotational potentials in orientationally disordered molecular crystals from Bragg data. For magnetic systems, measurements of the magnetic diffuse scattering in the paramagnetic phase enable one to determine the exchange and anisotropy constants as exemplified below. For diluted magnets or spin glasses, the determination of the average exchange constants,which thus becomes possible at least in the paramagnetic phase, is essential for model calculations of phase diagrams etc.

The method applied by us is based on the calculation of the paramagnetic neutron scattering cross section in the quasi-static and mean field approximations. While the latter is known to give wrong predictions for the phase transition, it provides an exact solution in the limit $T \rightarrow \infty$. Thus the two approximations should hold sufficiently for calculations of the neutron scattering cross section for neutrons with energy $E >> \langle J \rangle$ and temperatures $T >> \langle J \rangle / k_B$ (where $\langle J \rangle$ is an effective average exchange integral).

The approach has been applied to the antiferromagnetic garnet $\{Ca_3\}[Fe_2](Si_3)O_{12}$. Here the magnetic ions Fe^{3+} are in a $^6A_1$ state in the quasi-octahedral crystalline field and thus the spin dynamics can be described in a Heisenberg model with negligible anisotropy. From symmetry considerations, we expect the first neighbour interaction in this garnet to be spatially anisotropic and distinguish two nearest neighbour exchange interactions (J_1 and J_1'). Only the average $(J_1 + 3J_1')/4$ enters all macroscopic quantities, so that neutron diffraction as a microscopic technique is needed to reveal the spatial anisotropy. Fig. 32a shows the paramagnetic intensity distribution in a (1, 1, 0) reciprocal lattice plane around (3, 1, 1) as measured on D10 in the two-axis mode. The magnetic part of the scattering has been extracted by calculating the difference of the cross section at two temperatures. Fig. 32b shows a corresponding model calculation of the differential cross section. To obtain the exchange parameters up to the second nearest neighbours, we have measured the paramagnetic scattering along several main directions and determined our model parameters by a least-squares refinement. The parameters thus obtained (J_1 = - 0.43(10) K, J_1' = - 0.26(6) K, J_2 = 0.39 K) show the expected difference between the first neighbour exchange interactions and are in rough agreement with recent spin wave measurements in the long range ordered phase. Therefore, within the experimental errors no temperature dependence of the exchange integrals could be observed. This is a reasonable result, since the interatomic distances remain practically constant in the temperature range studied. Having thus shown the feasibility of the approach, we now intend to apply it to study the exchange interaction in disordered magnets. (Collaboration with the University of Tübingen).

Spin density measurements in the high T_c superconductor $YBa_2Cu_3O_{6+x}$

One of the key problems in the understanding of the high T_c perovskite-type superconductors concerns the localization of electrons and holes on the different copper and oxygen sites. Unpaired electrons or holes, under the action of a magnetic

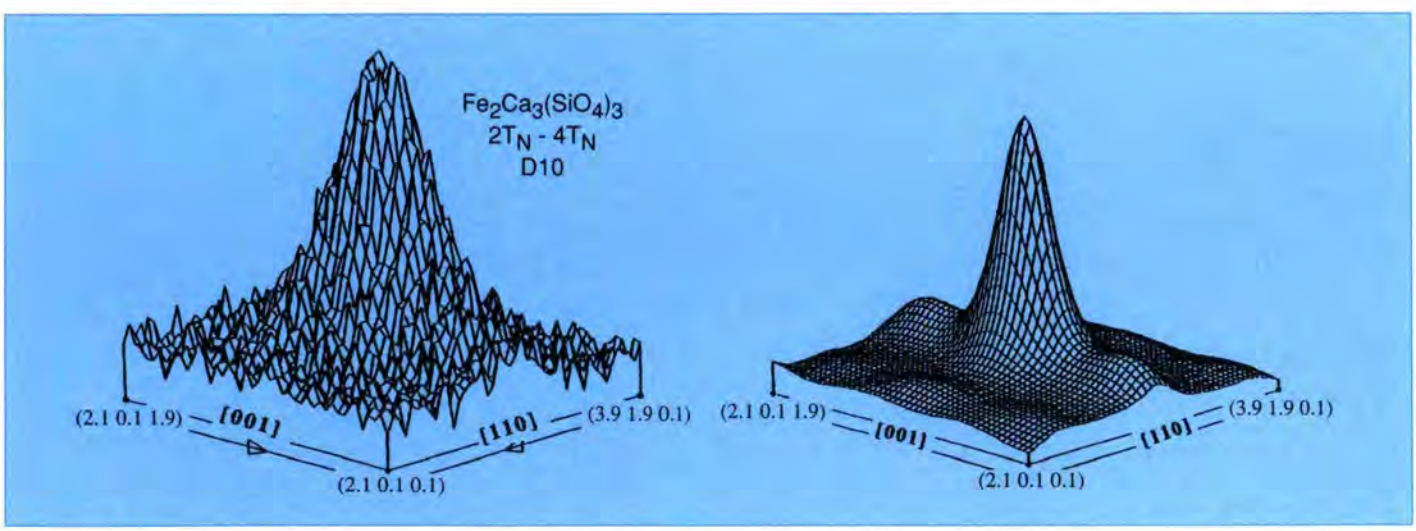

Fig. 32a: The paramagnetic intensity distribution measured on D10.

Fig. 32b: Model calculations of the magnetic neutron scattering cross section. For this plot, no convolution with the instrumental resolution has been performed.

field, result in a spin density which can be investigated by polarized neutron diffraction.

Three oxygen compositions were investigated on the spectrometer D3B, two in the AF state (x = 0.15 and 0.37), and one in the superconducting state with x = 0.9.

A typical result of magnetization densities projected along [110] and measured at T = 30 K in a magnetic field H = 4.6 T applied along [110], is reported in Fig. 33 for x = 0.37 and x = 0.9. In a first approximation the main part of the magnetization is concentrated on copper ions in Cu(1) and Cu(2) sites, as shown in Table 1. The contribution on the oxygen site is no larger than the experimental accuracy, i. e. not more than 10% that of copper. In a field H = 4.6 T, the induced magnetization is quite small ($\approx 10^{-3}\ \mu_B$) reflecting the weak susceptibility ($\approx 10^{-4}$ emu/mol Cu) which makes the experiments quite difficult.

The magnetic moments on the 2 copper sites, induced by the 4.6 T magnetic field are reported in the table for the 3 compositions.

x	0.15	0.37	0.9	T
$m(Cu_1)$	2.7 (4)	5.4 (4)	3.5 (4)	1.5 K
$m(Cu_2)$	1.1 (3)	1.0 (2)	0.8 (3)	
$m(Cu_1)$	0.8 (1)	1.0 (1)	0.9 (2)	30 K
$m(Cu_2)$	0.6 (1)	0.7 (1)	0.3 (1)	

Table 1: Magnetization (in $10^{-3}\ \mu_B$) induced by a field H = 4.6 T applied along [110] in Cu(1) and Cu(2) sites for $YBa_2Cu_3O_{6+x}$.

One striking feature is the strong depression of the susceptibility of Cu(2) below T_c indicating that spin fluctuations are frozen by the opening of the superconducting gap. The second feature is the strong increase of the magnetization on cooling down to T = 1.5 K which occurs mostly in Cu(1) sites. This contribution could arise from oxygen ordering effects in Cu(1) chains, Cu(1) vacancies or stacking faults. More accurate experiments are foreseen, in particular above T_c, and they are expected to give information on the magnetization density on oxygen sites. (Collaboration with CEN Grenoble).

Schwinger scattering in semiconductors with the GaAs structure.

Using the polarized beam diffractometer D3 experiments have been made which exploit the Schwinger effect to obtain information about the charge distribution in III-V compounds. This group of compounds, which includes many of the technologically important semiconductors, has been the subject of much experimental and theoretical study. The materials have the zinc-blende structure in which the lack of a centre of symmetry provides a polarization dependent term in the cross-section, due to Schwinger scattering, which is sensitive to the charge distribution. X-ray diffraction studies of charge densities in the III-V compounds are difficult because of the large number of participating electrons and the high absorption. The Schwinger scattering on the other hand depends on the difference between the nuclear charges and the electron form factors so that the valence electrons contribute a higher proportion of the scattering at low angles; additionally, absorption does not imply a correction to the measured flipping ratios.

Over the past few years meaurements have been made on GaAs[1], InSb, GaSb and InP also, most recently, on CdTe and InAs. For all these compounds we have measured flipping ratios for a group of low angle reflections including the special reflection 222 which would have no polarization dependence if the atomic charge distributions were centrosymmetric. The differences from unity of the flipping ratios are given in the ideal case by:

$$R-1 = 4\mathrm{Real}(N^*X_s)/N^2$$

where N^* is the complex conjugate of the nuclear structure factor and N its modulus. The Schwinger structure factor X_s is proportional to

$$\Sigma_j f_{sj}(k)\exp(\vec{k}.\vec{r}_j) \text{ with } f_{sj}(k) = Z_j - f_j(k)$$

the summation being over all the atoms (subscripted j) in the unit cell. In the absence of a model for the charge density, it is difficult to interpret the polarization ratios. The differences from unity of almost all those we have measured, apart from the 222, are smaller than would be calculated for a free atom model using UHF wavefunctions.

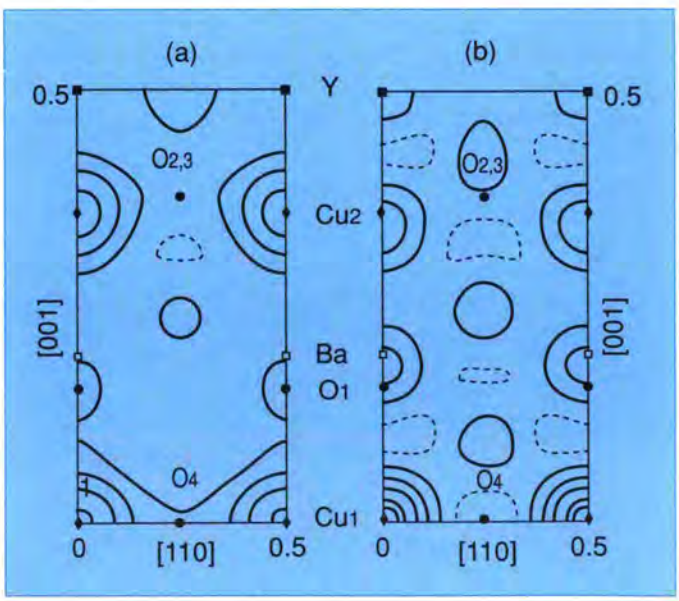

Fig. 33: Projection along [110] of the magnetization density induced by an applied field H = 4.6 T at T = 30 K for $YBa_2Cu_3O_{6+x}$ with x = 0.37 (a) and 0.9 (b).

The measurements on InAs complete the quartet of compounds between In, Ga and Sb, As; that on CdTe is the first on the series of isomorphous II-VI materials. Because extinction in our samples is significant and introduces an important correction to the polarization measurements, we have measured sets of integrated intensities on D9 at several wavelengths. The multi-wavelength refinement of the D9 data gives excellent R factors of 12% with a single mosaic parameter in the Becker-Coppens treatment [2]. For CdTe, due to its high absorption at thermal wavelengths, the optimum intensity was obtained at 0.48 Å, but the absolute scattered intensity at this wavelength was an order of magnitude smaller than that from similarly sized crystals of the other materials at 0.84 Å. For this reason, only the 111 and 222 reflections from CdTe have been measured and the measurement precision is rather less than that for the other materials.

Although at first sight it might seem possible to combine the results for the same high angle reflection in the quartet of compounds GaAs, GaSb, InAs, InSb, to obtain the individual Schwinger form factors for each element, subject to the assumption that no chemical effects are present at these angles, the four equations obtained are not linearly independent and so the data must be compared with theoretical models. One would expect that free-atom form factors could be used to calculate the Schwinger scattering adequately at values of $\sin\theta/\lambda > 0.3$ Å^{-1} where chemical and solid state effects should be very small. It is found however that the experimental results for the higher angle reflections are on average 20% lower than expected. Possible sources of systematic error have been examined, in particular the corrections made for extinction and beam polarization. The internal consistency of measurements at different wavelengths gives confidence in the extinction correction which is in the worst case about 30%. At the moment there is no proper explanation for this discrepancy between experiment and theory. Further measurements concentrating on obtaining more accurate values for a few high angle reflections as a function of wavelength will be made before seeking a novel physical origin for this effect.

[1] *Brown P. J. and Forsyth J. B. (1988) Proceedings of Neutron Scattering Symposium-Advances and Applications, Sydney, Australia August 1987.*

[2] *Becker P. J. and Coppens P. (1974) Acta Cryst A30, 129.*

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College 6

Liquids, Disordered Materials and Metal Physics

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Summary

The scientific work in college VI has concentrated on the traditional areas, employing the full range of the ILL instruments, even pushing the limits where possible. By volume, the studies of glasses and amorphous materials are still the first, followed by the investigations on metal physics, hydrogen in metals and the various liquid systems. The following overview reflects the progress in selected fields in terms of new methodology, new instrumentation, new or better materials of application and, of course, new ideas. We shall have a look, for example, at the very fundamental studies concerning excitations in quantum liquids and simple gases that maintain a continuous output of interesting results, often associated with instrumental development as in the case of Brillouin scattering in dense gases. The instrument and the analysis reach their current limits in the examination of collective excitations in a molecular liquid, deuterated methanol. In the field of dynamics of disordered systems, the characterization of fractal dynamics is strongly dependent on the understanding of preparation silica aerogels that have been studied in several experiments. In the search for general characteristics of the glass transition the results on polymer, van der Waals and network glasses are confronted with the mode coupling theories. The discovery of a new high-quality icosahedral phase opened a wide variety of structural studies associated with the parallel development of quasi-crystal structure solving methods. At the other extreme of the field of metal physics is the study of single crystal superalloy turbine blades that marks the level in the material development in applied research.

Scientific Trends and Highlights in 1989

Structures of molecular liquids

The structure of molecular liquids continues to attract considerable attention (Alvarez, Bermejo, Enciso, Garcia). A highly polar fluid, SO_2, has been studied. After detailed recoil corrections to the interference pattern the molecular structure is obtained. Evidence for strong short range orientational effects is found in the intermolecular pair correlation function which is difficult to explain in terms of simple pair potentials. In the case of a complex liquid such as 1,2 dichloroethane the long intermolecular distances are very difficult to isolate from the intermolecular contributions. However, a combined study on D4B with isotopic substitution of the chlorine and on LAD (at ISIS) up to very large momentum transfer has given the distribution of internal dihedral angles related to the torsion of the molecule. Again strong short-range correlations are found for the intermolecular structure. This work is a typical case for the study of the complementarities between D4B and LAD.

The equimolar mixture of CCl_4 and CS_2 whose pure components possess no permanent electric dipole moments has been studied by molecular dynamics simulation as well as neutron scattering (Mittag, Samios, Dorfmüller, Günster). Here the agreement between the experimental intermolecular functions obtained for several chlorine isotopes and the computer simulation is remarkably good.

Critical scattering

The metal-ammonia system which undergoes a liquid-liquid phase separation in the vicinity of metal to non-metal transition has for many years been studied by SANS (Damay, Leclercq, Chieux).The latest and most precise measurements in the vicinity of the critical point have given the critical scattering function and the critical index η to an accuracy not yet achieved in SANS measurements ($\eta = 0.030 \pm 0.0015$). The very strong contrast between the scattering of ammonia and that of alkali metal, the good optimization of the investigated $q\xi$ range (ξ = correlation length for fluctuations) and the elaborate method of data analysis have been critical factors of this success. These results reconcile neutron scattering with light scattering and are in favour of renormalization group theory predictions for the three-dimensional Ising model.

Proton diffusivity in acidic solutions

The proton dynamics of aqueous solutions of sulphuric acid have been compared to those of pure water and of cesium sulfate solutions in order to study the abnormal proton diffusivity expected to occur in acidic solution (IN6, Lassegues and Cavagnat). A marked slowing down of the translational diffusion results when salt or acid are added to water. The rotational motion is much less affected. In H_2SO_4 solutions corresponding to the maximum of specific conductivity, some evidence is obtained for a weak and broad quasi-elastic component, not present in pure water or in Cs_2SO_4 solutions. This additional component assigned to the abnormal proton diffusivity contains about 12% of the total intensity in agreement with the percentage of protons involved in H_3O^+ species. In a H_2SO_4 solution of 3.2 M at 263 K, mean water diffusion can be characterized by a diffusion constant $D_t = (0.53 \pm 0.03)\ 10^{-9}\ m^2s^{-1}$, whereas the fast proton diffusion process is characterized by $D^+ = (2.2 \pm 0.4)\ 10^{-8}\ m^2s^{-1}$. Thus for the first time, a signature of the abnormal proton mobility is observed by neutron scattering.

Excitations in methanol

Collective excitations in deuteromethanol (CD_3OD) have been studied at 200 K by inelastic coherent scattering on the triple-axis instrument IN8 (Bermejo, Batallan, Enciso, Garcia-Hernandez, Alonso and Martinez). The results obtained from either direct plots of maxima (ω_M) of S(Q, ω) or fits to the two models (linear hydrodynamic and viscoelastic) are shown in Fig. 34. The harmonic frequency ω_j and the normalized second moment ω_0 are in reasonable agreement up to $Q \approx 0.6$ Å^{-1}, and they start to diverge afterwards. The near equivalence at low Q-values is easily explained if we take into account that both the hydrodynamic and viscoelastic approaches are valid in this region and therefore both sets of parameters have a physical meaning. The rather flat shape of the Q-dependence on ω_M can be explained by the fact that such a quantity does not represent a physical frequency.

The shape of the ω_0 and ω_1 curves displayed in Fig. 34 shows the correct trend (narrowing when approaching the maximum of the first liquid-structure peak, at $Q \approx 1.78$ Å^{-1}), and the magnitudes of both quantities are in agreement with the deconvoluted data. Although further refinements can be introduced, especially for the calculation of the relaxation time, it is now clear that future experiments should be analysed within a framework able to extend its domain of validity well into the kinetic region. By extrapolation of the low-Q part of the ω_j versus Q curve a value of 2450 ± 215 ms^{-1} is obtained for the slope (see broken line in Fig. 1 (b)). This is well above the estimated adiabatic velocity for this temperature (1420 ms^{-1}).

Although it is not possible to assert whether this mode is a continuation towards large momentum transfers of ordinary sound (positive dispersion) or represents a high-frequency excitation specific to multicomponent fluids, the present data indicates that the results obtained from deconvolution or analysis in terms of the viscoelastic model can be accommodated within the "positive dispersion" phenomenon predicted by the generalized hydrodynamic theory.

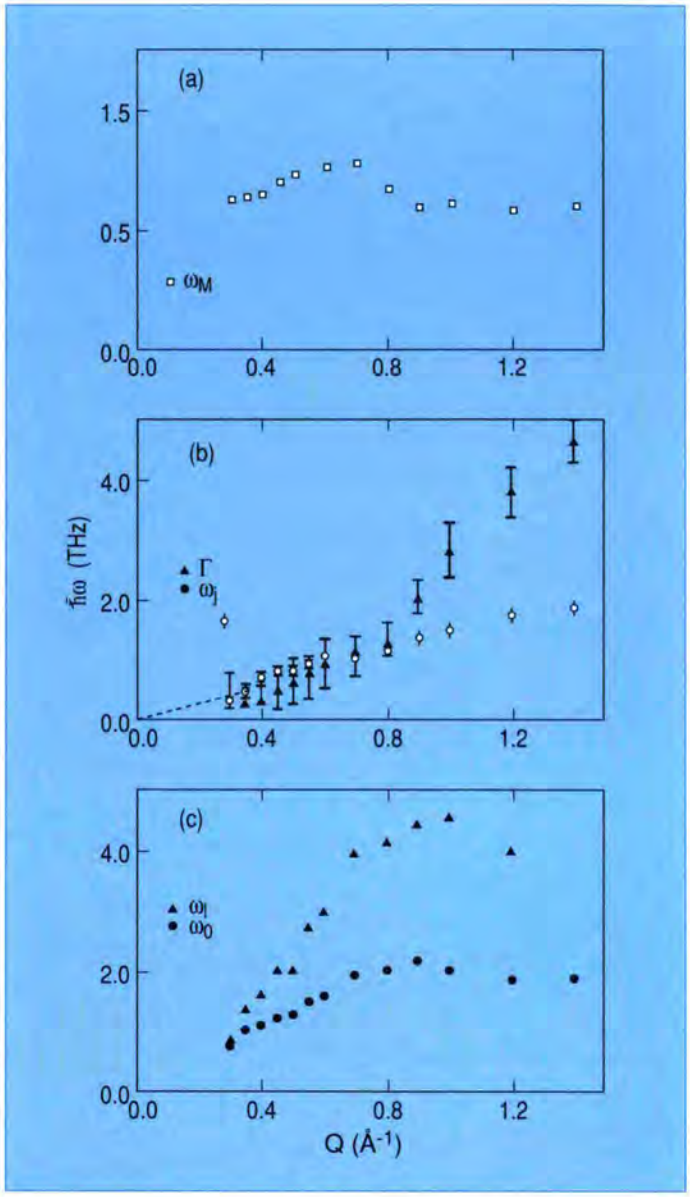

Fig. 34: *a) Position of the maximum of S(Q,ω) versus Q, taken from the deconvoluted spectra.*
b) Harmonic frequency ω_j and damping factor Γ versus momentum transfer for the damped harmonic oscillator model. Broken line indicates the extrapolation to the origin, in order to calculate a sound velocity (see text).
c) Square root of the normalized frequency

Brillouin scattering on dense gases

Study of dynamics of gases has continued in the low-Q regime with the IN5 instrument rigged for Brillouin scattering. Considerable improvement has been achieved, particularly in the reduction of background scattering and the positioning of the detector. This led to about an order of magnitude improvement in the quality of the data in dense nitrogen gas and allowed experiments with strongly absorbing samples of Kr gas where $\sigma_s / \sigma_a \sim 0.1$ (Egelstaff, Suck, Youden and

Mutka). The results have been compared with the Navier-Stokes theory of hydrodynamics using macroscopic transport coefficients. There is reasonable agreement for nitrogen but poor agreement for krypton. Room-temperature ^{36}Ar was also studied (Bafile, Barocchi, de Graaf, Suck, Verkerk, Mutka) at four densities (between 0.5 and 5 nm^{-3}, 20 to 200 bar). The large density range (low-density measurements are allowed by the large scattering cross-section of ^{36}Ar) makes it possible to study the whole range of dynamical behaviour from the Boltzmann regime to hydrodynamics, and will give information on the transition regime.

The 20-bar data show an overall ideal-gas-like behaviour with slight but systematic deviations. These can be compared, for instance, with a hard-sphere theory (Kamgar-Parsi et al.) which for $kl_0 > 3$ (l_0 is the Boltzmann mean free path) describes $S(k,\omega)$ as the sum of the free-gas gaussian expression plus the first correction term in a power series of $(kl_0)^{-1}$, whose coefficient is a known function of ω/k. In Fig. 35 the comparison between theory and experiment is reported for this function using data in the range $1.23 < kl_0 < 2.05$. The agreement is good, although the errors are rather large due to the subtraction of the dominant free-gas term. However, it seems that such a first-order correction accounts well for the experimental intensity for kl_0-values even smaller than what is predicted for hard spheres. At larger kl_0 the agreement is still good but the uncertainties become larger.

The 200-bar data clearly show Rayleigh-Brillouin triplet. The experimental symmetrised $S(k,\omega)$ when compared with a fitted linearilised hydrodynamic model, shows some systematic deviations in the frequency region between the central and the side peaks, which are not yet clearly understood.

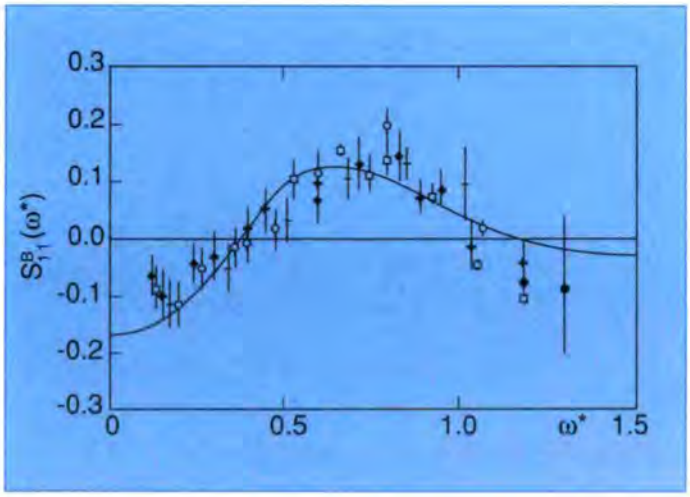

Fig. 35: The deviation from the free-gas behaviour in Ar: $S^B_{11}(\omega^*)$ as a function of reduced frequency $\omega^* = (\omega t_0)/kl_0$ where t_0 and l_0 are the Boltzmann free time and path, respectively. The solid line is the hard-sphere theory and the experimental points are collected at five values of kl_0 between 1.23 and 2.05.

Self diffusion in hydrogen

A comparison of the finite-k and the k = 0 diffusion constants in H_2 gas has been carried out on the IN11 spin-echo spectrometer (Verkerk, Bafile, Farago Mezei). The aim of the experiment was the determination of the coefficient of self-diffusion D in H_2 at 120 K and 750 bar (particle number density 21.04 nm^{-3}). The spin-echo spectrometer IN11 was modified with an additional set of 2.5 cm long Larmor coils complete with $\pi/2$ spin flippers in order to extend the lower limit of the accessible time range from 30 to 5 ps for 0.6 nm incident neutrons. This was necessary because of the relatively large self-diffusion coefficient of approximately 0.06 nm^2ps^{-1} in the hydrogen sample.

The data for the three scattering angles corrected for background and resolution were fitted with the expression $A \exp(-Dk^2t)$, simultaneously with all data. In this way the uncertainty in the normalization A at the individual k caused by the impossibility of determining $F_s(k,t = 0)$ is reduced. The result is $D = 0.0543 \pm 0.0021$ nm^2ps^{-1} in hydrogen at 120 K and 750 bar. It was demonstrated that the neutron spin-echo method can be used for the determination of such relatively large diffusion constants in high pressure samples. The lower limit of the accuracy is 4%.

Dynamics of silica aerogels

Several groups have been interested in the dynamics of silica aerogels, porous solids with fractal structure in a length scale about 1 to 100 nm that depends on the preparation conditions. The vibrational density of states is expected to reflect the fractal character with a frequency dependence of the type $G(\omega) = \omega^{d-1}$ where d is the spectral (or fracton) dimension. The frequency range of the fracton behaviour was shown to extend over three orders of magnitude in certain samples (studied by neutron backscattering on IN13 by Coddens, Pelous, Woignier, Vacher, Courtens and Williams). This frequency range is dependent on the scale of the static fractal structure (measurements on IN13, Reichenauer, Buchenau, Conrad, Frick and Fricke).

This relation between the microstructure and the dynamics was also studied by neutron spin-echo measurements on samples with different characteristics (Schaefer, Brinker, Richter, Farago and Frick). The variation of the dynamic characteristics (spectral dimension d and phonon-fracton crossover frequency ω_0) with the structural parameters listed in the table I and the relaxation S(Q,t) is shown in Fig. 36. A and B are deuterated polymeric samples with a fracton-like density of states reflected in the decay of S(Q,t) over four orders of magnitude in time. The pyrolyzed sample C and the non-fractal colloidal sample D show a more concentrated time-decay corresponding to a density of states peaked around 20 μeV. The sintered, however microporous sample E shows no relaxation indicating the elimination of the low-frequency modes due to hardening.

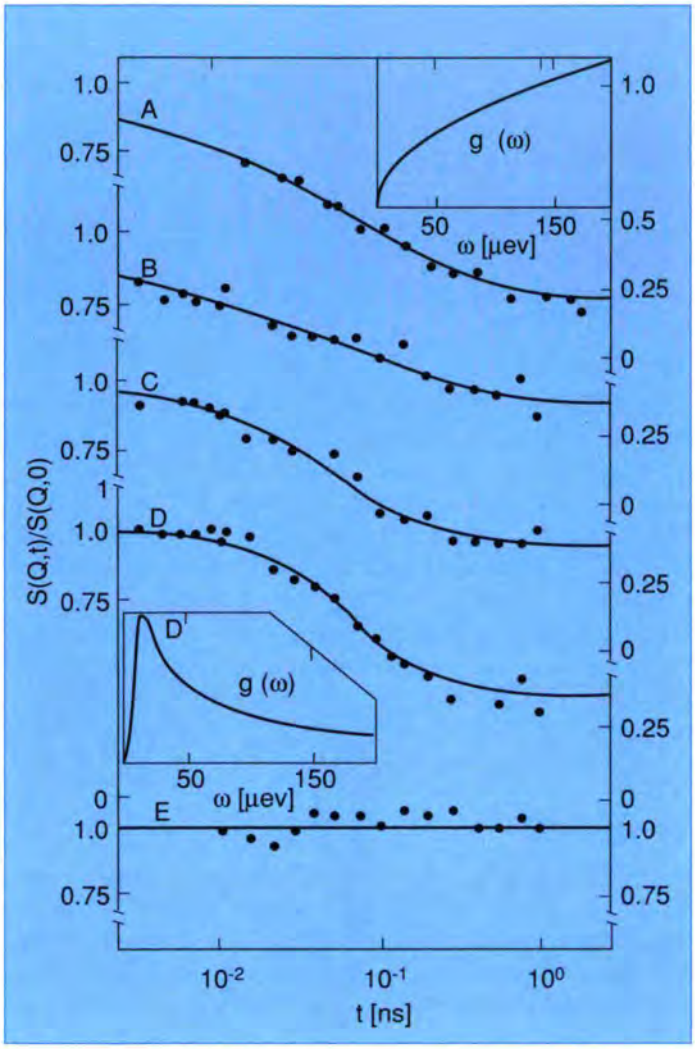

Fig. 36: Neutron spin-echo spectra for aerogel samples with different characteristics. The table shows how the fractal properties depend on the preparation conditions.

Quite recently a first attempt to observe the fracton modes by coherent inelastic scattering was carried out on IN5 in the Brillouin set-up (Mortensen, Pedersen, Posselt, Richter, Kearley and Mutka). The observation of the dispersion requires a delicate matching of the resolution, the Q-range and the incident energy with the sample density. Detailed analysis of the data is necessary before one can judge if this was done successfully.

SAMPLE	CLASS	POROD SLOPE	DENSITY [g/cm^3]	d	ω_0 (μev)
A	TWO-STAGE	2.4±.1	0.16	1.54±0.9	2.0±0.5
B	SINGLE-STAGE	2.9± 2	0.15	1.70±0.6	1.0±1.4
C	PYROLIZED	2.5±.2	0.19	1.22±.14	5.4±2.8
D	COLLOIDAL	4.0±.5	0.19	0.14±.28	9.0±2.8
E	SINTERED	4.0±.4	0.75		

Dynamics of disordered systems

The recent discovery of phonon softening in pressure-quenched crystalline Al-Si alloys (Chevrier, Suck, Coppens and Perroux) reminiscent of a similar softening in metallic glasses and accompanied by a glass-like linear specific heat term in the superconducting low temperature phase, stimulated an investigation in the related Al-Ge system. The interest concentrated on the frequency region between 100 GHz and 1 THz, where glasses exhibit a mixture of sound waves and additional modes with strongly anharmonic temperature dependence. No such behaviour, however, was found in the non-equilibrium Al-Ge system in spite of a thorough search on IN6 (Koleshnikov, Buchenau and Frick). The temperature dependence of the inelastic intensities between 5 and 300 K showed no deviation from the harmonic-oscillator picture in the whole frequency range. The dynamic structure factor revealed only sound waves peaked at the (111)-reflection.

While these findings do not contradict a softening of the transverse phonons as in Al-Si (that region is obscured in Al-Ge by a strong resonant mode of the heavy Ge atom in the host of lighter Al atoms), they discourage the hope of analysing glass problems within such a simple fcc crystal.

Among other subjects in the broad field glassy systems, we can mention the study of AgI doped silver borate glasses, in relation to the fractal properties (IN6, A. Fontana, Rocca, M. Fontana, Dianoux). Comparing Raman and neutron results, the frequency dependence of the electron-vibration coupling function was determined.

The problem of vibrational localization was examined comparing a-Si and a-Ge results from IN4 (Kamitakahara, Gompf) with computer simulation. The role of under-coordinated (2 or 3 instead of 4) atoms in the localized vibrational modes was identified (Biswas, Bouchard, Kamitakahara, Grest and Soukoulis).

The low frequency density of states of dried opals, built up by ~ 200 nm a-silica spheres on regular lattices (e.g. fcc) was studied on IN6 (Reichenauer, Sosnowska, Graetsch, Ibel, Frick, Buchenau). Structurally the opals must be classified between highly porous aerogels and amorphous SiO_2. An extraordinary enhancement of low frequency density of states with respect to a-SiO_2 has been observed and is interpreted as vibrations from small particles.

Glass transition

The studies on the glass transition have continued in connection with the mode coupling theories of liquids, trying to quantify the non-ergodic behaviour. For the liquid-glass transition at a critical temperature $T_c > T_g$, as one of its essential results, the theory predicts spontaneous ergodicity breaking followed by a subsequent $\sqrt{(T_c - T)}$ increase in the non-ergodic spectral contribution or the non-ergodicity parameter f(Q,t).

Neutron scattering couples directly to the density fluctuations and therefore is uniquely suited to scrutinize the theoretical predictions. In a neutron spectrum, the frozen correlations display themselves as an elastic spectral component. Above T_c in the supercooled liquid state, as a result of structural relaxation processes the elastic fraction broadens. Its spectral contribution is described by f°(Q), the value of the non-ergodicity parameter at T_c, and should only be weakly dependent on temperature.

Coherent quasielastic neutron spin-echo (NSE) experiments on the temperature dependence of the non-ergodicity parameter of simple glasses have been carried out by two groups. Farago, Frick and Richter have studied polybutadiene, a polymer consisting only of a backbone without sidegroups. The results seem to be in quantitative agreement with the theory. They show a cusp-like behaviour of f(Q,T), and a $\sqrt{T_c}$-T singularity with T_c = 216 K is found 35 degrees above T_g = 181 K. A similar T_c can be obtained from a power law of viscosity data at higher temperatures.

Similarly, the NSE results on the van der Waals glass deuterated orthoterphenyl by Bartsch, Fujara, Petry and Sillescu show a critical behaviour of the non-ergodicity parameter. The critical temperature is in agreement with the one deduced earlier by incoherent scattering experiments on IN13.

Other work on the network glass Se on IN6 and IN13 (Phillips, Buchenau, Nücker, Dianoux and Petry) suggests a slightly different picture. The occupation of low-energy states is explained by a temperature-dependent density-of-states. The quasielastic broadening of the elastic line above T_g is fully explained by the known long-range diffusivity.

Liquid metals and alloys

Up to now no quantitative agreement was obtained between the theoretical and experimental structure factor of liquid gallium. Therefore, high-precision measurements of the structure factor have been undertaken over a large momentum transfer range (Bellissent, Levesque, Weis, Chieux). Then the effective pair interaction was successfully obtained by the use of an inversion procedure. It establishes that the effective potential is positive and repulsive in the domain of distances corresponding to the first nearest neighbour shell.

In the field of binary alloys, the isotopic substitution method continues to be applied to produce the partial structure factors. The liquid AlNi has now been compared to the quasicrystalline glass former Al_{80} $(Mn_x(FeCr)_{1-x})_{20}$ previously studied by the isomorphous substitution technique. The comparison unexpectedly shows equivalent chemical short range order but a topological order quite reduced in AlNi. A possible explanation is related to the type and size of the different polyhedra which are formed in these systems, but icosahedral ordering in liquid AlMn remains to be proved (Maret, Pasturel).

Quasicrystals

The discovery of a high quality new stable icosahedral phase in the ternary AlCuFe system has opened a wide variety of possible structural studies (de Boissieu, Dubois, Janot, Pannetier). The Al_{65} Cu_{22} Fe_{12} alloy has been identified as a face centred icosahedral phase issued from a chemical ordering

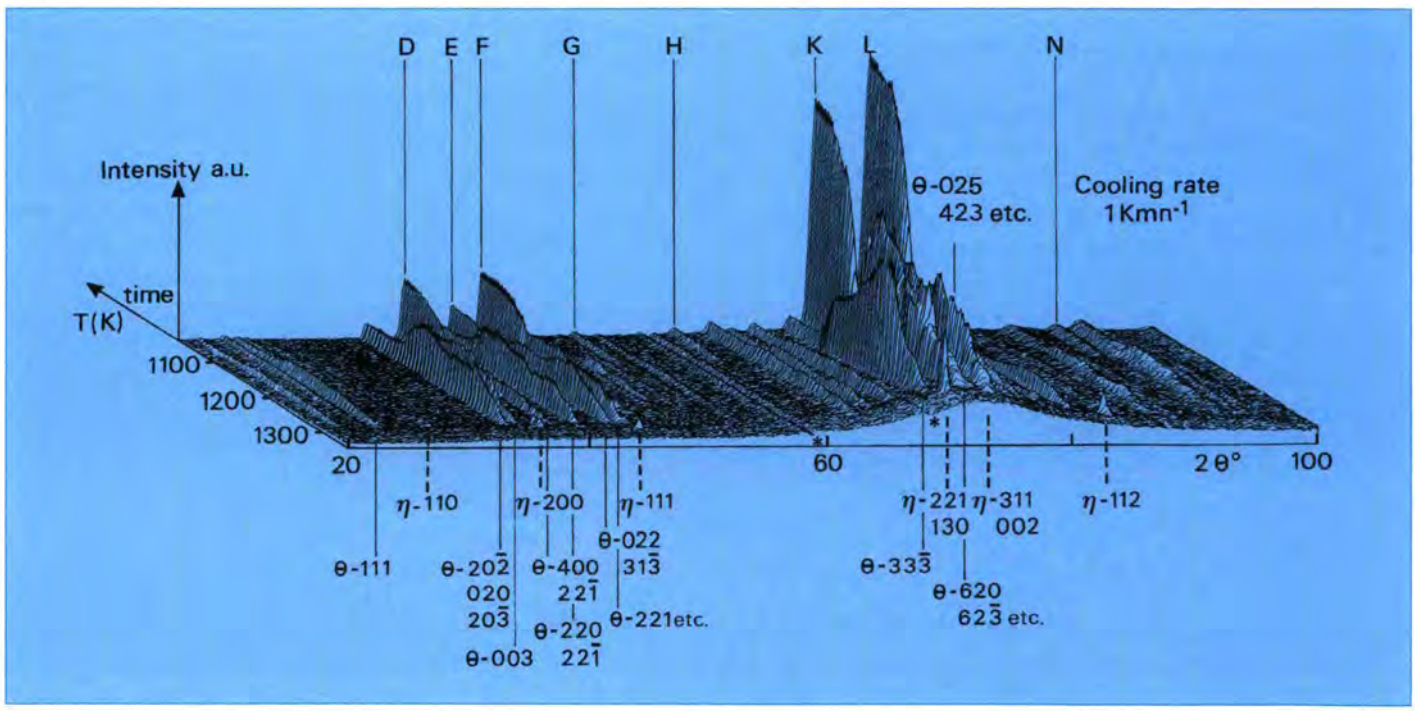

Fig. 37: Pseudo-three dimensional perspective view of the path from liquid quasicrystal measured on D1B (orthorhombic η-Al_5Fe_2, monoclinic θ-$Al_{13}Fe_4$ phases are indexed; the quasicrystal peaks are labelled D, E, F, ...).

of a primitive 6-dim. hypercubic lattice. A typical aspect of this system is that the icosahedral phase forms by peritectic reaction from a monoclinic $Al_{13}Fe_4(Cu?)$ primary phase (Fig. 37). On the other hand, quality and even basic structure seem to be strongly influenced by detail in the thermal history of the samples. Depending on annealing temperatures, cubic, monoclinic and icosahedral phases can nucleate; their further stabilization is then related to the growth of phase domains up to minimum sizes. When correctly prepared, this quasicrystal shows very sharp peaks in neutron diffraction, with the existence of features revealing chemical ordering.

