The ILL Millennium Symposium and European User Meeting

Grenoble, April 27 – 29, 2006

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Scientific Committee

D. Dubbers (Honorary Chair)
C. Carlile
W. Press
C. Vettier
R. Wagner

Conference Secretary: B. Standke

Local committee

W. Press (Chair until 28/2/06)
R. Wagner (Chair from 01/3/06)
S. Claisse
P. Fouquet
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G. McIntyre
P. Henry

1. SCOPE

Five years ago the ILL convened the first Millennium Symposium in order to launch an ambitious modernisation programme of instruments and infrastructure known as the ILL Millennium Programme. After five years of activity we have decided to run a second such Symposium. The objectives of this Symposium are to demonstrate the achievements of the Millennium Programme up to now and to develop ILL's plans for the decade to come with the input and help of the ILL user community.

The scientific programme of this Millennium Symposium will address the following points:

- Instrumental and scientific achievements enabled by the Millennium Programme.
- Trends in science and engineering and the implications for the ILL.
- Scenarios for future instrumentation and user support facilities.
- The scientific priorities of the user community.

The programme will consist of presentations of scientific results and achievements in methods and techniques. Furthermore, the ILL's scientists and engineers will present ideas and plans for the next decade to the users. A document "Perspectives and Opportunities for ILL" is in preparation which will include projects for instruments, infrastructure and user interface facilities as well as renewal plans of key components for the ILL's reactor, moderators and neutron guides. Our users will be encouraged to express their views either on line through the Symposium web site, or during the Symposium itself, which will be summarized at the wrapping up session. Time will be dedicated during each parallel session to listen to the comments of our user community on the ILL's goals.

2. SCIENTIFIC PROGRAMME

The three-day symposium will take place at the Europole site in Grenoble, starting on Thursday morning and ending on Saturday afternoon. Around 200 participants will attend the meeting.

The symposium will consist of plenary talks, parallel topical sessions each with oral presentations and a poster session. In addition, there will be a user feedback forum at the end of each of the parallel sessions on Friday morning and the Scientific Co-ordination Office (SCO) will also hold a feedback forum during the poster session on Friday afternoon.

Plenary Sessions

There will be seven plenary sessions focussing on general themes, scientific advances, achievements of the Millennium programme and future directions for instrumentation and the ILL in general.

Parallel Sessions

Over 40 oral presentations are organised into seven separate parallel sessions covering the following topics:

A. Nuclei and Particles
B. Materials science and diffraction
C. Magnetic structures
D. Biology and life sciences
E. Large structures
F. Fluctuations and dynamics
G. Neutron methods

3. PRACTICAL INFORMATION

Conference Address

The Symposium will take place at

Europole Grenoble Centre de Congrès
1, Place André-Malraux, BP297, 38016 Grenoble Cedex 1, France
Telephone: +33 (0)4 76 28 28 80
Fax: +33 (0)4 76 28 27 95
http://www.europole-congres.com

Transport to Grenoble

Details of how to get to the symposium site in Grenoble by car and timetables for the airport shuttle bus Lyon-Grenoble and a timetable for the TGV-train Paris-Grenoble can be found on the website: http://vitraill.ill.fr/symposium/venue.jsp

Local Transport

For local transport we recommend Grenoble's very efficient tram system, which operates until midnight. There are tram stops near both Europole and the main Railway Station, where tickets can be bought from a machine. You must stamp your ticket using the machine at the tram stop before boarding the tram. You can transfer freely between different tram and bus routes up to one hour after first stamping the ticket.

Internet Access

Internet access will be available throughout the conference using the six computers provided. The access point can be found in the Atrium of the conference venue.

4. SOCIAL EVENTS

The lunches and conference dinner will take place on the symposium site. Participants are free to make their own dinner arrangements for the Thursday evening. There will be no separate official programme for accompanying persons, although Grenoble offers many possibilities for those not directly attending the symposium.

We look forward to welcoming you to the symposium!

Thursday 27 April

11:00 - 14:00 **REGISTRATION** (Europole, Everest Room)

12:30 - 13:30 **Lunch** (Atrium)

14:00 - 15:30 **PLENARY SESSION – SETTING THE SCENE** (Auditorium)
Chairperson: D. Dubbers

14:00 - 14:30	**C.J. Carlile**	*Perspectives and Opportunities*
14:30 - 15:00	**D. Richter**	*Views from the Scientific Council*
15:00 - 15:30	**P. Radaelli**	*The ILL on the world scene*

15:30 - 16:00 **Coffee Break**

16:00 - 17:30 **PLENARY SESSION – SCIENTIFIC ADVANCES 1** (Auditorium)
Chairperson: D Richter

16:00 - 16:30	**C. Alba-Simionesco**	*Is there a correlation between the viscous slowing down of liquids and the fast dynamics of their glasses?*
16:30 - 17:00	**A. Harrison**	*Magnetism and polarized neutrons*
17:00 - 17:30	**P. Schurtenberger**	*Soft matter and neutrons*

17:30 - 18:00 **Coffee Break**

18:00 - 20:00 **EVENING SESSION** (Auditorium**)**
Chairperson: C Carlile

18:00 - 18:40	**D. Dubbers**	*The Institute Laue-Langevin and the role of Neutron Science*
18:40 - 19:20	**A. Frank**	*Searching for additional dimension in the universe with neutron experiments*
19:20 - 20:00	**H. U. Güdel**	*Molecular nanomagnets and neutrons*

20:00 - **Free Evening**

Friday 28 April

08:30 - 10:00 **PLENARY SESSION – MILLENNIUM PROGRAMME ACHIEVEMENTS AND PERSPECTIVES** (Auditorium)
Chairperson: Th. Brückel

08:30 - 09:00	**R. Wagner**	*The Millennium Programme : Achievements for the benefit of ILL's user community*
09:00 - 09:30	**C. Vettier**	*Instrument Review and Scientific Horizons*
09:30 - 10:00	**R. Gähler**	*Possible instruments and new concepts for the future MILLENNIUM programme*

10:00 - 10:30 **Coffee Break**

10:30 - 12:45 **PARALLEL SESSIONS** (see individual sections for room allocation)

12:45 - 14:00 **Lunch** (Atrium)

14:00 - 14:15 **K. Andersen** *Enabling the Millennium Programme: Advances in instrumentation* (Auditorium)

14:15 - 16:00 **POSTER SESSION AND DISPLAYS** (Atrium)

16:00 - 16:30 **Coffee Break**

16:30 - 18:00 **PLENARY SESSION – SCIENTIFIC ADVANCES 2** (Auditorium)
Chairperson: A. Harrison

16:30 - 17:00	**A. Boothroyd**	*Magnetic correlations in metallic Na_xCoO_2*
17:00 - 17:30	**J. Durrell**	*Nuclear physics at ILL*
17:30 - 18:00	**W. Kuhs**	*Time-resolved powder diffraction experiments*

20:00 - 23:00 **SYMPOSIUM DINNER** (at Europole, Atrium)

PARALLEL SESSIONS

PARALLEL SESSIONS A. Nuclei and Particles (Cervin)

Chairperson J. Jolie

10:30 - 10:40	**J. Jolie**	*Introductory comments*
10:40 - 10:55	**K. Protassov**	*The GRANIT experiment*
10:55 - 11:10	**P. Geltenbort**	*Ultra-cold neutrons: past, present and future*
11:10 - 11:25	**G. Simpson**	*Nuclear structure studies of neutron-rich nuclei at ILL*
11:25 - 11:40	**G. Mana**	*Towards an atomic realization of the mass unit: high-precision γ spectroscopy and the measurement of the molar Planck's constant*
11:40 - 11:55	**H. Abele**	*Parameters of neutron β-decay*
11:55 - 12:10	**M. van der Grinten**	*A new limit for the electric dipole moment of the neutron measured at the ILL*
12:10 - 12:45	**J. Jolie**	*User feedback (applause & boos)*

PARALLEL SESSIONS B. Materials Science and Diffraction (Mont Blanc 1+2)

Chairperson P. Henry

10:30 - 10:40	**P. Henry**	*Introductory comments*
10:40 - 10:55	**A. Steuwer**	*Salsa and FaME38 - Materials Science and Engineering at the ILL*
10:55 - 11:10	**S. Klotz**	*High pressure and low temperature for neutron diffraction*
11:10 - 11:25	**Y. Nishiyama**	*Neutron and X-ray fibre diffraction of cellulose polymorphs*
11:25 - 11:40	**M. M. Günther**	*In situ diffraction studies of lanthanum gallate superionic conductors*
11:40 - 11:55	**P. Salmon**	*Glasses and hot neutrons*
11:55 - 12:10	**J. Cole**	*New chemical trends with VIVALDI*
12:10 - 12:45	**P. Henry**	*User feedback (applause & boos)*

PARALLEL SESSIONS C. Magnetic Structures (Mont Blanc 3+4)

Chairperson C. Ritter

10:30 - 10:40	**C. Ritter**	*Introductory comments*
10:40 - 10:55	**J. A. Blanco**	*A non-collinear magnetic structure for GdB_4 determined using spherical neutron polarimetry*
10:55 - 11:10	**R. K. Kremer**	*Helicoidal magnetic ordering of frustrated antiferromagnetic Cu spin chains*
11:10 - 11:25	**J. Schefer**	*Complex magnetic ground state of CuB_2O_4*
11:25 - 11:40	**S. Bramwell**	*Spin ice: A laboratory for statistical physics*
11:40 - 11:55	**J. Goff**	*Spin correlations in the paramagnetic phase of quantum magnets*
11:55 - 12:10	**V. Simonet**	*Magnetic competition in a manganese-free radical chiral chain*
12:10 - 12:45	**C. Ritter**	*User feedback (applause & boos)*