Some aspects of the structure become visible on the 6-dim Patterson function (PF) that can be calculated using the neutron diffraction data. Thus it has been possible to derive a structural model whose pair distribution function compares quite well with its experimental counterpart.

Microstructure of superalloy single crystals

Better performance of aircraft turbines is linked to research on improved materials. The chosen solution for the high-temperature parts of the engine is the use of single crystals of Nickel-based superalloys as turbine blades. The high mechanical performance of these alloys are due to the presence of precipitates of an ordered phase which block the motion of the dislocations (structural coarsening). Thermal treatment which modifies the size and shape of the precipitates is used to improve the mechanical properties of the materials. By the use of single-crystalline turbine blades, it is possible to take further advantage of the anisotropy of their properties.

The influence of annealing has been studied using the instrument D11 (Bastie, Bellet, Legrand). Figure 38 shows the ordering and coalescence of the precipitates before and after two and eight hours of annealing at T = 1050°C. The precipitates are aligned along the <100> and <010> cubic axes. Their average interdistance increases from 290 nm to 365 nm and 415 nm. The analysis of the asymptotic behaviour of I(q), along several crystallographic directions is consistent with a shape of the precipitates like a cube with truncated corners.

After 1.5% creep deformation at high temperature (950°C, 280 MPa), the shape of the precipitates is strongly modified from cubic to raft-like.

The microscopic origin of this behaviour is related to the misfit of the lattice parameters between the γ phase matrix and the γ' phase of the precipitates. High resolution diffraction measurements have been performed on the instruments S21, IN10 and LI3. They revealed a tetragonal deformation of the γ' phase at high temperature.

Diffusion of metallic solutes

Metallic solutes such as Co or Fe diffuse anomalously fast in the bcc phase of the group 4 elements ß-Ti, ß-Zr and ß-Hf, i.e. diffusivities are observed which are two orders of magnitude higher than the already fast self-diffusion. Previous quasielastic studies on IN10 and IN5 yielded jump frequencies, however, corresponding diffusivities were about 1 order of magnitude lower than the one obtained from measurements of the total transport of mass. In order to shed light on this discrepancy the so far unknown solute site of Co in bcc-Zr-1.5at% Co was investigated by measurements of the diffuse elastic scattering intensity at 1000°C on D7 and D10 (Heiming, Petry, Trampenau, Chevrier, Schärpf). Experimentally such measurements are difficult to perform, because single crystals of the bcc phase are destroyed due to a martensitic phase transition at 883°C where a transformation from the bcc phase into the hcp phase occurs. Single crystals needed for the investigations had to be grown in situ by the zone melting technique on the diffraction instruments in a combined single crystal growth and measuring furnace. The TOF spectra are characterized by an extremely high inelastic background below the elastic signal due to the low-lying phonon branches which are very broad in energy. Because of this phonon intensities could be found even at zero energy transfer. For a detailed analysis of the truly elastic diffuse scattering the inelastic contributions had to be subtracted from the intensities measured elastically. Diffuse elastic intensities are found as a ridge in between the (110) and (200) Bragg reflexions. The comparison with model calculations shows clearly that all

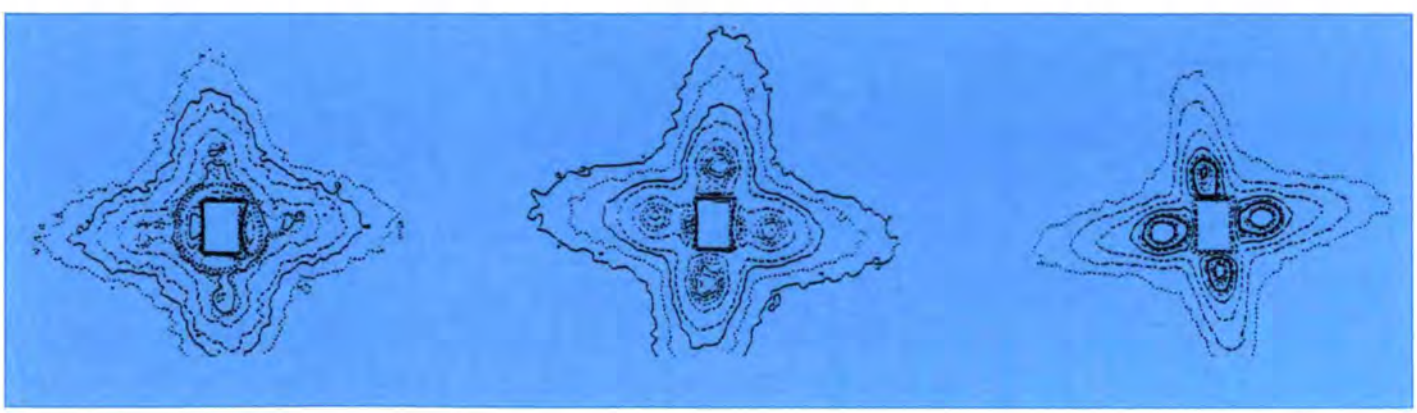

Fig. 38: Iso-intensity map for three samples (from the same single crystal) annealed for: a) 0 hours; b) 2 hours; c) 8 hours on D11, λ = 10 Å, D = 35 m.

observed intensities can fully be explained by substitutionally solvated Co atoms that induce an isotropic contraction of the host matrix.

For the diffusion of Co in bcc-Zr it is thus concluded that solute migration occurs for the majority of Co via a vacancy mechanism. This causes line broadenings in the quasielastic spectra as observed on IN10 and IN5. In order to explain the high diffusivity it is proposed that a small fraction of less than 10% migrates extremely fast and causes thus most of the transport of mass.

Diffusion of H in metals

Investigations on H diffusion in YH_x under high H-concentrations ($1.7 \leq x \leq 2.1$) have been carried out on IN10 between 350°C and 950°C (Stuhr, Steinbinder, Wipf, Frick). The H-atoms occupy mainly tetrahedral sites but also about 20 % octahedral sites in the cubic face centred Y lattice. The IN10 results show that diffusion takes place mainly by jumps on the octahedral sites.

Previous experiments showed that the quantum diffusion of light interstitials in metals at low temperatures is controlled by the direct non adiabatic interaction with the conduction electrons. According to Kondo the jump rates of the interstitials are determined by $\nu \sim J^2\ T^{2K-1}$, where J is the effective tunnelling matrix element and K is the electron interstitial coupling parameter. Recent investigations of the quantum diffusion of trapped H in $Nb(NH)_x$ between 10 and 150 K were concentrated on the specific influence of the tunnelling matrix element on the H jump rates. In comparison to $Nb(OH)_x$ the matrix element was measured as reduced by about 30% (IN6, T = 1.5K). Therefore the jump rates in the $Nb(NH)_x$ system are expected to be reduced by about 50%. The results from experiments on IN6 (Steinbinder, Wipf, Neumaier, Richter, Magerl) are in excellent agreement with theoretical predictions.

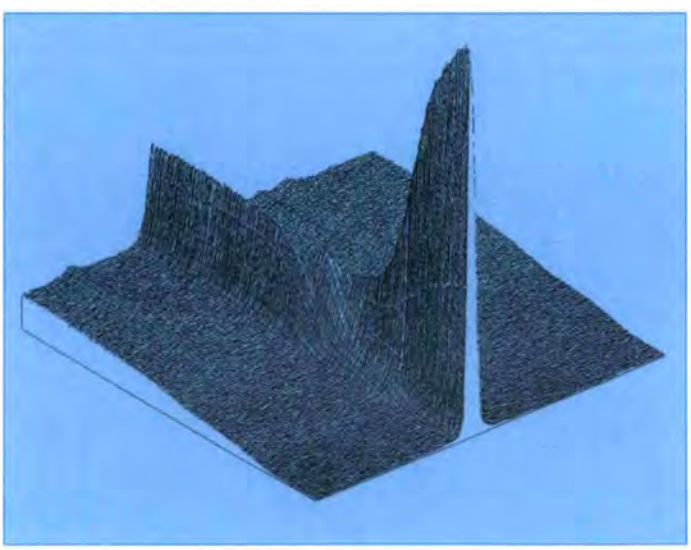

Fig. 39: The intermediate phase in $TiNiH_x$ during desorption of hydrogen while heating.

Structural and dynamic studies in $TiNiH_x$

Intermetallic hydrides with high hydrogen content that are very interesting materials for negative electrodes in high energy density batteries have been studied by Anne, Poinsignon and Frick on IN10 and IN6. The quantity of electrochemically active hydrogen has also been obtained from 'in situ' investigations of structural modifications occurring during charge/discharge of the hydride electrode on D1B. On IN10, following the variation of elastic intensity with increasing temperature (window test) a strong increase of intensity is observed at low Q between 550 K and 750 K and also confirmed by IN6 data. Another view on these phenomena is given by a time resolved experiment under heating on D1B. Structural transformations occurring in $TiNiH_x$ during desorption of hydrogen go through an intermediate phase, well shown on the 3D plot given in Fig. 39, and probably responsible for the anomalous intensity increase observed on 1N10 spectra.

Secretary : H. Mutka

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Ripplons in ^{4}He films

H.J. Lauter, V. Frank, H. Godfrin, P. Leiderer.

Quantized capillary waves (ripplons) are the elementary excitations of a free liquid surface. Their existence in bulk ^{4}He and in films has been predicted by theory and indirectly confirmed by experiment [1,2]. The ripplon dispersion relation is easily evaluated using hydrodynamic relations for an incompressible fluid:

$$\omega^2 = (\alpha_0/\rho_0)\, k^3 \qquad (1)$$

where a_0 is the zero temperature surface tension, ρ_0 the ^{4}He density at zero pressure and k the wavevector. This expression, only valid at small wavevectors, can be used to calculate the very low temperature thermal properties of the helium surface (entropy, heat capacity). At higher temperatures, however, the thermal occupation of high wave vector ripplon states is important, and a more realistic dispersion relation must be considered. Thermodynamic measurements, therefore, are an indirect test for different models of the ripplon dispersion relation.

Detailed measurements [3] of the temperature dependence of the surface tension $\alpha(T)$ revealed a much larger temperature dependence than expected from formula (1). Several modified dispersion curves have been proposed which differ mainly for wavevectors above 0.5 Å^{-1}. Edwards et al. [1,3], taking into account the curvature dependence of a, were able to fit the experimental excess surface entropy data. Their model involves two parameters: a length $\delta = d(\ln \alpha_0)/dK$ where $K = (r_1^{-1} + r_2^{-1})$ is the curvature of the surface, and an area $a = d\delta/dK$. Within the precision of the entropy data, several sets of parameters have been used ($a = +1.5$ Å^2, $\delta = 0$ [3] and $a = +1.0$ Å^2, $\delta = 0.036$ Å [1]), the latter giving a somewhat better agreement. Such a large variation in the parameters corresponds to very different ripplon dispersion curves at wavevectors ~1 Å^{-1}, with a common trend indicating the presence of a downward curvature.

Little direct experimental evidence is available[4], however, on the ripplon dispersion curve at these wavevectors. Such a study requires a microscopic probe-like inelastic neutron scattering (INS), but due to the low neutron cross-section of ^{4}He the measurement cannot be performed on the free surface of bulk liquid He. A way to circumvent this severe restriction is using samples with a large surface to volume ratio. This can be accomplished adsorbing He on exfoliated graphite sheets oriented in such a way that their adsorption surface is contained in the scattering plane. The total surface area can be determined by adsorption isotherms and neutron diffraction. In the present sample it was 730 m^2 ± 2%, and the ^{4}He monolayer coverage (0.112 at Å^{-2}) was 304cc STP.

The measurements were performed at the time of flight spectrometer IN6 using a wavelength of 5.12 Å. The elastic energy resolution is slightly Q dependent due to sample size effects, increasing from 80 to 110 μeV with scattering angle.

The data obtained before any ^{4}He was adsorbed were used as background and subtracted from subsequent measurements performed at several coverages between one and five monolayers. Finally a scan with the cell filled with bulk superfluid ^{4}He was performed.

The structure of the first adsorbed layer is known, from previous diffraction experiments [5,6], to be solid at all the coverages studied here. The inelastic spectrum from the first layer does not show any detailed structure in the measuring range. The second layer solidifies in the presence of a third liquid layer and its density is well known [5,6] (1st layer = 0.115 at Å^{-2}, 2nd layer = 0.094 at Å^{-2}). Thus, for high coverages (more than two layers) 0.209 at Å^{-2} correspond to the solid; the remaining amount of ^{4}He corresponds to the liquid layers (the mean density of a liquid layer is 0.078 at Å^{-2}). Cieslikowski et al. [7] observed layerwise growth of liquid films up to 9 layers on a solid hydrogen substrate.

Due to the large amount of data it is not possible to show here individual spectra for all the coverages. A general overview of all channels and detectors is given in Fig. 40 (see page 75) as a contour plot [8,9]. One can easily recognize two excitation branches. The higher energy one agrees well with the phonon-roton dispersion relation of bulk liquid ^{4}He (solid line in Fig. 40). The lower branch, located at about half the energy of the previous one, is the ripplon mode. Evidence of the existence of this branch has been given previously on measurements [4] done on a different substrate (Vulcan III graphite powder), together with the observation of dispersionless modes.

To determine the origin of the lower excitation branch a measurement was performed with the cell filled with bulk liquid. This procedure suppresses the liquid-vapour interface, but does not affect the adsorbed solid-liquid one. As seen in Fig. 41 (see page 75), the phonon-roton part is strongly enhanced due to the large amount of bulk liquid, while the ripplon excitation branch is suppressed. Clearly, the lower energy excitation originates from the free surface of the liquid.

The experimental ripplon dispersion curve displays a strong downward curvature and seems to merge with the bulk roton minimum for Q ~ 2 Å^{-1}. Due to the high intensity of the roton signal it is difficult to follow the ripplon peak at these wavevectors. Below Q = 1.5 Å^{-1} our result agrees well with the calculation of Edwards and Saam [1].

In conclusion, the ripplon spectrum at large wavevectors has been measured for the first time. This result is relevant for microscopic calculations of the interfacial properties of ^{4}He, in particular the phonon-ripplon and roton-ripplon coupling, the shape of the free surface, and sticking coefficients. They also concern some practical applications, as for example, the neutrino detector based on the quantum evaporation of superfluid ^{4}He.

Biological Structures and Dynamics

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Introduction

The activity in neutron scattering studies of biological material remains high, and as usual there has been a strong demand from external visitors and the group on the small-angle scattering facilities. Parallel to this, there is a growing request for beam time for studies of membrane systems, which mainly involve D16, and the number of low-resolution, single-crystal projects on DB21 is increasing. It is also gratifying to observe that more groups are getting involved in inelastic studies. A number of instruments are now being used by several teams and a more coherent picture of protein dynamics is emerging.

Despite its small size the college has had some housing problems, and during the year there have been a number of reorganisations on the second floor of ILL20 in order to accommodate everybody. It has also been possible - by sacrificing the ladies' washroom - to create a room for crystallisation, which will be of importance for the single crystal work.

As usual, there is a close contact and collaboration with the EMBL, including sharing of seminars, and a first contact is established with the ESRF. The EMBL changed head during the year as Bernard Jacrot completed his tenure as director, and we welcome him back to the ILL. He was replaced by Stephen Cusack, who for a number of years already has been very active both in crystallography and protein dynamics, where he is a much appreciated user of different instruments for inelastic neutron scattering.

Scientific Trends and Highlights in 1989

Techniques

The college has also been active in the discussions that will lead to a proposal for a modernisation programme. Members of the college were engaged in the working groups, and in parallel a proposal has been put forward - in collaboration with the EMBL - for the construction of a Laue diffractometer for protein crystallography. The principle of this instrument is to accept the small size of protein crystals, and to balance this by use of a larger wavelength band combined with several independent position-sensitive detectors. Because of the small crystal size, high spatial resolution would naturally be required. The detector would be smaller and thus more compact, and at present the choice of the most suitable available system is being investigated.

Work has also been done on ab initio structure analysis based mainly on neutron contrast variation combined with direct methods (collaboration between LURE and ILL).

Contrary to the single and multiple isomorphous replacement techniques (SIR,MIR) used at high resolution with X-rays, the contrast-variation technique does not provide a solution of the so-called structure factor phase problem. In addition, SIR and MIR do not work at low resolution where the diffraction is dominated by the contrast between the average molecular scattering length density and the solvent scattering length density. Up to now the phasing of low-resolution data can be made only using models as starting point. To find a new way out, direct phasing with techniques used with small molecules is presently under investigation. After "F to E" initial normalisation, the method consists in using the program MITHRIL (MULTAN) to generate, in two contrasts, a number of phase-sets with good figures of merit. The best couple of phase-sets is then selected by comparing the average phase difference between the two phase-sets and the average phase difference obtained from the contrast variation data. The results

obtained up to now with this technique, applied on model data as well as on real data, are very encouraging. A method for refining and extending these phases will have to be worked out as a next step.

Nucleic acids, transcription and protein synthesis

DNA, the molecular storehouse of genetic information, is usually depicted as a linear double-helical polymer. However, in vivo the axis of this duplex chain usually forms a higher-order helix or superhelix. Virtually every biological, physical and chemical property of DNA is altered by supercoiling. The structure of superhelical DNA is not well characterised and has usually been idealised as either a toroidal ring, rather like a coiled telephone cable, or as a rod consisting of two interwound duplex chains (see Figure 42). It was found that covalently closed rings of supercoiled DNA can form liquid crystals and, using neutron diffraction, they were shown to consist of a hexagonally packed array of rod-like particles over a range of concentrations. This provides the first clear evidence for the existence of an interwound conformation in solution. It was also possible to deduce approximate values for the pitch angle, the pitch and the radius of the interwound superhelix. The advantage of neutrons in this study is that they do not cause chemical damage which could progressively destroy the covalently closed nature of the molecules under investigation.

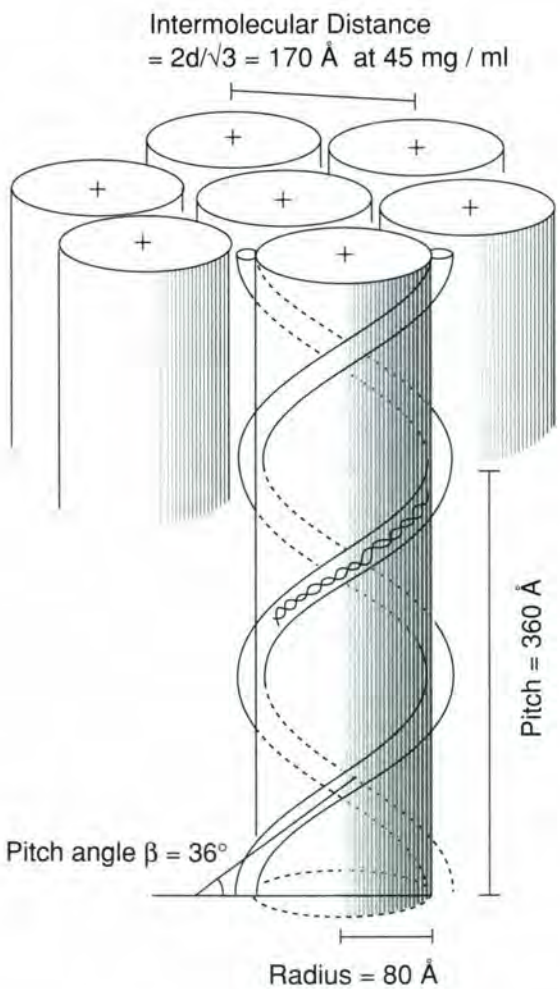

Fig. 42: Sketch of the interwound superhelix showing the approximate value of the parameters derived. The packing dimensions are shown for a concentration of 45 mg/ml. The superhelical density was 0.05 (i.e. the number of superturns per 10 base pairs).

When DNA is transcribed into base-complementary RNA a key enzyme, present in all living organisms, is RNA polymerase (RNAP). The spatial arrangement of this enzyme (from the bacterium Escherichia Coli) with respect to DNA has been studied in situ using neutron scattering (collaboration between MPI, Martinsried and ILL). RNAP of E.Coli is an elongated, trigonally shaped molecule with asymmetrically located subunits (MW = 450,000). The model for the quaternary structure of the RNA polymerase-promoter complex previously evaluated by neutron scattering shows that the long axis of RNAP runs parallel to the DNA axis.

The question is then how RNAP is oriented with respect to the direction of transcription, and to answer this question, distance measurements were made from RNAP to a point of reference on the DNA. The point chosen was the Tet repressor molecule, and a specifically designed DNA fragment of 126 base pairs was used, which carried the Tet repressor binding site. The centre-to-centre distance of 150 Å from RNAP to the Tet repressor is consistent with only one of the two possible orientations of RNAP. The base of the trigonally shaped RNAP faces the downstream direction while the tip of RNAP points in the up stream direction.

Finally, at the end of the process the code (messenger RNA) is transferred to the ribosomes where the proteins are synthetized. These particles are large molecular assemblies 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 ribosomal RNA) and a very long one (23S rRNA), and more than 30 proteins.

A long-term project conducted by scientists of the Max-Planck-Institut 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. The study had begun with the larger ones on the 50S proteins. In the meantime, some of the smaller 50S proteins, and some of the proteins in the small (30S) subunit (S1 to S21) have been included in the investigation. Recently, also a few inter-subunit protein distances have been determined in order to clarify the orientation of the subunits with respect to each other.

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 distance table obtained from the more than 120 different 50S pair-distance measurements collected to date

(some of them repeatedly) should result in a three-dimensional arrangement of 24 of the 50S proteins. A number of critical distances, however, need yet to be verified, since they are of insufficient quality or cannot be reconciled with the consistency control furnished by the redundancy of distances in the model-building procedure.

In recent years these protein factories have also been crystallized, and all the available techniques for structure analysis are now being used in order to give further information about the ribosome structure. One method to be used is low-resolution (30 Å) single-crystal neutron analysis with H_2O/D_2O contrast variation, and work has been undertaken on crystals of the large subunit from Halobacterium marismortui grown at the MPI in Berlin (collaboration with MPI, Hamburg and ILL). They were then soaked in buffers containing different D_2O concentrations to perform the contrast variation experiments. The crystals are very thin plates (0.5 x 0.5 x 0.1 mm^3); because of their high water content they are very fragile and do not even support the touch of a hair. As a consequence of the small size of the crystals the diffraction peaks are very weak and one data collection takes about 3 weeks. It is very difficult in these conditions to control rapidly the quality of the crystals and several data sets have to be collected for one contrast before good data are obtained. Up to now a fairly good intensity set was obtained for 100% D_2O; several 100% H_2O data were collected and the integration is in progress.

Various components of the cellular protein synthesis apparatus are also being studied, and the results from the SANS contrast variation study of seryl-tRNA synthetase and its interactions with $tRNA^{ser}$ (EMBL-Grenoble and ILL) have been interpreted by using the crystal structure of the protein which is now almost completely solved (EMBL-Grenoble). It is an elegant illustration of the usefulness of complementary approaches to the study of a complex problem. A similar study has been initiated on glutaminyl-tRNA synthetase (Yale University and ILL). Since the molecular biology of seryl-tRNA synthetase is also well developed (EMBL-Grenoble), a promising future project is to combine protein engineering and different structural studies of this protein-nucleic acid system.

Finally the study of the complex of E. Coli elongation factor Tu with GTP and amino-acyl tRNA (Pustchino-USSR, EMBL-Grenoble and ILL) has continued after initial studies showed the applicability of the triple isomorphous replacement contrast- variation method proposed by the Russian group.

Protein-membrane interactions

Phospholipid-protein interactions are common in nature, and are now extensively studied with neutrons. As for many other studies using neutrons the essential experimental feature relies on H_2O/D_2O contrast variation. Both small-angle scattering and crystallographic techniques are used. The lipid-storage protein lipovitellin from Lamprey oocytes has been extensively studied by X-ray crystallography. This dimeric protein contains some 60 - 70 molecules of bound phospholipid. Each subunit contains 3 polypeptide chains comprising some 1300 amino acids. The electron density maps at 2.8 Å resolution show clearly the conformation of the protein but no density is interpretable as phospholipid. This is now being sought using neutron crystallography with H_2O/D_2O contrast variation to a resolution of 13 Å (Minneapolis, ILL and EMBL-Grenoble). Preliminary results indicate that the phospholipid is mainly located within a cavity in the protein which in the X-ray maps is an area of extremely low density. That amino acid sequence is currently being determined in order to understand the interactions which mediate protein-phospholipid interactions.

Colicins are bacterial proteins which kill sensitive E. Coli cells. Colicin A belongs to the group of colicins which collapse the membrane potential by forming voltage dependent channels. The C-terminal domain of colicin A has been crystallized and the structure of its soluble form solved. A model has been proposed whereby on binding to the membrane the protein inserts a helical part of its structure into the membrane and at the same time oligomerizes. Such a membrane-bound conformation can be found in a complex of the pore-forming domain of the protein with the negatively charged phospholipid DMPG. Neutron small-angle scattering studies are being carried out to determine the distribution of protein and lipid within this complex (EMBL-Heidelberg and ILL).

Another important feature of structural studies on membrane proteins is the understanding of the parameters which control crystal growth in these systems. To date all successful crystallisations of membrane proteins have been by manipulation of protein/detergent complexes. The precise role of the detergent and the reasons for which particular detergents are more or less efficient is not as yet understood. Neutron scattering has been used to characterise some of the more useful detergents in terms of micelle size and aggregation number. More recently the effects of small amphiphiles, which are commonly used as cofactors in crystallisation, has been investigated. In the case of the detergent dodecyl diamine oxide (LDAO) it has been shown that the micelle curvature can be finely tuned by the addition of the appropriate amount of small amphiphile. The radius of curvature of the attached micelle may well be one of the important factors in determining whether a membrane protein can form 3-dimensional crystals (Freiburg and ILL).

The photosynthetic reaction centre has been in the centre of interest these last years as it was the first membrane-protein complex to be determined to atomic resolution by X-ray diffraction. This work has now been followed up in a collaboration between Munich, Gif-sur-Yvette and ILL to answer some specific questions concerning the membrane/protein interaction.

The Photosynthetic Reaction Centres of membranes of bacteria are solubilised from the bacterial membrane with detergents (LDAO for the bacteria *Rhodopseudomonas Viridis* or octyl-glucoside for *Rhodobacter Sphaeroides*) before crystallisation. The structure of the protein and chromophores can be determined by X-ray crystallography, but not the structure of the detergent which appears disordered at atomic scale. The structure of the detergent has been determined using neutron diffraction at low resolution (Bragg d-spacings > 15 Å) and the H_2O/D_2O contrast-variation technique. The data collection was performed using the low-resolution diffraction facilities

with first D17, then DB21. The phasing of neutron diffraction data was made by combining the known atomic structure of the protein and chromophores, and the contrast variation data, using a joint probability distribution of Fcalc's and Fobs's developed for contrast variation technique. In both cases (*Rhodopseudomonas Viridis* and *Rhodobacter Sphaeroides*), the detergent appears in these crystals in the form of rings encircling each reaction centre molecule in the same region i.e. around the transmembrane helices of subunits H, L, and M (see Fig. 43, see page 75 and front cover). These rings (one ring/molecule) are connected two by two through detergent *bridges*. The rings therefore form continuous chains. All chains are parallel to a common crystallographic direction. There are no connections between neighbouring parallel chains. The regions of protein-protein contact not being located in detergent regions, one can conclude that the stability of these crystals is based on both direct protein-protein interaction and detergent structure. The exact comparison of the size and shape of the rings in the two systems under investigation is in progress, as well as a detailed hydrophobic/hydrophilic analysis of the protein-detergent interface.

Work has also continued on the purple membrane of Halobacterium halobium, which occurs naturally as two-dimensional crystals. The labelling study of the membrane protein, bacteriorhodopsin, which was a collaboration between Paris, Yale and ILL, is now completed, as well as the study of the structural differences between the ground state of the protein, which is a light-driven proton pump, and its most long-lived excited state (Berlin and ILL). Dynamic studies are also under way as discussed below.

Although sodium dodecyl sulphate (SDS) is not itself of much biological interest, its wide spread use in biological preparations largely justifies studies of SDS-protein interactions. Analysis of the complexes formed by a bifunctional two-domain enzyme (isomerase:synthase) with SDS molecules has shed further light on the disputed structure (ILL, Basle and Uppsala). The isomerase:synthase chosen has 452 amino acids, and complexes with 216 SDS molecules. By analysing the distance distribution function at the match-points of the hydrocarbon moieties and deuterated protein/sulphate moieties for the intact protein/SDS complex, the structure was deduced to be a linked triple-micellar structure, with each micelle being composed of a hydrocarbon core with a thin shell consisting of the polypeptide chain and sulphate groups. Figure 44 shows the protein-decorated micelle model as seen by neutrons using D_2O and H_2O, and exemplifies well the power of contrast-variation studies.

Viruses, protein stability, water and dynamics

Bacteriophage T7 is an isometric particle (with a small tail) which contains ~ 50% by weight DNA. Various physical techniques indicate that when this virus is transferred to a low ionic-strength environment a major structural change takes place. Small-angle scattering with contrast variation is currently being used to investigate this effect. Preliminary results indicate that a large part of the DNA is released from the particle and that some change in the protein may also take place (Budapest, Moscow and ILL).

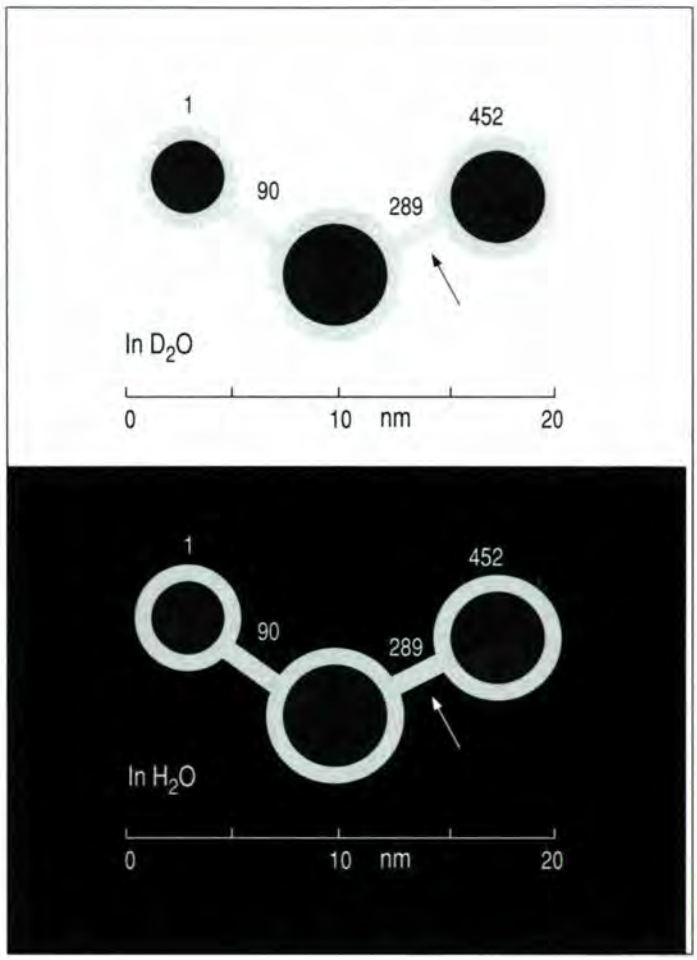

Fig. 44: Model for SDS/isomerase:synthase complex. The interior is hydrocarbon while the exterior is decorated with protein (deuterated) and sulphate groups. In D_2O the deuterated and sulphate parts are invisible, revealing the hydrocarbon core, while the opposite is true in H_2O.

Experiments have also continued on the release of RNA from particles of Turnip Mosaic Virus (TYMV) on freezing/thawing. These experiments, carried out at 80 K on D11 confirm that the RNA is released during the thawing rather than the freezing process (Strasbourg and ILL).

The protein P1 encoded by the yeast retrotransposon Ty is capable of self-assembly into multimeric structures referred to as virus-like particles (VLP's). Fusion proteins based on P1 retain the ability to form VLPs and are being used as a carrier system for recombinant viral antigens such as the HIV antigens gp120, TAT etc. The structural analysis of VLPs is an important step in the understanding of these particles.

Small-angle neutron scattering has recently been used to characterise the generic VLP particle made from the N-terminal 386 amino acids of P1. This particle, apart from the proteins, also contains a piece of RNA which through contrast variation has been located in the interior of the protein. In addition, the overall dimensions and distribution of the protein have been determined (Oxford and ILL).

College 8

The stability and shape of a protein depends on both its state and the solvent environment, and a number of studies relate to this subject. An example of the first kind are the studies of the stability of halophilic proteins, which continue in a multinational collaboration involving teams from Israel, India, France and the ILL, not only using SANS, but also other biophysical methods.

An example of the second kind is experiments on the cAMP dependent protein kinase suggesting that a major conformational change takes place on binding of the inhibitory peptide ITP. This results in a radius of gyration change of 1-2 Å. A similar phenomenon was observed in the past for yeast hexokinase on binding of glucose, and the present observation seems to confirm the hypothesis that the substrate inducing closing of the catalytic cleft is a general feature of all kinases (Montpellier, San Diego and ILL). Preliminary experiments were also carried out on the restriction enzyme EcoRV in order to investigate possible conformational changes on DNA binding (Hamburg, EMBL-Grenoble and ILL).

Water arrangements have equally come under close scrutiny, but are best studied in ordered systems. In the case of DNA, diffraction studies on ordered fibres of Calf-thymus DNA using isotopic substitution of H_2O by D_2O have been used to locate water positions around the DNA double helix. Fig. 45 shows scattering patterns recorded on the D19 multidetector from DNA in the A form in H_2O and D_2O solvents. Using a model of ADNA derived from X-ray diffraction, a Fourier difference synthesis between the two systems has been performed. A projection of the resultant density map, representing ordered water in the major groove, is shown in Fig. 46 (see page 75). The ability of DNA, under appropriate ionic conditions, to undergo humidity dependent transitions between conformations with possibly different functional roles makes the relation between ordered water and molecular conformation of particular interest. The A form, also adopted by RNA double helices and RNA-DNA hybrids, has been associated with the transcription of genetic information (Keele and ILL).

Single crystals give the most detailed structural information on water structure. Work was concentrated this year on a high resolution study to a resolution of 1 Å undertaken on vitamin B_{12} in a collaboration between Birkbeck College, Karlsruhe and ILL in an attempt to learn more about water order/disorder. For this reason the data were collected at 15 K, following up the very successful study at room temperature executed over a decade ago. A total of 15400 Bragg reflections were recorded on D19, giving 5500 independent reflection data with an overall statistical precision of 5%. Analysis is now underway.

Most of the dynamical studies of proteins concern soluble proteins (lysozyme, myoglobine, etc.), and this has triggered a wish to elucidate the dynamical behaviour of membrane proteins.

A very suitable candidate, well known to the group, is the bacteriorhodopsin of purple membrane where a first experiment was done using temperature scans on IN13 (ILL). Comparison to similar scans of hydrated samples of myoglobin (EMBL-Grenoble, Munich and ILL) showed remarkable differences. For myoglobin, a transition takes place around 180 K, which can be attributed to excitations of non-vibrational motions (corresponding to torsional transitions between two different energetic states of the protein). A similar change is not seen for the protein embedded in phospholipid. The evolution of the amplitudes of vibrational motion as a function of temperature, and for quasi-similar hydration of the membrane/protein complex, is much smoother. This is not yet completely understood, but hints at a rather hard coupling between lipids and bacteriorhodopsin. Attempts are now underway to work on membrane free bacteriorhodopsin.

Secretary: M.S. Lehmann

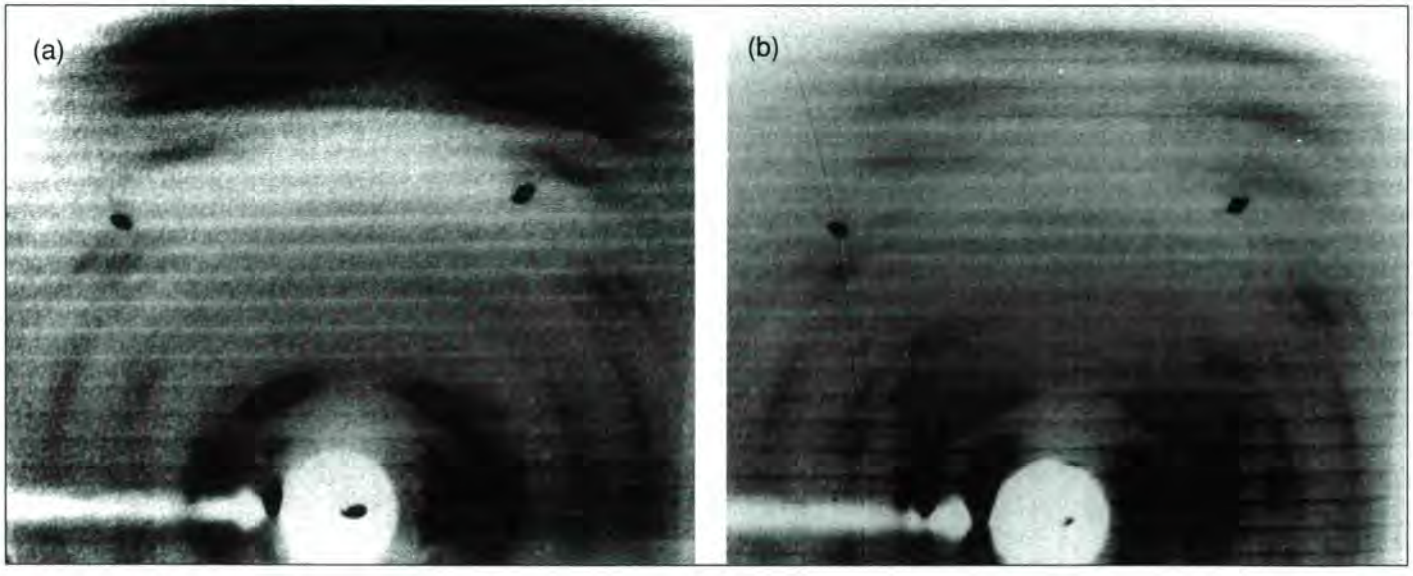

Fig. 45: Neutron diffraction data: (a) A-DNA with D_2O and (b) A-DNA with H_2O.

Molecular Spectroscopy, Surfaces and Mesophases

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Summary

Following a considerable decline in the years 1985-1987 the number of proposals submitted to College IXa has increased markedly again for the last two subcommittee rounds. Inelastic and quasielastic scattering continue to be the main techniques used, IN5 and IN6 remain heavily overloaded. The chemical systems studied get more sophisticated, and a tendency towards the study of dynamical processes in zeolites and inclusion/intercalation compounds can be noted. Surface studies using QNS, TAS and diffraction methods continue to be a main subject in College IXa, and the combination of several techniques proves very useful to advance our knowledge of the parameters governing the surface-adsorbate and adsorbate-adsorbate interactions. As a new field of scientific activity one has to mention the studies on liquid-air and liquid-solid interfaces using neutron reflection on D17.

Scientific Highlights in 1989

Tunnelling

The isotope effect of tunnelling of coupled methyl groups was studied in lithium acetate dihydrate (LIAC) by high-resolution inelastic neutron scattering (ILL, Braunschweig, Erlangen). LIAC is the model system for coupled pairs of methyl groups because they occur in pairs with a common axis of rotation in this sytem. Fully protonated, fully deuterated and mixed LIAC samples were investigated on IN10 and IN13. Tunnelling spectra from mixed LIAC samples $(CH_3)_c(CD_3)_{1-c}$ $COOLi.2D_2O$ were measured on IN13. A fit with a simple model was made in which it is assumed that the single particle potential hindering rotation is increased by a factor of 1.5 by deuteration, whereas the coupling potential is almost unchanged. The strong increase of the single particle potential by deuteration is tentatively explained by a model of phonon mediated coupling. The latter model is also capable explaining the spin temperature dependence of tunnelling spectra of LIAC(H) published earlier.

IQNS study of highly oriented fibres of copper laurate

Binuclear copper (II) complexes of fatty acids exhibit a phase transition from a lamellar-crystalline lattice to a liquid-crystalline mesophase above approx. 400 K. The latter is of the columnar type : columns made of stacked binuclear units, each unit being surrounded by four alkyl chains, are arranged in a two-dimensional hexagonal lattice. Copper laurate can be processed into oriented fibres by melt spinning of its thermotropic columnar mesophase. X-ray diffraction shows a high degree of orientation of the spun fibres in the solid state which upon heating results in columnar liquid-crystalline fibres of high anisotropic order.

Fibres of dicopper laurate were analysed using the high-resolution backscattering spectrometer IN10 (Saint-Martin-d'Hères, Grenoble, ILL).

Several measurements were carried out with different orientations of the fibres with respect to the incident neutron beam. The geometry is illustrated in Fig. 47. At the particular value of the scattering angle $2\theta = 90°$, the momentum transfer vector Q is either parallel ($a = 135°$) or perpendicular ($a = 45°$) to the direction of the columns of stacked molecules. In the former case, quasielastic scattering results only from motions of the alkyl chains along the directions of the columns (while $Q.d_T = 0$). Conversely, motions about the column axes yield a broadening of the spectra recorded with the latter geometry, the longitudinal motions resulting in pure elastic scattering ($Q.d_L = 0$). The difference between the spectra obtained for both geometries clearly showed a preferential motion of the alkyl chains around the axes of the columns.

Molecular dynamics of a van der Waals complex

The charge distributions of the simple aromatic molecules benzene and hexafluorobenzene are of considerable interest, their symmetry implies that all odd electric moments vanish and that there is just one independent quadrupole moment.

The large values and the difference in the polarity of the quadrupole moment for benzene and hexafluorobenzene implies that the interaction of these two molecules will be particularly strong. This is indeed what is seen, simple mixing of an equimolar quantity of C_6H_6 and C_6F_6 results in a

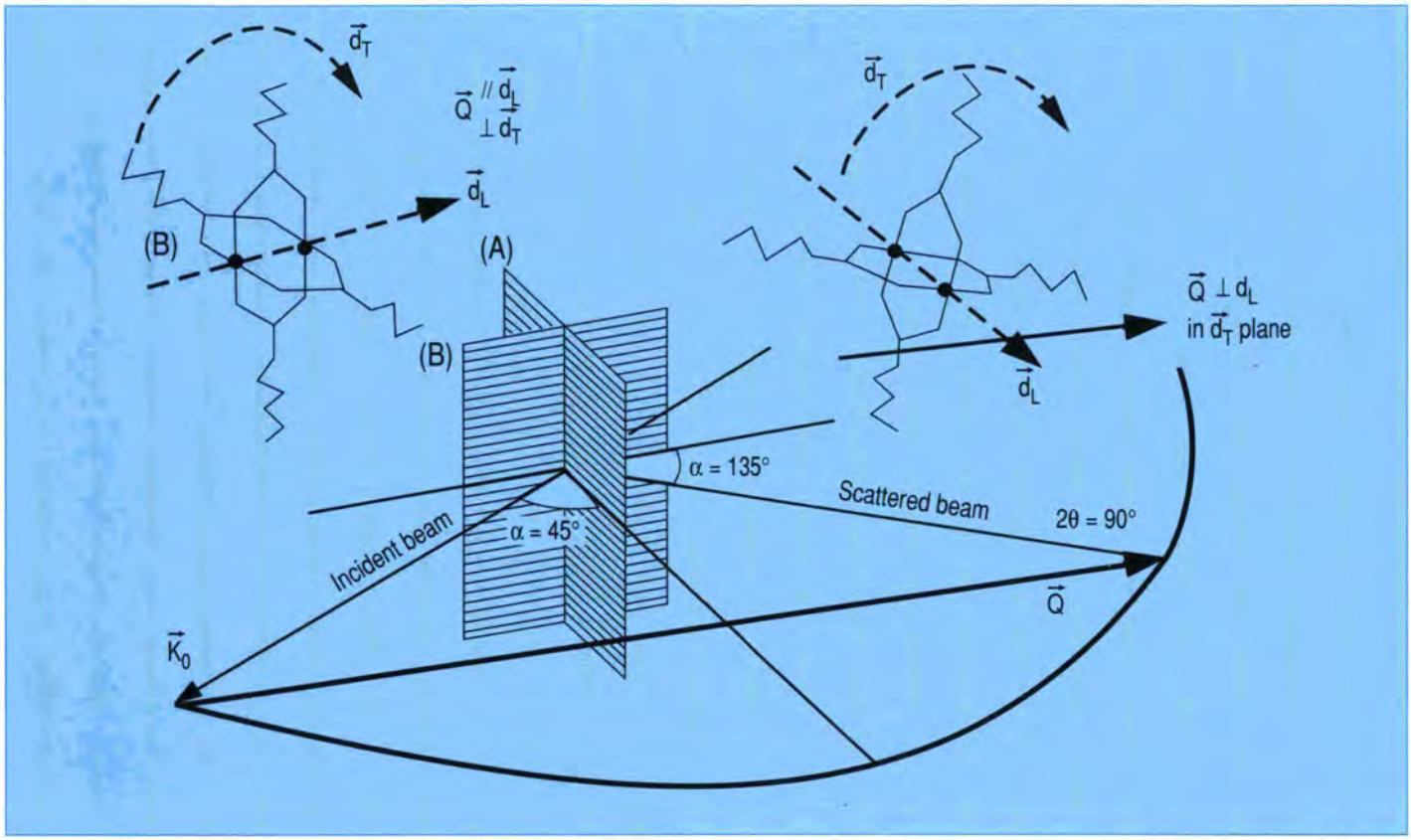

Fig. 47: The geometry of the IQNS-experiment on oriented fibres of copper laurate.

crystalline solid which has a melting point of 24°C. Motional processes were investigated on IN13 using a powdered sample. A fixed window scan reproduced 3 phase transitions already known from calorimetric data. The mean proton displacement evaluated for the T range 150 K - 299 K showed discontinuities at 208 K, 252 K and 273 K. The nonlinearity of the $\ln S(\bar{Q},w)T$ versus $\bar{Q}_2$ plot above 273 K indicated the presence of more than one dynamic process. This was confirmed by quasielastic data suggesting the onset of motion on a polymolecular level some 20 degrees below the melting point.

Dynamics of benzene and methane adsorbed in Zeolite ZSM-5

The quasi-elastic neutron scattering of benzene adsorbed at two different loadings in H-ZSM-5 has been studied in the temperature range 90-400 K (Villeurbanne, St. Martin d'Hères, ILL). The translational motion is too slow to be observed on the timescale of the experiment so that only the rotational motions can be characterized. The model of uniaxial rotation in an N-fold cosine potential is used to interpret the experimental data

The EISF for a powdered sample is given by

$$A_0(Q) = \frac{1}{\pi I_0^2(\gamma_N')} \int_0^\pi j_0(2Q\mathrm{r}\sin x)\, I_0(2\gamma_N' \cos Nx)\, dx$$

where I_0 is a Bessel function of the first kind, N the number of wells and γ_N' is related to the potential barrier by

$$\gamma_N' = V_N/2K_BT$$

where $$V(\phi) = -\frac{V_N}{2}\cos(N\phi).$$

The order parameter γ_N' is defined as the average value of $\cos(N\phi)$

$$\gamma_N' = \langle \cos(N\phi) \rangle = \frac{I_1(\gamma_N')}{I_0(\gamma_N')}.$$

It has been shown that from the general expression both the EISF of the rotational diffusion model on a circle and the EISF of the circular jump model among N sites can be derived. Calculated EISFs are shown in Figs. 48(a) and (b) as solid lines.

With decreasing temperature there is a progressive blocking of the molecules for both loadings, but the amplitude of motion is more restricted at higher loading, at the same temperature, indicating benzene-benzene interactions. Isotropic spherical rotation is not observed, in agreement with NMR results, and the C_6 uniaxial rotation is as fast as in the liquid, with a correlation time $\tau = 3.2 \times 10^{-12}$s at 300 K.

The translational and rotational motions of **methane adsorbed at different loadings in NaZSM-5** have been studied by

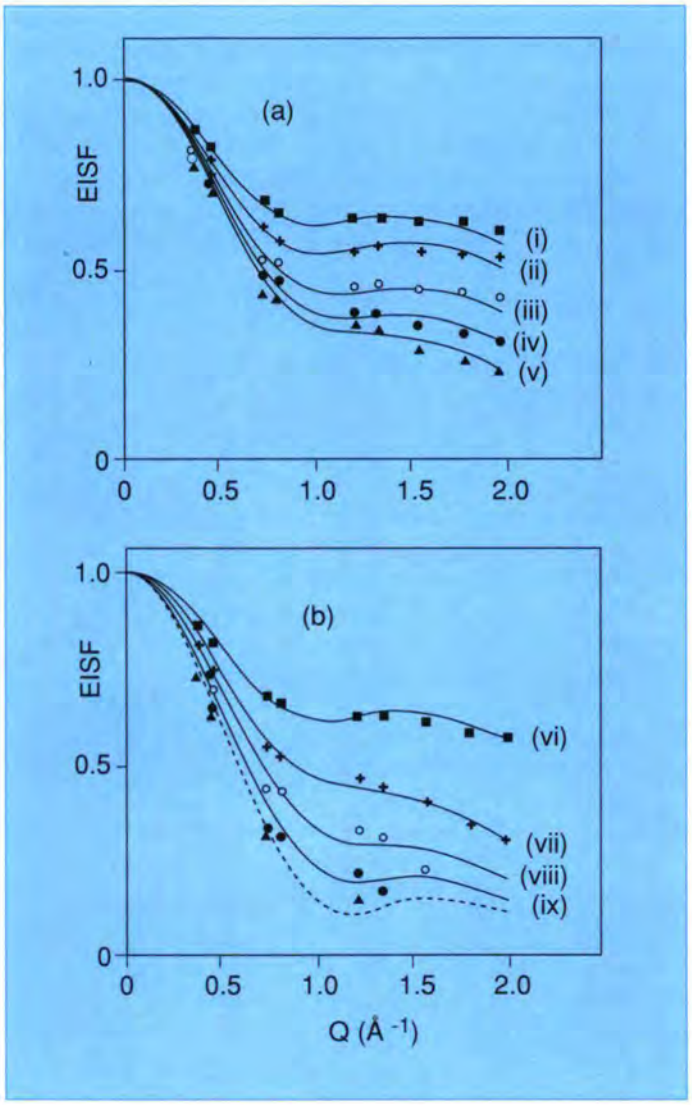

Fig. 48: EISF values of benzene adsorbed at different temperatures in ZSM-5; (a) θ_2, (b) θ_1. The solid lines are curves calculated with the model described in the text, $\Delta\phi$ being an average angle of rotation. The dashed line in (b) corresponds to the C_6 uniaxial rotation of benzene with jumps of 60°. Values of $\Delta\phi$: (i) 13°; (ii) 16°; (iii) 23°; (iv) 28°; (v) 32.6°; (vi) 14°; (vii) 22°; (viii) 36°; (ix) 48°; T/K : ■, 90; ✚, 150; ○, 220; ●, 300; ▲, 400.

quasi-elastic neutron scattering at two temperatures : 200 and 250 K. The translational motion does not simply follow Fick's law, but a jump diffusion model with a Gaussian distribution of jump lengths satisfactorily simulates the experimental results. The diffusion coefficient that is obtained for long-range translational motion does not vary much on the loading in the range that was studied. It ranges from 2.7 x 10^{-5} cm^2 s^{-1} at 200 K to 5.5 x 10^{-5} cm^2 s^{-1} at 250 K. Good agreement is found between the neutron and NMR results for this motion, but large discrepancies are observed with the macroscopic measurements.

The isotropic rotational diffusion coefficients of methane, D_R, deduced from the FWHM of the rotational broadenings, are shown in table 1 as a function of temperature and loading. Comparison with D_R values obtained for methane adsorbed on graphite (6 x 10^{11} s^{-1} at 55 K) or with the value obtained for bulk solid methane (10^{12} s^{-1} at 21 K) shows that the rotational motion of methane is much slower in the zeolite, which indicates interactions of the molecule with the framework.

	T = 200 K		T = 250 K		
Loading (molecule/u.c.)	FWHM (meV)	D_R x 10^{-10} (s^{-1})	FWHM Loading	D_R x 10^{-10} (meV)	(s^{-1})
2	0.066	2.5	1.5	0.12	4.6
4	0.1	3.8	3.8	0.124	4.7

Table 1: Values of D_R, the isotropic rotational diffusion coefficient of methane, as a function of temperature and loading.

Surface studies

Gases physisorbed on adequate substrates present a large variety of phases and phase transitions. Graphite has been one of the most studied substrates, since good characterized samples with a large surface to mass ratio can easily be produced. The observed phase transitions are the result of a delicate balance between the interaction of the adsorbed gas and the substrate, and between the adsorbed molecules themselves. Unfortunately, not enough is known about the details of these interaction potentials since not many experimental techniques are available. The adsorption potential itself has been determined mainly with molecular beam scattering, but the magnitude of the in-plane corrugation of the adsorption potential is very difficult to determine in this way. It is this corrugation that forces some physisorbed substances into a commensurate phase and, due to the lost translational invariance, produces an energy gap at the zone centre in the acoustic branches of the phonon spectrum. Thus, the determination of this gap is a direct measure of the adsoprtion potential corrugation. The temperature renormalization of the phonon spectrum gives insight into the anharmonic terms of the adsorption and intermolecular potentials.

The inelastic neutron experiments that determined the phonon gap and its dependence on temperature were performed on the TAS IN3 and IN14 (Konstanz, ILL). The gases studied can be grouped mainly into two classes according to their quantum character. The hydrogen isotopes (H_2, HD, D_2) and ^3He are typical quantum gases; their interaction potential is weak, they present a large zero-point motion and a very large compressibility. Nitrogen (N_2) and deuterated - methane (CD_4), on the other hand, are much heavier molecules, less compressible and with a smaller zero point motion. These differences are shown in their 2-dimensional phonon spectrum. The quantum gases present very little dispersion and resemble Einstein oscillators in a first approximation. Due to their strong

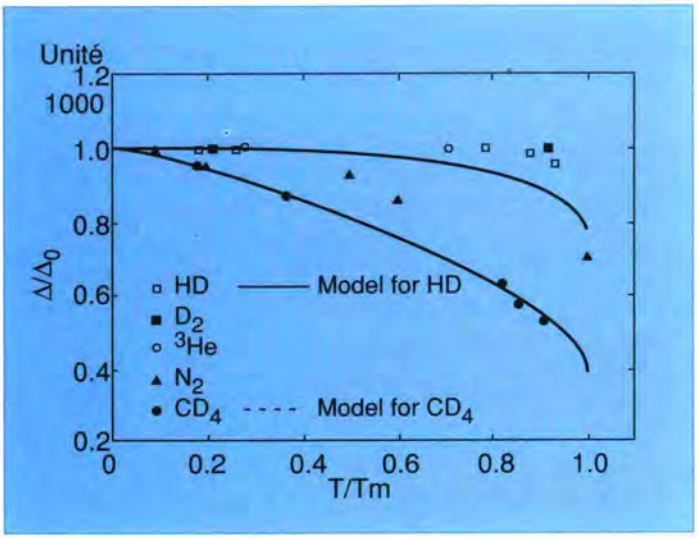

Fig. 49: Normalized zone centre phonon gap vs. reduced temperature for several gases. The lines are the result of the model calculation. Δ stands for the zone centre phonon gap).

interaction between adsorbed molecules, the dispersion curves of N_2 and CD_4 cover a wider energy range.

The Fig. 49 shows the temperature renormalization of the phonon gap due to the strong anharmonicity of the adsorbate potential for the available data. The q = 0 mode depends only on the curvature of the adsoprtion potential and not on the intermolecular forces. The effective curvature is a weighted average over, say, the root mean square amplitude of vibration, which is in turn determined by the effective curvature of the potential. This quasi-harmonic approximation must then be solved in a self-consistent way. On the other hand, the intermolecular potential is also anharmonic and can be developed in terms of the two particle correlation function. This further anharmonicity renormalizes the whole frequency spectrum of the phonons. The agreement between the data and the model is reasonable taking into account the poor knowledge of the potential parameters involved. In this treatment, a mean field approach has been used which should break down near the melting transition. But the qualitative features of the temperature dependence of the phonon gap are well reproduced. For the quantum gases, the rms vibrational amplitude is determined by their zero-point motion and is little affected by thermal population of phonons. On the other hand for the heavier gases the melting temperature lies well above the cut-off energy of the phonon DOS and the melting transition is driven by thermally excited phonons.

The structure of an iodomethane monolayer adsorbed on graphite was studied on the powder diffractometer D1B (Oxford, ILL)

The halomethanes are of particular interest because of their large dipole moments and the variation in molecule-molecule and surface-molecule interactions down the series.

The structural characterisation of these adsorbed layers usually rests upon fitting the positions and intensities of the experimental reflections with unit cells corresponding to a range of trial structures. The analysis may be limited because a single X-ray or neutron pattern often contains only one or two reflections, which leads to ambiguous results. One of the advantages of combining X-ray and neutron diffraction, with the consequent change of relative scattering of the elements, is that very few trial structures will be able to fit both patterns simultaneously.

The X-ray diffraction pattern from a layer of iodomethane (0.8 of a monolayer; 100 K) could be indexed on a small incommensurate unit cell containing two molecules. Because X-rays are only sensitive to the heavier halogen atoms, the positions of the methyl groups were not determined. Figure 50(a) gives the experimental neutron diffraction pattern from an adsorbed layer of iodomethane (same temperature and coverage as in the X-ray experiment) as obtained on D1B. Two of the reflections in this neutron pattern cannot be assigned on the small unit cell of the X-ray pattern. Doubling of the cell in the 'a' direction enabled all the reflections in both X-ray and neutron patterns to be assigned. The larger unit cell is required because of the lower symmetry of the methyl groups that were not shown in the X-ray pattern. The structure that gave the best fit to both patterns simultaneously is given in Fig. 51; the calculated neutron diffraction pattern is given in Fig. 50(b).

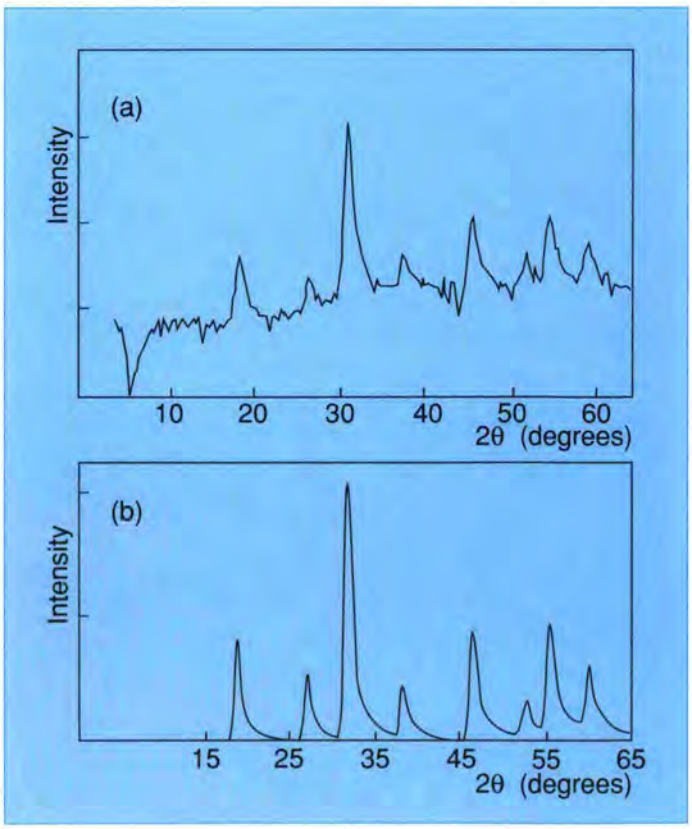

Fig. 50: Observed (a) and calculated (b) neutron diffraction patterns of CD_3I on graphite, (background of graphite subtracted), coverage 0.75 monolayers, temperature 100 K, and wavelength 0.252 nm.

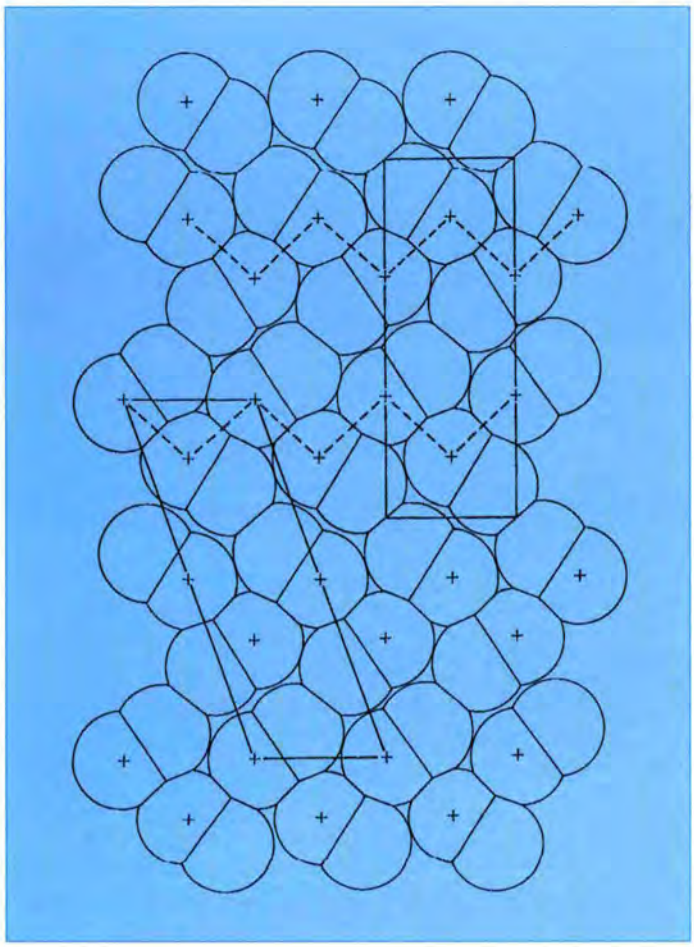

Fig. 51: The structure required to fit the X-ray and neutron patterns. Iodine atoms are indicated by crosses. Two unit cells are given to demonstrate the relation between the results deduced separately from X-rays and neutrons.

The structure of the adsorbed layer of iodomethane may be considered to be zig-zag chains of molecules in a head to head arrangement. Adjacent chains alternate in direction, thus the monolayer is antiferro-electrically ordered overall. There is evidence of dipolar ordering in the layer but strong halogen-halogen non-bonded interactions appear to dominate. The molecules are six-coordinate with space group pgg. This space group is consistent with the close packing requirements of incommensurate two dimensional layers.

Neutron reflection

Experiments on D17 have for the first time used neutron reflection from a solid-liquid interface to determine the structure of surfactant molecules adsorbed on a solid surface (Oxford, Rutherford, Port Sunlight, ILL). Neutrons were passed through an amorphous block of silica and reflected at the silica/water interface. Measurements of reflectivity as a function of angle were used to determine the structure of the adsorbed layer of dodecyl hexaoxyethylene ether ($C_{12}E_6$).

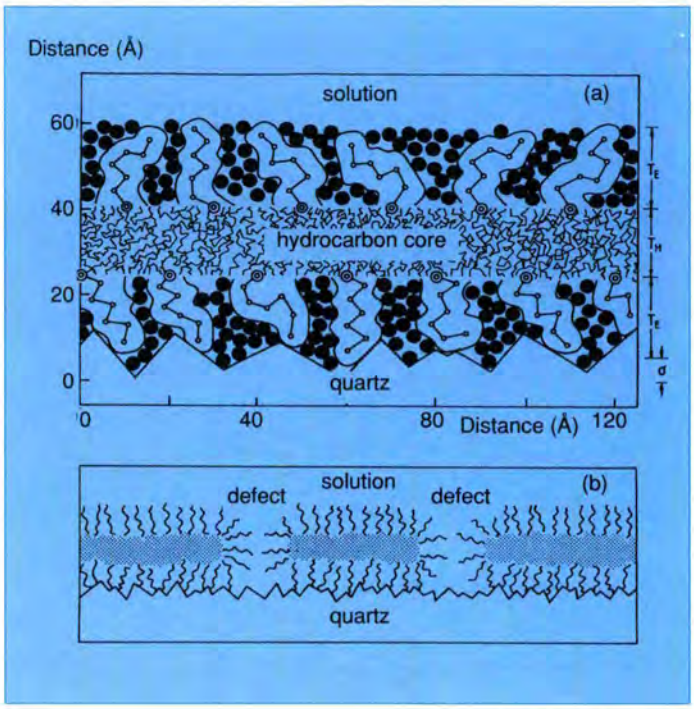

Fig. 52: Schematic diagrams of the structure of a layer of $C_{12}E_6$ at the quartz/water interface at the c.m.c. (a) is drawn approximately to scale and also shows some of the parameters used to characterize the model used to calculate the reflectivity profiles.

By varying the solvent contrast with isotropic substitution sufficient information was obtained from the reflectivity profiles to show that $C_{12}E_6$ adsorbs as a bilayer. These detailed measurements have allowed us to draw a surprisingly detailed model for the structure of this layer which is shown schematically in Fig. 52. Further experiments have investigated the effects of pH and coverage on this structure.

Secretary: C. Ritter

A new aspect of quantum motion of light particles in condensed matter: methyl tunnelling and quantum sine-Gordon breather in 4-methylpyridine crystal at low temperature

F. Fillaux, C. J. Carlile and G. J. Kearley

High resolution neutron scattering techniques have proven to be effective in direct observation of tunnel split ground states for a wide range of compounds containing rotating methyl groups with various potential barriers. At first, the single particle approximation [1] appeared consistent with experiments showing single bands for methyl tunneling. However, the improvement of spectrometer resolution and more thorough studies have revealed finer structures indicating possible rotor-rotor coupling. Here, we review new experiments on 4-methyl-pyridine (C_6H_7N, or γ-picoline), including isotopic mixtures of fully hydrogenated (4MP-h_7) and fully deuterated (4MP-d_7) species, showing that methyl-methyl coupling may extend over infinite chains in the crystal and give unusual dynamics.

Inelastic neutron scattering experiments

4MP was one of the first examples of direct observation of methyl tunnelling in a crystal [2]. The tunnelling frequency of 512 μeV is the highest known for a methyl group and a sixfold potential with a weak barrier was proposed. Recently, new spectra obtained on IRIS at ISIS have shown that beside the main transition at 516 μeV there is a weaker transition at 468 μeV and an unresolved shoulder near 535 μeV [3]. The spectrum obtained on IN5 at ILL with a better resolution (Fig. 53) clearly shows the three components.

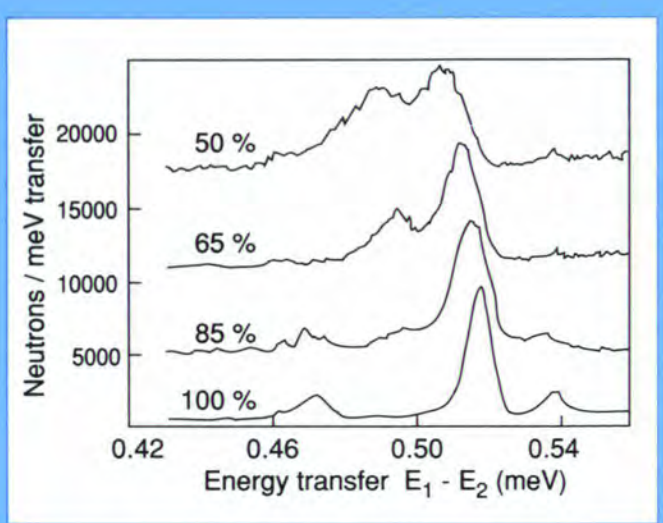

Fig. 53: High resolution IN5 spectra of 4MP-h_7 in isotopic mixtures of 4MP-h_7 and 4MP-d_7. Temperature is 0.5 K for the 100% 4MP-h_7 sample and 1.8 K for the others.

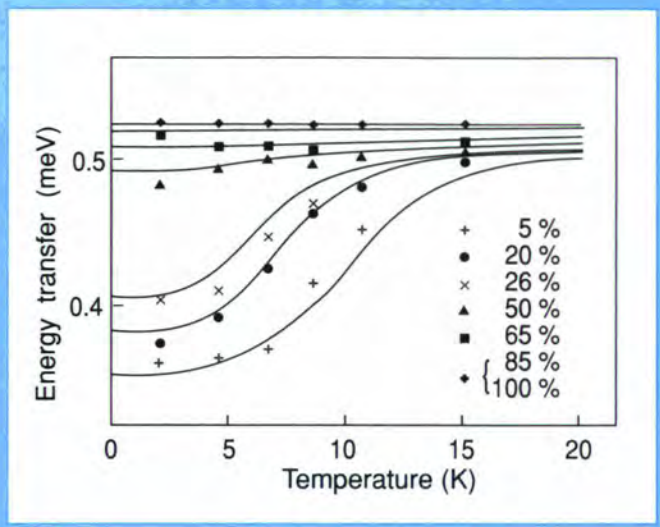

Fig. 54: Isothermal variation of the frequency at maximum intensity for 4MP-h_7 in isotopic mixtures of 4MP-h_7 and 4MP-d_7 measured on IRIS. The curves were calculated according to the proposed breather mode dynamics.

Since all the molecules in the crystal are equivalent [4, 5], these bands are due to inter or/and intramolecular coupling and in order to distinguish these couplings we have obtained the spectra of 4MP-h_7 in isotopic mixtures of 4MP-h_7 and 4MP-d_7. High resolution spectra of mixtures containing less than or 50% of 4MP-d_7 (Fig. 53) show a new band near 490 μeV which is assigned to mixed pairs of coupled methyl groups (CH_3-CD_3). A plot of the frequencies of the band maxima of 4MP-h_7 in isotopic mixtures at 2.5K containing up to 95% of 4MP-d_7 shows a spectacular decreasing of the frequency, down to 360 μeV, for concentration larger than 50% in 4MP-d_7 (Fig. 54). This frequency shift is extremely sensitive to temperature and vanishes above about 10-15K. 4MP-h_7 itself shows no frequency shift with temperature.

To our knowledge, such a complicated behaviour has never been reported for methyl tunnelling and it appeared impossible to rationalize these data with the theoretical models usually proposed.

The quantum sine-Gordon theory

A theoretical model for the collective rotation of methyl groups in 4MP is the infinite chain of coupled tops

$$H = \sum_j \left[-\frac{i}{2I_r}\frac{\partial^2}{\partial\theta_j^2} + \frac{1}{2}V_0\left(1-\cos(3\theta_j)\right) + \frac{1}{2}V_c\left(1-\cos\left(3i(\theta_{j+1}-\theta_j)\right)\right)\right] \quad (1)$$

This Hamiltonian is equivalent to that of the sine-Gordon potential [6, 7] if is restricted to small amplitudes. Then the coupling term can be linearized :

$$H \approx \sum_j \left[-\frac{i}{2I_r}\frac{\partial^2}{\partial\theta_j^2} + V_0\left(1-\cos(3\theta_j)\right) + \frac{1}{2}V_c\left(\frac{9}{2}\left((\theta_{j+1}-\theta_j)^2\right)\right)\right] \quad (2)$$

In this system phonons (or rotons), kinks (or solitons) and breathers are elementary excitations. Breathers can be viewed either as soliton-anti-soliton bound states or as anharmonic phonons. In the sine-Gordon system, these excitations have infinitely long lifetime and can propagate along the chain without deformation. At very low temperature, only breathers survive.

The spectra of pure 4MP-h_7 and 4MP-d_7 and 4MP-d_7 interpretated in terms of tunnelling and breather modes in a threefold quantum sine-Gordon potential. The weaker bands at 535 and 468 μeV in 4MP-h_7 (Fig. 53) are assigned to in-phase and out-of-phase tunnelling transitions, respectively. The energy spectrum calculated for the travelling motion of the breather is in good agreement with the band observed at 516 μeV.

Breather dynamics in isotopic mixtures

In isotopic mixtures of 4MP-h_7 and 4MP-d_7 the molecules are distributed randomly among the crystal sites. Therefore h_7 and d_7 molecules are distributed as clusters of various sizes which form a very inhomogeneous medium for the breather dynamics. We presume that deuterated clusters play the role of reflective walls for breathers in h_7 clusters, and vice-versa. As the cluster size decreases the energy of the ground state with respect to that of the infinite cluster increases. The first excited travelling state, on the other hand, is not affected. Therefore, the transition frequency decreases. Temperature effects are consistent with the existence of thermally populated breather-roton states. A simple calculation including the cluster size statistic and a first order law for the thermally activated process provides a nice fit for the experimental data (Fig. 54) which strongly support this interpretation.

At the present stage, the quantum sine-Gordon theory provides a very compact and elegant tool for interpreting the INS spectra and for describing the peculiar dynamics of methyl torsion in 4MP. Is this theory the only one capable of such a comprehensive description of the methyl dynamics in 4MP? The answer is probably yes. However, some aspects are not yet clearly settled and it is hoped that this work will stimulate further theoretical developments. Besides, it is suspected that the existence of breathers and solitons must be related to some unusual physical properties which have not yet been observed. So far, we do not know whether 4PM is unique and we are actively looking for new compounds with similar methyl dynamics.

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Large Molecules

Members

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Introduction

The College life continued to be very active as in recent years. The number of proposals stayed about constant. There seems to be a regain of interest in polymer science, especially in the field of gels and networks. The shear and real-time measurements continue to attract interest on the small-angle instruments. D11 and IN11 have still the heaviest overdemand, about a factor 2.5.

Scientific Highlights in 1989

Trapped chains in a deformed polymer network

A certain number of reactive sites (chemically measured) are first fixed randomly on long polystyrene chains and then connected two by two by a difunctional reagent. This cross-linking reaction produces a network. It is also possible to incorporate some polystyrene chains with no reactive sites, which after cross-linking, will just be trapped (without being linked). These chains are chosen deuterated. The result of this mixing prepared in solution is a polystyrene sample, which after drying can be deformed above its glass transition temperature. The response of the system to deformation and its evolution towards equilibrium under strain can thus be observed by SANS, through the spatial correlation of the perdeuterated chains.

We present in Fig. 55 one of the most striking spectra obtained in the conditions of equilibrium under strain, with rather long trapped chains, (100000), and high cross-linking degree (1 site for 44 monometers), and an elongation ratio of three. The intensity pattern, on the X, Y detector, exhibits an "8"or butterfly shape similar to the one first observed by Oeser and Rennie. The stretching axis is horizontal. The lobes of the 8 are vertically elongated ellipses. In the middle of each lobe a peak of intensity appears clearly. Similar figures, although less pronounced, have been observed this year on hydrogenated gels swollen by deuterated solvents, stretched in a swollen state, which is a very interesting result (LLB Saclay, ICS Strasbourg).

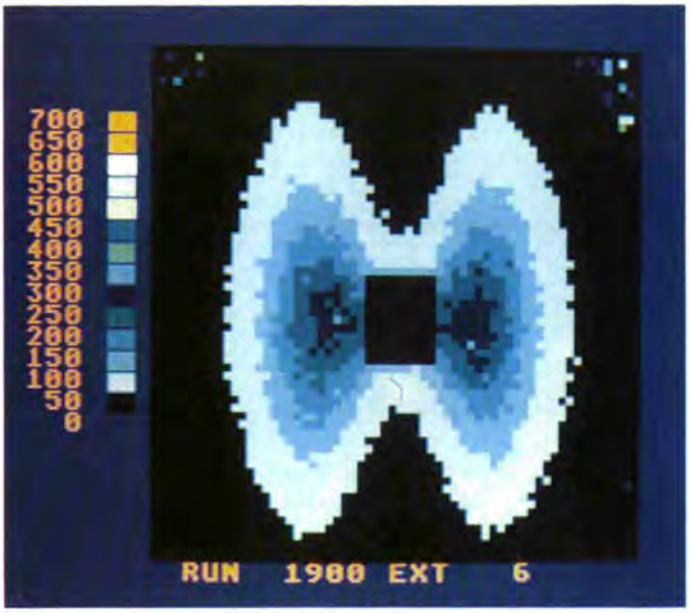


Fig. 55: Trapped deuterated polystyrene chains in a protonated polystyrene network under strain.

Topologies of polymer networks

Polymer networks are widely used as material for various applications. Their properties are closely related to their knotting topology, e.g. the geometrical scheme of how the polymer chains are arranged by the crosslinks. In recent years, a way has been developed to model networks by smaller substructures, so called μ-gels or μ-networks. This procedure has many advantages compared to their macroscopic pendants: well defined topologies can be more easily synthesized and purified. Further more, these structures can be characterized by the classical methods of polymer analysis in solution.

Fig. 56 shows the form factor of a spherical polystyrene micro-network, made by suspension polymerization (cross-linking density 50, i.e. 50 monomer units between cross-links) and dissolved in toluene-d8. Measurements were done at D11 at 5 sample-to-detector distances (2.5m - 36m) at a wavelength of 0.6 nm (Q-range : $0.02 < Q/nm^{-1} < 1.5$). Clearly seen is the particle form factor of a sphere at lowest and intermediate Q-values, including the oscillations. This indicates an only moderate polydispersity of the particles. At higher Q-values the Q^{-4}-scattering of a sphere is modified towards a scattering behavior that is determined by the liquid-like near ordering of the network meshes.

Fig. 57 shows the scattering behavior of specially structured microgels in a Kratky representation. These samples were prepared by a cross-linking reaction.

a) in the presence of a non-precipitating solvent (lower curve),
b) in the presence of a precipitating solvent (upper curve).

This latter case (upper curve) indicates that a spinodal decomposition in two phases is superposed upon the cross-linking reaction. Networks prepared in this way are called "macroreticular" and are, due to their porosity, the basis of all

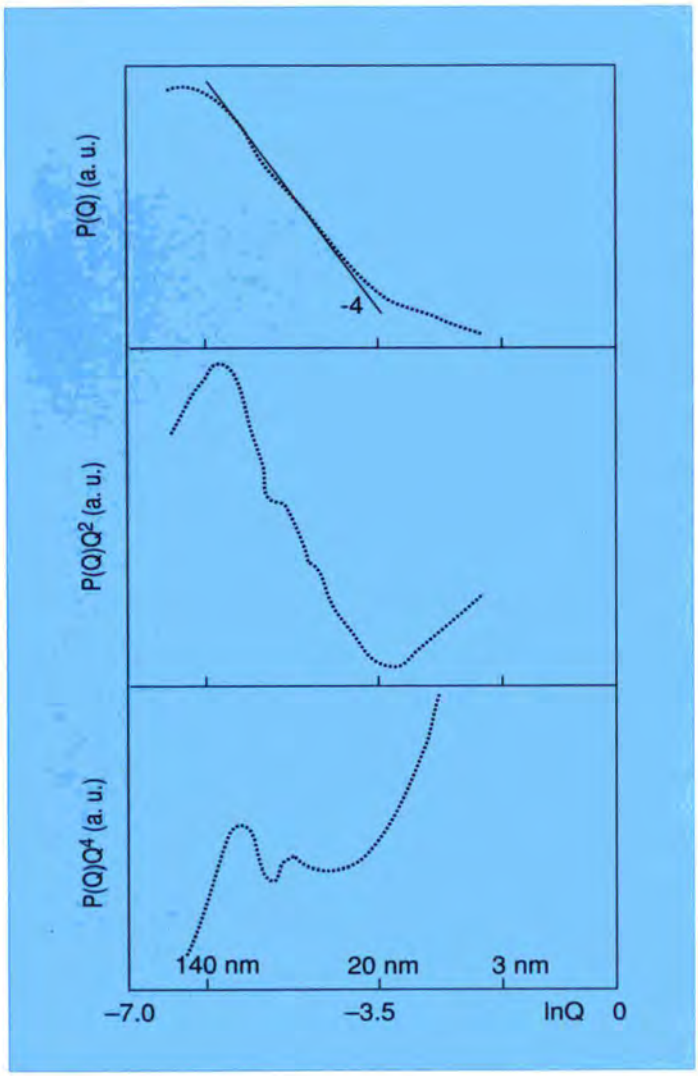


Fig. 56: The form factor of a spherical polystyrene micro-network in different representations.