PARALLEL SESSIONS D. Biology and Life Sciences (Auditorium)
Chairperson I. Parrot

10:30 - 10:40	**I. Parrot**	*Introductory comments*
10:40 - 10:55	**N. Fukuhara**	*SANS studies of the tRNA nuclear export complex*
10:55 - 11:10	**M. Budayova-Spano**	*Neutron crystallographic study of recombinant urate oxidase enzyme complexed with 8-azaxanthin*
11:10 - 11:25	**F. Gabel**	*Protein dynamics measured by incoherent elastic neutron scattering*
11:25 - 11:40	**M. Ferrand**	*Internalization of the translocation domain of the diphtheria toxin in model phospholipid bilayers : A neutron reflectometry study*
11:40 - 11:55	**M. Haertlein**	*The ILL-EMBL deuteration laboratory – a platform for isotope-labeling of biological macromolecules*
11:55 - 12:10	**L. Meinhold**	*Proteins in the beamline - a simulation analysis*
12:10 - 12:45	**I. Parrot**	*User feedback (applause & boos)*

PARALLEL SESSIONS E. Large structures (Kilimandjaro 1+2)
Chairperson I. Grillo

10:30 - 10:40	**I. Grillo**	*Introductory comments*
10:40 - 10:55	**J. Oberdisse**	*Structure of silica aggregates in a soft polymeric matrix*
10:55 - 11:10	**A. Rennie**	*Reflectometry - The needs for FIGARO*
11:10 - 11:25	**S. Förster**	*Block copolymers*
11:25 - 11:40	**P.Müller-Buschbaum**	*Surface induced order in thin triblock copolymer films*
11:40 - 11:55	**T. Cosgrove**	*Looking at colloidal interfaces*
11:55 - 12:10	**M. Ballauf**	*Structure of dendrimers in solution*
12:10 - 12:45	**I. Grillo**	*User feedback (applause & boos)*

PARALLEL SESSIONS F. Fluctuations and Dynamics (Kilimandjaro 3+4)
Chairperson M. Böhm

10:30 - 10:40	**M. Böhm**	*Introductory comments*
10:40 - 10:55	**H.B. Braun**	*Emergent soliton chirality in a quantum antiferromagnet*
10:55 - 11:10	**M. Braden**	*Magnetic fluctuations in Sr_2RuO_4 studied by polarized neutron scattering*
11:10 - 11:25	**S. Rols**	*Structure and dynamics of carbon nanostructures: How can neutrons help*?
11:25 - 11:40	**L. Bove**	*Neutron studies in liquid metals*
11:40 - 11:55	**A. Meyer**	*A microscopic view on mass transport in silicate melts*
11:55 - 12:10	**H. Rønnow**	*Exploring novel quantum magnets - the advent of IN8c and prospects for multiplexing*
12:10 - 12:45	**M. Böhm**	*User feedback (applause & boos)*

PARALLEL SESSIONS G. Neutron Methods (Makalu)
Chairperson L. P. Regnault

10:30 - 10:40	**L. P. Regnault**	*Introductory comments*
10:40 - 10:55	**J. Beaucour**	*The life expectation of neutron guides or Do neutron guides live forever?*
10:55 - 11:10	**M. Meiβner**	*New areas and limits of sample environment: Magnetic field and temperature*
11:10 - 11:25	**F. Fraga**	*MILAND (MIllimeter Large Area Neutron Detector) - developments and status*
11:25 - 11:40	**M. Enderle**	*Beyond 15 tesla*
11:40 - 11:55	**E. Lelièvre-Berna**	*Update on polarised ^{3}He*
11:55 - 12:10	**B. Schillinger**	*The European scene of high-quality neutron imaging facilities*
12:10 - 12:45	**L. P. Regnault**	*User feedback (applause & boos)*

Saturday 29 April

08:30 - 10:30 **PLENARY SESSION – SCIENTIFIC ADVANCES 3** (Auditorium)
Chairperson: C. Vettier

08:30 - 09:00	**T. Salditt**	*Collective dynamics of multilamellar lipid membranes: Inelastic neutron and X-ray scattering*
09:00 - 09:30	**O. Zimmer**	*Particle physics with ultra-cold neutrons*
09:30 - 10:00	**D. Oesterhelt**	*Solving signal transduction in biology: a quantitative model for an archaeal signal*
10:00 - 10:30	**Ph. Bourges**	*Spin dynamics in the high-T_c cuprates*

10:30 - 11:00 **Coffee Break**

11:00 - 12:30 **FINAL PLENARY SESSION** (Auditorium)
Chairperson: R. Wagner

11:00 - 11:30	**P. Timmins**	*Partnerships on the ILL Site*
11:30 - 12:15	**W. Press**	*Feedback from the user community (animated by W. Press)*
12:15 - 12:30	**C. Carlile & D. Dubbers**	*Closing remarks*

12:30 **Close of Meeting**

12:30-14:00 **Lunch and Good-byes** (Atrium)

Symposium Programme Abstracts

PLENARY SESSION - SETTING THE SCENE

Thursday 27 April, 14:00 - 15:30

14:00

PERSPECTIVES AND OPPORTUNITIES

C.J. Carlile [1]

[1]*Institut Laue-Langevin, Grenoble, France*

Following the successful launch of the Millennium Programme in the year 2000, ILL has seen a significant improvement to its instrument suite. Infrastructure aspects such as the neutron guides and sample environment equipment have also been enhanced. For the past 18 months ILL and its User community have been examining the possibilities for further improving the instrument suite. This has lead to the proposal for a 10-year programme of development of the instruments and the infrastructure, which will be implemented in two consecutive 5-year phases. The first phase would see the installation of thermal neutron guides to feed 4 flagship instruments - DRACULA, PASTIS, VIVALDI and SALSA - together with the rebuild of the IN16 back scattering machine and the construction of a new high intensity spin-echo spectrometer. The second phase would see the construction of a third cold source which would feed cold neutrons to the currently underused thermal guides in the first guide hall. This will allow purpose-built instruments to be situated at the end of this set of guides, which would be uncompromised in term of intensity and would be dedicated to measurements from samples in high magnetic fields (up to 35 T). The inclusion of a high density Ultra Cold Neutron source is also planned. A new small angle scattering instrument would in addition be built, as would a polarized sample Laue diffractometer for biological materials. These proposals form part of a Perspectives and Opportunities document for which funding is being sought. Included within these plans are joint laboratories for soft condensed matter and material science and engineering in collaboration with the ESRF. Additional comments and suggestions from the ILL User community are welcome.

14:30

VIEWS FROM THE SCIENTIFIC COUNCIL

D. Richter [1]

[1]*Institut für Festkörperforschung, Forschungszentrum Jülich, Germany*

In my talk I will discuss a European Neutron Strategy ensuring the best possible science with neutrons. Such a strategy bases on the ensemble of neutron facilities in Europe. It needs a top quality source with an ambitious and worldwide competitive instrumentation program, where the flux of knowledge is going in both directions to and from the ILL. This strategy will need to ask for an increase in the cooperation with universities and will base on a growing community also in areas where neutrons are commonly not used. In this context interface laboratories are key elements creating a viable scientific environment at ILL and ESRF. They will enable new science and attract contributions from laboratories presently not active at ILL.

15:00

THE ILL ON THE WORLD SCENE

P.G. Radaelli [1]
[1]*ISIS Facility, Rutherford Appleton Laboratory, UK*

The quantity and quality of the scientific output from a single instrument or a whole facility depend on a variety of factors, such as the strength of the user community, the quality of available samples and the competence of the scientific and technical staff. Nevertheless, objective "metric" criteria are useful to identify areas where the ILL and ISIS can most effectively compete with and even outperform next-generation neutron sources such as SNS and J-PARC. To this effect, I will illustrate and employ the concept of peak brilliance as a tool to assess the potential of pulsed and steady-state sources for diffraction and spectroscopy.

PLENARY SESSION - SETTING THE SCENE

Thursday 27 April, 16:00 - 17:30

16:00

IS THERE A CORRELATION BETWEEN THE VISCOUS SLOWING DOWN OF LIQUIDS AND THE FAST DYNAMICS OF THEIR GLASSES?

C. Alba-Simionesco[1], B. Frick[2], A. Chauty[1], K. Niss[1], F. Casas[1], A. Sokolov[3], F. Lequeux[4], H. Montès[4]

[1]Laboratoire de Chimie Physique, Bât 349, Université Paris-sud , Orsay, France, [2]Institut Laue Langevin, Grenoble, France [3]Dpt of Polymer Physics, Akron University, USA, 4Laboratoire de Physico-chimie des Polymères et Milieux Dispersés, ESPCI, Paris,France.