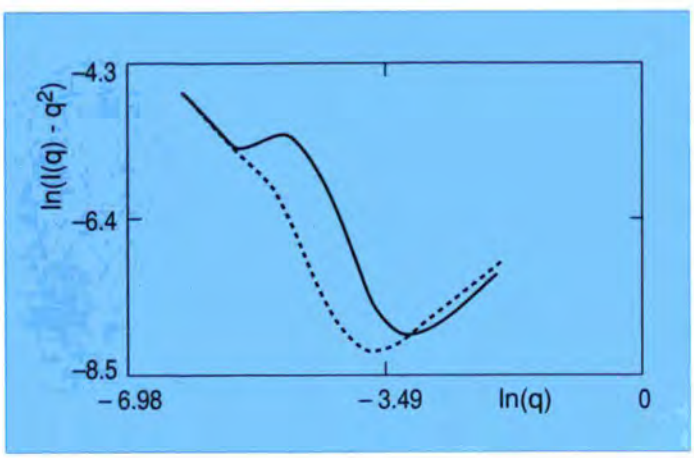


Fig. 57: The scattering curve in the Kratky representation of a micro-gel in the presence of a non-precipitating solvent (lower curve) and in the presence of a precipitating solvent (upper curve).

exclusion-chromatographic techniques (e.g. gel permeation chromatography GPC). Both samples (result a and b) are macroscopically identical. SANS shows, however, a broad scattering peak (sample b) which is correlated directly with the quasi-periodic demixing structure within the gel particle. This direct method therefore allows determination of pore sizes and, moreover, optimization of reaction conditions leading to very well defined materials. (Institut für Physikalische Chemie Mainz and ILL).

Polymeric thermoreversible organo-gels

Physical gelation of synthetic polymers is a growing field of basic research, not to mention the potential applications in the fibre industry. Current studies deal with the gelation mechanism and the molecular structure.

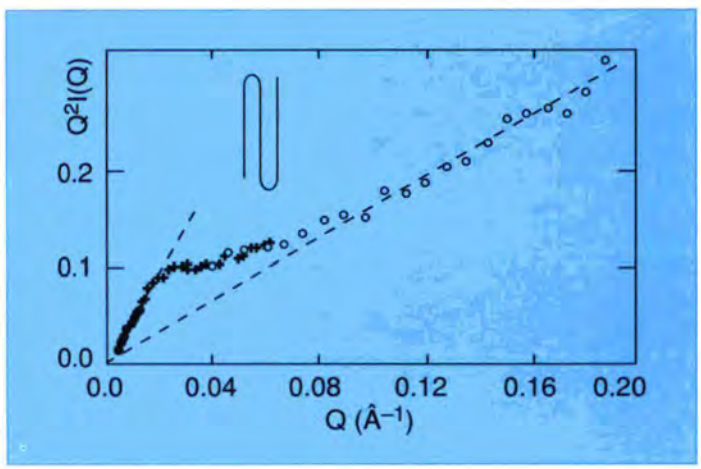


Fig. 58: SANS pattern of isotactic polystyrene / cisdecalin.

These past few years we have been investigating the system isotactic polystyrene/cis-decalin. Below the gelation threshold a fibre-like network is formed and it has been shown from SANS that the chains take on a worm-like conformation with a statistical length of about 8 nm. This length is about four times the statistical length in the amorphous state. The chain conformation in the gel is, therefore, intermediate between the one in the amorphous state and the one in the crystalline state. Diffraction experiments have shown the gel to display order in only one dimension thus resembling a nematic structure.

Recently, we have shown that just above the gelation threshold spherolites are formed which, however, possess the same melting point as the gel. Diffraction experiments have revealed that, in spite of the macroscopic order (spherolites), the crystallographic order is poor and rather reminiscent of that encountered with smectic arrangements. The chain trajectory in these spherolites has been investigated by SANS (see figure 58) and found to be rather close to a twice-folded hairpin (Q^{-1} behavior at very small angles and at larger angles with slopes in a ratio close to 3). This conformation is unusual for isotactic

polystyrene in the sense that chain-folding occurring in the crystalline state involves at least 30 to 40 folds for the same molecular weight. This result shows a new and unexpected aspect of the chain ordering with a polymer which is not intrinsically liquid-crystalline. It also opens up a new field of research in the vicinity of the gelation threshold which now appears as a kind of critical transition (ICS Strasbourg).

Surfactant organo-gels

We have investigated two thermally reversible gels in organic solvents: the steroid/apolar hydrocarbons which is a model system for low-molecular weight gelifying surfactants in apolar solvents and the 12-hydroxystearic acid and derivatives/organic solvents (polar and apolar) which, apart from the fundamental interest, is used in lubricating industries (ELF).

In both cases, we have noticed a large solvent-dependence of the structures of the aggregates which constitute the solid-like gel network. Small-angle neutron scattering experiments on the D11 spectrometer have clearly established that usually the gel network is fibrillar and that the constitutive chains are rod-like and very rigid (up to several thousand Å which is considerably higher than polymeric gel systems).

For the steroid system (see ILL Annual Report 88), the diameter, monodispersity and rigidity of the fibres can be strikingly increased by very minor sterical variations in the solvent structure (for instance trans → cis decalin or cyclohexane → methylcyclohexane). This is common behaviour for physical gels of isotactic polystyrene in organic solvents (Strasbourg).

For the stearic system, gels can be studied in polar solvents. A lamellar organization at two structural levels is found. First level: the initial rod-like constitutive fibres have an internal bilayered structure reminiscent of that of the crystalline solid (triclinic subcell of the parallel hydrocarbon chains). At Q = 0.15 $Å^{-1}$, the Bragg diffraction peak is in agreement with twice the hydroxy-stearic molecular length (47 Å). Second level: depending on the concentration (octane), or the solvent type (fluorobenzene as opposed to benzene) or the cation (H, Li as opposed to Na) the scattering curves exhibit a plateau in a logarithmic representation $Q^2I(Q)$ versus Q, typical of the existence of lamellae. Further analysis is in progress.

The mechanism of physical reticulation within the junction zones of these physical gels can be detailed. The steroid system gives one-dimensional bundles of fibres packed in an amorphous way. The fibres are only entangled or helically entwined together. As a result, the critical gel → sol temperature is low (30-50°C) and has no correlation with the crystalline solid state. By contrast, the crystalline fibres of the stearic system aggregate to give crystalline lamellar junction zones or heterogeneities. As a result, the gel melting temperature is high (160-170°C) and is typically the so-called "waxy" transition temperature of the thermotropic solid crystalline phase.

The influence on the rheological properties of the shape of the heterogeneities will be studied. (ILL).

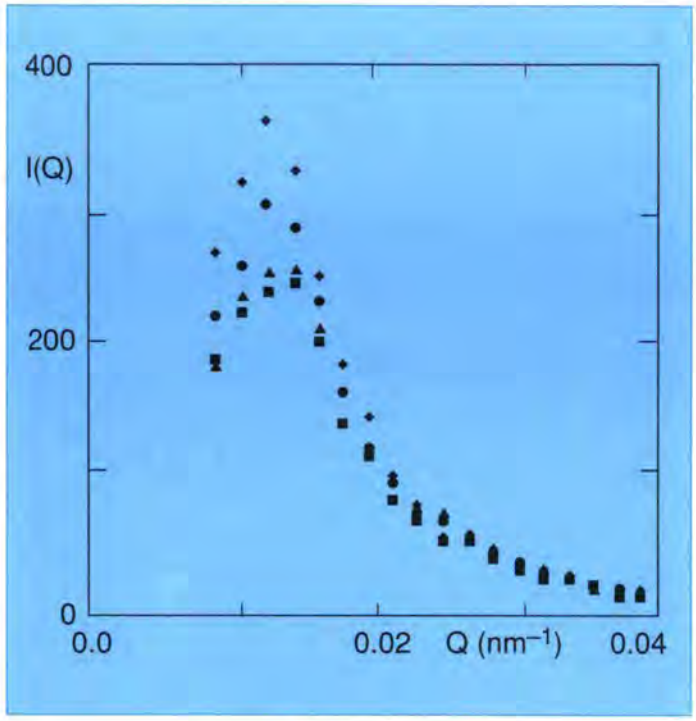


Fig. 59: Scattered intensity as a function of applied electric field : ■ Vcm^{-1}, ▲ 900 Vcm^{-1}, ● 1800 Vcm^{-1}, ◆ 3800 Vcm^{-1} for a PMMA latex in dodecane direction perpendicular to the field.

Latex ordering in organic solvents in an electric field

Work continues on colloidal systems that order under the influence of applied fields. Recent experiments involved the application of an alternating electric field to a dispersion in an organic solvent (Bristol, ILL). It is perhaps remarkable that when a small amount of calcium octanoate is added to a poly - (methyl methacrylate) latex stabilized with poly(12-hydroxystearic acid) in dodecane it becomes slightly charged. This gives rise to a small positive electrophoretic mobility and a significant change in the structure factor measured in small-angle neutron scattering measurements. This tendency to order is increased when an a.c. field is applied, as seen in Fig. 59. The absence of any large change in the position of the peak, but increase in intensity, is tentatively interpreted as an increase in order due to enhanced interparticle interactions without a change in the average separation. (Bristol, ILL).

Conformationally disordered phases in crystalline fluoropolymers

Linear chains of polyolefins (with different degrees of fluorination) generally crystallize into well ordered structures, but upon heating they may also exhibit intermediate "plastic-like" or "condis" crystalline phases below the melting point.

At one edge of the series: in Polyethylene $[(-CH_2-)_n]$, a "condis" phase is observed, but only under high pressure ($P > 4$ kbar). At the other edge of the series: in Polytetrafluoroethylene $[(-CF_2-)_n]$, such a disordered phase extends from 303 K up to the melting temperature (600 K).

In the intermediate range of substitution, one can find many

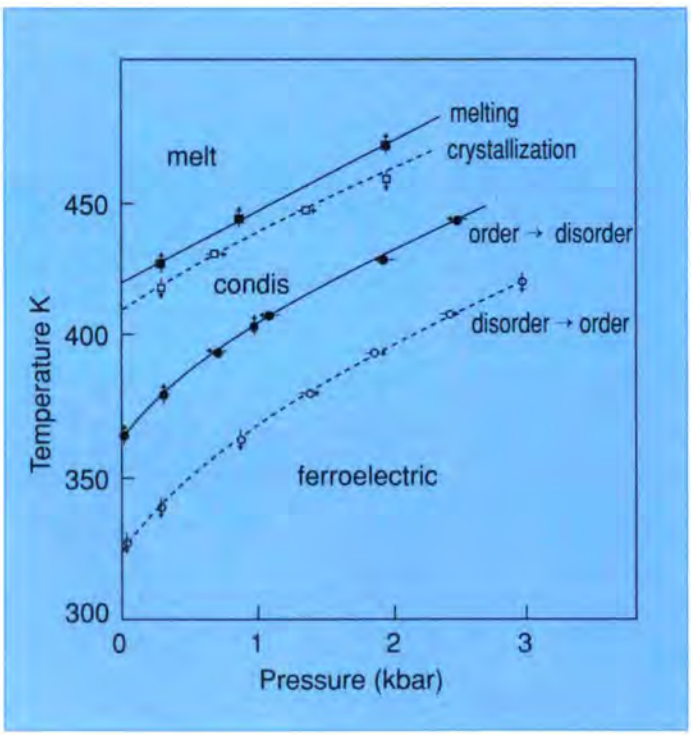


Fig. 60: Phase diagram of P(VDF-T_rFE) copolymer (70/30 mol %) under hydrostatic pressure.

other polymers of industrial interest like PVDF $[(-CH_2-CF_2)_n]$, "Tefzel" $[(-CH_2-CH_2-CF_2-CF_2)_n]$ and random copolymers of vinylidene fluoride $(-CH_2-CF_2)$ with trifluoroethylene $(-CH_2-CF_2)$. These latter copolymers can be obtained with a high degree of crystallinity and their structure at room temperature is ferroelectric. In these new materials, X-ray diffraction and neutron scattering techniques have revealed, below the melting temperature, a Curie transition from the ordered (ferroelectric) phase to a conformationally disordered one (paraelectric).

In comparison with polyethylene, it appeared interesting to analyze the effect of pressure on the phase transition. Neutron diffraction studies under high hydrostatic pressure were recently performed on D20 to determine the phase diagram, the changes in the lattice parameters and the compressibility of both ordered and disordered phases.

The phase diagram is presented in the Fig. 60. It shows that the domain of stability of the "condis" phase decreases under pressure (contrary to the case of polyethylene). In addition, it is worth noting the non-linear increase of the Curie temperature versus pressure.

In considering the Clausius-Clapeyron relation: $\partial T_c/\partial P = T_c\Delta V_c/\Delta H_c$, this effect can be related to a decrease in the volume change ΔV_c or to an increase of the enthalpy change ΔH_c under increasing pressure. The determination of the lattice parameters indicates that the volume change is almost constant versus pressure and this implies that the enthalpy change would be about twice as large at 2 kbar than at atmospheric pressure. (ILL, ICS Strasbourg and University Grenoble).

Reptation

Using neutron spin echo spectroscopy and rheometry, we investigated the melt dynamics of poly(ethylenepropylene) alternating copolymers.

The most celebrated theory of viscoelasticity which is based on the concept of an intermediate dynamic length scale, the reptation model, assumes that long scale motions transverse to the chain contour are forbidden and that the chain moves in a snake-like manner or reptates, confined in a tube along the chain profile. The tube diameter d_T is identified with the distance between entanglements.

The entanglement distance as an intermediate dynamic length scale is of central importance for the understanding of polymer viscoelasticity, it has never been observed experimentally in terms of microscopic dynamics.

Here, investigating polymers which have been tailored to cope with the accessible time and momentum transfer range of neutron spin echo, we present the first direct microscopic observation of this intermediate dynamic length scale in melt dynamics which shows the entanglement distances directly. Comparison with rheological measurements shows good agreement with an interpretation in terms of the Doi-Edwards theory.

If the chains could intersect freely the chain dynamics and could be described by the chain motion in a heat bath which interacts via a friction coefficient ζ_0. In this so-called Rouse model the diffusing chain segment performs a random walk on the random walk given by the chain profile. This convolution of two random walks leads to a mean square segment displacement $\langle r^2(t)\rangle \equiv \sigma^2\ (Wt)^{1/2}$ with the Rouse rate $W = 3kT/\zeta_0\sigma^2$, σ being the segment length. Besides the overall chain dimension, σ is the only length scale in the problem. Consequently, the time dependent intermediate scattering function $S(Q, t)$ for internal chain motion is a function of only one variable $u = Q^2\sigma^2(Wt)^{1/2}$ where Q is the momentum transfer during scattering.

The presence of a second dynamic length scale d_T changes the scaling behaviour of $S(Q, t)$ which now depends on two scales

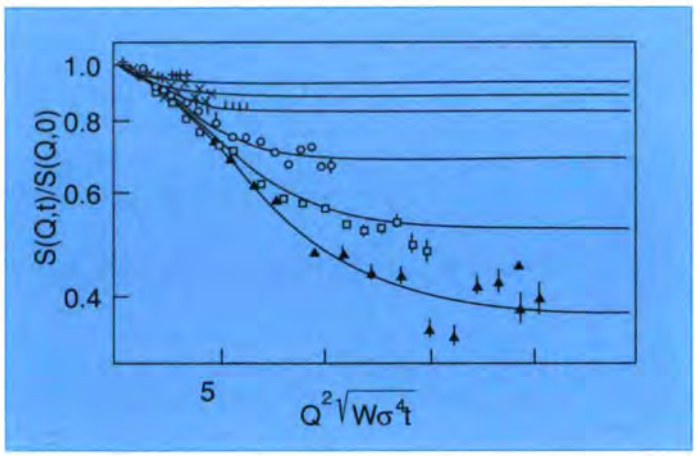


Fig. 61: NSE data of PEP plymer melt in the scaling representation.

$Q\sigma$ and Qd_T. Thus the entanglement distance or the tube diameter in reptation theories as an additional dynamic length scale is expected to cause systematic Q-dependent deviations from the Rouse scaling behaviour.

The neutron spin echo (NSE) experiments were performed using the NSE spectrometer IN11

All observed scattering functions are characterized by an initial decay followed by a plateau regime in time. Thus, qualitatively the observed relaxation dynamics have the feature of a long lived non-decaying contribution as predicted.

Fig. 61 presents the data at 492 K in a scaling representation, they are plotted vs the Rouse variable $Q^2 = (Wo^4t)^{1/2}$. The upper part presents the fit with Ronca's model. In contrast to previous experimental results the data do not scale with u but split into Q-dependent plateau levels. Rouse-like scaling is only observed at the initial decay at short times. The fit with the Ronca model represents an excellent description of the experimental data reproducing the experimental line-shape, the relatively sharp cross over and the Q-dependence of the long time plateau. The tube diameter deduced d_T = 47.5Å is in excellent agreement with the tube diameter obtained for rheological measurement (43Å). (ILL, Exxon).

Secretary: B. Farago

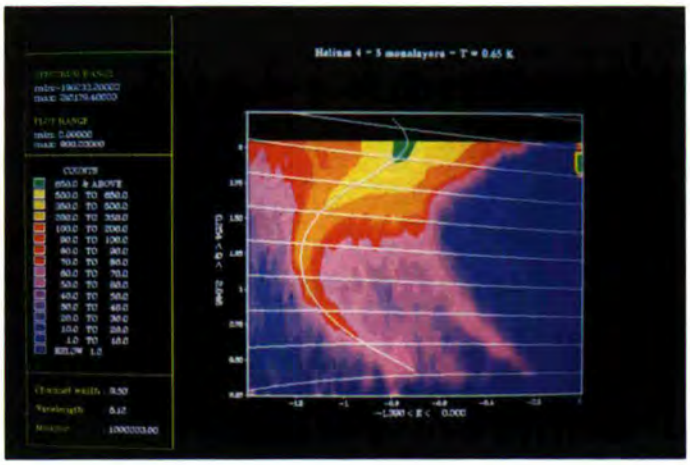


Fig. 40: (College 6), Contour plot for a coverage of 0.448 at $Å^{-2}$ at T = 0.65 K. The solid line is the bulk ^4He phonon-roton dispersion relation. The elastic Q-values are given in abscissa, constant Q lines are indicated by solid lines in the graph. The lower branch, located at about half the energy of the previous one, is the ripplon mode.

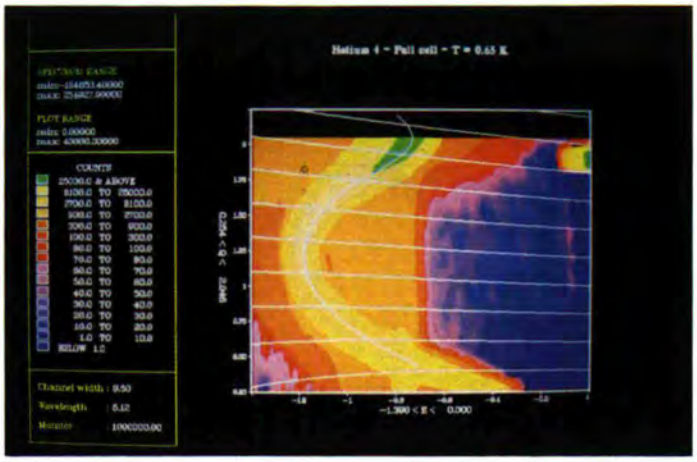


Fig. 41: (College 6), Contour plot of the cell filled with liquid ^4He at T = 0.65K. The solid line is the bulk ^4He phonon-roton dispersion relation. The elastic Q values are given in abscissa, constant Q lines are indicated by thin solid lines in the graph. The constant energy mode seen at 0.8 μeV is due to a double scattering process (elastic scattering at the 0002 peak of the graphite substrate and creation of a roton excitation in the liquid).

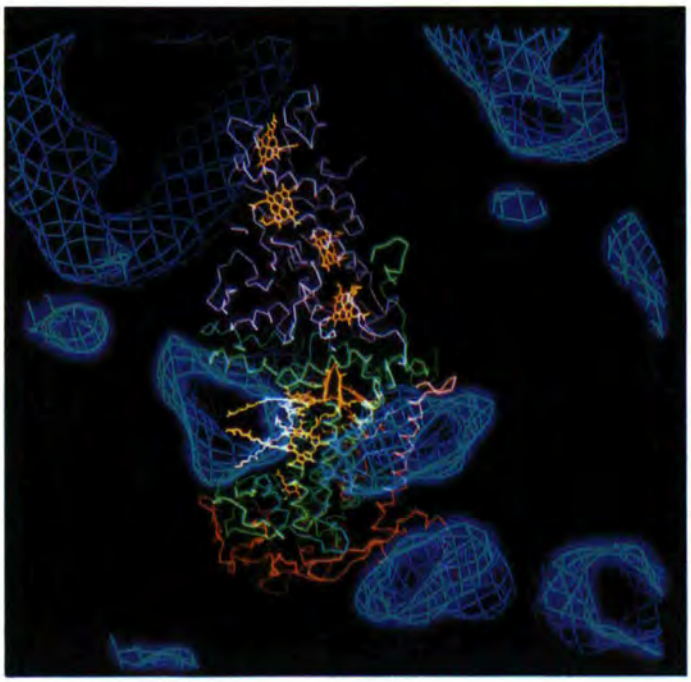


Fig. 43: (College 8), Section through the reaction centre. Subunits are indicated by colours red (H), green (L) and (M) and mauve (cytochrome). The prosthetic groups are orange. The detergent mimicking the membrane is seen in blue.

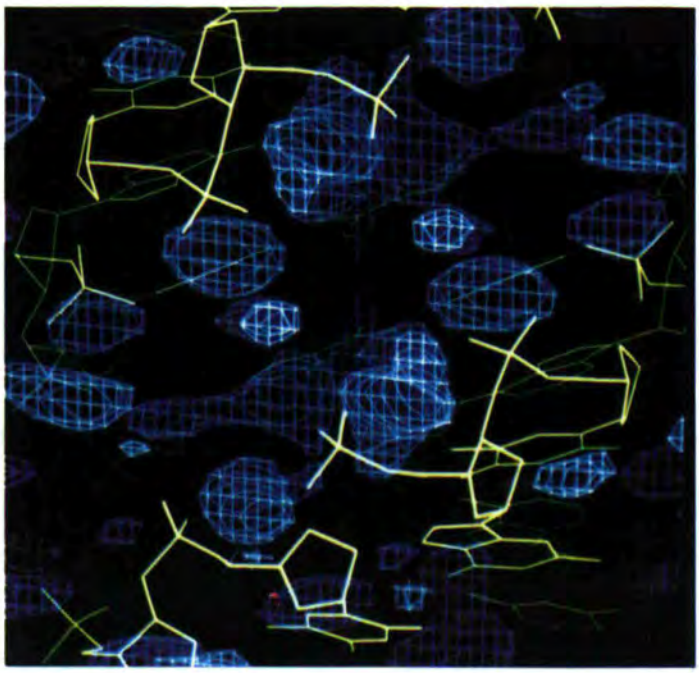
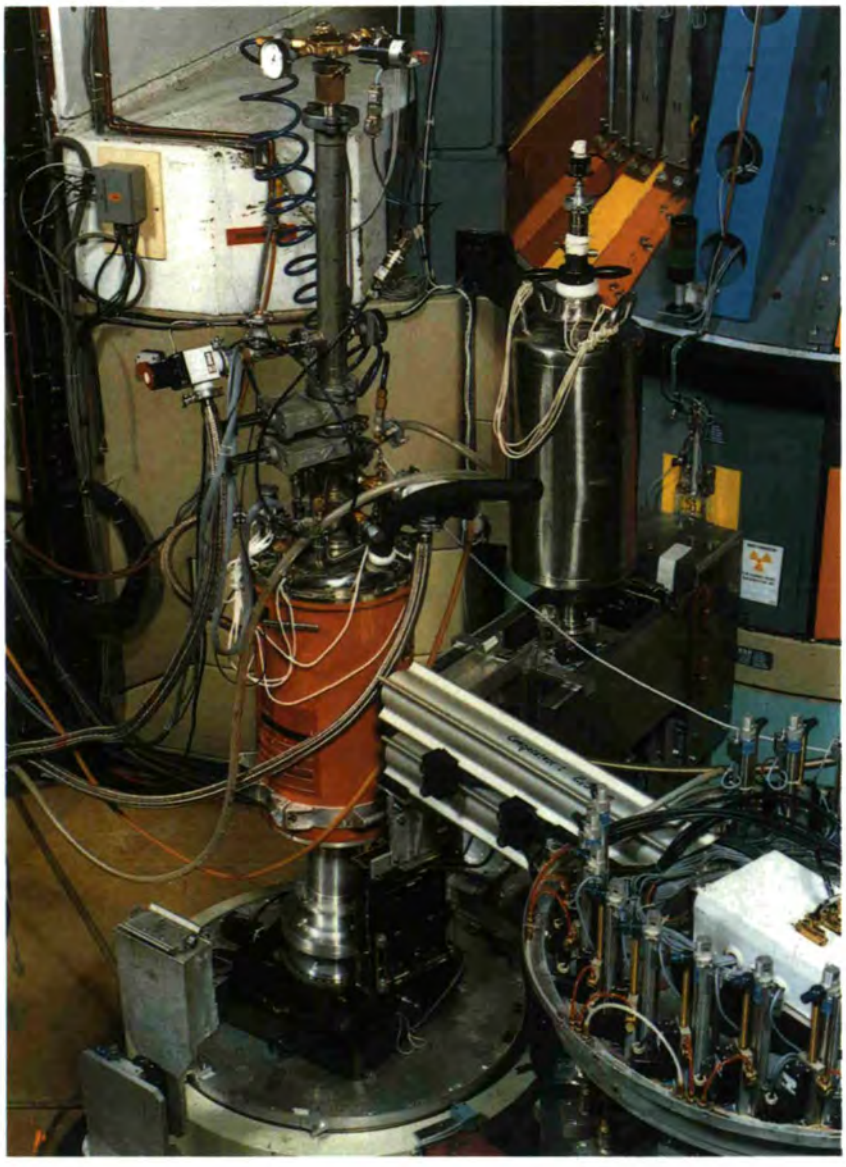
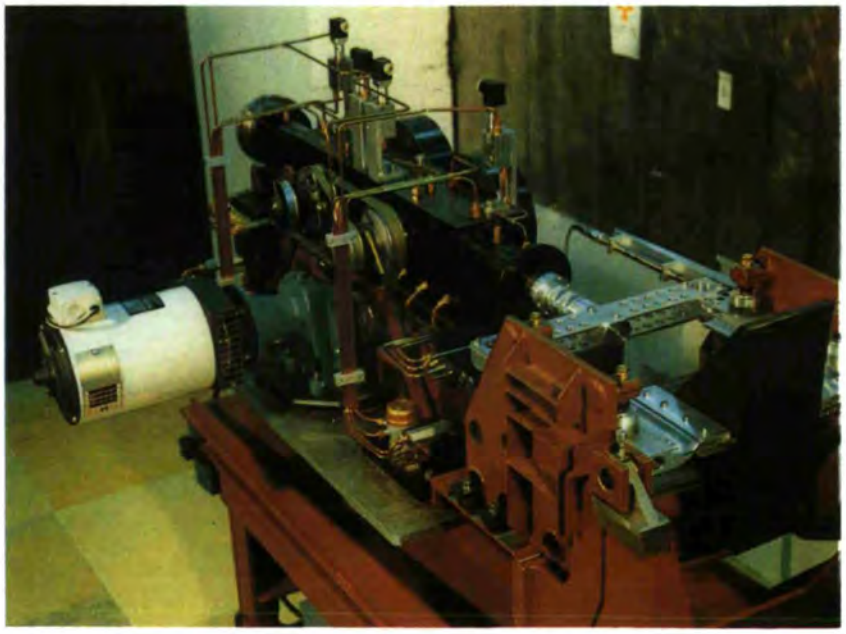


Fig. 46: (College 8), Projection into the major groove of A-DNA, showing a skeletal representation of the A-DNA (green) and difference density (blue) associated with ordered water.



A cryostat for transuranium samples on IN14.



View of IN10C, the new Backscattering Spectrometer at the 2nd Cold Source (see section "Instrument Group TOF, High Resolution and Diffuse Scattering).

Assembly of the large 64 x 64 - 15 multidetector for HMI-Berlin.

Precession coils and sample table on IN15.

The SUSSEX-NIST experiment on the neutron lifetime, mounted at the beam position SN7. The neutron beam enters from the left. The decay protons are trapped in the cylindric bottle on the right (superconducting solenoid and electric fields). The high tension part in the middle contains the proton counters.

View of EVA (Evanescent Wave Spectrometer at the 2nd Cold Source, (see "Special Instruments")

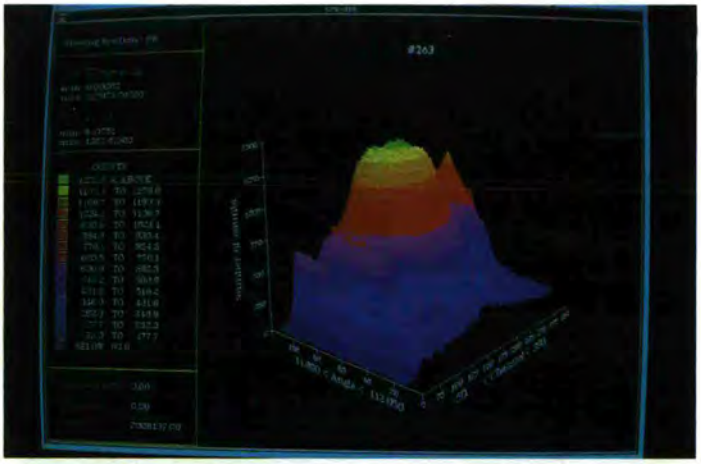
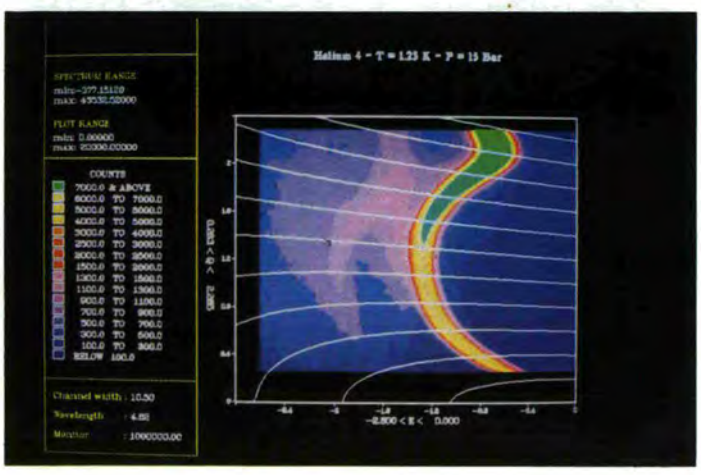
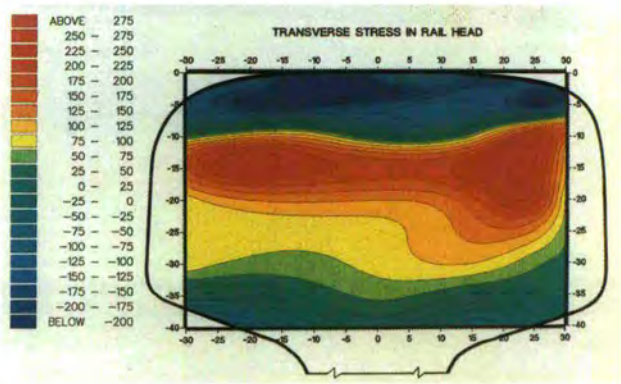
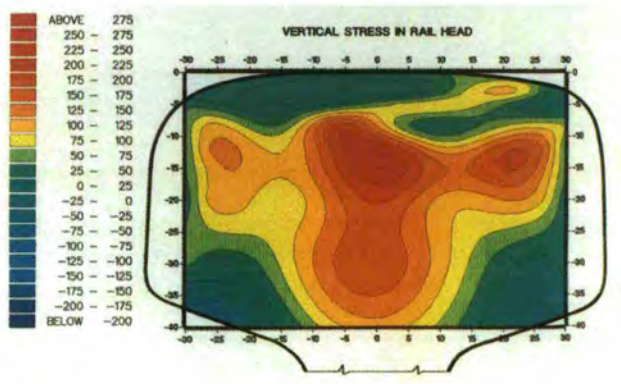


Fig. 62: 3D view of the inelastic response (upscattering region) of a metallic glass (top left). The elastic peak is centered at the channel 313 and thus not seen in this plot (result from IN6).

Fig. 63: 2D view of the scattering law of ^4He at $T = 1.23$ K and $P = 1.5$ MPa (bottom left). The roton minimum is clearly seen. The grid represents constant Q lines (result from IN6).







Stress in railway rail heads (by P.J. Webster et al. Salford University and Imperial College). The stress contours are in MPa (results from D1A).

Instrument Operation Department

Instrument Operation Department

Introduction

The operation of six reactor cycles this year created a heavy workload on all services and groups of the Instrument Operation Department. The day-to-day running of instruments and experiments did not leave much time for improvements and development. This was especially true for the 'High Temperature - High Pressure' group which was faced again with an increased number of experiments. Heavy workload problems occurred also in the 'Vercors Group' due to the fact that their new instruments in the second neutron-guide hall (IN10C, IN15 and D22) need more and more technical support. Some very encouraging events happened during the year 1989 and should be mentioned: the dilution refrigerator insert for the triple axis cryomagnet is now operational: 30 mK at 6 Tesla is now available! A prototype four-circle dilution refrigerator reached 200 mK (collaboration with the CRBT, Grenoble). The second neutron-guide hall was extended by the addition of 100 m^2 of workshop and laboratory space. The vacuum laboratory, the standard cryogenics laboratory and the chemistry-biology laboratory were substantially improved.

Advanced Cryogenic Service

Thermometry and Instrumentation Group

A final batch of five ILL precision temperature controllers have been ordered. Preliminary studies are being made into a new model which could replace the existing stock of controllers by 1995. A new, much more reliable type of helium level gauge for reservoirs has been tested and seems to fulfil all requirements. Work on the automatic cold valve is continuing in an attempt to make it more reliable under all circumstances. The stock of Allen-Bradley carbon resistors, used as the ILL standard for the measurement of temperatures below 50 K, have almost all been consumed. A decision was made to keep using this type of sensor since, apart from maintaining the present standard, uncalibrated ones are very cheap and can be used as throw-away thermometers for certain measurements where high accuracy is not necessary. A batch of 1000, all from the same production run, have been purchased and a certain number are being calibrated by the ILL.

Superconducting Magnets and Very Low Temperatures Group

A renewal of interest in horizontal magnetic field experiments has been observed. The dilution insert for the TAS cryomagnet has been tested and achieved a base temperature of about 30 mK in a field of 6-Tesla. The dedicated gas handling system for this insert is now operational and a project to automate it is being studied. A computer controlled sample rotating device has been fitted to the Thor 7-Tesla cryomagnet allowing accurate angular positioning.

23 experiments have been carried out at temperatures between 0.5 K and 20 mK involving more than 150 days of measuring time and 39 different samples. The ease and speed with which a sample can be changed is a facility very much appreciated. The construction of a low temperature dilution cryostat ($T \geq 5$ mK) is well advanced. The gas handling system and the basic cryostat have been completed and tested. A second 4-circle cryostat has been made for D10, preliminary tests for the dilution section have been undertaken.

Central Service

The Central Service consists of several groups, for which the principal activities in 1989 can be summarized as follows.

- General organization and maintenance of the experimental halls.
- Assistance and support for existing instruments and sample environment.

General Intervention Group

- Improvement of the shielding of the H5 horizontal cold source beam line,
- Continuation of the campaign to reduce the acoustic noise level in the experimental halls,
- Improvement of the neutron and gamma background levels by additional shielding on GAMS4, PN4, D9B, D19, H53, EVA, nn̄, IN5 and D17.
- Installation and commissioning of machine tools and equipment in the mechanical workshop in ILL22, and assistance with the commissioning of a new preparation laboratory in ILL22.
- Regular assistance to the 'S' instruments (nn̄, EVA, H17, SN7, T12, T16, S42),
- Improvements on D19, DB21, PN2,
- Maintenance of the nuclear physics evaporator.

Specific Intervention Group

- Modification and extension of the SADI network,
- Monitoring of transurania experiments on D3, IN14, D2B and SN7.
- Computerisation of technical drawings for the instruments using 'AUTOCAD' system,
- Assistance with the beam distribution control panel projet for the guides H53, H511, H512 (shielding, shutter equipment).
- Measurements of neutron and gamma background levels on the new H5 guides and on the instruments IN14, GAMS, IN10C, D9B, D19, EVA, nn̄, and IN5.

Sample Environment Groups

Standard cryogenics group

In 1989 the standard cryogenics laboratory has been modified and modernized to incorporate a new test laboratory and office facilities.

Cryogenic development has included the design of a new "Top loading" cryorefrigerator using the latest Edwards cold head and compressor. The performance of the prototype machine was encouraging, giving a base temperature of 10 K with a cooling down time of less than 3 hours as compared with 15 K and 7 hours using existing equipment. Two new machines have been ordered and will be added to the pool of cryostats available on request to the cryogenics laboratory. Cryofurnace development has continued. Other projects completed or in hand include:

- A new sample stick with an adjustable sample position,
- A redesigned manual cold valve eliminating the fragility and subsequent frequent damage encountered with the previous model,
- An anti-return valve for the helium recuperation lines,
- A new 3-way valve to replace the existing exchange gas valve,
- The replacement of the vacuum valve on the standard orange cryostat with a valve less subject to leaks.

The consumption of liquid helium rose by more than 20% in 1989 principally due to the increased number of reactor operating days. The recuperation rate remains very high at 88% despite losses due to a compressor fault.

Vacuum group

In 1989, the vacuum laboratory layout was totally modified in order to improve functionality and efficiency.

The computerized stock control is now operational. The present stock of ILL equipment includes 530 primary pumps, 34 turbo pumps, 30 helium tables and 11 leak detectors. During the year 120 pumps and pump groups were repaired. The oil was changed on over 500 pumps. More than 200 leak tests were carried out, both in the laboratory and on site. 52 Penning gauges were repaired. New helium detectors were purchased which are lighter and less bulky, and can be used more easily in the experimental halls.

New developments have included:

- Four helium tables which have been put into service,
- A special transurania pumping group,
- A universal leak detection system which has been made and installed, together with a calibration bay for vacuum equipment.

High temperature - high pressure group

In 1989, this group with a staff of 3 technicians provided an assistance in the operation of high pressure cells and high temperature furnaces which operated for about 6000-7000 hours on different instruments.

Other tasks were:

- Maintenance, repairs and technical improvements to existing equipment,

- Realisation of a stock of spare parts,
- Manufacture of replacement thermocouples,
- Commissioning, repairs and modifications of outside equipment, which often necessitated the manufacture of interface parts to provide compatibility with ILL standard equipement.

This left little time for development work. Nonetheless, the following projects were undertaken:

- Special furnace for D4B,
- Special furnace with sapphire window for D11,
- Standard base furnace Room Temperature to 2000°C,
- CuBe 3 Kbar cell for operation with the cryofurnace.

Chemistry laboratory

A serious effort has been made to improve the existing chemistry laboratories. Special cupboards for storage of solvents and acids and bases have been installed. The Precision Measurements Laboratory has been reorganized to be more functional and to have more working surfaces. An air-conditioned room is now available for growing crystals. The D11 laboratory is now well-equipped with benches, fume cupboards, system for demineralized water, cupboards for storage of solvents and acids. There is now also a room in the basement of ILL20 for short-term storage of visitors' samples.

Building Maintenance and Modifications Service

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

Maintenance, Repairs and Improvements

The main purpose is to keep in an operational state the ILL site (road network, fences, open spaces and drainage system), the buildings (masonry, wood and metal joinery, water proofing) and the technical installations (electricity, plumbing, heating, air conditioning, ventilation, handling) associated with buildings and experiments. To reach this end, systematic maintenance is planned in order to prevent faults, repairs are executed to minimize 'down time' and improvements are realized to increase reliability.

The interventions are carried out using the workshops of the group or by placing external contracts.

Construction, Renovation, Modification and Equipment

Site and buildings

At the request of the Directors, the group designs and follows up the construction, renovation and modification of buildings, offices, laboratories and technical installations. The principal work in 1989 included the external repainting of the ILL7 building, the extension of the ILL22 building to create a workshop and laboratory, a new fence around the modified ILL site, the raising of the roof of the ILL18 building and realisation of a garage in the ILL11 building. Modifications have been made to the vacuum laboratory and the ILL20 chemistry laboratories. A new "clean workshop" for the welding of aluminium and stainless steel has also been constructed.

Experimental positions

In collaboration with the Central Service, the Reactor Department and the Instrument and Methods Department, the Group defines and organizes the construction and assembly of

the biological shielding and infrastructure required around the instruments in the experimental halls. The principal projects carried out in 1989 were the completion of the infrastructure around $n\bar{n}$ and IN14, the fitting of a chemistry/biology preparation laboratory near D11, and continuing work on the equipping of the IN10C, IN15, D22 and EVA experimental positions and improvements to the instrument computer cabins.

Technical Assistance

General services

The self-service workshop and the main sheet metal workshop were used to carry out modifications or production of items which were difficult to subcontract or were needed at short notice or which required on the spot presentation and adaptation. The group supervises the general cleaning of buildings and open spaces, the clearing of snow and waste removal; the supply of furniture, and office and laboratory transfers.

Services for external organisations

The group carried out maintenance of the building and technical installations of the EMBL outstation. In collaboration with the ESRF, it successfully managed the site modifications necessary for installation of the synchrotron buildings, and participated in studies for a common library and canteen building.

Fundamental and Nuclear Physics

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

PN2 Beta spectrometer (BILL) on the vertical beam-tube V3 (B. Krusche, S. Judge).

PN3 Three curved crystal spectrometers (GAMS 1,2,3) and one flat crystal spectrometer (GAMS4) on the through going beam-tube H6-H7 (H. Börner, S. Robinson, P. Schillebeeckx, 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 Cold polarized neutron beam at end position of guide H14 (K. Schreckenbach, D. Dubbers).

PN8 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), (J.P. Bocquet): prompt gamma activation analysis (H22E), (S. Robinson, R. Oliver); γ, γ angular corrections (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, R. Bender, A. Steyerl).

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

Fission Research

PN1

The 6-parameter data acquisition system based on an Atari PC proved to be reliable and was therefore improved for easy use and convenient syntax for the PN1 user groups. A new compiler was installed which increased the speed of the graphics display for the 1000 x 1000-matrices and projections by a factor of 3. An on-line transfer via a parallel interface to the microvax computer was installed, allowing future on-line handling and display of any combination of the multiparametric data.

It was decided to implant the standard IEEE philosophy on Lohengrin to perform the instrument control. For the moment the reference voltages controlling the electrical condensor fields, the magnet and the regulation loop for the magnetic field are controlled via the bus, which is connected to a personal computer. Because IEEE is going to be standard also for a variety of NIM modules which are extensively used on Lohengrin, we will also perform the experiment control via this bus in the future. At present a convenient environment for the PC is in the programming stage.

An effort was made to replace the slow regulation loop for the high tension generators by a newly designed module in NIM standard. With the implantation of this module, the last part of the high tension improvement will be finished and the almost 15 year old regulation units will have been totally redesigned.

In view of the second modernisation programme at the ILL, projected for the coming years, the specification and design of a third magnetic field on the Lohengrin spectrometer were worked out. The dipole magnet proposed would allow for an increase in particle density at a new focal plane of a factor of 2 to 3, together with a major decrease of background components by several orders of magnitude. Specifications of the proposed magnet are summarized in the table.

Characteristics of the proposed third magnet at PN1	
Area of pole piece	$S = 0.7\ m^2$
Field homogeneity	$\Delta B/B = 5 \times 10^{-4}$
Deflection	$\varphi = 90$ degrees
Deflection radius	$r_m = 100$ cm
Maximum field strength	B = 1 Tesla
Gap height	1 = 5 cm
Gap length on entrance side	L = 40 cm

PN8

Due to the efforts in the past, the instrument Cosi Fan Tutte (PN8) operated completely satisfactorily again in 1989 and only minor modifications had to be done. As a consequence of the smooth running of the instrument, a new test facility for selfmade and very delicate polypropylene foils was built and assembled. The foils are made by stretching them over a heated mushroom-shaped piece of teflon down to about 1/1000 of their original thickness. They should be as thin and as homogeneous as possible, but still gas-tight, as they are used as entrance windows for the gas-filled ionization chambers on Cosi Fan Tutte. The test stand consists of a high vacuum part with a turbomolecular pump and of an ionization chamber, including automatic pressure and gas flow control systems. It allows a straightforward quality check of the handmade foils under experimental conditions without interrupting a running experiment on Cosi Fan Tutte.

Spectroscopy

PN2

The beam-time at the high resolution beta spectrometer BILL was again shared between nuclear spectroscopy experiments on nuclei ranging from ^{76}As to ^{243}Pu and positron scattering experiments.

In the previous years the data acquisition system for the investigation of Bhabha scattering (electronics, microvax etc.) was borrowed from the GSI, Darmstadt. The transport and installation of this system for each experiment involved a considerable effort. However, in 1989 a complete multi-parameter list mode data acquisition system was incorporated into the normal BILL data acquisition system. A set of amplifiers, diverse electronics units and CAMAC ADCs were bought and the instrument computer was upgraded from a PDP 11/23 to a PDP 11/73.

A complete software system to run this kind of multi-parameter experiment was developed and tested in spring 1989. It was successfully used for six weeks beam-time. It consists of four interacting programs. The first of them controls the spectrometer and the CAMAC ADCs and passes the buffered events (10 ADCs per event, 4096 channels per ADC) to a subsequent program. In this second program the events are compressed (for a typical event only 2-4 ADCs are involved) and densely written to tape. A third program performs an on-line analysis of as many data buffers as possible (typically 80-90%) without slowing down the list mode data acquisition and creates up to 30 1K spectra from different coincidence requirements. These spectra may be displayed and analysed with the fourth program. Thus a full on-line control of the list mode data taking is possible.

For the search for neutral particles in Bhabha scattering a new set-up was used (see scientific part) which was particularly sensitive to longer lifetimes. It was based on the fact that neutral particles with lifetimes longer than 3.5×10^{-12} (the lower limit deduced from the previous experiments) would decay outside the scattering foil. The detectors at one side of the foil were shielded by a scintillator from the direct view to the tilted foil and thus the high background from prompt Bhabha events was almost completely suppressed. This method together with a further two-fold increase in the positron beam intensity (at present 3×10^6 mono-energetic positrons per second in 10 x 1 cm^2 of the focal plane at 2 MeV), allowed the lower lifetime limit to be pushed up by about an order of magnitude.

The development of the intense positron source also provides the possibility of studying the interaction of positrons with matter, for example investigating positron annihilation in flight. For this purpose the γ-radiation emerging from a scattering target has to be studied with detectors positioned around the target. However, as the process of interest has a very small cross-section, the γ-ray background of the reactor hall raises a serious problem. It is envisaged to overcome this problem by placing a transmission multiwire proportional counter in the direct positron beam in front of the target. Thus, the

background can be reduced by requiring a coincidence with the incident positron. This counter is currently under development and will be tested in December 1989. It consists of a plane of 32 anode wires, 2 mm apart, with two planes of wires to act as the cathode. The positrons enter the counter through a thin mylar window, ionise the counting gas as they pass through and leave the counter through a second mylar window to hit the target.

PN3

GAMS2/3 has obtained a new blockhouse in order to improve shielding against background from neighbouring instruments. Additionally the shielding of GAMS4 has been improved. A background level as small as 0.01 counts/sec/keV has been obtained for the 1 MeV region. A new temperature stabilization and control system has been installed at GAMS2/3.

A microvax station replaced the PDP11 system for data evaluation.

The new Ge detector for PN4, with a fast baseline restore feature, has been installed, with a consequent improvement in resolution at high count-rates.

Fundamental Physics

A variety of fundamental physics experiments were performed in 1989 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 SN7, the new cold beam for $n\bar{n}$ and several dedicated experiments at thermal beams (H22, S50). 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). The neutron lifetime was determined precisely with a fluid wall neutron bottle (ILL).

A neutron gravity monochromator was used for the investigation of the Fermi potentials for material walls (SUSSEX). First experiments were performed with the long base line neutron interferometer for 100 Å neutrons (Vienna-Munich).

SN5

The SN5 ultra-cold neutron beam has been used as a test facility for various preparatory experiments.

H17

Work on the superthermal Helium source for ultra-cold neutrons has been continued by the Berlin group and the ILL.

SN7

The SN7 beam position was used in 1989 for experiments with chopped, continuous and polarized neutrons. Two different experiments on the neutron lifetime were carried out: chopped neutron beam experiment with the electron spectrometer PERKEO (Univ. Heidelberg, ILL), and a continuous beam experiment with a proton trap (SUSSEX, NIST; see page 77). In the last reactor cycle of 1989 an experiment is being mounted to measure the A coefficient in the neutron decay by means of a TPC in coincidence with plastic scintillators (LAPP, Chambéry, ILL).

Two experiments on parity-non-conservation (PNC) in polarized neutron induced fission were running on the same polarized beam during the 3rd and 4th reactor cycles. The ITEP-Kurchatov Institut collaboration (Moscow) investigated PNC in ternary fission. A group from the University of Tübingen looked into PNC as a function of the fission fragments.

$n\bar{n}$

The neutron-antineutron oscillation experiment is running continuously.

S50

The long baseline experiment for a precise determination of h/m_n is operational at the monochromatic thermal beam S50 (PTB Braunschweig).

T16

The monoenergetic 8 Å neutron beam at H14 was used for parity-non-conserving spin-rotation experiments (Univ. Seattle).

Coordinator: K. Schreckenbach

Three-Axis Spectrometers

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

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

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

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

IN20 3-axis spectrometer for neutron polarization analysis on the thermal beam-tube H13 (C. Vettier, A. Severing, H. J. Heuer).

Instruments

IN1 Hot source three-axis spectrometer (H8).

The instrument has operated reliably over the scheduled period which has been slightly extended at the expense of the Be-filter spectrometer. A new cabin will be installed in 1990 to provide a quieter working area for users for data treatment during experiments (to be shared with IN1 Be-filter and D4).

IN1 Be-filter (H8).

The Be filter is used in conjunction with the Cu(200) and Cu(220) monochromator crystals in order to match the 5 meV resolution of the filter itself. The interchange of crystals can be performed automatically by the instrument computer. The Be-Graphite combination filter with a resolution better than 2 meV requires the use of the Cu(331) monochromator crystal. The instrument has operated without major problems during the last few cycles.

IN8 Three-axis spectrometer on the thermal guide H10.

The high neutron flux available and the flexibility and reliability of the instrument have been of prime importance for many studies, in particular in the case of cuprate layered compounds which are also known as high T_c materials. As a consequence the large number of research proposals accepted has made the scheduling of experiments very difficult on IN8. It is hoped that in the future, more time can be allocated to instrument tests or repairs. Some improvements are being implemented. The vacuum box which reduces air scattering for low-angle experiments can be mounted without removing the beam stop. The local computer memory capacity will be increased to 40 Mbytes. A video system will allow the remote control of instrument movements and reduce the radiation exposure for users.

IN12 Three-axis spectrometer on the cold guide H142.

IN12 continued to operate reliably throughout the year. The main improvement implemented this year was the replacement of mechanics connected with the first spectrometer arm. With the new, more robust, system the instrument can be run in the constant-kf mode.

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

IN14 has been made available to external users for a total of 145 days in 1989. Several scheduled experiments have demonstrated the capabilities and performance of this new instrument. A non-exhaustive list would include the study of the vibrational spectrum of ^{3}He adsorbed on graphite using the horizontally focussing PG(002) analyzer, the investigation of critical magnetic behaviour in EuO, NpSb and NpAs, as well as the line-shape analysis of spin-waves in reentrant spin-glasses.

The remaining reactor time was used for tests, calibrations and electronic maintenance and upgrade. The incident neutron beam will be polarized by using a supermirror bender; a horizontally focussing Heusler crystals analyzer is already available. Test measurements are planned for December 1989.

The variable-wavelength l/2 filter and a vertically focussing Si(311) monochromator for high resolution in the thermal range studies are still in construction.

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

The instrument was fully operational during 1989. An apparent drop in the beam time demand for inelastic work can be explained by the low neutron flux for incident energy in the range 50-80 meV. An increase in flux can be achieved with a new design of the Heusler monochromator and analyzer. New permanent magnet circuits will be tested. Further improvements will include magnetic shielding of flippers which are sensitive to fringe fields from electro- and cryo-magnets used on the instrument. A quiet room is now available for the users next to the instrument.

Coordinator: C.Vettier

Time-Of-Flight, High Resolution and Diffuse Scattering

IN4	Time-of-flight spectrometer on thermal tube H12 (A. Murani, H. Mutka, A. Dorn (technician)).
IN4B	New TOF spectrometer with a Brillouin option (H. Mutka)
IN5	Multichopper spectrometer on cold guide H16 (G. Kearley, F. Rieutord, H. Blank, S. Jenkins (technician)).
IN6	Focussing TOF spectrometer on cold guide H15 (A.J. Dianoux, R. White, S. Jenkins (technician), Y. Blanc (technician)).
IN10	New backscattering spectrometer on cold guide H15 (B. Frick, S. MahlingEnnaoui, P. Joubert (technician)).
IN10C	New backscattering spectrometer at the horizontal cold source (project) (A. Magerl, J.L. Coquin, Y. Blanc (technician)).
IN11	Spin-echo spectrometer on 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) (C. Lartigue, F. Mezei, D. Richter, F. Douchin, J.F. Barthélémy (technician)).
D7	Diffuse scattering instrument with polarization analysis on cold guide H15 (O. Schärpf, W. Just, R. Rebesco (technician)).
D11	Small-angle scattering diffractometer on cold guide H15 (P. Timmins, R. May, R. Baker (technician)).
D17	Low Q, low-resolution diffractometer on cold guide H16 (A. Rennie, R. May, M. Cruz (technician)).
D22	Project of small-angle scattering diffractometer on cold guide H512 (R. May, M. Thomas, R. Gay (technician)).
	Group engineer: F. Douchin

IN4 TOF spectrometer on the thermal beam H12

The long awaited modification of the flight box to obtain a shorter flight path was carried out during the reactor shutdown in January. This involved essentially decoupling of the outer part of the original 4 m flight box along its joint in the middle. IN4 now has a single row coverage of detectors at scattering angles ranging continuously from -60° to + 100° with sample to detector distance of 2.1 m.

The instrument operates with a single monochromator oriented for the take-off angle of 38° and two background choppers, the second of which also pulses the beam by means of a slit package incorporated in its axis. Use of the currently available graphite and Cu(220) monochromators enables selection of a discrete set of incident energies namely 17, 68, 115 and 153 meV, the last of which is obtained with the (006) reflection of graphite and gives about 10 % of the intensity of the first order (002) reflection.

Despite the shortened flight path the original energy resolution of the double monochromator mode of operation is maintained with a net gain of flux (~ 300%) for Cu(220) and C(004) reflections resulting from the use of the single monochromator). This is in addition to the increase of the solid angle per available detector due to the shortened flight path. Furthermore the possibility of rotating the choppers at high speeds (30000 rpm) now enables us to achieve even higher resolutions than previously possible ($\Delta E/E$ ~ 3.5% at 17 meV). We have installed adjustable diaphragms which provide the necessary collimation conditions for the primary spectrometer if the required size (height) of the incident beam is not too large (< 1.5 cm). For larger beam sizes use of Soller collimators is preferred.

Another major upgrade was the installation of a micro-VAX computer to replace the old PDP11. Simultaneously the control and acquisition software was also renewed. The system, although fully operational, is still being under refined. The speed and reliability of the new computer has already been greatly appreciated.

After a modification of the IN4 cryostat it is now possible to reach temperatures down to 2.5 K (previously 5 K). The sample change has also been made much easier and quicker with a new insertion device.

IN4B New TOF spectrometer with a Brillouin option

This high efficiency thermal TOF spectrometer is designed for the (Q,w)range from 0.1 to 10 Å-1, 1 to 100 meV, with a resolution adjustable in the range from 2 to 5%. It uses a large area, variable curvature monochromator with variable takeoff angle ($20° < 2Q < \theta < 75°$) for flexible optimization of incident energy, intensity or resolution that is still missing on the present IN4. With three rows of detector tubes on an angular range of about 130° the counting rates will be up to 50 times higher than on the present already improved IN4 in similar resolution conditions.

The incident energy range of the instrument starts from the upper limit of IN5/IN6. The resolution is also similar as shown by results from a MonteCarlo simulation that includes time-focussing. The result illustrates the performance that can be attained at low incident energy, i.e. $\Delta E/E \approx 1.6\%$ FWHM at 5.5 meV.

The Brillouin option working parallel on the same beam hole is aimed for low angle inelastic experiments with good resolution at thermal incident energies (10 to 50 meV), in the range 0.01 $Å^{-1} < Q < 0.2\ Å^{-1}$, 0.1 meV < ω < 5 meV where no standard instrumentation exists at present. A doubly curved monochromator focussing on the detector through a conical collimator is necessary to maintain acceptable intensity in spite of the stringent wavelength and angular resolution requirements.

IN5 Multi-chopper spectrometer on the cold guide H16

IN5 continues to be in great demand, the main users coming from colleges 9, 6 and 4. The attractions of this spectrometer seem to be its clean resolution function and its flexibility. Since the advent of programmable choppers and a near complete detector bank, users have taken to experimenting with the instrumental set-up on a routine basis. We had hoped to replace our rather pedestrian PDP11 with a microVax during the year but due to the heavy instrument demand we were obliged to run a full instrument schedule until 1990.

Use of the spare D11 multidetector for high-resolution small-angle experiments has progressed well. During the year there have been 4 such experiments studying Brillouin scattering in dense gases, critical narrowing in liquid metals, and fracton-phonon crossover in aerogels. The instrumental set-up is now well defined and requires less than a day to install. An evacuated conical flight-path is being constructed which should be installed around August 1990.

Users of cryostats have appreciated the automatic filling and control facilities. We have also installed *in situ* unblocking of the cold valve; this also seems to work well. The new furnace designed specially for IN5 should be available in 1990.

IN6 Focussing TOF spectrometer on the cold guide H15

The instrument has worked satisfactorily during this year, permitting a record number (52) of experiments. The only subject of worry is the aging CAMAC electronics which caused two instrument stops this year. It is hoped that in the very near future the new VME electronics will be ready.

The same facilities as on IN5 for operating the cryostat have been implemented and numerous users have appreciated the automatic filling and temperature changes.

A new program (TOPODIS) is available on the IN6 microVax GPX workstation. This program produces 2D and 3D colour plots of data collected on the instrument. Originally written by V. Frank to use the NAG library of graphics routines and work in monochrome, it has been altered by D. Youngs to produce 8 or 16 colour graphics using the DISSPLA library. Two examples of such graphs are given in figures 62 and 63 (see page .78).

IN10 Backscattering spectrometer on the cold guide H15

IN10 operated successfully in 1989. The 33 scheduled experiments covered mainly scientific problems of Colleges 6, 9 and 8. Besides the "classical" problems, studied quite often on IN10, like H-diffusion in metals and tunnelling experiments, measurements were carried out on aqueous solutions, proton conductors, proteins, lipids, diverse glasses and polymers as well as lattice distortions and jump diffusion of metal atoms.

On the spectrometer side the new Si(0.9) Ge(0.1) monochromator combined with Si(111) analysers allow measurements up to about 30 μeV energy transfer, thus measuring asymmetrically around the elastic peak. The advantage of this SiGe monochromator over the CaF_2 monochromator is that the elastic peak still remains within the energy window. The monitor flux of the SiGe monochromator in comparison to the unpolished Si(111) monochromator is roughly reduced by a factor 2. A new Si(111) analyser plate with ~ 0.7 μeV energy resolution is also available.

Some further improvements on the spectrometer side were improvements of the adjustment devices for the small angle analyser circles. In the sample environment, the sample table and the cryofurnace have been renewed.

The instrument, operating on VME electronics as a pilot project, generally worked well. Some difficulties caused by the link between VME and the microVax seem to be solved now.

The instrument is now running by default with 256 energy channels. For test purposes the data inspection program "GENIE" (RAL) was installed (Kearley). Furthermore, a new program for user defined model fits - refining all detectors simultaneously - has been implemented. In situ data evaluation is now largely facilitated by a fast fitting routine FIR (R. Ghosh).

IN10C New backscattering spectrometer at the horizontal cold source (project)

The construction of IN10C has progressed normally during 1989. The primary shielding including the first deflector, the secondary shutter, the focussing guide and the Be filter are completely installed and aligned (Fig. 64). All associated movements are operational. The neutron optical performance of this part of the spectrometer is as expected.

The construction of the Doppler drive has been finished. First tests have shown that the drive mechanism works well for the entire dynamic range. However, the guide system of the monochromator support which is based on an air cushion design needs to be reconstructed. A large part of the electronic equipment and the computer system with a VME/VAX configuration has been installed on site and many components are operational by now. Some development still remains to be done, such as control and protection of synchronized running of the two choppers on IN10C or programming and

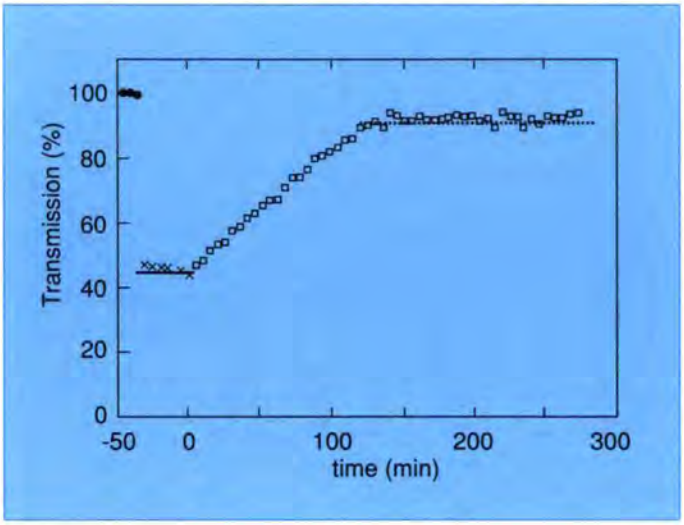


Fig. 64: Measured transmission of Be filter at IN10C. The solid circles, crosses and open rectangles represent the neutron intensity measured without the filter (reference value), the filter at ambient temperature and after cooling the Be filter, respectively. Cooling in a liquid nitrogen dewar started at t = 0. The solid line and the dotted line give the calculated transmissions at ambient and liquid nitrogen temperature, respectively.

commissioning of an amplifier with automatic adjustment of the amplification. The help of the KFA Jülich for support in the construction and for making the large scale analyzer plates is acknowledged. There will be two sets of analyzers with a surface area of 7 m^2 each. They will be covered entirely with Si crystals of an individual size of 4 x 4 mm^2. An appropriate technique for gluing these small crystals with correct orientation onto the supports made by Jülich has been developed and gives very satisfactory results.

The secondary spectrometer remains the last major structural component to be built. An order will be placed before the end of 1989. The planning calls for a finished construction on site by the beginning of summer 1990, and we expect that first tests with neutrons on a largely finished IN10C can start after the summer holidays.

IN11 Spin-echo spectrometer on cold guide H15

In the hope of availability in the near future of the very high resolution NSE spectrometer IN15, the efforts on IN11 are oriented mostly toward higher flux improvements. In fact up to now essentially the 6 - 8.5 Å wavelength band was used and the old analyser supermirror set was known to have decreasing reflectivity starting from ≈ 4 Å. This limitation had little effect as the actual velocity selector can work only in the $\lambda > 4.7$ Å range. The following improvements are in progress:

1. With the advent of the availability of a large number of CoTi supermirrors (Schärpf type) the analyser is planned to be changed during January 1990.
   From a preliminary measurement the expected gain factor in intensity is:

Wavelength	Gain factor (new flux / old flux)
4.5 Å	2.8
5 Å	2.3
5.5 Å	2.0
6 Å	1.7
7 Å	1.3
8 Å and higher	1.1

   Final numbers will be available in January.
2. A new shorter Gobert type selector is under construction which should extend the wavelength range down to 3.5 Å (the peak flux of the guide is ≈ 4.5 Å). Due to the better luminosity, it is expected to bring an increase of ≈ 10% of the flux. Probable installation October 1990.
3. Similar or even better improvements are expected from the installation of a new transmission polarizer and a prepolarizing guide between the selector and the polarizer. Expected installation October 1990.

The instrument computer was equipped with an IEEE interface which allows us to connect easily user supplied auxiliary equipment for specific experiments.

The extension of IN11 with an optional multidetector bank covering simultaneously ≈ 30° scattering angle was approved by the Instrument Subcommittee. The expected resolution is about 1/2 - 2/3 of IN11. The project is waiting for money, otherwise ready to start.

IN13 Backscattering spectrometer for short wavelengths on the thermal guide H24

Over the last twelve months IN13 has operated satisfactorily. There have been no large-scale changes to the spectrometer itself. However, a number of improvements are under way. Also a new cryofurnace has been built and inaugurated with high temperature measurements on both polymer samples and on the inorganic glass $Ca_{0.4}K_{0.6}(NO_3)_{1.4}$. It can be used to control and regulate the temperature of such samples in the range 100 to 670 K.

Of considerable importance for the future is the addition of a new collimator bank allowing a resolution of $\Delta Q = 0.1$ - 0.025 $Å^{-1}$ for the available Q range of 1.0 - 5.5 $Å^{-1}$. Delivery is expected early in 1990. In addition, a new electronic system for temperature measurement and regulation at the calcium fluoride monochromator is being constructed and interfaced to the instrument computer.

Over the last year the spectrometer has been used for a wide variety of investigations. Among the more traditional type of tunnelling experiments was the study of the pressure dependence of the methyl group tunnelling in acetylacetone. A series of new measurements on the van der Waals solid formed between benzene and hexafluorobenzene was begun. These experiments included fixed window or elastic scattering measurements, which clearly showed the three phase transitions which occur in this material between 200 K and its melting point at 300 K, which are probably the result of increasing levels of orientational disorder. Inelastic scans were also made which allowed the identification and analysis of the dynamic behaviour in the two lowest temperature phases. This material is a good example for demonstrating the unique properties of IN13, i.e. high energy resolution over a large dynamic range and the possibility of observing an EISF at the largest Q.

The investigation of coherent quasielastic scattering has continued with experiments on the oligomer of Teflon, C20F42 and on the orientational glass $KBr_{1-x}KCN_x$. In both these cases the measurements are only possible on IN13 requiring good Q resolution in the high Q range, hence the necessity for the new collimator with much improved angular resolution.

Another experiment performed on IN13 in 1989 on a subject of considerable current interest was the study of the density of states of fractals in aerogels. These quasielastic scattering measurements on the vibrational density of states in neutrally reacted silica aerogels suggest that fractons are now observed over more than two orders of magnitude in frequency.

IN15 High-resolution spin-echo spectrometer for long wavelengths (project)

The design of the instrument has been completed and the assembly work is continuing on site.

Most mechanical parts for the sample table and secondary spectrometer have been assembled in the guide hall. The intermediate part is being installed: a 12 m long Ni guide with a magnetic guide field (neutrons being polarized upstream) on a beam designed to allow the change from the normal to the focussing mode of operation (to be added later).

The normal procedure for balancing the non-magnetic velocity selector developed at the ILL (helical lamellae) was started on site and led to two important modifications; the external collar was replaced since it showed a continuous deformation with increasing speed of rotation; the support structure which was giving a high level of vibrations at 8000 rpm has been considerably reinforced. The selector should be ready to be installed again on site in January 1990.

The Larmor precession coils are due to be delivered before the end of the year: high precision winding was much more tricky than expected by the manufacturer.

Most of the 25 power supply units will be delivered by the end of the year: tests for stability were made at the ILL on a few prototypes before acceptance.

The detector shielding has been delivered.

VME modules for TOF data acquisition and motor control are available at the ILL. Electronics will start to be installed at the beginning of next year.

D7 Diffuse scattering instrument with polarization analysis on cold guide H15

In 1989, a small angle scattering option with polarization analysis operating simultaneously with the wide-angle part was implemented on D7. It uses a standard D7 analyzer, but mounted with the Soller slits in the vertical direction. Thus the small-angle scattering is not influenced in the horizontal direction (with the exception of mirror reflection), and is collimated in the vertical direction, avoiding slit corrections.

This set-up was used for small-angle scattering measurements on polymer samples. As in the wide-angle case, measuring the scattering with both neutron spin orientations allows us to determine quantitatively the incoherent scattering contribution. This can serve as an internal standard, because it can be related to the hydrogen cross-section of the sample, which is often well known. The combination of small-angle with wideangle measurements has been successfully applied to a study of the properties of ionomers, where the full scattering angle was important for obtaining exact quantitative results.

The next step will be an extension of the application of these options to the investigation of magnetic effects, especially of samples showing strong small-angle scattering. Such studies require a special coil for the rotation of the neutron spin in the three orthogonal directions x, y and z for separating the magnetic contribution.

Extensive measurements of the magnetic behaviour of powders and single crystals revealed the limits of such measurements as well as the advantages of combining polarization analysis and the conventional method. One example of such a study is that on the "Shirane ridge" in a La_2CuO_4 single crystal and its magnetic and inelastic properties. At the moment of writing this report, we are looking at a Sr-doped single crystal of $T_c \approx 33$ K, where we also find this ridge, and the change in its behaviour, together with a group from Brookhaven.

For the near future, the inclusion of all 64 detectors in the polarization-analysis option and an improvement of the highenergy transmission of the analyzers without the need for more mirrors are being prepared.

D11 Small-angle scattering diffractometer on cold guide H15

D11 has operated routinely throughout the year with 111 scheduled experiments being carried out.

Several "state-of-the-art" experiments have been performed. Magnetic flux lines were observed for the first time by neutron diffraction in the mixed state of the High Temperature Superconductor $YBa_2Cu_3O_{7-8}$. The experimental data indicate the existence of a vortex at low temperatures. Using the full 35 m sample-detector distance and 10 Å neutrons diffraction has been observed from photochemically prepared hologram gratings of 3617 Å period. An increased number of experiments now require special sample environments such as pressure, shearing, turbulent flow or kinetic facilities.

At the end of last year it was clear that the detector electronics were suffering from an unacceptable level of parasitic noise.

The electronics were entirely renewed in December/January and have since functioned satisfactorily.

A number of improvements have been carried out at the level of sample environment. A furnace for samples up to 13 mm diameter, operating at temperatures up to 250°C, has been constructed and is currently under test. It can take up to 4 samples and be used on the standard slideway controlled by the standard sample-changer software. A control box for manual positioning of sample changers at the sample area has been installed.

The wide bandwidth velocity selector Adèle ($\Delta\lambda/\lambda$ = 40%), which has been unused for some years, has been renovated and is now available if requested at the time of scheduling. Due to radiation constraints it may only be installed or removed in the first few days of a cycle.

Two major improvement projects have been initiated; the construction of a new velocity selector and the replacement of the collimation system. The velocity selector, which should be delivered early in 1990, is an ILL design in lightweight material and will give a wavelength resolution of 10% (FWHM). The collimation system will be replaced over the 20 m section back from the sample position. This will enable users to better adapt the collimation length to the sample-detector distance and thus optimize the flux for a given configuration. The housing will be in aluminium which will provide a non-magnetic environment for IN11 and hence allow the dynamic range of that instrument to be extended beyond 1000. This modification will be installed during the October shutdown of the reactor in 1990.

The D11 sample preparation laboratory has now been completely renovated and re-equipped. There are two ventilated hoods as well as most equipment necessary for preparation of samples immediately before and during experiments.

D17 Low-Q, low-resolution diffractometer on cold guide H16

At the beginning of 1989 the large D17 multidetector (128 x 128 x 5 mm^2) was out of service following damage caused by the failure of a high voltage supply. With the cooperation of the technical services at the ILL a small detector (16 x 8 cm) was installed and used for some reflection experiments and tests. Although good use was made of the beam during this time (some of the first results on solid-liquid interfaces are described elsewhere in the report), for small angle scattering a large multidetector is indispensable. The full normal programme of experiments was resumed in the middle of June when the final adjustments of the rebuilt detector were completed on the D17 beam position.

Much of the first half of the year was largely occupied with tests of either the small detector or the rebuilt large detector. However, some further instrument developments have been made during the year. A third velocity selector is now available for experiments that require a high flux and can use conditions of relaxed resolution. Although previously available on D11, such an option had fallen into disuse. Renewed interest in experiments with very low scattering contrast has led to further recent demand which because of the relatively easy access to the selector on D17 has already proved useful in accurate measurements of dimensions of polymers. A wide variety of experiments during the year have exploited many of the possibilities of this flexible small-angle spectrometer. Time of flight measurements, polarization and spin flipping experiments as well as many reflection experiments have led to many modifications of the sample environment equipment. For the coming year it is expected to continue this steady modification; major plans include the purchase of a replacement detector - the detailed specification is under discussion at the time of writing.

D22 New low-Q diffractometer on cold guide H512

The project of a new small-angle scattering instrument on the horizontal cold source, D22, has made substantial progress in 1989.

The collimation unit has been assembled in the factory and has been delivered to the ILL together with the detector tube (2.54 m diameter and 20 m length) and the detector carriage mid December, 1989. These two major components of the new instrument should be installed on site by the end of February, when the neutron guides should arrive.

Due to budget problems, the 1 m x 1 m detector with 128 x 128 detection elements of 7.5 x 7.5 mm^2 has not yet been ordered, but there is an offer corresponding to our specifications. Since its construction will take 14 months, the complete instrument cannot be commissioned before early 1991. We should be able, however, to start test runs with the spare D11 detector in the second half of 1990.

The acquisition electronics, and most of the encoded shaft controls, will be in the VME standard. The other movements and the vacuum system will be controlled by a programmable automat. A final choice of the instrument computer, probably of the microVax family, has not yet been made, but it will certainly be identical with the future computers of D11 and D17.

Contrary to the prediciton in last year's report, a Dornier high-tech velocity selector with 10% resolution has not yet been obtained, but according to the latest information, it should be available in 1990.

At the moment, the protection around the wavelength-selection zone is being designed; the sample zone and the beamstop mechanism will complete the mechanical set-up.

Development of small-angle scattering programs

The revision of the small-angle scattering data treatment programs was completed during the year with the issue of a new computing guide. It is clear that all users and instrument responsibles are grateful for the good collaboration with the Computing Department on this project.

Coordinators: A. Dianoux
R. May

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 H4
(F. Tasset, M. Vrtis, 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, M.S. Lehmann, J. Archer).

D10 Four-circle triple-axis spectrometer on thermal guide H24
(C.M.E. Zeyen, 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, J.M. Reynal).

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

D20 High-flux multidetector diffractometer 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
(M. Roth, C Wilkinson (EMBL), P. Agnes).

CRYOPAD Cryogenic Polarization Analysis (F Tasset, V. Nunez, P. Feder)

D1A High resolution powder diffractometer on the thermal guide H22

D1A is fully scheduled, but 42 days/year are pre-allocated to the MPI Stuttgart in return for their paying the salary of a full time instrument scientist (Dr. J. K Cockcroft). Demand for D1A beam-time has continued to increase with the saturation of D2B. Because of the absence of short wavelength contamination due to its guide tube position, D1A is unique for high resolution work at longer dspacings, for example for magnetic order. The long wavelengths are also an advantage for work on zeolites, and of course D1A has continued to be important for work on high temperature superconductors. Stress measurements have also been a strong growth area (see photo on page 78), with several groups from Britain (London, Salford, Harwell etc.), Germany (Stuttgart, Dortmund, Karlsruhe etc.) and more recently France.

The success of the 160° multidetector on D2B has encouraged planning for a large detector bank on D1A. This could be accomplished with commercially available detectors and collimators, and would increase the efficiency of the machine by a factor of 2.5 for many experiments, and make possible rapid scans of temperature, of particular interest for phase transitions. It is hoped that the new detector bank can be installed early in 1990, reusing the existing D1A detectors and collimators.

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

D1B continues to be a very reliable and versatile instrument for studying powders or partially oriented samples under widely differing environmental conditions. With 70 officially scheduled experiments successfully carried out in 1989 the habitual overload on this machine was stabilized at a factor of 2 (user demand/available time). Besides routine experiments using the normal orange cryostat or standard furnace, several studies were undertaken to study magnetic structures in the milli-Kelvin region using a dilution cryostat, and to study phase transitions above 1300 K with a special furnace. Texture studies are now carried out in a routine way and an adaptation to allow a furnace to be used for studies with the Eulerian cradle is in preparation. Three experiments used the polarized neutron option and proved again its power to reveal small ferromagnetic moments.

A novel type of experiment was the study of the sequence of phase transitions in a partially oriented polymer sample using ω-T scans. The oscillating Soller collimators used to exclude scattering from the cryofurnace were adapted to allow the latter to rotate freely about its axis. Data were collected with both 2.52 and 1.28 Å wavelengths which enormously increased the accessible Q-range; thermokinetic studies with 1 λ = 1.28 Å, allowing a pattern to be recorded every three minutes, are a new departure for D1B.

D2B High resolution powder diffractomer on the thermal beam H11

D2B was heavily scheduled in 1989, the average experiment lasting roughly 3 days.

The machine is used exclusively in its high flux mode enabling data collection times of 34 hours per sample. Improvements under way are a new monochromator and graphite filters.

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

In 1989 D3B has been operating extremely successfully in its enhanced electronic and mechanical configuration (cf. 1988 ILL annual report p 109). In particular the renewed data acquisition system based on a PDP11/73 and a DEC Camac Crate controller has proved to be 100% reliable. The new facilities such as automatic change of wavelength and on-line control of the magnetic field have been of great help for some experiments.

A precious heritage from D5 is the very good Heusler monochromator crystal cut in transmission geometry. It delivers a neutron flux which gives peak counting rates which are at best 7.5 times those obtained with the CoFe monochromator, and even at high angles are 3 times higher. The combination of this high flux with the 10 Tesla CENG magnet was particularly valuable in the difficult experiment on high T_c superconductors.

Almost the whole of the D3B experimental program relies on the availability of the 15 year old 4.6 Tesla cryomagnet. Although it was successfully modified ten years ago to incorporate a variable temperature sample chamber, it now shows signs of aging. Any breakdowns of this magnet, such as the leak which developed recently, imply disruptions of the experimental program so long as there is no replacement available.

D4B Disordered-materials diffractometer on the hot beam H8

Room temperature measurements for the isotopic substitution method are now routinely obtained with an accuracy of about one part per thousand. Progress is slowly being made to achieve this accuracy with more difficult experimental conditions (high or low-temperature, pressure etc.). At high temperature, one is still limited by, yet unmastered, aging of the containers (vanadium, sapphire ...) and tests are continuing to obtain a better understanding of these problems. Improvement in mechanical reproducibility of positioning the pressure equipment has allowed us to obtain good results. The machine is also very successfully used for magnetic structure determination of absorbing powders (e.g. Gd compounds ...); the resolution is then improved using a 3 meter sample to detector distance, there is however a growing need for redesign of the whole instrument to increase the data collection rate.