The understanding of the viscous slowing down of liquids and polymers, the glass transition and the nature of the glassy state is an old and unsolved fundamental problem, but it remains an exciting branch of condensed matter physics with strong direct or indirect implications in many areas. It is not clear what governs the viscous slowing down of the structural relaxation time or the viscosity as the glass transition is approached by cooling; its increase is in almost all cases found to be much more dramatic than the expectation for a simple activated behavior. Moreover its T-dependence differs largely from one system to another one, and accordingly, liquids have been classified by introducing the concept of fragility. One of the striking results is the relation between the fragility and the fast dynamics of the undercooled liquid close to the glass transition and the vibrational properties of the corresponding glass. There is a hidden connection between the flow process on a time scale of seconds and the processes seen in a pico- nano time scale experiment, more than ten decades faster. A number of different results suggest that the glassy dynamics and the fragility of the liquid might be intimately related; among them, it has been observed that an increase in fragility correlates with - the increase in mean square displacement (msd) as temperature rises above Tg (Buchenau 1992), - the intensity of the boson peak or an excess in the vibrational density of states VDOS (Sokolov 1993), the temperature dependence of the high frequency shear modulus (Olsen 1998), the non-ergodicity (fq) factor at Tg (Scopigno 2003), and the Poisson ratio in the glass (Novikov 2005). The results are still controversial and satisfactory theoretical explanations for the different relations are lacking. We propose here to use the knowledge gained within the last decade on the msd, the fq, the excess of VDOS in order to clarify their relation to the viscous slowing down via the relative contributions of the temperature and the density on the relaxation processes. We have investigated by inelastic neutron scattering (time-of-flight, backscattering and neutron spin echo) the dynamics of glass-forming polymers and molecular liquids in the wave-vector range of the main diffraction peak known from elastic measurements; the temperature ($2K < T < 400K$) and pressure ($Patm < P < 1.5$ GPa) conditions used cover the glass and the supercooled liquid regions, whose thermodynamic properties were characterized independently. Finally recent approaches suggest to rationalize these findings by introducing either a growing length scale encoded in the fluctuations of the liquid dynamics (Berthier 2005) or a correlation length; defined as a limit for the applicability of continuous elasticity theory (Leonforte 2005, Barrat 2006); it is very likely that the existence of this latter length could be related to the excess of VDOS. Such a length scale was newly observed for the first time in structural experiments of a stretched polymer.

16:30

MAGNETISM AND POLARIZED NEUTRONS

A. Harrison [1]
[1]*The School of Chemistry and the Centre for Science at Extreme Conditions, Edinburgh, UK*

The study of magnetic materials and magnetic phenomena through elastic neutron scattering is a cornerstone of the scientific reputation of the ILL. It has benefited greatly from groundbreaking and creative developments in techniques and instrumentation, as well as the pioneering spirit of its scientists and collaborators. The Millennium Programme is already enhancing that tradition, though the provision of greatly improved diffractometers that will reveal magnetic correlations in single crystals, powders or nanostructured samples with greater sensitivity, resolution or range of length-scale than previously possible. Complementary developments in the capability to provide neutron polarization analysis add a further dimension to this work that is unsurpassed in many important areas of condensed matter science. Some of the new science that is already emerging from the Programme will be reviewed, together with the promise that planned instruments and techniques hold.

17:00

SOFT MATTER AND NEUTRONS

P. Schurtenberger [1]
[1]*Department of Physics and Fribourg Center for Nanomaterials, Fribourg, Switzerland*

Soft condensed matter represents a rapidly expanding field of research, in which one primarily focuses on three different complementary areas: colloids, polymers and surfactants. Soft condensed matter science is not only an attractive area of modern basic research, but is of considerable technological importance in areas such as, for example, the manufacturing of synthetic dispersions for coatings, ceramics fabrication, polymer processing, corrosion phenomena, environmental pollution, food technology, pharmaceutical industry, biocompatible materials, and biotechnology. A major goal is to understand the formation processes, structure, and functional properties of supramolecular systems that play an important role in real life. Among the experimental techniques to characterize complex fluids neutron scattering has played a unique and successful role. This is mainly for two reasons (i) neutrons access the proper length and time scales: especially small-angle neutron scattering and reflectometry for structural and kinetic studies and neutron spin echo for dynamic investigations. (ii) For hydrogen-containing substances the exchange of hydrogen by deuterium facilitates labeling on a molecular scale, an extremely important method to decipher complex structures in multicomponent materials. In this short review I will give a number of examples for successful neutron studies, covering different areas such as aggregation and gelation in concentrated colloidal dispersions, the formation of polymer-colloid nanocomposites, and structural and dynamic properties of dense protein solutions. I will point out the importance of complementary techniques, and give an outlook on future developments.

PLENARY SESSION - EVENING SESSION

Thursday 27 April, 18:00 - 20:00

18:00

THE INSTITUTE LAUE-LANGEVIN AND THE ROLE OF NEUTRON SCIENCE

D. Dubbers [1]

[1]*U. Heidelberg, Germany*

As is well known, world-wide the ILL is still the standard reference with respect to neutron flux and to instrument performance, and the intention of the Millennium renewal programme is to keep it this way also in the future. What is less well known is that ILL also pioneered a new way of how central facilities are being used by the scientific community, by an open access strategy which was at least as important to the success of ILL as was its high neutron flux, and which, too, has served as a model for many later facilities.

18:40

SEARCHING FOR ADDITIONAL DIMENSIONS IN THE UNIVERSE WITH NEUTRON EXPERIMENTS

A. Frank [1]

[1]*Instituto de Ciencias Nucleares, Universidad Nacional Autónoma de México*

Is the Newtonian theory of gravity (or, more precisely, Einstein's General Relativity) valid all the way from microscopic to astronomic scales? Surprisingly, this has not been confirmed below a distance of about a tenth of a millimeter. The assumption that the same law holds all the way down to the Planck scale involves more than 30 orders of magnitude, with no experimental evidence to support it. Gravity seems to be many orders of magnitude weaker than the gauge forces. Why is gravity so faint? String Theory finds the need for additional dimensions, closed around themselves with a characteristic length of the order of the Planck scale, where gravity becomes strong enough to be unified with the gauge forces. But recent theories conjecture that the extra dimensions could be as big as a fraction of a millimeter, invisible to us because they can only be probed via the feeble gravitational interactions. Their existence, however, would imply modifications to the gravitational force. In this talk I discuss this problem and present a simple derivation of the compactification lengths of additional dimensions (which depend on the number of them) as well as an explicit form of the modified gravitational law. Neutron scattering experiments are proposed that may catch a glimpse of possible modifications of gravity at very short scales. The question remains whether we can listen to this whisper in the nuclear background roar.

A. Frank, P. Van Isacker, J. Gomez-Camacho, 'Probing additional dimensions in the universe with neutron experiments', Physics Letters B, 582, 15-20 (2004).

19:20

MOLECULAR NANOMAGNETS AND NEUTRONS

H. U. Güdel [1]

[1]*Department of Chemistry, University of Bern, Switzerland*

Single Molecule Magnets (SMM) are the smallest units to store a bit of information at cryogenic temperatures. The observation of SMM properties in the molecule Mn12-acetate has triggered a flurry of transdisciplinary research between chemistry and physics. Inelastic neutron scattering is a very powerful tool for the study of exchange and anisotropy interactions in spin clusters. The tunneling of the magnetization in Mn12-acetate and related SMM clusters can be studied as well as the tunneling of the Neel vector in antiferromagnetic rings. Examples from our own work shall be used to illustrate the power of neutron scattering in the area of molecular magnetism.

PLENARY SESSION - MILLENNIUM PROGRAMME ACHIEVEMENTS AND PERSPECTIVES

Friday 28 April, 08:30 - 10:00

08:30

THE MILLENNIUM PROGRAMME: ACHIEVEMENTS FOR THE BENEFIT OF ILL'S USER COMMUNITY

R. Wagner [1]

[1]*Institut Laue-Langevin, Grenoble, France*

In order to maintain the scientific value of the ILL to its broad user community throughout Europe and beyond, in 2000 the Millennium Programme was launched to boost the quality of the experimental facilities. The ongoing renewal programme has been directed towards renewing some of the neutron delivery systems – neutron guides and beam tubes -, towards improvement of sample environment and installation of user-friendly data acquisition/ handling systems, and in particular towards upgrading of neutron instrumentation. Hitherto, nine instruments with significantly improved efficiency and great advances in the instruments' performance have been completed. Already at this stage of the Millennium Programme, this will pay great dividends to ILL's users in terms of scientific opportunities and results.

09:00

INSTRUMENT REVIEW AND SCIENTIFIC HORIZONS

C. Vettier [1]

[1]*Institut Laue-Langevin, Grenoble, France*

The ILL is evolving in a constantly changing environment. As a user facility, the ILL must respond to the expressed needs by optimizing neutron instruments and also by offering new tools and methods to neutron users. On the one hand, the review of ILL public instruments has stimulated the coherence of neutron instrumentation at ILL and has led to prioritization of the instrument and infrastructure programmes. On the other hand, the ILL should exploit innovative techniques to expand the scientific base of neutrons. Furthermore, the ILL will provide interface facilities to enable users' novel scientific programmes. These developments will strengthen the value and scientific output of neutron methods, but also underpin and extend ILL's leadership in neutron science.

09:30

POSSIBLE INSTRUMENTS AND NEW CONCEPTS FOR THE FUTURE MILLENNIUM PROGRAMME

R. Gähler [1]
Institut Laue-Langevin, Grenoble, France

We discuss some potential projects for the Millennium Programme of ILL: The two key projects are a 3rd cold source and a high field laboratory. Their realization would have strong impacts on the future instrumental scene. In addition, we present some visions on a new hot diffractometer, a forth SANS instrument and an option to measure life times of phonons. Finally we outline a new efficient beam modulation technique and discuss its possible applications in neutron science.

PARALLEL SESSION A. NUCLEI AND PARTICLES

Friday 28 April, 10:30 - 12:45

10:40

THE GRANIT EXPERIMENT

K. Protassov [1]

[1]*Laboratoire de Physique Subatomique et de Cosmlogie, CNRS-UJF, Grenoble, France*

Gravitationally bound quantum states of matter were observed for the first time thanks to the unique properties of ultra-cold neutrons (UCN). This phenomenon and the related experimental techniques could be applied to various domains ranging from the physics of elementary particles and fields (for instance, spin-independent or spin-dependent short-range fundamental forces, or the search for a non-zero neutron electric charge) to surface studies (for instance, the distribution of hydrogen in/above the surface of solids or liquids, or thin films on the surface) and the foundations of quantum mechanics (for instance, loss of quantum coherence, quantum-mechanical localization, or experiments using the very long path of UCN matter waves in medium and in wave-guides).