D9 Four-circle diffractometer on the hot beam H3

D9 has for the most part operated very smoothly this year with an interesting mix of structural crystallographic experiments, of magnetic studies of Gd compounds, and of more esoteric investigations of dynamical diffraction near resonance and bonding deformation via Schwinger scattering. A crucial aid in many of these experiments was the small position sensitive detector which has been in nearly constant use since March. This detector which has 32 x 32 pixels and subtends 8 x 8 deg. at the sample has proven to be as reliable as the conventional single detector. Users have been happy to trade off the lower efficiency of 75% against the better knowledge of the peak positions and limits, and the much quicker change-around of experiments afforded by this detector. It was also proven invaluable for studies of twinned crystals, poorly crystalline samples and phase transitions.

Tests with the horizontally-focussing Be (110) monochromator have continued. These indicated a three-fold increase in intensity and a two-fold improvement in resolution at high scattering angles compared with the present Cu (220) monochromator. It is hoped that this monochromator will soon be available for routine use. A new gas-flow cooling device is under development for the pressure cell to minimize consumption of liquid N_2. Modifications are being made to the furnace to improve the insulation at its high-temperature limit of 850°C.

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

This year there have been a surprisingly high number of experiments on D10 dedicated to study the rather complicated magnetic structures of rare earth elements (Ho, Dy, Nd, Tm, Er) and their compounds. D10 lends itself to these experiments, since with the analyzer it is able to resolve the close lying satellites in these systems. Another group of experiments, namely the study of elastic diffuse scattering from alloys and of critical magnetic diffuse scattering took advantage of the low background on D10. There also has been one purely inelastic scattering study. D10 has an unique energy and momentum resolution at rather high momentum transfer that is not available on other triple axes instruments at the ILL.

The new four-circle cryostat has been working to the greatest satisfaction. Its temperature stability is better than that of an orange cryostat in the full temperature range (1.7 K to 450 K) independent of the χ setting. The four-circle dilution cryostat has been successfully tested on the Eulerian cradle and in its present state can reach temperatures down to 200 mK. It will, however, be available for users only in the middle of next year when the worn out Eulerian cradle is replaced. With the new cradle, severe geometrical constraints for the dilution cryostat can be overcome and we expect to reach even lower temperatures.

By using the movement of the two axis detector as an ω-turn-table, we are now able to work on D10 with heavy sample environment devices. This option has been welcomed for experiments with special furnaces and heavy cryomagnets (e.g. the CENG 10T superconducting magnet).

With the increase in computing power due to the installation of the MicroVAX instrument computer, we were able to improve the software available on the instrument appreciably. The operating system (LSD) is now more user friendly. An independent simulation program (SIMLSD) and a program to calculate the instrumental resolution (RESPLT) have been installed to help the user make an optimal choice of scans. The raw data treatment can be performed on line via the COLL5N or DIFFIT programs.

D15 Four-circle diffractometer on the inclined thermal beam IH4

Although nominally a four-circle diffractometer, D15 has operated for the whole of 1989 with normal beam geometry. In this configuration the lifting counter gives access to reflections with scattering vectors out of the horizontal plane. With this geometry large cryostats, furnaces and pressure cells can be mounted at the sample position and need only be rotated about a vertical axis to measure reflection intensities.

The wide range of experiments carried out during the year included a study carried out in the milli Kelvin range of nuclear spin ordering in HoF_3 in which the ordered spin structure found was quite different from that which had been predicted, another low low-temperature experiment demonstrated 3D magnetic ordering of erbuim in the high T_c type oxide $Er_2BaCu_3O_7$. High pressure studies were continued on KDP and related compounds, and on the behaviour under pressure of incommensurate magnetic structures with experiments on $EuAs_3$ and CuO.

For part of the year a small 32 x 32 multidetector such as that on D9 has been used on D15. This promises to bring considerable benefits to the measurement of weak reflections and the study of incommensurate phases. Unfortunately the efficiency of the present detector has not proved stable enough for it yet to be used routinely.

D16 Four-circle MK6 diffractometer on the cold guide H16.

There have been no major changes on D16 this past year. The diffractometer continues to be heavily booked for experiments requiring the specific combination of Q range and Q resolution that it offers. These experiments are in many different fields of study, ranging from biology via polymers and surfactants to magnetic studies and the physics of surfaces. There have been few single crystal experiments. Because of this, the full implementation of software for such studies was delayed, but this will be remedied very soon.

D19 Multidetector diffractometer for protein crystallography on the thermal beam H11

New D19 experiments in 1989 included successful tests of a high-pressure cell, and use of the Munich mirror furnace up to 2000 K, both in conjunction with the 4° x 64° multidetector. A fast-moving arm has been constructed for optional mounting of a single detector or a small D9-type position-sensitive detector for use at wavelengths around 1 Å. Construction of the new 20° x 64° curved detector, to replace the 4° x 64° one, will start in 1990; it will give a gain factor of 6 to 10 for large unit cell experiments and for fibre and liquid crystal diffraction.

A Microvax 3500 was installed without difficulty in June, and all compressed data are now automatically transferred to the central VAX cluster for archiving. Full software compatibility has already made the instrument much more user-friendly.

D20 High-flux multidetector diffractometer on the thermal beam H11

D20 in its current small detector version is now fully operational and has operated very smoothly in 1989. Owing to the limited range of its detector ($2\theta = 12.6°$), most experiments were run in the scanning mode. The beam-time was shared almost equally between college 5 and college 6. College 5 experiments covered many aspects of crystallography including powder diffraction under a wide range of experimental conditions (dilution cryostat, cryofurnace, cryomagnet, pressure cell), texture measurements, single crystal diffraction (phase diagram under magnetic field). In the fixed-position mode, the high flux of the instrument and its angular coverage make it extremely useful for fast data collection for stress measurements in engineering materials.

The body of large banana position-sensitive detector (160°) has been completed and the electrodes for the 1600 cells of the detector will be delivered at the end of 1989.

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

This instrument is dedicated to single crystal diffraction studies at low resolution with H_2O/D_2O contrast variation, mostly on biological macromolecules. DB21 was running in 1989 without major problems almost 100% of the time. Beam-time was allocated to low resolution studies on Photosynthetic Reaction Center from Rhodobacter Sphaeroïdes, Tumor Necrosis Factor, Seryl-synthetase, Expanded Tomato Bushy Stunt Virus and Ribosome 50S subunit from Halobacterium Mariis Mortui, plus a small amount to tests of new biological systems. The instrument is very reliable. Some troubles came from the photomultipliers of the 2-dimensional Position Sensitive Detector (Anger camera) which seem to suffer from ageing and have to be replaced from time to time. A new large capacity

disk, 50% dedicated to DB21 data, was purchased on the DIVA-VEGA cluster in order to allow extensive data storage, and data treatment on large series of spectra.

CRYOPAD Cryogenic Polarization Analysis Device

The CRYOPAD is an instrument which is used to carry out generalized polarization analysis of a scattering process (see ILL Ann. Rep. 1987 p. 49). It has been installed several times during the year on the triple axis spectrometer IN20 to investigate aspects of the magnetic structures of antiferromagnetic crystals. The original prototype system is still under development and many improvements have been made during the year. The nutation fields were remagnetised to optimum values following a detailed investigation of the strength of the outer Meissner screen. The power supplies feeding the precession coils which were insufficiently stable have been replaced by higher quality ones.

The small VIXEN computer has been reinstalled in a larger crate allowing addition of a magnetic tape streamer for backing up the system, and IEEE interface. Various mechanical improvements have been made to facilitate and speed up the installation and alignment on IN20. The acquisition program has been further developed to improve the precision of polarization analysis, and the data reduction now incorporates a geometrical correction for imperfect coil alignment. New terminals allow graphical display of the polarization directions in a stereographic representation. The next planned developments which are now well under way are automatic positioning of the outgoing precession coil at the Bragg angle and the dialogue with the computer of the host instrument.

Coordinator : J. Brown

Special Instruments and Experiments

Introduction

1989 was again a very successful year in the field of 'S'activites at the ILL: Two new instruments started operation: the evanescent wave diffractometer EVA (University of Munich) started its first test measurements after a very short construction period and the very cold neutron interferometer produced the first interferogram in a 50 cm size prototype set-up (University of Vienna - Technical University of Munich).

The UCN-VCN team was especially happy after the announcement of this year's Nobel prize awards: indeed, two of the three 1989 Physics Nobel Prize winners have been using the new source of very slow neutrons on level D over a period of years: Wolfgang Paul (University of Bonn) is the "father" of the superconducting neutron storage ring NESTOR (neutron lifetime measurement) and Norman Ramsey (Harvard University) has a most active role in one of the great experiments at the ILL, the search for an electric dipole moment of the neutron (EDM).

Overview of current 'S'activities at the ILL

The current 'S'activities are listed in the following table:

Beam	Experiment/Instrument	Labs concerned
Level C:		
H17	superthermal He UCN source	RAL/HMI
H18	quantum chopper	TUM
IH3	SN5 - UCN source for test and development work	ILL
H7	GAMS4 - very high resolution gamma spectrometer	NIST/ILL
Level D:		
TGV	'Tube Guide Vertical ' - vertical neutron guide for very cold neutrons	TUM/URI/ILL
TURBINE	Doppler shift device - production of ultracold neutrons	TUM/URI/ILL
ZS2	NESSIE - very high resolution gravity spectrometer	TUM/URI
ZS3	Very high resolution gravity diffractometer	TUM/URI
ZS4	EDM - search for an electric dipole moment of the neutron	Sussex Intern. coll.
ZS5	'Testleiter', neutron lifetime experiments	ILL
ZS6	VCN interferometer	Vienna/TUM

Neutron guide hall ILL 7:

H142	S16	Cold neutron beam (proposals)	ILL
H142	SN7	Polarized neutron beam (proposals)	ILL
H21	S50	Precision measurement of λ/m	PTB
H21W	thermal beam for test and development work		ILL
H22	S10	n-α reactions (proposals)	ILL
H22	S34	γ- γ correlations (proposals)	ILL
H22	S51	Activation analysis (proposals)	ILL
H24	S20	Topography	CNRS
H24	S42	Laue diffractometer	CNRS/ILL
H25	S30	Depth profiling	HMI
H25	S18	Interferometer (thermal neutrons)	Dortmund/ Vienna
H25	S21	Double crystal diffractometer (proposals)	ILL

Neutron guide hall ILL 22:

H53	EVA	Evanescent wave diffractometer	Univ. Munich
H53	$n\bar{n}$	Neutron-antineutron oscillations	Padua/Pavia/ Heidelberg/ILL

Progress on instruments in 1989

Progress on 'S'-activities in 1989 is summarized below (see also Instrument Sections of College and College Secretaries' reports for scientific results):

S18 The neutron interferometer and diffractometer on the thermal guide H25 was in routine operation. Tests on a new (220) 45 degree interferometer and examination of a forbidden reflection on a quartz crystal have been carried out. Replacement of the original electronic equipment by an IEEE-system including a PC is in progress. A new X-ray generator was installed near the optical bench.

S20 The neutron topography instrument has been reconstructed. It was thus possible to initiate new lines of research, and new groups of users became interested in collaborations. A group from the Nuclear Physics Institute in Prague took advantage of the high resolution, the possibility of

switching easily from the polarized to the unpolarized neutron set-up and the continuously variable wavelength to perform experiments on nearly perfect crystals (vibrating crystals, magnetic crystals). These experiments lead to interesting comparisons with recent extinction theories. Scientists from the Kurchatov Institute used the new automatic control system of sample orientation, magnetic field and temperature to investigate details of the Morin transition in high quality crystals of hematite (α-Fe_2O_3). Other investigations, e.g. the dendritic structure of super-alloys or the chirality domains in helimagnets were pursued in collaboration with external groups and ILL thesis students.

S42 The Laue diffractometer has been heavily used (148 users / 6 cycles) for orientation of single crystals and testing of crystal quality. The apparatus can be used in self-service mode. It has been equipped with a monitor; improvement of the beam shielding is underway. Tests of a 2-dimensional detector based on a neutron-to-light converter, light intensifiers and photomultipliers have been started under the view for a feasibility study of a quasi-Laue diffractometer.

S50 The apparatus for the precision measurement of h/m has now reached a level of precision of 4×10^{-7} (original aim: 1×10^{-6}). Attempts will be made to push the limit to 1×10^{-7} by further improvements of the apparatus.

GAMS4 The very high resolution gamma spectrometer (2 axes, flat crystals) was heavily used during 1989. However, some amount of time and effort has been devoted to improving GAMS4. New silicon crystals with a thickness of 2.5 mm were manufactured and tested. Gamma-ray profiles obtained with these crystals agree with dynamical theory predictions to within about 0.01 arcsec. Some of the electronic equipment used for servo-control of the angle interferometers was upgraded. A small measurement error (hysteretic in character) was discovered in the polarization angle interferometers. Extensive diagnosis was performed to understand this error including use of a two frequency angle interferometer. Measurement errors were reduced by a factor of about 4 with the two frequency angle interferometer. Conversion of GAMS4 to this type of angle interferometer is being considered.

EVA The mechanical parts of the evanescent wave spectrometer EVA were assembled on site in February 1989. At the same time the computer system (PDP11, AT) and the electronic equipment were installed and tested. Software for full computer control of the instrument is available. First tests with neutrons revealed the expected resolution of the linear position sensitive detector to be 1 mm and provided information to optimize detector protection and beam tubes. The instrumental background was brought down to 0.1 n/sec over the whole detector area of 100 cm^2 after installation of the improved detector protection, evacuated beam tubes and additional shielding at the instrument site, and will be further reduced. The spectrometer is aligned and first test measurements on a Si(110) surface - looking simultaneously for the reflected and Braggs.

The photograph (see page 78) shows the current state of EVA: at the left the position sensitive detector (200 cells) in its shielding, at the right the specular beam detector and - towards the sample the vacuum tube with the internal collimation of 1 mrad.

In the **neutron-antineutron** oscillation experiment the neutron beam-line had to be shielded carefully against the earth's and other environmental magnetic fields because magnetic fields would suppress the oscillation process. This is not an easy task because the standard shielding process with high permeability mumetal shields alone is not sufficient here: for long mumetal tubes there is no shielding of the axial field component B_z (B_z = 11 μT= 11 μT, as shown in Fig. 65a). Compensation of B_z by the field of a solenoid wound around the beam tube brought B_z down to $B_z \approx 1$ μT (Fig. 65b), but this value is still far from the goal of $B_z < 10$ nT. Only a procedure called "idealisation" of the shield helps to suppress the residual field by the required factor of 10 000 from B_{earth} = 46μT to an average of B = 5nT (Fig. 65c). The residual short length fluctuations of B do not disturb the oscillation process. The "quasifree" oscillation efficiency in the residual field of Fig. 65c is 99.8%. The set-up is the largest high quality magnetic shield in existence.

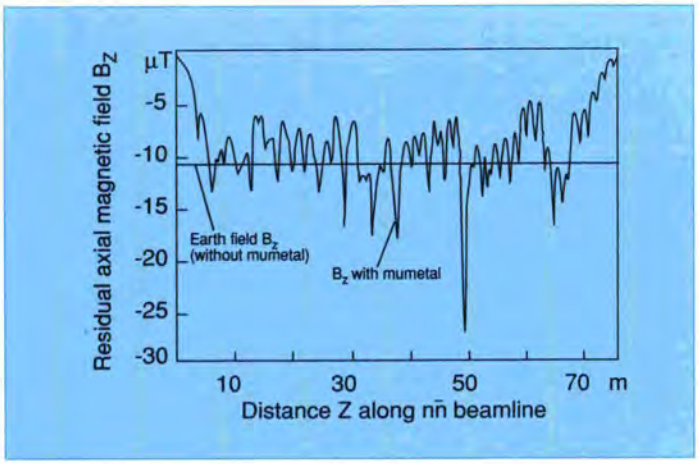
On H18, a group from the TU Munich has tested a first version of fast choppers and the beam transport system of the **FOTOF** spectrometer. Work will be continued in 1990.

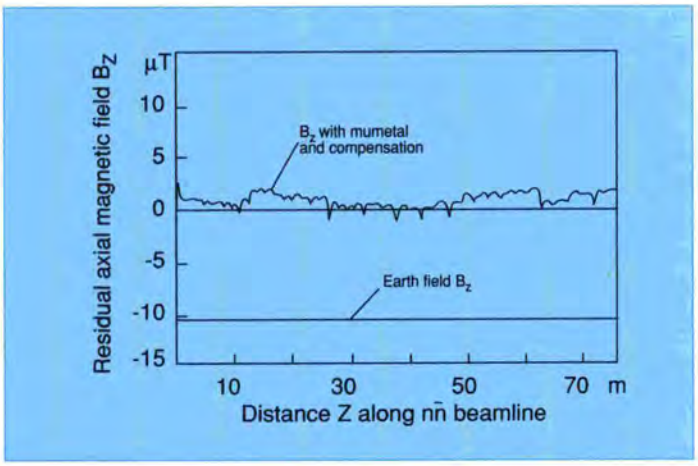
Activities in the field of very cold and ultracold neutrons

VCN interferometer: at the very cold neutron beam on level D a large (6 m x 1.2 m) vibration isolated optical table has been installed. The neutrons there have a wavelength of 100 Å and are ideally suited for experiments analogous to many classical optical experiments. The instrument presently under development on the optical table is a large (4 m long) interferometer, a prototype with 0.5 m length has recently been tested successfully. The new interferometer uses diffraction gratings as beam splitter devices. These gratings have a grating constant of 2 μm and for intensity reasons they are designed as phase gratings.

The **EDM** experiment is being rebuilt as described below.

Firstly, to increase the sensitivity, a larger neutron storage volume is under construction. This will be installed in a cylindrical vacuum chamber fitted along the axis of the magnetic shield. The vacuum chamber has a coil wound on its outer surface which will produce a vertical B_0 field of





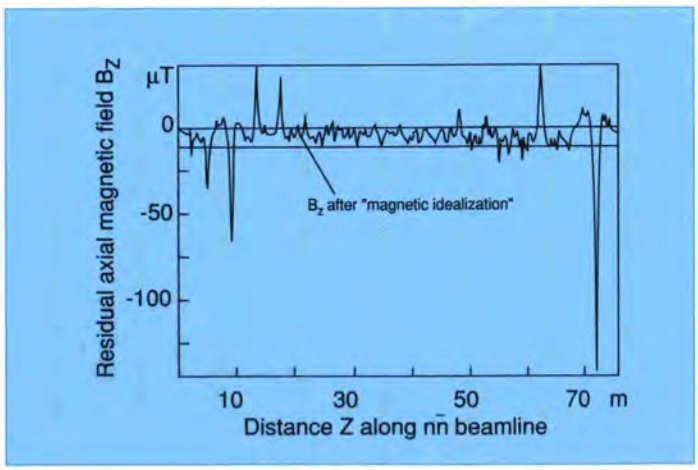


Fig 65: Plots of the residual magnetic field along the neutron beam of the neutron-antineutron experiment:

a) The mumetal magnetic shield alone has no axial shielding effect; on the contrary, it strongly disturbs the initially uniform earth field.

b) Additional field suppression by a compensating current-coil

c) Residual field after "magnetic idealization" of the shield. Note the change in scale !

10 mgauss. The innermost mumetal cylinder has been removed from the 5 layer magnetic shield to provide space for these changes. The remaining 4 mumetal layers have been thermally and electrically insulated to improve the overall shielding stability.

Secondly, the new experiment is planned to include a Hg vapour magnetometer system, the polarised Hg atoms will be stored in the neutron storage cell. This system is designed to eliminate systematic errors found in the previous data due to uncertainties in the average value of the magnetic field in the neutron storage volume.

In order to maximise the number of neutrons counted in the experiment, the neutron storage bottle is to be raised by 2 metres to compensate for having 2 gas-tight membranes in the turbine exit guide. The details of the Hg installation are in the design phase.

On the **UCN diffractometer** surface studies of various samples have been performed. Linewidths of 6.5 neV (FWHM) have been observed in total reflections of UCN on a liquid Fomblin surface. Computer simulations give a theoretical resolution of 5.2 neV. Some effort was devoted to studying the diffusion of the components in sandwich structures after heat treatment and to understanding the influence of vibrations of the instrument. Currently, the instrument is being modified for use with polarised neutrons; a furnace is under development to allow studies near the Curie temperature.

NESSIE - the gravity spectrometer produced its first data. The 3-dimensional Brownian diffusion of polystyrene spheres (Latex) in D_2O has been chosen as test object. Due to the large contrast between the hydrogenous Latex spheres and its solvent (D_2O), the coherent scattering from a 0.01% solution could be studied as a function of temperature in the energy range from

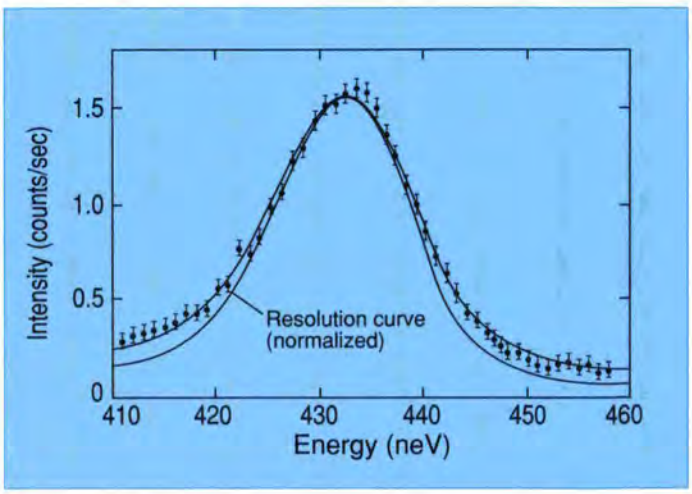


Fig. 66: Resolution curve together with quasi-elastic scattering from a soluion of polystyrene spheres in D_2O.

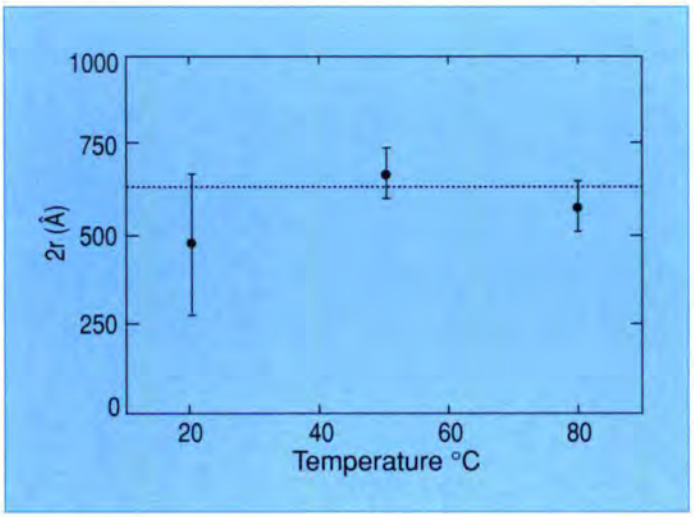


Fig. 67 Particle diameter as determined from neutron scattering.

390 to 560 neV. The fig. 66 shows a typical curve for particles of 640 Å diameter at T = 80°C; the dot-dashed line is the instrument's normalised resolution curve (BeO), whereas the solid line is the result of a least squares fit (a slightly modified version of the CERN MINUIT program is used for the convolution of a Lorentzian with the numerical resolution curve and the fit). The following values for the linewidth of the Lorentzian were obtained:

T = 20°C: $\Gamma = (0.74 \pm 0.3)$ neV

T = 50°C $\Gamma = (1.1 \pm 0.12)$ neV

T = 80°C $\Gamma = (2.2 \pm 0.28)$ neV

The agreement between the particle diameter and these values of the linewidths - via the Einsteinon-Stokes relation - is fairly good (Fig. 67) .

Other UCN-activities

Level D

During the reconstruction of the EDM apparatus, the available UCN beam is being used to perform systematic UCN reflectivity studies with the UCN monochromator developed by D. Richardson. Experiments with an energy band of only 5 neV are feasible.

Efforts have been undertaken to reduce the γ-background produced in the turbine, and the thermal neutron background has been mapped in order to optimize the shielding for future high sensitivity/low background experiments.

Level C

The superthermal He UCN source on H17 has been used to study the interaction of ultracold neutrons with superfluid He^4. For this purpose a correlation chopper was constructed and brought into operation including all the necessary control and analysis software for measuring the spectrum of upscattered UCN in the presence of a rather high background (signal/background ≈ 1/3) and low counting rates (≈ 1/3 s^{-1}). First observations of the temperature dependent time-of-flight spectrum of upscattered UCN were made.

Coordinator: W. Drexel

Scientific Coordination and Public Relations

Statistics of the Scientific Programme

With 1989 we come to the end of a decade. This provides an opportunity to look back at the 80 s. Fig. 68 shows the number of experiments allocated for the whole of the instruments for each year. The decrease in 1984 and 1985 can be explained by the long shut-down. The improvements on the different instruments over the last few years have resulted in an increased number of experiments allocated.

Fig. 69 shows the details of the instrument statistics. The total beam-time requested was on average twice the time available. Due to the postponement of the 6th cycle of 1988 into 1989, the instrument IN3 is included. However, IN3 is now a special beam instrument (see details in the 'special beam' section). An overall total of 5072 instrument days was allocated. The distribution of these experiments amongst the different Colleges is presented in Fig. 70. In 1989 the number of experiments allocated for the new member countries Spain and Switzerland increased. Fig. 71 shows the beam-time allocation for the five member countries. All instruments and all instruments except nuclear physics and scheduled special beam instruments are shown separately in Fig. 71.

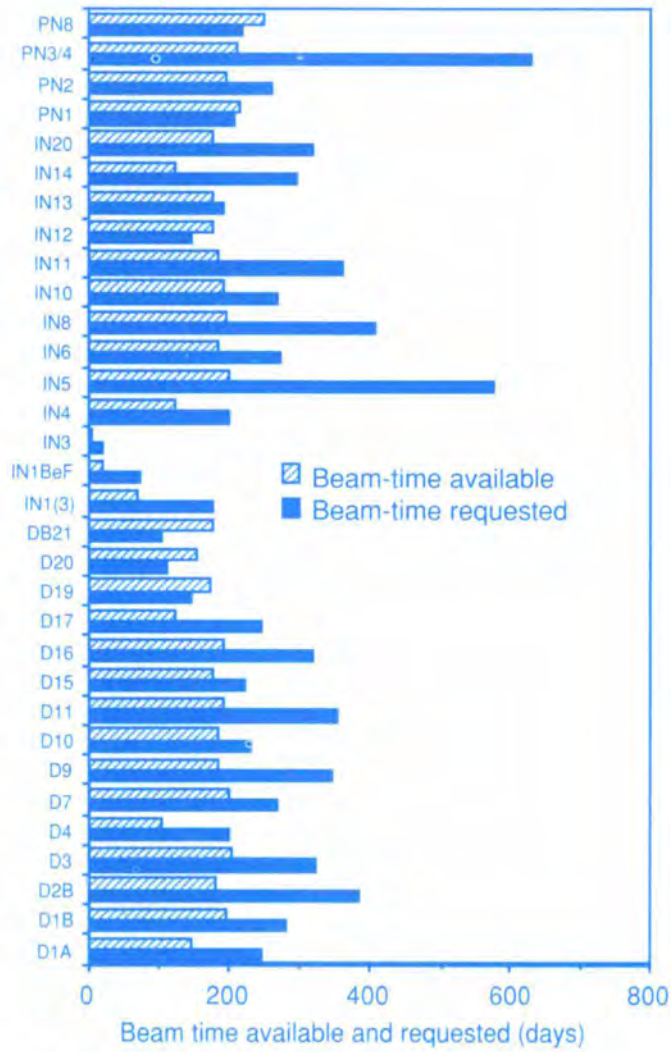


Fig. 69: Instrument statistics 1989

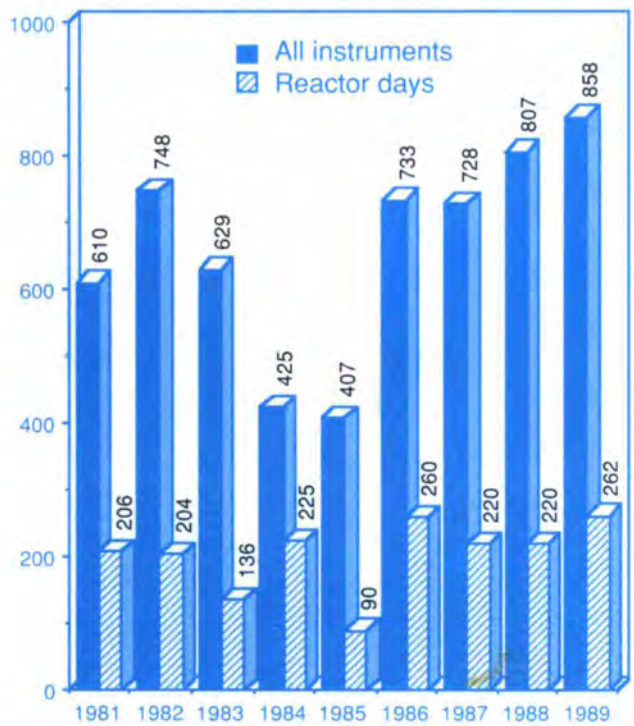


Fig. 68: Number of experiments in the 80's

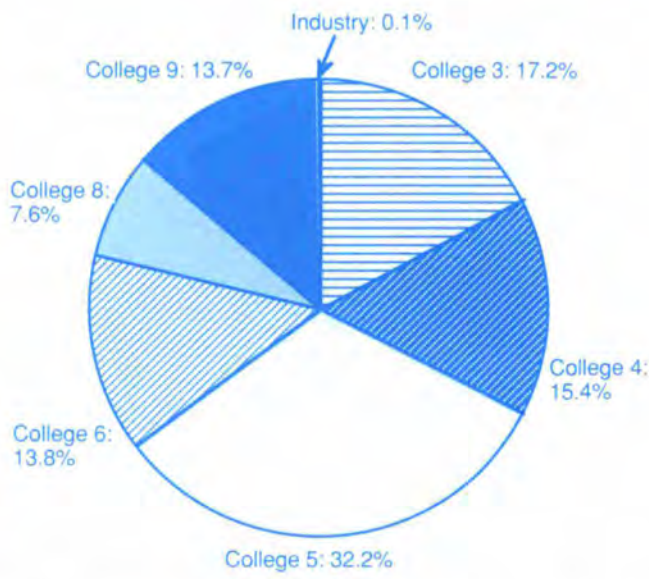


Fig. 70: Instrument days allocated per College 1989 (total of 5072 days)

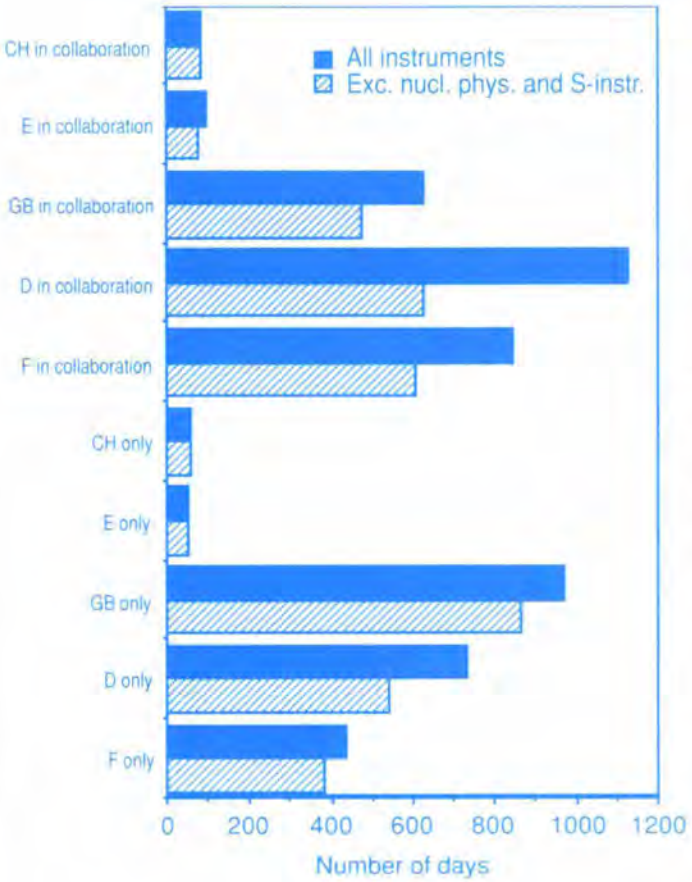


Fig. 71: Beam allocation for the five member countries

Library

Library Budget 1989: 789 KF

The library provides ILL and ESRF users with information and scientific literature. The increase in the budget (inflation plus 6%) combined with the reduction in the cost of binding and the complete stop of the purchasing of reprints helped to meet the increase in the cost of scientific journals (more than 10% between 1988 and 1989). The rate of acquisition of books could not be maintained.

Half-time secreterial help was given by the ESRF in order to deal with the increase in the administrative work.

- 350 purchase orders were typed and processed (250 for the ILL and 100 for the ESRF)
- 620 books were purchased and processed: 350 for the ILL Library, 120 deposited with ILL departments, 150 deposited with ESRF.
- 650 volumes of journals were bound.

Computerization of holdings began using "Hypercard" on Macintosh microcomputer: references of 1000 books were entered.

In close connection with the scientific work of the ILL

- 500 ILL publications
- 500 ILL experimental reports

were registered (Hypercard on Macintosh).

Collaboration with ESRF

The project for a joint ILL/ESRF Library which wil be housed in the ESRF/ILL joint building is taking shape. As a first step, the participation of the ESRF in Library expenditure should begin in 1990.

Safety, Medical and Health Physics Group (D.SPS)

The main function of the units responsible for General Safety, Health Physics, Works Medical Service and Safety Officer is to assist ILL staff, guest scientists and employees of outside firms working on the ILL site. For all activities involving a risk, their work makes it possible to define working conditions to ensure that the risks are limited, and to implement appropriate monitoring and inspection facilities.

These units also provide technical support for the Committee on Health, Safety and Working Conditions, and for the Internal Safety Commission (CIS).

Instruments and Methods Department

Instruments and Methods Department

Introduction

The activity of the Instruments and Methods Department (DIM) in 1989 shows certain trends:

With a view to developing engineering techniques in the Project Office, the ILL is starting to use a finite element method numerical simulation programme in cooperation with ESRF.

In the field of development of methods it should be noted that

- A scientist has been nominated to augment the team responsible for the development and maintenance of multidetectors;
- The transfer of technology for multiwire detectors to an external firm has been successfully carried out. This firm is now capable of supplying complete detectors.
- The construction for HMI of a detector with 64 x 64 cells at 15 mm intervals. The success of this prototype has enabled work to be started on the D22 detector.
- The success of the technology of microstrip anodes permitted a start to be made on the assembly stage of the 1600 cell banana detector for D20.

For the first time for many years no new instrument project has been started, despite some reflections on a future IN4B.

The construction of the instruments on the horizontal cold source (IN15, D22, IN10C) has continued actively. All the main components have been designed and ordered, and assembly on site has started (IN15).

The Department was responsible for the organisation and construction of a joint stand with ESRF at the Société Française de Physique Exhibition in Paris. Various items of technical equipment developed at ILL were presented on this occasion.

Project Office

Finite element method numerical simulation group

In 1989 the new "ANSYS" program (operating on the VAX 8650) was introduced, which is much more powerful than the previous "CADSAP" program (operating on PC AT 386). This very high powered program was chosen with a view to our cooperation with ESRF, which has been using it since autumn 1988.

After a running-in period of 3 months (July to September 1989), real problems arising at ILL were studied:

- deformation study of a beam subject to multiple loads for IN15 (static elasticity);
- study of vibration modes in the chassis supporting the IN15 velocity selector (dynamic elasticity);
- beginning of a study for a new hot source for the reactor (stationary and non-stationary thermal study);
- study of the crystal support structure of the IN10C Doppler machine (deformations, strains and vibration modes).

Neutron guides

There were major projects on:

- replacement of the guide H53B
- completion of the line H5 for an acceptance inspection by the Instrument Operation Department (primary beam shutters, electro-pneumatic equipment, etc.)
- installation of a first 12 m section of guides H511 for the instrument IN15.

Electronics Group

This group of 18 staff is responsible for the maintenance of all control and data acquisition electronics on all the instruments used at ILL (more than 50 if the "S" and "Test" instruments are included).

It nevertheless devotes part of its time to the development of VME standard modules for:

- the new instruments on the horizontal cold source
- the long awaited replacement of the CAMAC time-of-flight electronics used since the start of the ILL, the technology being now out-dated.

In 1989:

- the final VME controls for IN10A were commissioned
- the controls for the future D22 were assembled and the first tests carried out
- the tests of prototypes for future modules to control choppers, for time-of-flight analysis, and for axis control were completed
- the controls of the new instrument T13A for testing polarising monochromators were designed and commissioned during the year.

Mention should finally be made of the maintenance and loan group, which has initiated on Macintosh the preparation of a general inventory of all the electronic equipment with a view to economic control of:

- the stock of equipment for loan
- the optimum renewal of the modules in use
- corrective and preventive maintenance of the above equipment and the associated tests

This group has also dealt with a number of jobs on request:

- reference current source
- automatic temperature control
- interface cards
- magnetic field detectors, etc.

Mechanical construction

The mechanical construction and maintenance group comprises three parts:

- drawing office, with 6 staff dividing their time between design studies and intervention work on instruments
- mechanical construction workshop, which deals with the majority of requests for urgent intervention work for the whole of the ILL
- test workshop, which is particularly well equipped for the various fields of mechanical and optical measurements and for special production work.

Drawing office

A considerable part of the work in 1989 was still devoted to the projects IN10C, IN15, D22 and the rebuilding of T13A, which are in their final phase.

A major training plan has been initiated to accompany the introduction of CAD (with EUCLID software). In particular two draughtsmen are attending refresher courses on the strength of materials.

With the recent purchase of a second workstation for EUCLID it will be possible to start the design of an instrument with this very powerful tool.

Workshop

In addition to numerous projects for the reactor, reference may be made in the instrument field to:

- fabrication of components for IN15
- production of the motor for the IN10C Doppler machine with the aid of subcontracting, development of Kevlar carbon fibre chopper disks and reflector supports.

Test workshop

All the intervention work on the guides was carried out on a regular basis by test workshop staff.

Reference should also be made to:

- testing and balancing of choppers (new composite material selector for IN15)
- production of sintered LiF beam shutters, scintillators, etc
- assembly of IN10C and IN15
- contribution to study for control of certain instrument functions by commercially available programmable controllers (in collaboration with and under the responsibility of the electronics group).

Multidetector Group

As in the past, the work of the multidetector group has again been very widespread. A lot of time has been - and will be - devoted to all kinds of interventions on the various neutron detectors and on the numerous instruments and their associated electronics to ensure their smooth and reliable running during all reactor cycles. Only the major tasks in this respect may be listed here:

- complete recabling of the 128 x 128 multidetector for D17 after repair at LETI and its successful installation on the instrument;
- partial renewal of the commercial photomultiplier tubes of the DB21 scintillation multidetector and then tuning of the complete detector;
- development, tests and installation of new LS hybrid circuits for the D11 electronics.

Fortunately, apart from this maintenance work, time was left for development and construction of some detectors. Among other things the first (128 x 128 wires at 1.5 mm intervals) multidetector for colleagues at Saclay has been successfully installed at their reactor ORPHEE, while a second detector of the same type but with a new spherical window will be finished by the end of this year.

For IN15 and IN10C slim (total thickness 10 mm) neutron monitors with 0.5 mm thin aluminium windows have been developed, to keep neutron losses and neutron diffraction as small as possible. They have an active area of 60 mm x 75 mm and are filled with 1 bar of the standard Ar-CH_4 (10%) mixture.