In the present talk we focus on transitions between the quantum states of neutrons in the gravitational field, consider the characteristic parameters of the problem and examine various methods for producing such transitions. We also present the future experiment GRANIT (GRAvity Induced Neutron Transitions), which will study these quantum transitions and their optimization with respect to particular physical goals.

10:55

ULTRA-COLD NEUTRONS: PAST, PRESENT AND FUTURE

P. Geltenbort & C. Plonka

Institut Laue-Langevin,Grenoble, France

Due to their outstanding property to be storable and hence observable for long periods of time (several hundreds of seconds) in suitable material or magnetic traps, ultra-cold neutrons (UCN) are an unique tool to study fundamental properties of the free neutron. A short history of UCN sources will be given while the existing UCN installation at the ILL will be described in detail. This source offered greatly improved sensitivity and systematics compared to experiments done with cold neutrons. After many breakthroughs those storage experiments are now mainly limited by the low UCN statistics. Alternative UCN production schemes such as down scattering of cold neutrons into UCN in superfluid helium or in other cold solid moderators such as solid deuterium or deuterated methane have been successfully demonstrated. They are potentially attractive methods to achieve orders of magnitude higher UCN densities. Latest results will be presented and possible scenarios for new UCN sources at the ILL will be discussed in detail, to keep ILL's leading position in physics with UCN.

11:10

NUCLEAR STRUCUTURE STUDIES OF NEUTRON-RICH NUCLEI AT THE ILL

G. Simpson[1], J.-A. Pinston[1], J. Genevey[1], W. Urban[2], A. Scherillo[3], R. Orlandi[4], A.G. Smith[4]
[1] LPSC Grenoble, [2] University of Warsaw,[3] University of Cologne, [4] University of Manchester

The properties of neutron-rich nuclei around the doubly magic ^{132}Sn have been studied in detail at the Lohengrin spectrometer of the ILL, using microsecond isomers. Nuclei around shell closures have a particularly simple structure, which makes them suitable for interpretation using the nuclear shell model. These detailed studies show that the properties of exotic neutron-rich nuclei in this region can be generally well described by the nuclear shell model for $Z > 50$, but less well for $Z < 50$ [1][2]. These studies of very rare nuclei have only been possible due to the upgrade of gamma-ray detection facilities under the Millennium Project.

The neutron-rich mass 100 region has also been investigated using a combination of Lohengrin data and spontaneous fission data. Here it is seen that just a few orbits play key roles in the onset of deformation [3] and that many different shapes can co-exist in these nuclei.

Several new techniques have been introduced at the ILL to measure pico-to-nanosecond lifetimes and magnetic moments of excited states in very neutron-rich nuclei at Lohengrin. In addition experiments have been carried out at the PF1 neutron guide to search for isomeric states in the lifetime range 50 nanoseconds to 2 microseconds. These new developments allow the properties of exotic neutron-rich nuclei to be studied in greater depth.

[1] J.A. Pinston and J. Genevey, J. Phys. G 30 (2004) R57.
[2] A. Scherillo et al. Phys. Rev. C 70 (2004) 054318.
[3] W. Urban et al. Eur. Phys. J. A 16 (2003) 11.

11:25

TOWARDS AN ATOMIC REALIZATION OF THE MASS UNIT: HIGH-PRECISION γ SPECTROSCOPY AND THE MEASUREMENT OF THE MOLAR PLANCK'S CONSTANT

G. Mana [1]
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A definition of the mass unit based on a conventional value of the Planck's or Avogadro's constants, h and N_A, or of the mass of an atom is highly desirable. An attractive way to do that is through a nucleus whose Compton's frequency mc^2 / h is given a conventional value.

In nuclear reactions, the energy variation is high enough to allow a measurement of the mass difference between the exited and ground state. Consequently, in principle, nuclear transitions can set time, length, and mass units via the frequency and wavelength of the emitted γ rays and the mass difference between the relevant energy levels. Although, for what concerns time and length measurements, this is far beyond today capabilities, as regards mass, it opens the way to precision measurements of atomic masses in terms of frequency measurements; in other words, to measurements of the Compton's frequencies of nuclei.

Metrologists are measuring h via the comparison of electrical and mechanical powers and N_A by counting the number of atoms in a crystal mole of ^{28}Si. The difficulties and the potentials for undiscovered systematic effects are demonstrated by the present discrepancy between the h and N_A measurement results. Therefore, accurate measurements of nuclear binding energies, which can be used to determine the product N_A h – the molar Planck's constant, represent an important step towards an atomic definition of the kilogram.

11:40

PARAMETERS OF NEUTRON β-DECAY

H. Abele [1]
[1]*Department of Physics, University of Heidelberg, Germany*

We review the status of precision measurements in neutron β-decay with focus on angular correlation coefficient measurements. The results are related to the Standard Model description of particles and fields. Particular attention is paid to the presently poorly satisfied unitarity condition for the CKM matrix and to the ratio $\lambda=g_A/g_V$, a fundamental quantity in its own right. Besides that, a new instrument being planned is presented. It is a joint project (called PERC) of the Universities Heidelberg, Mainz and Munich and it will considerably improve statistical and systematic errors at the same time. The neutron beam can be monochromatized, polarized or pulsed according to the need of the quantity under study.

11:55

A NEW LIMIT FOR THE ELECTRIC DIPOLE MOMENT OF THE NEUTRON MEASURED AT THE ILL

M. van der Grinten [1]
[1]*University of Sussex, UK*

The search for the electric dipole moment (EDM) of the neutron plays a prominent role in particle physics because of its direct bearing on CP and T violation: a non-zero value of the neutron EDM would be evidence of CP and T violation. The neutron EDM is of particular interest because it is very sensitive to CP violation beyond the Standard Model. The region that is probed by past experiments is already putting tight constraints on models such as Supersymmetry, additional Higgs fields and Left-Right symmetric models.

We report on the results of the nEDM measurement carried out at PF2 at the ILL. The experiment has been taking data over a period of six years and has subsequently been running for one year devoted to systematic studies related to the experiment. The new limit on the nEDM from these measurements will be presented along with an outlook of the new cryogenic EDM experiment that has been constructed at ILL's H53 beam and will start taking data in Summer 2006.

PARALLEL SESSION B. MATERIALS SCIENCE AND DIFFRACTION

Friday 28 April, 10:30 - 12:45

10:40

SALSA AND FAME38 - MATERIALS SCIENCE AND ENGINEERING AT THE ILL

A. Steuwer
Institut Laue-Langevin, Grenoble, France

The development and implementation of advanced materials for engineering applications requires equally advanced tools for their characterisation. Neutron diffraction is a unique tool for materials engineering science as it can provide valuable material information, ranging from microstructural information to residual stresses, non-destructively and in the bulk.

In this talk we review progress at the ILL in view of the commissioning of the new dedicated materials engineering beam line SALSA, as well as the joint FaME38 support and research facility.

10:55

HIGH PRESSURE AND LOW TEMPERATURE FOR NEUTRON DIFFRACTION

S. Klotz[1], G. Hamel[1], C. Th. Strässle[2], N. Kervananois[3], M.M. Koza[3]
[1] IMPMC, Université P&M Curie, Paris,France, [2]Laboratory for Neutron Scattering, ETH Zürich and Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland, [3] ILL, Grenoble, France

As part of the Millennium Program, the ILL has an ongoing project to enable high-pressure neutron studies in the 10 GPa range and at low temperature down to 4 K as a standard user facility. The setup consists of a "panoramic" VX5 Paris-Edinburgh press with a capacity of 130 tn to compress samples of typically 80 mm^3 to 10 GPa, in conjunction with a powerful closed cycle refrigerator to cool the 30 kg press to the required temperature in a reasonable time. In this talk we present the basic features of this device and report on the first online measurements done with it in 2005, shortly before the long shutdown. In these measurements the vibrational spectrum of H_2O ice Ih (ordinary ice) was investigated by incoherent inelastic neutron scattering on IN6 up to ~2 GPa, in the temperature range 4-100 K. A specific requirement of these measurements was that all pressure changes needed to be made below 130 K. We find mode softening of low-energy acoustic phonons as predicted by extrapolation of previous measurements using coherent inelastic scattering on single crystals up to 0.5 GPa [1]. The potential of these experimental possibilities as well as remaining development issues will be addressed.

[1] Th. Strässle, M.A. Saitta, S. Klotz, M. Braden, Phys. Rev. Lett. 93, 225901 (2004).

11:10

NEUTRON AND X-RAY FIBER DIFFRACTION OF CELLULOSE POLYMORPHS

Y. Nishiyama[1], P. Langan[2], Masahisa Wada[3], Junji Sugiyama[4], H. Chanzy[1]
[1] CERMAV/CNRS Grenoble, France, [2]LANL Los Alamos, USA, [3]Univ. of Tokyo, Japan, [4]Kyoto Univ., Japan.

Cellulose, the most abundant and renewable biopolymer on earth, is daily produced and extruded through enzyme complexes on the cell membrane of plants. They form crystalline nanofibrils with completely extended chains. Once the native cellulose (cellulose I_α, I_β) dissolve or swell in different medium, cellulose can take other crystalline forms of different physical and chemical properties. With three hydroxyl groups per residue, hydrogen bonding plays an important role in its structural stability. We succeeded in preparing uni-axially oriented specimens of cellulose microcrystals with large lateral size (~20 nm), from certain algae and tunicate, that allowed us to obtain good resolved X-ray and neutron fiber diffraction at 1Å resolution. Further more, the hydroxyl groups inside the crystal could be stably deuterated without affecting the crystal structure. Using the phase of the X-ray structure, the difference in amplitude of neutron diffraction obtained from deuterated and native specimen gave us directly the position of hydrogen atoms that are involved in hydrogen bonding. The hydrogen-bonding scheme was in good accordance with polarized infrared studies and difference in physical properties of the crystal.