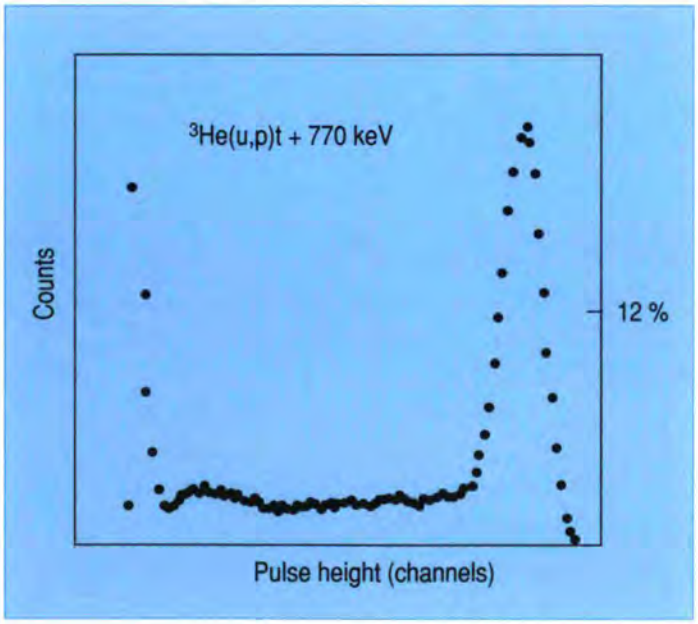


Fig. 72: Pulse height spectrum of the 64 x 64 - 15 multidetector, all anodes connected.

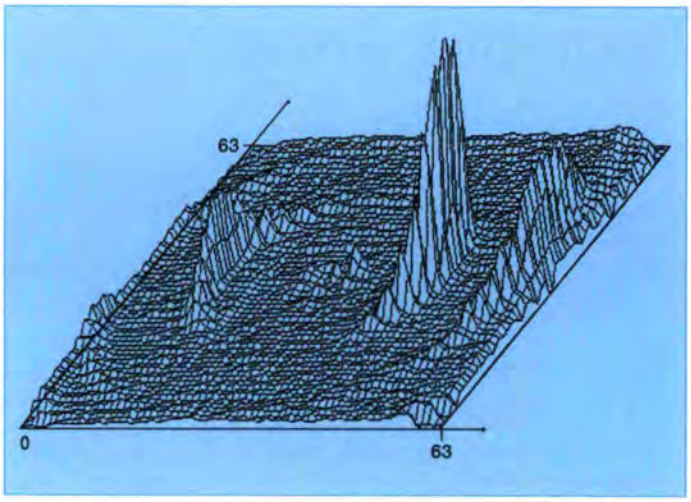


Fig. 73: Diffraction pattern of a carbon sample over a 1 m x 1 m active detector area.

The through-going neutrons are monitored via the ^{235}U(n,f) reaction by collecting the electrons created by the ionising fission fragments. Therefore these monitors operate at a low voltage of 100 V.

A replacement of the thin ^{235}U-layer by ^{3}He gas is envisaged.

A bigger and much more ambitious project, the construction of a 64 x 64 multidetector with a wire spacing of 15 mm for HMI-Berlin was successfully completed in the autumn. The detector has an effective area of 960 mm x 960 mm, at present the largest neutron multidetector in the world. It is filled with 1.65 bar ^{3}He and 0.35 bar Propane as stopping gas. With its detection gap of 28 mm, the measured efficiency for 2.5 Å neutrons is about 52%. The average intrinsic noise of the detectors is less than 1 count/h/cell. (see photograph on page 77).

By connecting all anodes, the overall performance of such a multidetector can easily be checked. By using an AmBe-source and applying - 1525 V to the anodes an energy resolution of about 12% was achieved as shown in Fig. 72. The resolution of single anodes is slightly better. Finally, the more or less perfect homogeneity of the detector's response is clearly demonstrated in Fig. 73, where the diffraction pattern of a small carbon sample is shown.

As this detector was initially foreseen as a prototype for the new ILL instrument D22, the construction of the D22 detector (half the wire spacing) by an external firm seems to be assured.

As already mentioned in last year's contribution, ILL has signed a licence agreement with an external firm for the transfer of the technology of standard gaseous multiwire neutron detectors. This arrangement has proved its usefulness

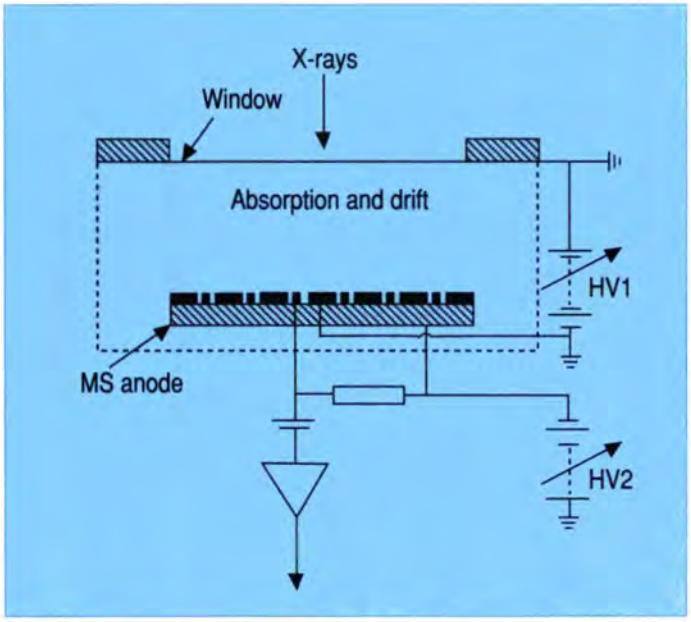


Fig. 74: Schematic set-up of the MS-detector.

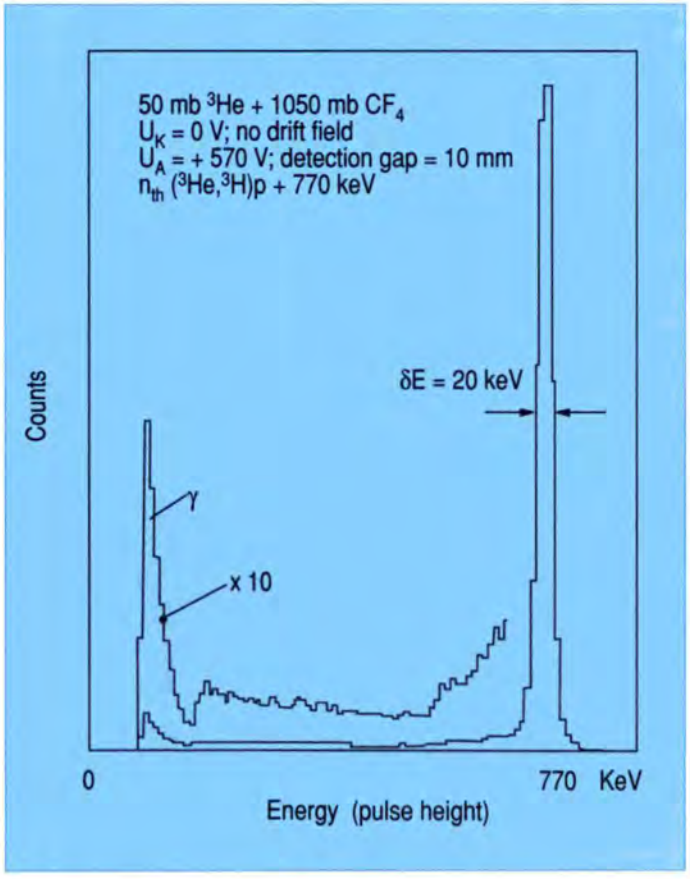


Fig. 75: Pulse height spectrum of the MS prototype detector for ultra-cold neutrons.

and a first multidetector for an external customer was delivered at the end of this year.

Besides these more technical applications, the lion's share of the research work has been devoted to further investigations of the properties of wireless microstrip proportional counters (MSPC), first proposed by A. Oed [*]

Such a MSPC can be used to detect not only neutrons, but all kinds of ionising particles, X-rays and even single photons may be detected. Its working principle is shown in Fig. 74. The entrance window in front can serve as a detector cathode in order to transport the primary electrons generated by the ionization towards the microstrip (MS) anode - alternating narrow and broad conducting strips - which replaces the wires of the usual multiwire counters.

The MS plate is produced by means of a photographic technique, as used in the semiconductor industry. With this technique strip structures in the micrometer range with a precision of 0.2 μm on up to (1400 x 400) mm^2 large glass plates can nowadays be made. The MS plate operates as a gas amplifier, just like a proportional counter. Holding the narrow strips (anodes) at a sufficiently high positive potential with respect to the broader ones (cathodes), electrons produced in the detector gap will drift towards the anode and undergo an avalanche amplification close to it.

For moderate potential differences (around 800 V) gas amplification factors up to 10^5 have been measured. A prototype detector for very cold and rather cold neutrons with such an MS plate and filled with ^{3}He has recently been developed and tested. Its pulse-height spectrum is shown in Fig. 75. This excellent energy resolution - just twice the

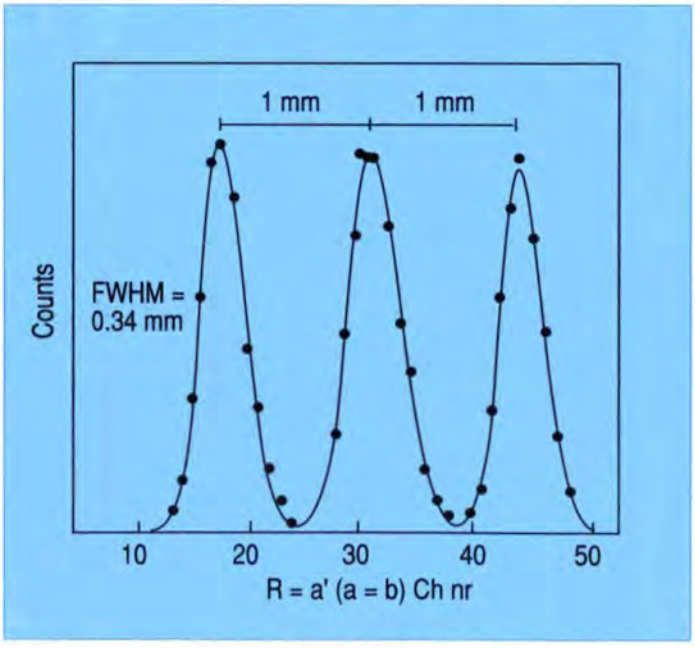


Fig. 76: Position determination using pick-up strips on the back of the glass substrate.

theoretical one - is nearly gain independent up to 10^4. It is also uniform over the whole detector area due to the high precision MS structure.

Furthermore, the limiting countrate of this detector is at least 10 times higher than for a common ^{3}He wire detector.

Moreover, such MS-plates can easily be used to build two-dimensional position sensitive detectors with promising resolution: either one uses resistive anode strips giving a rise-time dependence of the pulses as a function of the detection position along the strip, or one fixes mechanically or evaporates on the back of the MS plate thin metallic strips perpendicular to the structure on the surface and makes use of the induced signals on the rear electrodes.

So far only preliminary attempts have been made. In the first case, the resolution was close to 1 mm, while for the latter a vertical position resolution for ^{55}Fe X-rays of 0.34 mm was achieved as shown in Fig. 76.

Further research work will go on to test the attainable limit (μm-range) of these MS-plates.

[*] A.OED, NIM A 263 (1988) 35 & Patent 86 10810 France

Monochromators

As part of the activities of the group a number of monochromators or filters have been prepared, improved or realigned, such as a Heusler monochromator for IN12, a Si analyser and a single crystalline graphite filter for IN14 and a rotating deflector with 120 graphite crystals for IN10C. This graphite material was made at the ILL's own graphite facility. Also a beryllium test monochromator for D9 with a new mechanical mounting for precision alignment was built. It gave very good results at a wavelength of about 1 Å. However, an unexpected wavelength contamination was observed at about 0.5 Å which necessitates further studies on this monochromator before it can be finally transferred to D9.

The conditions for the growth of Beryllium single crystals for monochromators as a joint venture of the ILL, the MPI at Stuttgart and other interested neutron scattering centres, have improved during the year. Higher quality beryllium from AMT became available. Only about half of the number of zone refinements are necessary to obtain a sufficient purity for single crystalline growth. Studies on the plastic deformation of beryllium have concentrated on tensile stress at ambient temperature and compressive stress at higher temperatures. The first deformation mode gave very promising results and it is being pursued further. A particular problem concerned the solder between the beryllium and the steel holder needed for clamping the samples. It used to seize up frequently when a load was applied. We showed that this could be avoided by an appropriate geometry of the tensile specimen (see photograph). In spite of the progress achieved, the plastic deformation of the beryllium crystals cannot be considered as completely solved.

Beryllium single crystal prepared for a tensile experiment.

At present the measured neutron reflectivities are not yet as high as expected, probably due to an inappropriate microstructure, and further studies have been initiated to improve this situation.

The first instruments have received graphite crystals made at ILL. Although we have made top quality graphite of a few square centimetres, to date we have not succeeded in producing large size specimens comparable to ZYA material from Union Carbide. Efforts now concentrate on systematic studies on our samples including, in particular, a better characterization of the starting material to try to correlate process parameters with the quality of the final product.

The R&D project on the growth of $Si_{1-x}Ge_x$ single crystals came to an end this year. Upon request, crystals with a Ge concentration x up to 20 atomic % are now available on a commercial basis.

Further major activities of the group concerned the growth of Cu_2MnAl Heusler crystals in our own Bridgeman furnace to cope with the great demand for polarizing monochromators and a development for monochromators with extreme anisotropy of crystal mosaicity. This is advantageous for focussing optics and should improve the control of the quality of the crystals.

In addition the group frequently provides assistance to the user community for sample characterizations with both X-rays and neutrons.

Multilayer Laboratory

The equipment of the laboratory has suffered due to a fire on the air conditioning for the new control computer installed last year on the RIBER evaporator. The replacement of the improved control electronics is nearly finished. Some programming work is still necessary. The ELECTROTECH evaporator has operated without major problems.

The last 12 months were devoted mainly to the serial production of bender polarizer supermirrors: a small angle set-up for analysis on D7, a polarizer for short wavelengths (down to 2 Å) for IN14, an analyser with larger cross section for IN11 and a set of polarizer analysers for very short wavelengths (0.8 Å limit) for the zero field spin-echo test facility on H21 were made. A test of a normal D7 analyser on IN11 immediately gave a gain of a factor 2 for the intensity.

The development work, 33% of the time, was undertaken for a polarizer with high divergency, using 300-layer supermirrors with a factor of 3 for the cut-off angle [3]. Other developments are a focussing device with very high gain (>7) and a polarizing neutron bandpass filter used as a neutron splitter, allowing the use of half of the neutron spectrum with the wrong spin state in transmission. The splitter will replace a mechanical selector (collaboration with KFA Jülich).

The work for external laboratories, 15% of the time, consisted in the supermirror coating of neutron guide elements for GKSS Geesthacht and bender polarizers for RIT Stockholm and LLB Gif-sur-Yvette.

In the framework of a collaboration for industrial supermirror coating of neutron guides with the guide manufacturer CILAS-ALCATEL (France) and the laboratories ILL and LLB (France), HMI (Germany) and PSI (Switzerland), test evaporations on substrates with different treated surfaces were carried out. The aim is to optimize the substrate surfaces and the methods of deposition.

Publications and preprints:

[1] *R. Pynn, "Some comments on the use of supermirrors at the Institut Laue-Langevin".*
Thin-Film Neutron Optical Devices: Mirrors, Supermirrors, Multilayer Monochromators, Polarizers, and Beam Guides, Charles Majkrzak, Editor, Proc. SPIE 983,18 (1989).

[2] *B. Alefeld, J. Duppich, O. Schärpf, A. Schirmer, T. Springer, K. Werner, "New neutron guide laboratory at the FRJ-2 reactor in the KFA Jülich and its special beam forming devices".*
Thin-Film Neutron Optical Devices: Mirrors, Supermirrors, Multilayer Monochromators, Polarizers, and Beam Guides, Charles Majkrzak, Editor, Proc. SPIE 983,75 (1989).

[3] *O. Schärpf, N. Stüsser, "Recent progress in neutron polarizers".*
Nuclear Instruments and Methods, in press.

Reactor Operation 1989

Introduction

In 1989 the reactor schedule was planned to include 6 cycles, despite a difficult period due to a shortage of fuel elements. This necessitated the reduction of some of the short shutdowns between cycles to the minimum essential for reactor maintenance operations.

January 1989

Completion of the work scheduled for the shutdown, primarily on strengthening the prestressing of the reactor shell.

Cycle 1/89

Operation from 7 February to 23 March. The scheduled dates were respected and the cycle was completed without incident.

Cycle 2/89

Operation from 4 April to 20 May. The cycle was extended by two days to compensate for a shutdown with Xenon poisoning on 5 May due to failure of the refrigerator on the cold source.

Cycle 3/89

Operation from 30 May to 15 July. The end of the cycle was delayed by two days to compensate for a reactor shutdown with Xenon poisoning on 7 July, caused by a mains power failure on the EDF supply. On 19 June an interruption of the power supply and releases of the safety rods resulted in several brief reactor shutdowns followed by immediate re-starts.

Cycle 4/89

Operation from 20 July to 31 August. Shutdown from 24 to 26 August caused by failure of one of the two EDF power supply lines to ILL.

Cycle 5/89

Operation from 19 September to 2 November. The scheduled dates were respected. There was a brief shutdown on 21 September following a disturbance on the EDF power supply.

Cycle 6/89

Operation from 7 November to 21 December. The scheduled dates were respected and the cycle was completed without incident.

Data for 1989

Number of days originally scheduled	264
Actual number of days of operation	259.3
Number of equivalent days of full power	250
Actual operating time as proportion of year (%)	71
Actual operating time in relation to time scheduled (%)	98.3
Number of fuel elements used	6
Number of fuel elements despatched for reprocessing	0
Number of new fuel elements received	
Number of unscheduled shutdowns	9
including:	
brief shutdowns	6
shutdowns with Xenon poisoning	3

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.

Difficulties in the supply of fuel elements, due to delays in the supply of uranium, resulted in a shutdown of approximately two months up to the end of January 1989. This situation was a cause for concern for most of the year, but became easier towards the end of the year. However no shipments of used fuel elements to the reprocessing plant could be effected, due to administrative difficulties. Possibilities for temporary storage of these fuel elements are currently being investigated.

During the whole year particular attention has been paid to the reactor building. The upper part of the concrete structure has been strengthened with prestressing cables. This added 800 tonnes of additional prestressing, so that the building now conforms completely to the current requirements, and in particular to the earthquake regulations which have been amended since the reactor was built. Systematic checks and the necessary intervention work have been carried out to improve the airtightness of the reactor building. A series of measurements, necessitating the complete isolation of the reactor for several days, showed that its airtightness was better than required by the regulations.

The facilities necessary for the use of the pneumatic tubes were dismantled and reinstalled in the basement of the reactor building.

The emergency control room, which permits the reactor to be monitored and the essential manoeuvres to be carried out by remote control, was provided with a diesel generator to ensure that its operation is unaffected by fluctuations in the external electricity supply.

The Quality Assurance system, set up in 1984 and enhanced as necessary, was the subject of an external audit at ILL's request. It was found that the system in operation was in accordance with the legal requirements.

Computing Department

Computing Department

Introduction

A major reorganisation of the Department was put into effect at the end of 1988. The aim was to better respond to evolving requirements in the computing field during a time when available manpower is being reduced. The main changes were as follows.

A new Instrument Service has been created, with responsibility for the control of all condensed-matter instruments. Likewise, all data treatment for these instruments is centralised in one Group, which has also been given the task of identifying and promoting new development projects. In recognition of the gradual merging of all form of electronic information transmission, the Telecommunications Group has been integrated into the Central Computing Service to form a new Central Facilities Service.

These changes have been implemented smoothly, and seem to have been well received by both the people directly concerned and the users of the various services.

The only serious organisational difficulties arose in an area untouched by the above changes. The application of computers to administrative and office activities has posed problems over recent years because it has grown to become a significant activity just at the time when ILL has been cutting back on staff. In the latest effort to improve the situation the Computing Department has agreed to take overall responsibility for this area. Responsibility has been given to the Central Facilities Service in order that systems and operational support staff can cover the computers used.

Central Facilities Service

This new grouping constitutes a merging of the former Central Computer Service, Telecommunications Group and Management Information Services.

For the first full year since the start of the transfer from DEC10 to VAX, the users of the Computing Centre have had available an essentially homogeneous cluster of 2 VAXes (8700 and 8650). The majority of the software conversion was completed in the 3 previous years, and by 1989 this activity was practically non-existent.

In April the Service was given the responsibility for the operation of the four management information service machines and had to arrange to provide the necessary assistance to their users. This reorganisation resulted in a very considerable excess workload for the service and no long term solution to this problem has yet been found.

Operations

The Operations Group is responsible for operation of the scientific computers and management information systems, and provides all users with a first level assistance in the use of workstations and of a number of applications; it also controls the stocks of consumable materials.

The level of use of the Cluster (VAX 8650/VAX 8700) has been high this year: typically about 500 hours/month/CPU. The advantages of the cluster have been very evident: incidents were normally confined to one or other processor, and it was rarely necessary to shut down completely.

An important task of the group is the monitoring and management of the disk resources. The safeguarding and recovery procedures for files (software ARCHIVE2000) have become operational. The same software is also used for archiving expired visitors' files.

To ensure proper conservation of the data base, almost 300 old magnetic tapes were this year copied on to new tapes, and the experimental data on to optical disk.

Systems and Communications

The year 1989 was characterised by the transfer from version 4.7 to version 5.02, then 5.2 of the VMS operation system. To get the maximum benefit from the power of the Cluster, performance measurement tools were used in collaboration with DIGITAL. The connection has been made to the HEPNET network; the network software (DFS/DNS) has been installed.

The use of the JANET, EARN and TRANSPAC networks remains at a high level, and also necessitates maintenance and supervision at all times. A task detects possible anomalies in operation. Utilities for creation and recovery of tapes to communicate with the non-DIGITAL world have been written. Various Macintosh programs have been installed and procedures developed to permit the recovery of experiment data on Macintoshes. The use of optical disks and the writing of appropriate software improves reliability in the archiving of experiment data.

Several applications have been developed in the field of wordprocessing: MacTexindex (creation of an index under TEX on the basis of information produced by LaTEX), transfer of French texts written on WPS (Vax) to WORD (Macintosh).

Graphics

There is a rapid development of equipment in this area, and a variety of software necessitating tests and adaptation to the requirements of physicists.

Of the modelling software, CHEMX is available on Macintosh; the interface of SCHAKAL has been restructured with drivers available on BENSON, JUPITER, TEK4014, TEK4015, LN03 and Macintosh plotters and printers.

For the display of data DISSPLA enables experimentalists' graphics requirements to be dealt with; the library has been installed and 12 drivers are available.

The VIEW program permits very fast display of raw data and also provides numerous algorithms for image processing.

Mathematics

Version 13 of the NAG mathematics library is now in use. The specialised software MATLAB and MATHEMATICA are available on Macintosh.

Version 2.6 of the crystallographic software XTAL has also been installed.

The work commenced in previous years in the field of maximum probability algorithms for the treatment of diffraction data (ABFfit software) has continued, with the appearance of version 4 on Macintosh and an implementation on VAX expected in 1990. A two-dimensional adaptation is being studied in collaboration with ESRF. A graphics software ABFplot is associated with ABFfit. The validity of the least square procedures has been studied for the analysis of powder diffraction data, showing the interest of the maximum probability type approach. In the field of Laue diagram treatment, an IBM-PC version of the Laue program has been improved, permitting the orientation of monocrystals on the basis of a single Laue pattern with the aid of an indexation procedure and a simulation of diagrams on a graphics screen. A Vax version is also available.

Administration and Office Computing

The reconstitution of this activity (formerly Management Information Services) within the Central Facilities Service has posed a number of organisational problems. At the hardware and operating system level, the computers have been incorporated into the set of machines supported by the Service. Appropriate technical staff are available but evidently spread more thinly. At the applications and user support level there is a clear lack of suitable staff and the principle adopted has been to contract out as much of this work as possible.

The application of this concept has been most successful in the area of salaries and personnel management. The main programs of the package (PACHA) now run on the computers of the SOPRA company at Annecy, to which the staff of the Personnel Service are linked via a network of PCs.

In the finance and purchasing area it is recognised that problems arise due both to imperfections in the package as installed and to an insufficiency of hardware resources.

The long overdue modernisation of the MISSILL system (which supports the visitor programme and associated activities) is at last under way. This will run on a VAX 3500 using an ORACLE data base. The first phase is limited to the needs of SCAPRO, but if successful it is hoped to widen its range of application. In this area all programming is done under contract.

In the field of wordprocessing the supplier of the ILL standard package, ITOS, announced that no further development of the product would take place. To replace it we have adopted Microsoft's WORD, running on Macintosh, this being already a de facto standard amongst the scientists.

Telecommunications

- **Telephone:** the collaboration of this group with ESRF has been considerable. Work has been done to equip the ESRF buildings, particularly ESRF02. A working group has had the task of studying the possibility of a joint ILL/ESRF telephone service. A memorandum of understanding has been signed by the 2 Institutes on future collaboration in this area.

- **Computing networks:** the APPLETALK network now covers the main ILL buildings (80 Macintosh micros and 14 Laser printers). The Ethernet network has been extended to the complete site with some use of optic fibres. In parallel, the number of terminal servers on this network is now 29 (an increase of one third).

Instrument Service

This Service has as responsibilities

- computer systems for control of all condensed-matter instruments (i.e. IN and D series)
- supervision of the in-house computer network
- that part of computer maintenance which is carried out in house.

The main function of the Service has been the maintenance of hardware and software to ensure optimum availability of the instrument computers; this was successfully achieved, as the number of shutdowns on instruments due to computers during the year was very low.

Three main lines of development have been pursued:

- increased monitoring and regular analysis of the local network with installation of a network analyser and development of several software tests,
- further standardisation of program development tools on instrument computers, particularly VAXes,
- a considerable effort for development and improvement of VME units (VMS, OS9), in collaboration with DIM (Electronics Group).

The instrument IN10A is operational using VME.

The Service installed the following replacement computers in 1989:

- the Microvax 3500 on D19, permitting considerably better performance than the PDP11, and a particular effort was made on treatment in connection with D9 and D15 for multidetectors; a display unit was still to be installed,
- the VAX 3200 station on IN4 and on IN5,
- the PDP 11/73 computer on the gamma diffractometers.

Data and Projects Group

The role of the Group is to support current data treatment, and to examine future strategies for further development.

During the current year the primary access routines to data have been reviewed and partially documented: the PDP 10 archived data for many instruments may now be used transparently for data from 1978, and from 1974 in certain cases.

Looking to the future the UIS and X-windows software from Digital has been examined in some depth. The use of windowing systems for an easy-to-use interface is exemplified by the popularity of the Macintosh PC. ILL data have been interfaced to simple interactive display programs. Having acquired this basic expertise, the manpower costs for more practical projects can be assessed quantitatively. In parallel the Group has also examined several public domain and commercial display and calculation packages and has prepared demonstrations of these linked to ILL data. One such commercial package is being proposed to provide interactive raster display facilities for coloured surface plots in the immediate future, where alternatives lack performance and sophistication.

The basic treatment programs for the Vercors Group instruments have been completely revised for use on the VAX. The SANS programs have now an up-to-date documentation and a set of programs has been prepared for easy installation at sites external to the ILL. While the set of inelastic programs is now complete, the renewal of these programs is under study.

A new project of use in crystallographic measurements is the examination of the use of transputers in signal-analysis from multi-electrode detectors. The use of a fast processor to compute more precise positional information rather than simple hardware selection depends to a large extent on the amount of cpu power available and the bandwidth for handling large volumes of events. The transputer offers scalable amounts of both. Initial studies of the transputer and its software has involved collaboration with ESRF who have similar test facilities; both are based on VAX host computers.

Nuclear Physics and Special Instruments Group

On PN1 the modernisation programme has been completed with the installation of the DISSPLA graphics package and the VECTRA system to drive an IEEE bus for magnetic field control.

The situation on PN2 is now also considered to be stable with list-mode data acquisition and improved on-line data treatment.

On the complex of γ-spectrometers, PN3, the μVAX installed at the start of the year has significantly improved both instrument surveillance and data treatment.

No significant changes were made on the other PN instruments. Amongst these, PN8 is now considered to have the most urgent need for improvements.

From the computing viewpoint, the S instruments can be divided into two groups. There are those such as S3, S20, S21, S34, NESSIE, TGV, having an ILL scientist in charge, which tend to have standard ILL computer control systems. In these cases one aims to provide a level of support approaching that for the mainstream ILL instruments.

The second category comprise those constructed and run by external groups. In these cases our involvement is much more limited, although on $n\bar{n}$, work has been done providing connections to external networks.

In the area of development, considerable attention is being paid to the IEEE bus which is now being widely used for the connection of all sorts of peripheral devices.

Administration Department

Administration Department

Introduction

The following events and changes should be mentioned in the work of the Administration Department in 1989.

The negotiations on a new Collective Agreement were concluded in June 1989. The new Collective Agreement runs for a period of five years, and includes a number of measures (e.g. adjustment of the expatriation, adaptation and education allowances), designed to help improve the balance in the number of staff from the member states. The new Collective Agreement also incorporates many changes reflecting developments in the legislation and the structure of the Institut.

The cooperation with ESRF has continued to develop. In the Administration and infrastructure there continue to be many close aspects of cooperation. The Directors of the two institutes have decided to settle the main lines of this cooperation, the areas of responsibility and the financial questions on a long-term basis by the conclusion of inividual agreements (see chapter "ILL/ESRF Collaboration").

In the second half of the year negotiations were resumed with the Austrian Ministry for Science and Research on a scientific participation of Austria in ILL, on the model of the Spanish and Swiss agreements. Following the agreement of the Steering Committee on 24.11.89 to the conclusion of this agreement, it is expected to be signed at the beginning of 1990. The Austrian signatory is the Austrian Academy of Sciences.

The Steering Committee met at the beginning of June 1989 at the invitation of the French Associate CNRS at Vaux-de-Cernay near Paris, and in November 1989 in Grenoble, where it adopted the 1990 Budget with expenditure of 312.3 MF (1990 prices; including a reserve of 12.7 MF, particularly for fuel elements).

Comparison of 1988 and 1989 Budgets (Expenditure)

Expenditure	Expenditure 1988 MF	%	Estimated expenditure 1989 MF	%	Change %
1) **Staff costs**	151.5	54	158.4	55	+ 5
Other expenditure on personnel	2.0		2.0		
2) **Fuel elements**	34.3	12	34.0	12	1 -
Consumables	27.6	10	29.4	10	+ 7
Long term supplies and services	7.2	2	8.8	3	+ 22
Short term supplies and services	12.0	4	11.8	4	2 -
Travel	2.2	1	2.1	1	5 -
Miscellaneous administrative costs	7.5	2	7.7	3	+ 3
Taxes and fees	1.4	1	1.4	-	0
3) **Operation**	57.9	20	61.3	21	+ 6
I **TOTAL OPERATION**	**245.7**	**86**	**255.7**	**88**	**+ 4**
Buildings	0.6	-	0.8	-	+ 33
Equipment	6.2	2	7.0	2	+ 13
Instruments	21.0	8	16.4	6	20 -
Other investments	11.6	4	11.0	4	5 -
II **INVESTMENTS**	**39.4**	**14**	**35.2**	**12**	**10 -**
TOTAL EXPENDITURE	**285.1**	**100**	**290.9**	**100**	**+ 2**

Finance

Implementation of the 1989 Budget

The budget authorized for 1989 amounted to a total of approx. 303 MF (excl. taxes). Total expenditure in 1989 is anticipated at approx. 291 MF. The difference is mainly due to the impossibility of shipping fuel elements for reprocessing to the USA, and to the delay in the construction of the joint ILL/ESRF building, now planned for 1991/1992.

More detailed information on the expenditure and income in the ILL Budget 1989 is contained in the following tables, which permit a comparison with 1988.

The comparison of expenditure between 1988 and 1989 shows an increase in staff costs of 5%, which reflects general salary increases, increased social charges and new measures to improve the attractiveness of the Institut for non-French staff. Fuel element costs remained stable in 1989 compared to 1988. They were more than 8 MF lower than the envisaged expenditure, as it was impossible to ship used fuel elements to the reprocessing plant. Other operation expenditure increased by 6%, as there were 6 reactor cycles in 1989 in comparison with 5 cycles in 1988. The decrease of 20% in the scientific investments in 1989 is mainly due to lower expenditure for the Horizontal Cold Source instruments. The scientific investments in 1989 saw the continued development and construction of instruments on the Horizontal Cold Source (IN10C, D22 and IN15), the improvement of existing instruments (D20, IN11 and D11) and the development of monochromators.

Forward Look

The ILL's present medium-term investment plans in the scientific field are essentially as follows:

- group budgets for the existing instruments (approx. 5.1 MF/year);
- improvement of existing instruments and the replacement of old instruments (3.9 MF in 1990, 6.4 MF in 1991 and 8.2 MF from 1992 to 1994). The completion of the instruments on the Horizontal Cold Source (IN10C, D22, IN15) with an investment of 5.1 MF in 1990 and 1.8 MF in 1991.

Further important items in the medium term are:

- the replacement of equipment necessary for the safety and reliable performance of the reactor;
- continuation of the build-up of a reserve of three fuel elements in the years 1990 and 1991;
- the construction of joint ILL/ESRF building (library, offices for theoreticians, canteen/cafeteria); the construction of the joint building is now planned for 1991-1992 (ILL share: 6.5 MF).

Furthermore the Institut is preparing a Modernization Programme for the instruments and the reactor for the years after 1992.

Comparison of 1988 and 1989 Budgets (Income)

Income	Income 1988		Estimated income 1989		Change
	MF	%	MF	%	%
Collaboration with ESRF	0.213	0.1	0.800	0.3	+ 275
ILL's own income	10.244	3.6	8.465	2.9	- 10.0
Reabsorption of provision	-	-	0.764	0.3	-
Spanish and Swiss	-	-	-	-	-
Contributions	8.540	3.0	8.584	3.0	+ 0.5
Associates' contributions	267.590	93.8	269.546	92.6	+ 0.7
Carry forward 1987/88	13.958	4.9	-	-	-
Carry forward 1988/89	- 15.958	- 5.4	15.425	5.3	-
Carry forward 1989/90	-	-	- 12.662	- 4.4	-
TOTAL INCOME	**285.120**	**100.0**	**290.922**	**100.0**	**+ 2.0**

Purchasing

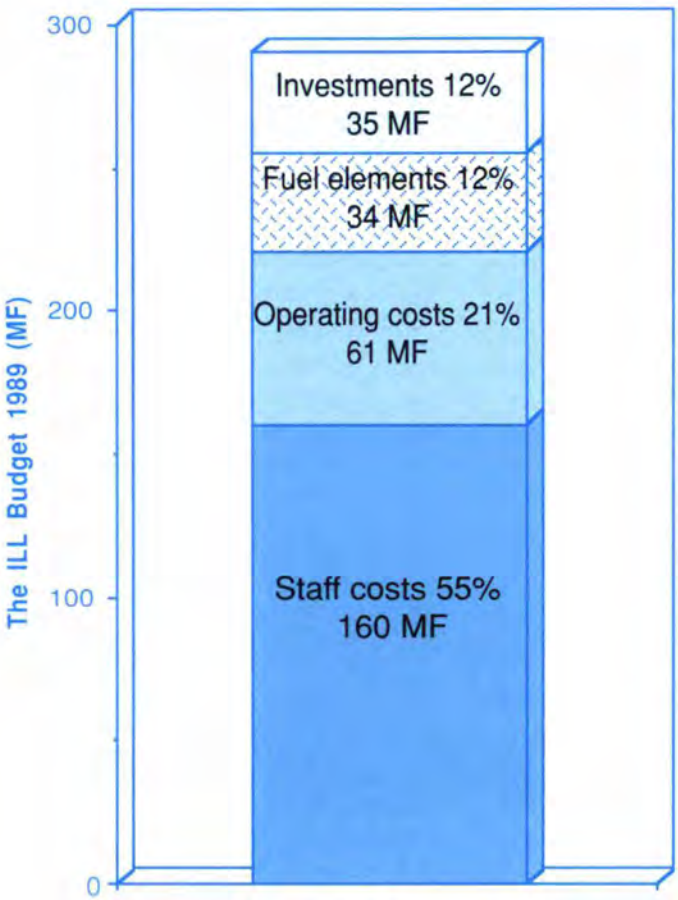


Fig. 77: Total expenditure 1989: 290,90 MF.

Considerable efforts are being made in the search for a new supplier of fuel elements to replace NUKEM (D) who ceased these operations in 1988. The Institut is studying fuel element supply possibilities in the UK and in the USA. In order to ensure future reactor operation and to build up a reasonable stock of fuel elements a contract was placed with CERCA (F) for the manufacture of 12 fuel elements to be delivered in 1990 and 1991. To ensure uranium supply, 32 kg of uranium (93% enriched) was purchased from NUKEM (D) who were also awarded a contract for the manufacture of 25 inner and outer cylinders for fuel element production.

An important order for the manufacture of 10 replacement absorber elements for the reactor was awarded to COMPTOIR LYON ALLEMAND (F) who will deliver them in 1990.

International invitations to tender were carried out for the procurement of major replacement parts for the reactor including:

- H1/H2 beam-tube awarded to NUKEM (D),
- H6/H7 beam-tube won by GIROD SISA (F),
- coupling sleeves awarded to PALY (F),
- and a convection valve ordered from NTG NUKLEAR-TECHNIK (D).

Also for the reactor, two replacement support tubes were ordered from BARRAS PROVENCE (F) later in the year.

Purchasing for the construction of new instruments was at a lower level than in previous years because IN14 spectrometer and the experiment are complete and operational; the major parts for D22 were already ordered in previous years and are in the process of reception and delivery, at the time of writing. Only the neutron guides for D22 were ordered in 1989. Some progress was made for the other new instruments; stabilized power supplies for IN15 have been produced by FUG (D); and we are currently studying offers for the construction of the analyser shielding for IN10C. As for the existing instruments, a notable order was placed with ANDRE CONSTRUCTIONS METALLIQUES (F) for the new collimation system for the small-angle scattering diffractometer D11.

In the computing area, five new Vaxstations 3100 for the instruments and a cluster controller for the central computer were ordered from Digital. Several Macintoshes were acquired and this has become a standard workstation at ILL.

As in previous years about one quarter of purchasing expenditure was spent on the electricity and telephone bills, cleaning, restaurant, and contracts with the CENG for heating, helium supplies and radioprotection services, as well as the contracts for maintenance of computers and other equipment.

Whenever possible, for major purchases, an international call for tenders was carried out; offers were compared on an ex-works basis so as not to disadvantage British, German, Swiss and Spanish firms compared with local suppliers. Nevertheless the distribution of purchases in the member states remains unsatisfactory and efforts are continuing to be made to try to improve the situation.

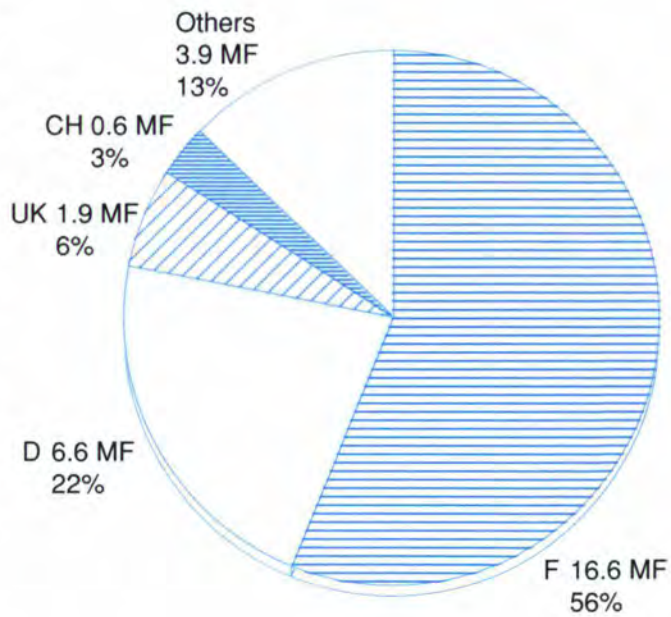


Fig. 78: Distribution of ILL purchases

The distribution of ILL purchases (orders exceeding 50 KF) in 1989 is shown in the diagram. The figures include purchases for which a free choice of suppliers was possible excluding therefore the fuel cycle, electricity and small purchases of less than FF 50 000.