11:25

IN SITU DIFFRACTION STUDIES OF LANTHANUM GALLATE SUPERIONIC CONDUCTORS

M. M. Günter[1], M. Lerch[2], H. Boysen[3], C. Korte[4], E. Suard[5]
[1] OSRAM GmbH, Berlin, Germany [2] Institut für Chemie, Technische Universität Berlin, Germany, [3] Universität München, Department für Geo- und Umweltwissenschaften, Sektion Kristallographie, Germany, [4] Physikalisch Chemisches Institut der Justus-Liebig Universität Gießen, Germany,[5] Institut Laue-Langevin, Grenoble, France

In-situ neutron powder diffraction investigations of the oxygen super-ionic conductors $La_{0.9}Sr_{0.1}Ga_{0.8}Mg_{0.2}O_{2.85}$ and $La_{0.8}Sr_{0.2}Ga_{0.8}Mg_{0.2}O_{2.80}$ were performed at 1460 K with and without an applied electric field (U = 3 V DC) resulting in lasting ionic currents of 180–270 mA. At this temperature both samples adopt the cubic perovskite structure ($Pm\bar{3}m$). Field-induced structural changes are evidenced by anharmonic terms in the Debye-Waller factors of oxygen only for the first sample. The corresponding probability density function maps indicate curved diffusion pathways around the Ga atoms shifted further into the direction of an octahedral void with applied field. In addition, double maxima appear in the direction of the Ga—O bond which are more prominent in the second sample. A tentative explanation of the observed phenomena is given in terms of long-range ordering of the corresponding potential minima and residual short-range order clusters persisting at high temperature [1]. In addition to the measurements with an external electrical field first in situ high temperature neutron scattering experiments under microwave irradiation have been carried out on this superconductor. A definite non-thermal microwave effect on the resulting crystallographic structures was discovered mainly derived from opposite changes of the lattice constants and the atomic displacement parameters. These effects are related to changes in the phonon density of states (DOS) due to coupling of the microwave field via (anharmonic) multi-phonon processes, limited phonon life times and local modes arising from the defects. The problem of defining a temperature in a microwave field due to the non-equilibrium DOS is discussed [2].

[1] M. M. Günter, H. Boysen, C. Korte, M. Lerch, E. Suard, Z. Kristallogr. 2005, 220, 1.

[2] M. M. Günter, C. Korte, G. Brunauer, H. Boysen, M. Lerch, E. Suard, Z. Anorg. Allg. Chem. 2005, 631, 1277.

11:40

GLASSES AND HOT NEUTRONS

P. S. Salmon[1], R. A. Martin[1], A. C. Barnes[2], P. E. Mason[2], G. J. Cuello[3]
[1] Department of Physics, University of Bath, UK, [2] HH Wills Physics Laboratory, Royal Fort, University of Bristol, UK, [3] Institut Laue-Langevin, Grenoble, France.

An experimental determination of glass structure is a formidable problem because the atomic sites are topologically disordered and the presence of two or more chemical species adds further complexity. In this talk, some new in-roads are reported that have emanated from an application of the method of isotopic substitution in neutron diffraction. Specifically, the topological and chemical ordering in several binary AX_2 network glasses is measured and two length scales at distances greater than the nearest-neighbour are identified. The interplay between the ordering on these length scales and the physical properties of network glasses is discussed.

11:55

NEW CHEMICAL TRENDS WITH VIVALDI

J. M. Cole[1], G. J. McIntyre[2]
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The single-crystal thermal-neutron Laue diffractometer, VIVALDI, was the first instrument commissioned in the ILL Millennium Program. The conception of VIVALDI came from trials in 1997, where LADI, a cold-neutron Laue diffractometer for studies of biological macromolecules, was placed temporarily on a thermal beam. In one trial [1], the crystal structure of the non-linear optical material, zinc (tris)thiourea sulfate, was determined on 'thermal-LADI' and compared with that obtained from the high-flux single-crystal neutron diffractometer, D9, also at the ILL. The exact hydrogen positions and details of the hydrogen bonds in this material were important to establish their roles in the non-linear optical properties. The same scientific conclusions were drawn from each experiment, but with 'thermal-LADI' showing a hundred-fold gain in efficiency. Thus, a thermal-neutron Laue diffractometer was proven to be extremely well suited to rapid determination of hydrogen positions.

The VIVALDI instrument is briefly described, together with illustrations of its capability in four quite different chemical studies: the location of H in the Li cage of an organometallic complex [2]; the C-H...F hydrogen bonding in a Zr-based organometallic catalytic complex [3]; a multi-temperature study of the zeolite, YUG, where knowledge of the disorder in its water contents is important in assessing its potential to adsorb guest molecules; and a charge-density study of the organic molecule, coumarin, a chemical precursor to many laser dyes.

[1] J.M. Cole, G.J. McIntyre, M.S. Lehmann, D.A.A. Myles, C. Wilkinson, J.A.K. Howard, Acta Crystallogr. A57 (2001) 429-434.
[2] S.R. Boss, J.M. Cole, R. Haigh, G.J. McIntyre, P.R. Raithby, R. Snaith, A.E.H. Wheatley, Organometallics, 23 (2004) 4527-4530.
[3] M.C.W. Chan, S.C.F. Kui, J.M. Cole, G.J. McIntyre, S. Matsui, N. Zhu, K-H. Tam, Chem. Eur. J. 12 (2006) 2607-2619.

PARALLEL SESSION C. MAGNETIC STRUCTURES

Friday 28 April, 10:30 - 12:45

10:40

A NON-COLLINEAR MAGNETIC STRUCTURE FOR GdB_4 DETERMINED USING SPHERICAL NEUTRON POLARIMETRY

J. A. Blanco[1] , J. Fernandez-Rodríguez[1], P. J. Brown[2], A. Stunault[2], K. Katsumata[3], S. W. Lovesey[3,4], F. Iga[5] and S. Michimura[5]

[1]Departamento de Física, Universidad de Oviedo, Spain, [2]Institut Laue Langevin, Grenoble, France, [3]RIKEN Harima Institute, Japan, [4]ISIS Facility, RAL, UK, [5]Department of Quantum Matter, ADSM, Hiroshima University, Japan

Recently, interest in the antiferromagnetic ordering on GdB_4 has been renewed by resonant X-ray scattering experiments at the Gd L_3 edge in which interference between magnetic and anisotropic charge contributions to the scattering were observed [1]. The X-ray scattering data were, however, unable to distinguish between collinear and non-collinear models for the magnetic structure. This ambiguity has been resolved using spherical neutron polarimetry at short wavelength (λ= 0.545 Å at D3) on ^{11}B enriched single crystals. The polarimetric measurements show unequivocally that the full tetragonal symmetry is preserved in the antiferromagnetic phase. The magnetic space group is P4/m'b'm' with the Gd magnetic moments of 7.2(2)μ_B lying in the *ab*-plane of the tetragonal structure on the 4 Gd ions in the unit cell parallel to the 4 different <110> axes.

[1] S. Ji et al. Phys. Rev. Lett. 91 (2003)257205

10:55

HELICOIDAL MAGNETIC ORDERING OF FRUSTRATED ANTIFERROMAGNETIC Cu SPIN CHAINS

R. K. Kremer[1] M. Banks[1], L. Capogna[1,2], M. Enderle[2], B. J. Gibson[1], G. J. McIntyre[2], B. Ouladdiaf[2], S. Pujol[2], J.-L. Raggazzoni[2], M. Rheinstädter[2]

[1] MPI für Festkörperforschung, Stuttgart, Germany, [2] Institut Laue-Langevin, Grenoble, France

Stimulated by the vivid search for a theoretical understanding of high-T_c superconductivity, the magnetic properties of low-dimensional quantum antiferromagnetic (afm) systems that contain S=½ moments on $Cu^{2+,}$ V^{4+} or Ti^{3+} ions have attracted particular attention. Unusual ground-state properties have been seen to evolve. They are due to the proximity of such systems to quantum criticality via mainly a considerable sensitivity to higher-order effects in the exchange coupling, but also to coupling to lattice or charge degrees of freedom.

We investigated several Cu^{2+} one-dimensional chain systems which contain CuX_2 (X=O, Cl, Br) ribbons. They all show an incommensurate helicoidal afm ordering along the chains which we ascribe to a competition of nearest and next-nearest neighbour superexchange interaction along the S=½ chains.

11:10

COMPLEX MAGNETIC GROUND STATE OF CuB_2O_4

J. Schefer[1], M. Boehm[2], B. Roessli[1], A. S. Wills[3], B. Ouladdiaf[2], E. Lelièvre-Berna[2], U. Staub[4] , A. Amato[5], C. Baines[5], and G. A. Petrakovskii[6]

[1]Laboratory for Neutron Scattering, ETH Zurich & Paul Scherrer Institute, Switzerland, [2]Institut Laue-Langevin, Grenoble, France, [3]Department of Chemistry, University College London, UK, [4]Swiss Light Source, Paul Scherrer Institute, Switzerland, [5]Swiss Muon Source, Paul Scherrer Institute, Switzerland, [6]Institute of Physics, Krasnoyarsk, Russia

The magnetic ground-state of copper metaborate CuB_2O_4 was investigated with unpolarized and polarized neutron scattering as well as Muon-spectroscopy at PSI (TASP, TriCS) and ILL (D10,D3) [1]. A phase transition was found at T_N=21 K to a commensurate weakly ferromagnetic state followed by a second transition at T*=10 K to an incommensurate magnetic structure. Neutron diffraction revealed a continuously changing magnetic propagation vector below T*, and unusually asymmetric magnetic satellite reflections. Additionally, diffuse scattering is observed in the temperature range 1.5 K<T<30 K. The magnetic structures of both phases determined from single-crystal diffraction analysis on D10 and refined by spherical neutron polarimetry on D3 are shown to be consistent with results of symmetry analysis. In particular, we find that only one of the two inequivalent Cu^{2+} sublattices fully orders down to the lowest temperature. Our results show that the complex magnetic behavior of copper metaborate is a consequence of mutual interaction between the two Cu^{2+} sublattices with different ordering temperatures. Detailed results are given in [2-4].