A joint ESRF-ILL purchasing group has been operating since 1986; in mid-1989 the ESRF established its own purchasing department which still operates on the ILL computerized system until the end of 1989. The two groups collaborate closely in their approach to suppliers and will continue to do so in the future in order to negotiate better discounts and exchange market information.

Stores

A joint ESRF-ILL stores facility is operating successfully and will continue for the foreseeable future, allowing economies for both partners. All deliveries of purchased equipment for ILL and ESRF were received and checked by the storemen who also carry out the despatch of samples, returned equipment, etc. and the provision of raw materials.

The careful stock control was confirmed by the annual stock inventory carried out in December 1989.

Personnel

Staff

A total of 482 staff complement posts were occupied at 31.12.89. This is a reduction in comparison to the figure at 31.12.88 (490 staff), due to recruitments in progress for personnel who will start early in 1990.

French	65.4%	(66.5%)
German	14.9%	(13.7%)
British	13.9%	(13.3%)
Others	5.8%	(6.5%)

The table above shows the percentage of staff of different nationalities at the ILL (in brackets the corresponding figures for 1988).

There was a decrease in French and other staff, and an increase in German and British staff. Following the measures adopted by the Steering Committee in June 1989 to improve the ILL's attractiveness to German and British nationals, it may be hoped that in future years there will be a greater increase in staff from Germany and the UK.

Collective Agreement

A new Collective Agreement was signed on 29 June 1989 for a period of five years between the Director and three unions (CFDT, CGT and FO), following lengthy negotiations (more than a year).

Salaries

By analogy with measures implemented by the CEA, salaries were increased by 1% at 1.4.89 and 1.2% at 1.10.89. In December 1989 an additional bonus was paid (0.5% of the total payroll) to be taken into account in the final settlement for the year, expected early in 1990.

Guest scientists

There were approximately 2 400 visits by 1 500 guest scientists to the ILL between January and early December 1989. Of these visitors 31% came from laboratories in France, 24 % from the UK, 27% from Germany and 18% from other countries.

Staff Complement Situation in 1989

(by categories and nationalities)

CATEGORIES	POSITION ON 31.12.88					POSITION ON 31.12.89				
	G	B	F	O	T	G	B	F	O	T
Cadres										
Scientists (permanent)	12	6	6	5	29	12(-)	5(-1)	8(+2)	6(+1)	31(+2)
Scientists (non-permanent)	13	8	15	9	45	12(-1)	8(-)	11(-4)	6(-3)	37(-8)
Engineers		2		2			2(-)		2(-)	
Total	25	14	23	14	76	24(-1)	13(-1)	21(-2)	12(-2)	70(-6)
Other 'Cadres'	13	8	42	-	63	15(+2)	8(-)	39(-3)	–	62(-1)
Total 'Cadres'	**38**	**22**	**65**	**14**	**139**	**39(+1)**	**21(-1)**	**60(-5)**	**12(-2)**	**132(-7)**
Thesis students	8	7	9	5	29	9(+1)	8(+1)	9(-)	3(-2)	29(-)
'Non-Cadres'										
Technicians	13	25	122	2	162	15(+2)	26(+1)	117(-5)	2(-)	160(-2)
Others	8	11	130	11	160	9(+1)	12(+1)	129(-1)	11(-)	161(+)
Total 'non-cadres'	**21**	**36**	**252**	**13**	**322**	**24(+3)**	**38(+2)**	**246(-6)**	**13(-)**	**321(-1)**
Grand total	**67**	**65**	**326**	**32**	**490**	**72(+5)**	**67(+2)**	**315(-11)**	**28(-4)**	**482(-8)**

G = German, B = British, F = French, O = Other, T = Total

The breakdown by sex remains practically unchanged (83% men, 17% women).

Welfare and General Services

Housing

ILL flats

ILL has 20 furnished flats, available for guest scientists staying for at least two weeks or for new ILL or ESRF staff on arrival in Grenoble. These flats were occupied for almost 95% of the year 1989; 89 persons or families made use of these facilities, including 70 from ILL, 16 from ESRF, 1 from EMBL, 2 from IRAM. It is not possible to satisfy all the demands. When the "Maison du Chercheur" is available within walking distance, this should make things much easier.

Finding accommodation

New arrivals at ILL and ESRF are helped as far as possible to find accommodation. Thanks to the good relations with a number of house agents in Grenoble, usefull offers are frequently received; we also regularly receive offers of accommodation from individuals. About 60 staff contacted us in 1989, including 38 from ESRF.

Employer's contribution to housing

This contribution permits the reservation of flats at a reasonable rent: 2 flats were reserved in 1989, there were numerous applications for loans, particularly towards the end of the year, 20 loans were granted (minimum: 6 000 F, reimbursed over 2 years; maximum 150 000 F, reimbursed over 15 years) using as intermediary the organisations to which ILL contributes.

Role of the Welfare Assistant

Mme Pennec, the welfare assistant, assists families with administrative formalities (e.g. for the family allowances, unemployment benefit, and contacts with job centres), or in case of occasional serious personal difficulties. She works closely with the various subcommittees of the Works Committee (e.g. those covering housing and holidays), 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.

Assistance for German Staff

For a period of 2 years from January 1989, Frau Hildebrandt, who is German and a psychologist, has been detached to ILL by the German Associate, the KfK.

She deals with questions of integration of German ILL staff and their families at a social and cultural level (employment for wives, recognition of qualifications, retirement problems, etc.). For this purpose she has met all the German families interested to analyse their problems and to seek solutions.

She has had many contacts with municipal departments in Grenoble and the employment exchange and with various associations or companies which may be able to offer employment to wives of German staff. There are already encouraging results and useful contacts made. Frau Hildebrandt's presence and her role are widely appreciated.

International Education

The international schooling facilities are extremely popular at Grenoble.

In September 1989 there were 54 children of English mother tongue and 23 of German mother tongue in the German and English "sections" at the International Primary School.

The Lycée International Stendhal now has 4 national "sections": English, German, Italian and Spanish. Its aim is to prepare French and foreign pupils, bilingual and with a dual cultural background, for the French Baccalauréat of their choice. Negotiations are in progress for preparation of an international baccalauréat. In September 1989 there were 50 German mother tongue pupils and 118 pupils of English mother tongue in the specific "sections" at the Stendhal Collège and Lycée. The first pupils who have attended the complete Lycée course will sit the Baccalauréat in June 1990.

For the school year 1989-90, ILL and ESRF have had to continue their administrative and financial support to permit this experiment to continue. Thus ILL prepared the contracts for the German teachers, being reimbursed by the German Ministry for Research and Technology; for the British teachers an agreement has been signed by the various partners, ILL, ESRF, Isère Department Council and the city of Grenoble, under which the last two partners pay a subsidy to ILL.

In accordance with the Convention on the construction and operation of the ESRF, the French Ministry of Education is due to take over for the September term in 1990.

Training

Training courses are essentially divided as follows:

Languages: French, English, German and Spanish courses account for about 28% of the training budget.

Technical and professional courses: these account for approximately 65% of the budget. Among the courses may be mentioned introductory and advanced courses on CAD using different software, a course on the strength of materials, for which M. Thomas, engineer in the Instruments and Methods Department, was responsible and an introduction to Quality Assurance for cadres staff, etc.

The remaining 7% of the budget is devoted to courses of general interest; for example four ILL staff attended a course on new technologies, organized by the Grenoble Social Sciences University.

College 2

Theory

"Field theory for the negative U Hubbard model".
R. OPPERMANN, ENS, Paris.

"Andreev-scattering".
P. WYDER, MPI, Grenoble.

"Recent studies of the d-d excitation model for high T_c superconductors".
W. WEBER, KFK, Karlsruhe.

"Apprentissage et dynamique dans des réseaux de neurones".
W. KRAUTH, ENS, Paris.

"Aspects granulaires des supraconducteurs à haut T_c".
G. DEUTSCHER, University of Tel Aviv and CRTBT, Grenoble.

"Bond and molecular orientational order in two dimensional liquid crystals".
"M. GINGRAS, University of British Columbia, Vancouver.

"Martensitic transitions, twin boundaries and superconductivity".
B. HOROVITZ, University of Ben Gurion, Israel.

"Perturbation theory of superconducting micronetworks near the phase transition boundary".
H.J. FINK, University of California, Davis.

"Direct microscopic observation of interacting colloids in two dimensions: association dynamics and phase transitions".
S. FRADEN, MPI, Grenoble.

"Fermions lourds ?".
H. CAPELLMANN, ILL.

"The role of fluctuation in electron pairing mechanisms".
N. ASHCROFT, Cornell University.

"Ordering of dipoles in a disordered system".
B. BERGERSEN, University of Bristish Columbia, Vancouver.

"Chaos in small quantum systems".
H.A. WEIDENMÜLLER, MPI, Heidelberg.

"Instabilités d'étalement".
J.F. JOANNY, ENS, Lyon.

"Génétique et épigénétique des fonctions neuronales".
M. KERZBERG, Jülich et CENG.

"Van der Waals theory of surface melting".
H. LÖWEN, University of Munich.

"Lois d'échelle pour les fractures".
H. HERMAN, Saclay.

"Nuclear magnetic resonance in quantum Hall effect systems".
I. WAGNER, MPI, Grenoble.

"Propriétés de surface de ^{3}He et ^{4}He".
F. DALFOVO, University of Trente and ILL.

"Magnetic resonances in non colinear and tensor magnetics".
V. MARCHENKO, ILL.

"Electron correlations and antiferromagnetism in high T_c superconductors".
A. OLES, Wroclaw.

"Some thoughts on the glass problem".
A.J. LEGGETT, University of Illinois.

"Boltzmann-Landau description of electronic localization in the presence of strong disorder".
G. STRINATI, Ecole Normale de Pise.

"Supraconductivité des phases à flux commensurable".
P. LEDERER, ETH, Zürich.

"Systèmes électroniques fortement corrélés en deux dimensions".
D. POILBLANC, ETH Zürich.

"Temperature dependence of rotational tunneling".
A.WÜRGER, ILL.

"Kondo lattice hamiltonian in high T_c superconductors".
C. di CASTRO, Rome.

"Slave particle theory for the $U = \infty$ Hubbard model".
F. OHKAWA, CNRS Grenoble and Université de Hokkaido.

"Front propagation into an unstable state in the presence of noise".
O. VALLS, University of Minnesota.

"Ordre atomique dans les quasicristaux : développements récents".
Ch. OGUEY, Ecole Polytechnique, Palaiseau.

"Aspects of Landau-level broadening".
H. LESCHKE, Erlangen.

"Apprentissage dans les réseaux de neurones (à unités cachées)".
P. PERETTO, DRF-CENG.

"Modèles théoriques et simulations numériques de la transition vitreuse".
J.L. BARRAT, Laboratoire de Physique, ENS de Lyon.

"Fluctuations de la réponse diamagnétique de métaux désordonnés".
E. AKKERMANS, CRTB-CNRS, Grenoble.

"Phases spirales dans un antiferromagnétique quantique Dopé".
T. DOMBRE, CRTBT-CNRS, Grenoble.

"The range of validity of the Migdal theorem".
A.B. KREBS, Moscow Physics Engineering Institute.

"Quantum Monte-Carlo simulation of strongly correlated Electrons".
W. Von der LINDEN, IBM, Rüschlikon, Suisse.

"A scaling approach to Pinning - Charge density waves and giant flux creep in superconductors".
T. NATTERMANN, Jülich.

College 3

Fundamental and Nuclear Physics

"Invariance d'échelle dans la fragmentation d'objets de taille finie".
X. CAMPI, IPN, Orsay.

"Time reversal non-invariance and the compound nucleus".
E. DAVIS, MPI, Heidelberg.

"CP violation in K decays".
D. FOURNIER, Orsay.

"Geology of the high himalayas".
P. LEFORT, CNRS/Institut Dolomieu, Grenoble.

"Testing the interacting Boson model in the N=84 isotones".
J. COPNELL, University of Manchester.

"Ultracold antineutrons".
R. GOLUB, TU, Berlin.

"High spin phenomena in the A=80 region".
K.P. LIEB, Göttingen.

"Radiochemistry at AWE".
P. THOMPSON, Awe Aldermaston.

"Neutron properties and their importance for GUTs and cosmology".
W. MAMPE, ILL.

"Experiments with monochromatic UCN".
D. RICHARDSON, University of Southampton.

"Laser spectroscopy at closed Proton shells far off stability".
G. HUBER, Mainz.

"Search for right-handed currents with a novel bhabba polarimeter
J. van KLINKEN, Groningen.

"Shell model and IBM descriptions of M1 transitions and β-decay in the $f_{7/2}$-shell".
M. ABDELAZIZ, University of Sussex.

"A polarized ^{3}He neutron spin-filter" and "Absolute flux measurement calorimetry".
T.E. CHUPP, Harvard.

"Electron spectrometer for the PIK reactor at Leningrad".
Yu. KHAZOV, Leningrad.

"Cold antiprotons in a trap : a new measurement of the antiproton mass".
G. GABRIELSE, CERN, Geneva.

"Applications of the interacting boson-fermion model to odd-mass nuclei".
P. van ISACKER, Daresbury.

"Review seminar on Lohengrin".
H. FAUST, ILL, Grenoble.

"Study of M1 strength in atomic nuclei".
C. de COSTER, Gent.

"$\sqrt{N}$-classification of reaction amplitudes and parity non conservation in neutron reactions".
V. FLAMBAUM, O. SUSKOV, University of Novosibirsk.

"Onset of collective motion in medium and heavy mass nuclei".
J. CIZEWSKI, Daresbury.

"A new method of nuclear picosecond lifetime measurements".
R. CASTEN, BNL.

"Microscopic self-consistent and collective model description of nuclear structure".
K. HEYDE, Gent.

College 4

Structural and Magnetic Excitations

"Polarized neutron reflection studies of ultra thin (epitaxial) ferromagnetic films".
T. BLAND, University of Cambridge.

"Neutron diffraction as a probe of Marijuana-Membrane interaction".
P. MARTEL, LLB, Saclay.

"Raman scattering from high T_c superconductors".
P. LEIDERER, Universität Konstanz.

"A computational method to determine superstructures : applications from alloys to high T_c superconductors.
K. MIKA, Jülich.

"Pattern formation and travelling waves in non-linear systems : excitable media in biology, chemistry and physics".
Th. PLESSER, MPI, Dortmund.

"Strontium and oxygen concentration effects on the electrical resistivity of $La_{2-x}Sr_xCuO_{4-y}$".
E. OSQUIGUIL, Bariloche, Argentina.

"Macromolecular alignment of ferrofluids".
R. PYNN, Los Alamos.

"Solar neutrinos and low temperature physics".
H. MARIS, Brown University, Providence, R.I.

"Magnetism in high T_c oxides".
G. SHIRANE, Broohaven National Laboratory.

"Pulse experiments with coherent and incoherent phonons".
O. WEIS, University of Ulm.

"Excitations in commensurably modulated magnetic systems".
J. JENSEN, University of Copenhagen.

"Ballistic propagation of O.7 THz acoustic phonons in GaAs".
M. FIESELER, Dortmund.

Two-dimensional spin correlations and magnetic phase transitions in Nd_2Cu0_4 and $Pr_{2-x}Ce_xCu0_4$ (x = 0, 0.08).
K. KAKURAI, Tohoku University.

"Triple axis spectroscopy with He beams".
C. STASSIS, Ames, Iowa.

"Soft modes and incommensurate phase transitions in BCCD (Betain Calcium Chloride Dihydrate)".
S. KAMBA, Czechoslovak Academy of Sciences.

"Monte Carlo molecular dynamics studies of 1D systems. Application to Peierls systems".
E. TUTIS, University of Zagreb.

College 5

Crystal and Magnetic Structures

"Permanent magnet materials".
D. GIVORD, Laboratoire L. NéeL, CNRS, Grenoble.

"Electron microscopy of high T_c superconductors".
Elizabeth A. HEWAT, LETI-CENG, and Laboratoire de Cristallographie, CNRS.

"Powder neutron diffraction at Risoe National Laboratory".
B. LEBECH, Risoe National Laboratory, Denmark.

"Least squares explained".
D.J. WATKIN, Chemical Crystallography Laboratory, Oxford.

"Application-oriented space group notation : importance to computer applications and data bases".
S.R. HALL, University of Western Australia and Röngtenlabor, MPI, Mülheim.

"Neutron and X-ray powder diffraction on $La_2CuO_{(4+x)}$ and $Pr_2NiO_{(4+x)}$".
P. ZOLLIKER, Brookhaven National Laboratory.

"How to do neutron scattering using X-rays".
P. SIDDONS, Brookhaven National Laboratory.

"Thermal neutron monochromators based on elastically-deformed silicon crystals".
P. MIKULA, Institute for Nuclear Physics, Rez-near-Prague, Czechoslovakia.

"Structural aspects of high T_c superconductors".
A. SEQUEIRA, BARC, Bombay.

"Rôle de la préparation thermomécanique de la magnésie dans le processus de cristallisation d'oxychlorures de magnésium à prise activée".
E. BURIOT, Centre Scientifique et Technique du Bâtiment, St. Martin d'Hères.

"Studies of the charge-density wave in alpha uranium: a comparison of neutron and synchrotron capabilities".
G. LANDER, European Institute for Transuranium Elements, Karlsruhe.

"Absolute configuration of chiral methylene groups using neutron diffraction".
R. BAU, University of Southern California.

"Everything you want to know about wavelets".
A. ANTONIADIS, Université Joseph Fourier, Université de Saint Etienne.

"Crystallography of intergrowth structures".
S. van SMAALEN, Inorganic Chemistry, Rijkuniversiteit, Groningen.

"Resolving synthetic hibschite... with multiplet peak fitting, multiphase Rietveld and Fourier-filtering techniques".
F. ROTELLA, IPNS Division, Argonne National Laboratory.

"Profile fitting of neutron powder data using the convolution equation".
H. TORAYA, IBM Research Laboratory, San José.

"Magnetic and crystallographic properties of rare earth disilicides".
J. PIERRE, Laboratoire L. Néel, CNRS, Grenoble.

"Hydride and oxide structures, high pressure equation of state for solid deuterium perfect magnetic crystals, neutron radiography using refraction constrast : a review of recent neutron diffraction results at the Kurchatov Institute".
S. Sh. SHILSTEIN, K. PODURETS, Kurchatov Inst. Moscow.

"Analysis of the diffraction patterns of γ-MnO_2 : a computer simulation of De Wolf's layer model.
M. RIPPERT, ILL.

"Magnetic and structural properties of some ferromagnetic halides, and some antiferromagnetic arsenates : the value of studying an homologous chemical series".
S.T. BRAMWELL, ILL.

"Investigation of metallic hydrides by pertubed angular correlations and muon spin rotation techniques".
P. BOYER, DRF-CENG.

College 6

Liquids, Disorder and Defects in Materials

"Medium range order in metallic alloys and glass formation".
J.M. DUBOIS, Ecole des Mines, Nancy.

"The structure of dense-packed oxide glasses - some recent neutron scattering results".
P.H. GASKELL, University of Cambridge.

"Evidence for fracton dynamics in silica aerogels".
R. VACHER, Université des Sciences et Techniques du Languedoc, Montpellier.

"Synthesis and characterization of HCP Fe/Ru superlattices".
M. MAURER, Laboratoire Mixte CNRS-Saint Gobain, Pont-à-Mousson.

"Of maps and monkeys - the maximum entropy method".
G.J. DANIELL, University of Southampton.

"Déformation plastique du Béryllium".
A. COURET, Laboratoire d'optique Electronique du CNRS, Toulouse.

"Microscopic theory of martensitic transitions".
J.A. KRUMHANSL, Cornell University, Ithaca, New York.

"Unusual palladium-hydrogen bonding in Li_2PdH_2 and Na_2PdH_2".
D. NOREUS, University of Stockholm.

"Local displacive atomic ordering in high T_c oxides determined by pulsed neutron scattering".
T. EGAMI, University of Pennsylvania.

"The structure of liquid and quenched sulfure".
P. EGELSTAFF, University of Guelph.

"Mirrors and multilayers".
I. ANDERSON, P. Scherrer Institut, Villigen, Suisse.

College 8 and EMBL

Biochemistry

"Un cytochrome multihaemique, le cytochrome C3. Structure et mécanisme de transfert d'électrons".
M. BRUSCHI, Laboratoire de chimie bactérienne, CNRS, Marseille.

"Measles virus fusion protein ; purification and immunological characterization".
P. de VRIES, RIVM, Bilthoven, Netherlands.

"Structure and function of a pore forming domain of colicin A".
F. PATTUS, EMBL, Heidelberg.

"X-ray structure determination of proteins interacting with ß-lactam antibiotics".
O. DIDEBERG, Université de Liège.

"Reflections on the structure of membrane proteins, bacteriorhodospin and porin".
G. BÜLDT, Freie Universität Berlin.

"Physical studies of the relationship between structure and function in connective tissues".
D. HUKINS, University of Manchester.

"The gene sequence of halophilic EFTu : what makes a protein halophilic".
G. BALDACCI, Laboratoire de Biologie Moléculaire de la Réplication, Villejuif.

"High resolution 13C-solid state NMR of bacteriorhodopsin : Structural implications of single site mutations on the surface structure".
M. ENGELHARD, MPI, Dortmund.

"Spectroscopic and structural studies of a membrane protein : the photosynthetic reaction center of rhodobactin spheroides strain Y".
F. REISS-HUSSON, CNRS, Gif-sur-Yvette.

"NMR investigations of proton exchange and base-pair kinetics, with applications to DNA structure".
M. GUERON, BIOP Polytechnique, Palaiseau.

"The structure of the Holliday junction in DNA".
D.M.J. LILLEY, University of Dundee.

"Virus-like particles of the yeast retrotransposon Ty : structural studies on a vehicle for polyvalent antigen presentation".
N. BURNS, Bristish Biotechnology Ltd, Oxford.

"New approaches in small angle scattering analysis for macromolecular systems".
D. SVERGUN, Institute of Crystallography, Moscow.

College 9

Chemistry

"X-ray reflectivity of multilayers and interfaces".
F. RIEUTORD, ILL.

"Surface premelting".
M. BIENFAIT, CNRS, Marseille.

"Molecular motions in Hydrocarbon chains in two dimensional disordered solid phases".
F. GUILLAUME, Laboratoire de Spectroscopie, Bordeaux.

"Rotational excitations of CH_4 molecules in rare gas matrices".
B. ASMUSSEN, Institut für experimentalphysik, Univ. Kiel.

"The origin of the barrier to rotation of the molecular hydrogen ligand in transition metal compounds".
J. ECKERT, LANSCE, los Alamos.

"An inelastic neutron scattering study of methyl tunnelling and the quantum sine-gordon breather in isotopic mixtures of 4-methyl-pyridine at low temperature".
F. FILLAUX, Laboratoire de Spectrochimie infrarouge et Raman, CNRS.

"Proton and muon dynamics in a large metal cluster compound".
P. DALLIN, University of East Anglia, U.K.

"The reorientational motion of the NH4+ ion in ammoniumtetraphenylborate : evidence for nearly free rotation".
M.P. ROBERTS, University of California, Berkeley, USA.

The application of the specular reflection of neutrons".
J. PENFOLD, Rutherford Appleton Laboratory.

"Static and dynamic light scattering from polymers of different architectures in semidilute solutions".
W. BURCHARD, Institute of Macromolecular Chemistry, University of Freiburg.

"What you can learn from computer simulations on polymers".
G. GREST, Exxon research and Eng. co.

"σ-conjugated polysilylenes - a new class of organic electronic materials".
J.M. ZEIGLER, Sandia Laboratory, Albuquerque.

"Enhancement of inhomogeneities in gels upon swelling and stretching".
J. BASTIDE, ICS-CRM, Strasbourg.

Thursday colloquia

"Dynamical properties of modulated sytems; longitudinal magnets, electrons in a magnetic field and lattice vibrations in incommensurate" crystals.
S. LOVESEY, Rutherford Laboratory.

"Valence fluctuations and heavy fermions".
D. WOHLLEBEN , Université de Cologne.

"Motion of light interstitial particles in metal lattices at low temperatures".
E. KARLSSON, University of Uppsala.

"Quantum mechanics and macroscopic realism".
A.J. LEGGETT, University of Illinois.

"Chemistry and physics of molecular-based compounds exhibiting a spontaneous magnetization".
O. KAHN, Laboratoire Chimie Organique, Université Paris-Sud, Orsay.

"Topological quantization of physical parameters in (2+1)-Dim theories".
V.M. YAKOVENKO, Physique des Solides, Université Paris-Sud, Orsay.

"Aspects of chaos in Nuclear Physics".
I. BOHIGAS, Institut de Physique Nucléaire, Orsay.

"Low frequency protein dynamics and ligand migration: a case of diffusion in fractal geometries".
R. TAHIR-KHELI, Temple University, Philadelphia.

"Time and spatial parity, non-conservation in atoms and nuclei".
V. FLAMBAUM, O. SUSKOV, University of Novosibirsk.

"The Oak Ridge advanced neutron source project".
J. HAYTER, Oak Ridge Laboratory.

Seminars for thesis students (Organized by ILL)

"Introduction to small angle scattering". C. JANOT.

"Introduction to particle physics with slow neutrons".
D. DUBBERS.

"Introduction to neutron spin echo techniques". B. FARAGO.

"The dynamics of the Griffiths phase in dilute magnets, investigated by neutron scattering". R. LLOYD.

"Biological applications of neutron small-angle scattering".
R. MAY.

"Neutron optics, extinction, topography". J. BARUCHEL.

"AlMnSi quasicrystals : where are the atoms ?".
M. de BOISSIEU.

Workshops Organized in 1989:

DUBBERS D., LIAUD P., MAIER B., MAMPE W., ROBINSON S.J., SCHRECKENBACH K.
I.L.L. Workshop on Fundamental Physics with Slow Neutrons, ILL, Grenoble, March 8-11, 1989.

SCHRECKENBACH K.
Meeting on the use of a high flux source of moderated positrons, held on June 27, 1989 at the Institut Laue-Langevin, Grenoble, France. (View-graphs, 89SC15T).

Workshops Published in 1989:

Dynamics of Disordered Materials. Proceedings of the ILL Workshop, Grenoble, France, September 26-28, 1988.
Richter D., Dianoux A.J., Petry W., Teixeira J., Eds. Springer Proceedings in Physics, Vol. 37 (Springer-Verlag, 1989), pp. 323. (ISBN 3-540-50942-9).

Fundamental physics with slow neutrons. Proceedings of the International Workshop, ILL, Grenoble, France, March 8-11, 1989.
Dubbers D., Mampe W., Schreckenbach K. Eds., Nuclear Instruments and Methods in Physics Research A 284 (North-Holland, 1989), pp. 232. (ISSN 0168-9002).

Molecular basis of polymer networks. Proceedings of the Fifth IFF-ILL Workshop, Jülich, RFG, October 5-7, 1988.
Baumgärtner A., Picot C.E. Eds., Springer Proceedings in Physics Vol. 42 (Springer-Verlag, 1989), pp. 223. (ISBN 3-540-51649-2).

Neutron scattering. Proceedings of the International Conference on Neutron Scattering, ICNS'88, Grenoble, France, July 12-15, 1988.
Gläser W., Rossat-Mignod J., Schweizer J., Vettier C. Eds. Physica B 156 & 157 (Elsevier Science Publ., 1989), pp. 934. (ISSN 0921-4526).

Theses

BOISSIEU M. DE
Structure atomique des alliages quasi cristallins AlMnSi et AlLiCu.
THESE, INSTITUT NATIONAL POLYTECHNIQUE DE LORRAINE, JUIN 1989.

CHAHID A.
Etude de la structure dynamique de quelques matériaux par diffusion de neutrons. Calcul numérique des lois de diffusion cohérente et incohérente.
THESE, INSTITUT NATIONAL POLYTECHNIQUE DE GRENOBLE, NOVEMBRE 1989.

COPNELL J.
^{138}Xe and the N =84 isotones.
THESIS, UNIVERSITY OF SUSSEX, DECEMBER 1988.

CRAMPIN N.
The polarisation of ultra-cold neutrons.
THESIS, UNIVERSITY OF SUSSEX, JUNE 1989.

GIBBONS E.P.
A study of the magnetic properties of neodymium and cerium.
THESIS, UNIVERSITY OF BIRMINGHAM, DECEMBER 1988.

GUILLAUME F.
Etude de la dynamique de chaines hydrocarbonées (alkylenediammonium, alkylammonium et n-alcane) en phases solides désordonnées par diffusion incohérente inélastique des neutrons.
THESE, UNIVERSITE DE BORDEAUX I, DECEMBRE 1988.

LLOYD R.G.
The dynamics of dilute magnets, studied by neutron inelastic scattering.
THESIS, UNIVERSITY OF MANCHESTER, 1989.

MELVILLE R.J.
Magnetic properties of Gd-Y and Gd-Sc alloys.
THESIS, UNIVERSITY OF WARWICK, JUNE 1989.

MOUZE G.
Recherches sur l'application de méthodes de coincidence à l'étude de la désexcitation du polonium 214.
THESE, UNIVERSITE DE NICE, NOVEMBRE 1987
(Experiment partly performed at the ILL).

POWELL D.H.
The structure of solutions of simple electrolytes in water and methanol.
THESIS, UNIVERSITY OF BRISTOL, AUGUST 1989.

RICHARDSON D.J.
The production of, and experiments with, monochromatic ultra cold neutrons.
THESIS, UNIVERSITY OF SUSSEX, FEBRUARY 1989.

SANDONIS J.
Estudio de la coexistencia de fases helimagnetica ferromagnetica en monocristales de Tb Y MnP mediante topografia con neutrones y radiacion sincrotron.
TESINA, UNIVERSIDAD DE CANTABRIA, 1989.

SEVERING A.
Über inelastische Neutronenstreuung an 4f- instabilen Verbindungen.
INAUGURAL-DISSERTATION, UNIVERSITÄT KÖLN, FEBRUAR 1989.

WILLIAMS A.P.
The determination of the neutron lifetime by trapping decay protons.
THESIS, UNIVERSITY OF SUSSEX, NOVEMBER 1989.

WUERGER A.
Zur Temperaturabhängigkeit des Rotationstunnelns.
DISSERTATION, UNIVERSITÄT ERLANGEN-NÜRNBERG, MAI 1989.

This list groups all the known publications resulting from the research at the ILL during 1989.
ILL Reports are listed first (number 1 to 99). They are followed by the list of publications in the scientific literature (journals, conference proceedings, books) with ILL authors and coauthors (100 to 999) and by publications related to experimental work performed by visiting scientists at the ILL but without ILL author or coauthor (1000 to 1200).

Internal Reports

(G = General Reports, T = Technical Reports)

89AL1T
ALBA M., CURRAT R., LEQUIEN S., KAISER W., BROCHIER A.
Preliminary-flux-measurements on IN14.

89GH2T
GHOSH R.E.
A computing guide for small angle scattering experiments.

89GH3T
GHOSH R.E.
Flexible data storage for large multi-channel experiments at ILL.

89BL4G
BLANK H., MAIER B.(EDS.)
Guide to neutron research facilities at the ILL. The yellow book.
(Available from SCAPRO).

89FR5T
FRANK V.L.P., GODFRIN H., LAUTER H.J.
IN3-IN14 Comparison.

89FR6T
FRANK V.
TOPO: Program to plot topographic maps of TOF data.

89CA7G
CASTETS C. (ED.)
1988 ILL Experimental Reports & Theory College Activities.

89GH8T
GHOSH R.E.
FITFUN. An interactive/Graphical fitting routine.

89GH9T
GHOSH R.E.
FIRR. Fitting simple models to inelastic scattering data.

89TO10T
TORRELLES X.
Introduction of the beam profile in the subtraction and attenuation corrections for liquid samples confined within two coaxial cylinders.

89DA11T
DAY P., DIANOUX A.J., DREXEL W., DUBBERS D., HEIDEMANN A., JANOT C., LAUTER H.J., MAGERL A., MASON S.A., RICHTER D., TASSET F.
Suggestions for the Second Modernisation Programme I.L.L. Scientists' "Get-Together", Allevard, January 18-20, 1989.

89JO12T
JOLIE J.
Recent progress in the application of extended supersymmetries to odd-odd nuclei.
CONTRIBUTION TO THE INTERNATIONAL CONFERENCE ON THE SPECTROSCOPY OF HEAVY NUCLEI, CRETE, 25.6-1.7.1989.

89AN13T
ANTONIADIS A., BERRUYER J., FILHOL A., HAMMERSLEY A.
A maximum likelihood 2-D fitting algorithm.

89DR14T
DREUILLET B., CABAU E.
Une méthode d'affinement relevant du principe de maximum de vraisemblance.
RAPPORT DE PROJET EFFECTUE AU DEPARTEMENT INFORMATIQUE DU 1.12.88 AU 15.6.89.

89SC15T
SCHRECKENBACH K.
Presented view-graphs of the "Meeting on the use of a high flux source of moderated positrons" held on June 27, 1989 at the Institut Laue-Langevin, Grenoble, France.

89VE16T
VETTIER C.
Diffraction magnétique des rayons X.
COURS PRESENTE A LA SESSION "LE RAYONNEMENT SYNCHROTRON" DE L'INSTN, AVRIL 1989.

89DR17T
DROUOT V.
Identification de modèles pour régulation P.I.D. et régulation numérique.
Rapport de stage, Année 1989.

89SU18T
SUMMERFIELD D.
Magnetic properties of $Cu_4OX_6L_4$.
Rapport de stage, Année 1989.

89AG19T
AGERON P., BOERNER H.G., BRUECKEL T., GAEHLER R., GOLUB R., HAMELIN B., JOLIE J., KEARLEY G.J., KOEGEL G., KRUSCHE B., LAUTER H.J., LEHMANN M.S., LISS D.K., MAGERL A., PETRY W., ROBERT A., ROBINSON S.J., SCHILLEBEECKX P., SCHRECKENBACH K., TASSET F., TRIFTHAUSER W., VETTIER C., WEBSTER P.J., WILKINSON C.
Proposals for the "3ème souffle". Presentation on 31 August 1989, Institut Laue-Langevin.

89FA20T
FAUST H.R.
Proposal for a focussing magnet on the Lohengrin spectrometer.
Part I : Technical case.
Part II : Scientific case.

Papers Published in Scientific Periodicals, Books and Conference Proceedings

1 - with ILL authors or coauthors

89FU101
FURRER A., GUEDEL H.U., BLANK H., HEIDEMANN A.
Direct observation of exchange splittings in $Cs_3Tb_2Br_9$ by neutron spectroscopy.
PHYSICAL REVIEW LETTERS **62**, 210-213 (1989).

89DO102
DORNER B., BELASH I.T., BOKHENKOV E.L., PONIATOVSKY E.G., ANTONOV V.E., PRONINA L.N.
Inelastic incoherent neutron scattering spectra from fcc $NiH_{1.05}$, hcp $CrH_{1.0}$ and hcp $MoH_{1.2}$ at 15 K.
SOLID STATE COMMUNICATIONS **69**, 121-124 (1989).

89AH103
AHMAD S.T., HAMILTON W.D., VAN ISACKER P., HAMADA S.A., ROBINSON S.J
Mixed-symmetry states and the structure of ^{200}Hg.
JOURNAL OF PHYSICS G **15**, 93-112 (1989).

89SC104
SCHILDBERG H.P., LAUTER H.J.
Lineshape calculations for two-dimensional powder samples.
SURFACE SCIENCE **208**, 507-532 (1989).

89KE105
KENNEDY S.J., MURANI A.P., COCKCROFT J.K., ROY S.B., COLES B.R.
The magnetic structure in the antiferromagnetic phase of $Ce(Fe_{1-x}Co_x)_2$.
JOURNAL OF PHYSICS : CONDENSED MATTER **1**, 629-636 (1989).

89RI106
RICHTER D., FARAGO B., HUANG J.S., FETTERS L.J., EWEN B.
A study of single-arm relaxation in a polystyrene star polymer by neutron spin echo spectroscopy.
MACROMOLECULES **22**, 468-472 (1989).

89NA107
NAJIB A., PIERRE J., BESNUS M.J., HAEN P., MURANI A.P., SIAUD E.
Correlations in heavy fermions close to magnetic instability: $CeInCu_2$.
JOURNAL OF MAGNETISM AND MAGNETIC MATERIALS **76** & **77**, 135-137 (1988). PROCEEDINGS OF THE SIXTH INTERNATIONAL CONFERENCE ON CRYSTAL-FIELD EFFECTS AND HEAVY FERMION PHYSICS, FRANKFURT, FRG, JULY 18-21, 1988.

89RA108
RAINFORD B.D., CUSSEN L., JENSEN J., FORT D.
Impurity mode dynamics of dilute erbium in praseodymium.
JOURNAL OF MAGNETISM AND MAGNETIC MATERIALS **76** & **77**, 399-400 (1988). PROCEEDINGS OF THE SIXTH INTERNATIONAL CONFERENCE ON CRYSTAL-FIELD EFFECTS AND HEAVY FERMION PHYSICS, FRANKFURT, FRG, JULY 18-21, 1988.

89GI109
GIGNOUX D., SCHMITT D., ZERGUINE M., MURANI A.P.
Paramagnetic spectral response of the Kondo-lattice compound $CePt_2Si_2$.
JOURNAL OF MAGNETISM AND MAGNETIC MATERIALS **76** & **77**, 401-402 (1988). PROCEEDINGS OF THE SIXTH INTERNATIONAL CONFERENCE ON CRYSTAL-FIELD EFFECTS AND HEAVY FERMION PHYSICS, FRANKFURT, FRG, JULY 18-21, 1988.

89QU110
QUEZEL S., BURLET P., JACOUD J.L., REGNAULT L.P., ROSSAT-MIGNOD J., VETTIER C., LEJAY P., FLOUQUET J.
Magnetic ordering in $Ce_xLa_{1-x}Ru_2Si_2$ solid solutions.
JOURNAL OF MAGNETISM AND MAGNETIC MATERIALS **76** & **77**, 403-404 (1988). PROCEEDINGS OF THE SIXTH INTERNATIONAL CONFERENCE ON CRYSTAL-FIELD EFFECTS AND HEAVY FERMION PHYSICS, FRANKFURT, FRG, JULY 18-21, 1988.

89RE111
REGNAULT L.P., ERKELENS W.A.C., ROSSAT-MIGNOD J., VETTIER C., KUNII S., KASUYA T.
Inelastic neutron scattering study of the rare earth hexaboride CeB_6.
JOURNAL OF MAGNETISM AND MAGNETIC MATERIALS **76** & **77**, 413-414 (1988). PROCEEDINGS OF THE SIXTH INTERNATIONAL CONFERENCE ON CRYSTAL-FIELD EFFECTS AND HEAVY FERMION PHYSICS, FRANKFURT, FRG, JULY 18-21, 1988.

89LO112
LOEWENHAUPT M., PRAGER M., GRATZ E., FRICK B.
Magnetic excitations in $CeCu_2$.
JOURNAL OF MAGNETISM AND MAGNETIC MATERIALS **76** & **77**, 415-416 (1988). PROCEEDINGS OF THE SIXTH INTERNATIONAL CONFERENCE ON CRYSTAL-FIELD EFFECTS AND HEAVY FERMION PHYSICS, FRANKFURT, FRG, JULY 18-21, 1988.

89KN113
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