[1] B. Roessli, J. Schefer, G. Petrakovskii, B. Ouladdiaf, M. Boehm, U. Staub, A. Vorontinov and L. Bezmaternikh, Formation of a Magnetic Soliton Lattice in CuB_2O_4 Metaborate, Physical Review Letters 86,9 (2001) 1885-1889.
[2] M. Boehm, B. Roessli, J. Schefer, A.S. Wills, B. Ouladdiaf,, E. Lelièvre-Barna, U. Staub and G. A. Petrakovskii, Complex Magnetic Ground State of CuB_2O_4, Phys. Rev. B 68, 024405-1-9 (2003).
[3] M. Boehm, B. Roessli, J. Schefer, B. Ouladdiaf, A. Amato, C. Baines, U. Staub and G. A. Petrakovskii, A Neutron Scattering and μSR Investigation of the Magnetic Phase Transition of CuB_2O_4, Physica B A74, S82-S85 (2002).
[4] J. Schefer, M. Boehm, B. Roessli, G. A. Petrakovskii, B. Ouladdiaf and U. Staub, Soliton Lattice in Coppermetaborate, CuB_2O_4, in the Presence of an External Magnetic Field, J. Applied Physics A 75, S1740-S1742 (2002)

11:25

SPIN ICE: A LABORATORY FOR STATISTICAL PHYSICS

S. Bramwell [1]

[1]University College London, Department of Chemistry, UK

Pauling's model of hydrogen disorder in water ice illustrates how zero-point entropy can occur in a practical system. "Spin Ice" is a precise analogue of Pauling's model in which proton displacement vectors are replaced by Ising spins and the "ice rules" are enforced by ferromagnetic coupling. The model is approximated almost ideally by several rare-earth pyrochlore magnets of general formula $R_2M_2O_7$ (R = Ho, Dy, M = Ti, Sn). These materials have a disordered low-temperature magnetic state with zero-point entropy. Application of a magnetic field to the low-temperature state
(at ~50 mK) allows the experimentalist to observe novel phase transitions between a rich variety of disordered, partially ordered and fully ordered magnetic phases. Neutron diffraction has played a key role in elucidating the properties of spin ice, as emphasized in this talk.

11:40

SPIN CORRELATIONS IN THE PARAMAGNETIC PHASE OF QUANTUM MAGNETS

J.P. Goff[1], A.M. Toader[1], M. Skoulatos[1], M. Enderle[2], J.R. Stewart[2], A. Murani[2], M. Roger[3], N. Shannon[4], E.E. Kaul[5], C. Geibel[5]

[1] Department of Physics, University of Liverpool, UK [2] Institut Laue-Langevin, Grenoble, France, [3] Service de Physique del 'Etat Condensé, Commissariat à l'Energie Atomique, Centre d'Etudes de Saclay, France, [4] HH Wills Physics Laboratory, University of Bristol, UK, [5] Max-Planck Institute for Chemical Physics of Solids, Dresden, Germany.

Frustrated quantum magnets exhibit a strongly correlated phase over a wide range of temperatures below their Curie-Weiss temperatures, before ordering long range. It is of great interest to study this spin fluid state, but it is always difficult to separate the weak neutron scattering signal from the background. The three-dimensional polarization analysis on the D7 and IN20 spectrometers allows the purely magnetic signal to be isolated. Improvements to the monochromator on IN20, and upgrades to the polarizer and detector bank on D7, as part of the Millennium Project, have facilitated the study of diffuse scattering from spin ½ systems, where quantum fluctuations are greatest. We shall describe recent experiments to study square-lattice Heisenberg antiferromagnets, emphasizing how the spin correlations in the paramagnetic phase give new information on the exchange mechanism. We find that the behaviour of La_2CuO_4 agrees with the predictions of the quantum non-linear sigma model, and that it is the first electronic material to exhibit ring exchange. Quantum order from disorder is observed for $Pb_2VO(PO_4)_2$, and we find ferromagnetic nearest-neighbour exchange J_1 and antiferromagnetic next-nearest-neighbour exchange J_2 of comparable magnitude, allowing the exploration of a new region of the J_1-J_2 phase diagram.

11:55

MAGNETIC COMPETITION IN A MANGANESE-FREE RADICAL CHIRAL CHAIN

V. Simonet [1], E. Lhotel [2], C. Paulsen [2] and E. Ressouche [3]

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The organic chemistry synthesis methods, applied in the field of molecular magnetism, allow to obtain original compounds with properties characteristic of both classical magnets and organic compounds. This is the case of the chain compound, (R)-3MLNN $Mn(hfac)_2$, formed by alternating Mn^{2+} ions carrying a spin 5/2 and free radicals with delocalized spin ½ which confer to the chain its chiral geometry.

Magnetometry measurements showed that the two magnetic species are strongly antiferromagnetically coupled along the chain axis leading to a model of ferromagnetic chains of effective moment M=4. There are two possible competing inter-chain coupling, ferromagnetic dipolar interaction and antiferromagnetic exchange interaction, which are estimated to be very low (≈mK). A transition to a 3D magnetic order occurs at 3K, announced by pre-transitional ferromagnetic fluctuations, and characterized by a magnetic anisotropy, the effective moment being tilted by an angle of 20° with respect to the chain axis.

Neutron diffraction experiments were performed on a single crystal in order to determine the nature of the magnetic order. Magnetic Bragg reflections are detected below 3 K which corresponds to a canted

antiferromagnet. In the chain direction, the magnetic moments are mainly oriented along the chain axis with a small antiferromagnetic component perpendicular to it. Surprisingly, the inter-chain coupling is antiferromagnetic. The apparent contradiction with the magnetometry measurements was lifted by an additional neutron diffraction experiment on a single crystal under magnetic field. The magnetic peaks observed in zero field, characteristics of the antiferromagnetic inter-chain arrangement, vanish in low applied field. At the same time, new Bragg peaks, characteristic of ferromagnetic inter-chain arrangement, rise rapidly with the magnetic field. These results show that in this quasi-1D molecular compound, a complex magnetic behavior results from the competition of two weak inter-chain interactions of opposite sign.

PARALLEL SESSION D. BIOLOGY AND LIFE SCIENCES
Friday 28 April, 10:30 - 12:45

10:40

SANS STUDIES OF THE TRNA NUCLEAR EXPORT COMPLEX

N. Fukuhara[1], J.Ebert[2], D. Lindner[2], M.-T. Dauvergne[3], M. Härtlein[3], P. Timmins[3], E. Conti[2], D. Svergun[4]

[1] Imperial College London, [2] EMBL-Heidelberg, [3] ILL, Grenoble, [4] EMBL-Hamburg

Nuclear transport receptors (importins/exportins) are responsible for the translocation of their specific cargo in or out of the cell nucleus through the nuclear pores. Most of these receptors, belonging to the importin ß family, are superhelically twisted macromolecules composed of alpha-helical HEAT repeats, and have molecular weights around 100 kDa. Import receptors bind their cargo in the cytoplasm and translocate it to the nucleus where the small GTPase Ran (predominantly in its GTP-bound form) dissociates the import complex. Oppositely, export receptors associate with their cargo in the nucleus, in the presence of Ran-GTP, forming a trimeric complex that is dissociated upon GTP hydrolysis in the cytoplasm. Crystallographic studies on importins have shed light on the mechanisms of nuclear import [1,2], but little is known on the mechanism of nuclear export. Two recent structures [3,4] have provided the first snapshots of the exportin Cse1 in its free and Ran/cargo bound forms.

The study we describe here was initiated before the first structure of an exportin was available. We first used X-ray small-angle scattering to reconstruct the envelope of the export complex Exportin-t/Ran/tRNA. We then carried out a full contrast variation experiment on the export complex reconstituted with deuterated Ran, and reconstructed the overall architecture of the ternary complex. The export factor has a compact shape similar to that of the Cse1 export complex. The tRNA appears as a density plugged in the center of the globular protein envelope, and the superhelical shape of the export complex can be clearly recognised. The position of Ran in this model is also consistent with that observed in other transporter/Ran structures. We are now trying to dissect the interactions taking place between the components of the export complex, using site-directed mutagenesis.

[1] G. Cingolani et al., Nature 399(6733), 221 (1999)
[2] Y. Chook and G. Blobel, Nature 399(6733), 230 (1999)
[3] Y. Matsuura and M. Stewart, Nature 432(7019), 872 (2004)
[4] A. Cook et al., Molecular Cell 18, 355 (2005)

10:55

NEUTRON CRYSTALLOGRAPHIC STUDY OF RECOMBINANT URATE OXIDASE ENZYME COMPLEXED WITH 8-AZAXANTHIN

M. Budayova-Spano[1,2], F. Bonneté[3], M. El Hajji[4], M.P Blakeley[1], F. Meilleur[2], B. Castro[4]
[1] EMBL Grenoble Outstation/[2] ILL, Grenoble, France., [3] CRMCN-CNRS, Campus de Luminy, Marseille, France, [4] Sanofi-Aventis, Montpellier, France.

Urate oxidase is an enzyme which catalyses the oxidation of uric acid to allantoin. It is produced as a protein drug to reduce toxic uric acid accumulation and to resolve the hyperuricemic disorders occurring during chemotherapy. A putative mechanism for the oxidation of uric acid has been proposed but the precise ionization state of the substrate during the reaction is not yet definitively established. A novel method and apparatus that can be used for the growth of large high-quality crystals, which are necessary to compensate for the weak flux of neutron sources, will be presented. Using a crystal (grown using the device) with volume 1.8mm^3 of hydrogenated urate oxidase in complex with its substrate analogue, 8-azaxanthin, neutron diffraction data were collected on the LADI instrument at the ILL to 2.1 Å resolution. Analysis of the neutron data clearly indicates the protonation states of active site residues and of 8-azaxanthin. The implications of these results in terms of the enzymatic mechanism of this therapeutically important enzyme will be discussed.

[1] M. Budayova-Spano, F. Bonneté, N. Ferté, M. El Hajji, F. Meilleur, M.P. Blakeley, B. Castro. (2006). Accepted for publication in Acta Cryst. F.

11:10

PROTEIN DYNAMICS MEASURED BY INCOHERENT ELASTIC NEUTRON SCATTERING

F. Gabel [1]
[1]Structural and Computational Biology Group, European Molecular Biology Laboratory, Heidelberg, Germany.

Incoherent elastic neutron scattering is widely used to measure atomic mean square displacements of biological macromolecules in powder and in solution [1]. The technique is particularly suited for weakly scattering systems. The influence of the instrumental energy resolution and the wave vector transfer (Q-range) on the time and length scales of observable motions are discussed. The possibility to focus selectively on protein intramolecular motions by elastic scans is outlined theoretically and illustrated by an experimental example, viz. hydrated human butyrylcholinesterase measured on IN16 [2, 3]. In the light of these results, implications on the choice of Q- and energy-ranges in various experimental situations are discussed.

[1] Gabel, F., Bicout, D., Lehnert, U., Tehei, M., Weik, M. and Zaccai, G. (2002). Protein dynamics studied by neutron scattering. Quart. Rev. Biophys. 35: 327-367.
[2] Gabel, F. (2005). Protein dynamics in solution and powder measured by incoherent elastic neutron scattering: the influence of Q-range and energy resolution. Eur. Biophys. J. 31(1), 1-12.
[3] Gabel, F., Weik, M., Doctor, B. P., Saxena, A., Fournier, D., Brochier, L., Renault, F., Masson, P., Silman, I. and Zaccai, G. (2004). The influence of solvent composition on global dynamics of human butyrylcholinesterase powders: a neutron-scattering study. Biophys J. 86(5), 3152-3165.

11:25

INTERNALIZATION OF THE TRANSLOCATION DOMAIN OF THE DIPHTERIA TOXIN IN MODEL PHOSPHOLIPID BILAYERS: A NEUTRON REFLECTOMETRY STUDY.

M. Ferrand[2], A. Chenal[1], V. Forge[2], G. Fragneto[3], M. Haertlein[3] & D. Gillet[4].

[1] Laboratoire de Biochimie des Interactions Macromoléculaires, Institut Pasteur, France, [2] Laboratoire de Biophysique Moléculaire et Cellulaire, Département de Réponse et Dynamique Cellulaires, CEA Grenoble, France, [3] Institut Laue Langevin, Grenoble, France, [4] Département d'Etudes et d'Ingénierie des Protéines, CEA Saclay, France.

The study of the membrane insertion process of the translocation domain (TD) of the diphtheria toxin can provide a precious insight into the interactions between proteins and membranes and the refolding mechanisms of membrane proteins. During intoxication of cells by the diphtheria toxin, and due to acidic conditions both present in the membrane vicinity and within the endosomes, the TD changes from a soluble state with a stable tertiary structure to a functional membrane-inserted state. In vivo penetration of the TD in the endosomial membranes has been approached by in situ neutron reflectometry experiments on model phospholipid bilayers. The internalization of the TD proceeds according to a two-step mechanism. At pH=6, the binding to model membranes involves the partial unfolding of the T-domain, with a penetration of some secondary structure elements at the interface between the outer polar lipid headgroup layer and the hydrophobic layer made of the lipidic tails. In more acidic conditions (pH=4), this protein sub-domain penetrates the core of the membranes whereas the rest of the TD fully reorganizes in the layer of the polar headgroups.

11:40

THE ILL-EMBL DEUTERATION LABORATORY – A PLATFORM FOR ISOTOPE-LABELLING OF BIOLOGICAL MACROMOLECULES

M. Haertlein[1], M.Moulin[1], V.Laux[1], M-T. Dauvergne[3], M.Weidenhaupt[3], M.Spano[1,3], I.Parrot[1,2], P.Callow[1,2], S.Teixeira[1,2], J.B.Artero[3], I.Hazemann[1], S.Miles [1,2] , R.Leal [2,4], V.T. Forsyth[1,2] and P.A. Timmins[1]

[1]Institut Laue Langevin, Grenoble, France, [2] Institute for Science and Technology in Medicine, Keele University, UK, [3] EMBL Grenoble Outstation, Grenoble, France, [4] ESRF, Grenoble, France

The ILL, in collaboration with the EMBL-Grenoble, has established a joint laboratory to support the deuteration of biological molecules for neutron scattering experiments. This initiative as part of the Partnership for Structural Biology Programme provides the tools and facilities required for the complete, partial or selective isotopic-labeling of complex bio-molecules such as proteins, nucleic acids, lipids and sugars. The laboratory has developed procedures for deuterium labeling in high cell density culture, primarily in E. coli and is testing the feasibility of alternative labeling strategies.

Access to the Deuteration facility is via a peer-review procedure, details of which can be found at http://www.ill.fr/deuteration. The facility's user program has to date provided a variety of deuterated samples for experiments in protein crystallography, fibre diffraction, small angle scattering and reflectometry. In October 2005 the platform was transferred to the Carl-Ivar Branden building (CIBB) where increased lab space including dedicated areas for fermentation, algae growth and for P2 work are available. Some examples of biological deuteration will be described.

11:55

PROTEINS IN THE BEAMLINE - A SIMULATION ANALYSIS

L. Meinhold [1]

[1]*Universitaet Heidelberg, IWR, Computational Molecular Biophysics, Germany*

Computer simulations are an important tool for understanding how the dynamics of a protein leads to function. Molecular dynamics (MD) simulations, in particular, have developed into an indispensable tool to bridge the gap between theory and experiment, as will be illustrated in this talk which focuses on the interpretation of X-ray and neutron scattering experiments using MD. In a first example, the X-ray diffuse scattering of a crystalline protein, which depends directly on the collective motions present, is analysed: individual scattering features are assigned to specific collective motions in the protein, and some of these explicitly involve potentially functional active site deformations. Then, in a second example, the effect of high hydrostatic pressure on the internal protein dynamics is investigated, revealing a qualitative change at ~4kbar. This change involves the existence of two linear regimes in the atomic mean-square displacement, reminiscent of the temperature-dependent dynamical transition, and a loss with increasing pressure of large-amplitude low-frequency collective motions. Inelastic neutron scattering is a particularly suited technique to experimentally study the dynamics below and above the pressure dynamical transition.

L Meinhold, and JC Smith. PRL 95:218103 (2005).
L Meinhold, and JC Smith. PRE 72:061908 (2005).

PARALLEL SESSION E. LARGE STRUCTURES

Friday 28 April, 10:30 - 12:45

10:40

STRUCTURE OF SILICA AGGREGATES IN A SOFT POLYMERIC MATRIX

J. Oberdisse [1]

[1]*Laboratoire des Colloïdes, Verres, et Nanomatériaux (LCVN), Université Montpellier II, France*

Some recent progress in the analysis of Small Angle Neutron Scattering intensities in the field of colloidal aggregation will be presented. Our experimental model system is made of small colloidal silica beads (radius < 10 nm) embedded by evaporation of the aqueous solvent in a soft polymeric matrix made from nanolatex beads. In the case of low pH of the precursor solutions, rather big silica aggregates are found, which demonstrates the need for high-flux/low-angle beamlines. The degree of aggregation was estimated using a simple model, using the inter aggregate structure factor, and then checked with a more elaborate combination of a Reverse Monte Carlo approach and a colloidal structure factor. The mechanical properties of the resulting nanocomposite films are found to be strongly dependent on the size of the silica aggregates.

10:55

REFLECTOMETRY – THE NEEDS FOR FIGARO

A. R. Rennie [1]

[1] *Department of Physics, Uppsala University, Sweden.*

Neutron reflection is a relatively young technique for investigation of interfaces between condensed phases or of a condensed phase with vapour. A wide range of applications for reflection experiments have developed across the fields that include thin-film physics, interface chemistry, biotechnology, environmental and medical sciences. These research fields are placing increased demands on instrumentation as the needs emerge to study smaller samples, determine changes in interfacial structure with time or simply to investigate specific types of surfaces. For example, liquid/vapour interfaces are studied widely as model two-dimensional systems having particular scientific interest. These surfaces are readily reproduced and provide excellent smooth materials. FIGARO, which is now under construction at the ILL, will provide a facility study for horizontal interfaces (for example, but not exclusively, liquid surfaces) for neutron reflection experiments that is optimised for the highest flux to permit a wide range of experiments. Examples of how recent work will be enhanced will be presented.

11:10

BLOCK COPOLYMERS

S. Förster[1], C. Schellbach[1], A. Timmann[1], P. Lindner[2]
[1] *Institute for Physical Chemistry, University of Hamburg, Germany,* [2] *Institut Laue-Langevin, Grenoble, France*

Block copolymers self-assemble into a variety of ordered structures on the nanometer to micrometer scale. Using external shear forces, these structures can be oriented into large ordered single crystalline domains. These domains can serve as templates for the preparation of highly ordered nanostructured surfaces and bulk materials.

We investigate the shear-induced orientation and ordering of spherical and cylindrical block copolymer micelles with small-angle neutron under shear (rheo-SANS). We find that cylindrical micelles show pronounced shear-thinning and development of high orientational order with increasing shear rates. The experiments allow to directly relate bulk properties like shear viscosity to molecular properties like orientational order.

Cubic phases of spherical micelles show a sudden shear-induced alignment into highly ordered structures leading to about 50 – 100 Bragg peaks. We show that most of these Bragg-peaks are quasi-forbidden and occur as a consequence of the low elastic moduli of soft materials. Highly ordered mesoporous single crystals derived from these phases are investigated by SAXS in a classical rotating crystal experiment (small-angle diffraction).

S. Förster, M. Konrad, P. Lindner, Phys. Rev. Lett. (2005), 94, 017803.

11:25

SURFACE-INDUCED ORDER IN THIN TRIBLOCK COPOLYMER FILMS

P. Müller-Buschbaum[1], E. Bauer[1], E. Maurer[1], R. Cubitt[2]
[1] *TU München, Physik-Department, Germany,* [2] *Institut Laue-Langevin, Grenoble, France*

Block copolymers self-assemble into well-controlled nanoscale structures ranging from spheres to cylinders to lamellae and to a more complex bicontinuous cubic phase. However, in contrast to A-B diblock copolymers, the mean-field phase diagram of A-B-A triblock copolymers is highly asymmetric as a result of the higher entropic penalty in deforming the central B blocks so as to accommodate the two outer blocks into the A domains. The phase diagram is dominated by the lamellar phase. The presence of external surfaces and the confinement effects in ultra-thin films may alter the morphology of materials. The effect of the free- surface is revisited with advanced scattering experiments making use of grazing incidence small angle neutron scattering (GISANS).

X-ray reflectivity, GISAXS, optical microscopy and AFM complement the investigation. The influence of two limiting interfaces present in confinement is compared to the presence of only one surface. GISANS allows for the detection of structures in the very limited sample volume of confined films as well as for a depth sensitivity to probe the near-free surface part of bulk films. With respect to the surface a perpendicular oriented lamella is observed. In contrast to the shrinkage of the characteristic lamellar spacing in confinement at the free surface a slight increase is determined.

11:40

LOOKING AT COLLOIDAL INTERFACES

T. Cosgrove [1]
[1]*School of Chemistry, University of Bristol UK*

The interface between colloidal particles and their environment is of paramount importance in describing their physical and chemical properties and one of major interests in our group is to discover the structure and dynamics of these inter-facial regions. In a series of papers [1, 2, 3] we have shown the level of detail that can be elicited from scattering and NMR about the structure of adsorbed polymer layers and some of these results will be highlighted. Examples of adsorbed polymer complexes with surfactants and proteins [4] and the invasion of high molecular weight polymers with nanoparticles will also be presented.

[1] Marshall, J. C.; Cosgrove, T.; Leermakers, F.; Obey, T. M.; Dreiss, C. A. Langmuir 2004, 20, 4480-4488.
[2] Hone, J. H. E.; Cosgrove, T.; Saphiannikova, M.; Obey, T. M.; Marshall, J. C.; Crowley, T. L. Langmuir 2002, 18, 855-864.
[3] Nelson, A.; Cosgrove, T. Langmuir 2005, 21, 9176-9182.
[4] Marshall, J. C.; Cosgrove, T.; Jack, K.; Howe, A. Langmuir 2002, 18, 9668-9675.

11:55

STRUCTURE OF DENDRIMERS IN SOLUTION

M. Ballauff[1], C. N. Likos
[1] *Physikalische Chemie I, Universität Bayreuth, Germany,* [2] *Institut für Theoretische Physik II, Heinrich-Heine-Universität Düsseldorf, Germany*

Dendrimers are well-defined organic molecules with a tree-like structure. The word “dendrimer” derives from the Greek word “dendron” for tree. The dendritic molecules can be dissolved in suitable solvents and represent objects with a diameter of a few nanometers only. Structural information on such partially or totally disordered systems can be obtained through small-angle neutron scattering (SANS). In our contribution we shall demonstrate that SANS in conjunction with molecular dynamics (MD) simulations can elucidate the spatial structure of dendrimers. The method developed here [1] are also suitable to analyze other supramolecular structures.

1. M. Ballauff, C. N. Likos, Angew. Chem. Intl. Ed. 2004, 43, 2998.

PARALLEL SESSION F. FLUCTUATIONS AND DYNAMICS

Friday 28 April, 10:30 - 12:45

10:40

EMERGENT SOLITON CHIRALITY IN A QUANTUM ANTIFERROMAGNET

H.B. Braun [1]

[1]*UCD School of Physics, Dublin*

Chiral matter is present in nature at every scale ranging from seashells through molecules to elementary particles. In magnetism, chirality maybe inherited from the asymmetry of the underlying crystal structure or it may emerge spontaneously. In particular, there has been a long-standing search for chiral spin states that emerge spontaneously with the disappearance of antiferromagnetic long-range order. We report here on experimental evidence for chirality associated with the quantum dynamics of solitons in antiferromagnetic spin chains [1]. The soliton chirality observed by polarized neutron scattering is in agreement with theoretical predictions and is a manifestation of Berry's phase. Our observations provide the first example of the emergence of spin currents and hidden chiral order that accompany the disappearance of antiferromagnetic order, a scheme believed to lie at the heart of the enigmatic normal state of cuprate superconductors.

[1] H.B. Braun, J. Kulda, B. Roessli, D. Visser, K.W. Kramer, H.U. Gudel, P. Boni, Nature Physics 1(3), 159 (2005).

10:55

MAGNETIC FLUCTUATIONS IN Sr_2RuO_4 STUDIED BY POLARIZED NEUTRON SCATTERING

M. Braden[1], P.Steffens[1], Y.Sidis[2], J.Kulda[3], P. Bourges[2], S.Hayden[4], N.Kikugawa[5] and Y.Maeno[5]

[1] *II. Physikalisches Institut, Universität zu Köln,, Germany,* [2]*LLB, CE-Saclay, France,* [3]*ILL, Grenoble, France,* [4]*H.H. Wills Physics Laboratory, University of Bristol, UK,* [5]*Kyoto University, Japan*

Magnetic excitations in superconducting Sr_2RuO_4 are dominated by incommensurate fluctuations arising from Fermi-surface nesting. The incommensurate nature of this magnetic instability, however, is difficult to reconcile with the p-wave symmetry of the superconducting phase. By polarized neutron scattering significant progress was recently achieved. The nesting fluctuations exhibit a sizeable anisotropy, but much smaller than that proposed or assumed in several theoretical models. In addition to the nesting fluctuations we find a very broad magnetic contribution around the Brillouin-zone centre. Combining these polarized neutron scattering data with NMR and susceptibility results we obtain a quantitative description of the full magnetic excitation spectrum, which may serve as a base to understand the superconducting pairing within magnetic models.

11:10

STRUCTURE AND DYNAMICS OF CARBON NANOSTRUCTURES: HOW CAN NEUTRONS HELP?

S. Rols[1], J. Cambedouzou[1], R. Almairac[1], J.-L. Sauvajol[1], H. Schober[2] and M. Johnson[2]
[1] *L. C. V. N, University of Montpellier, Montpellier, France* [2] *Institut Laue Langevin, Grenoble,*

In this communication, some results about the structure and dynamics of some new carbon nanostructures will be presented. First I will discuss the structure of alkali-doped (Li and K species) single-walled nanotubes (SWNT) based on neutron diffraction experiments where advantage of the isotopic substitution was taken. Then I will present a combined numerical and experimental investigation about the adsorption of Ar inside nanotubes bundles. Finally, I will present new results obtained on C_{60} encapsulated into SWNT. The structure and the vibrations of this "peapod like" molecular system will be discussed based on neutron/X-ray diffraction, neutron inelastic scattering measurements and molecular modelisations.

11:25

NEUTRON STUDIES IN LIQUID METALS

L.E. Bove [1]
[1] *Département de Physique des Milieux Denses, CNRS-IMPMC, Université Pierre et Marie Curie, Paris VI*

The interest of the study of the density fluctuations in liquid metals at the mesoscopic scale is twofold. On the one hand, the high frequency dynamics of these simple systems is similar to that of a wide class of more complex systems, from glasses to undercooled liquids. Understanding its connection with the local structure can thus shed light on the decay of the density fluctuations in a topological disordered system. This mesoscopic range, corresponding to a few interparticle distances (nm^{-1} wavevector range) and to THz frequencies, is now accessible with high-resolution small-angle Inelastic Neutron Scattering (INS) experiments. On the other hand, the understanding of the ultimate microscopic mechanisms responsible for the propagation of the collective ionic excitations is still a challenge in such systems where the dynamic behavior cannot be disentangled from the effects of the interacting electron gas.

A review of recent high-resolution INS studies of a wide class of systems (ranging from simple metals, alkaline-metal alloys, polyvalent metals, $Li(ND_3)_4$ solutions) with an appropriate choice of samples in order to enhance the role of either the electron-density or that of the ionic-core, is presented. These studies have shown that the velocity of the collective modes, always in excess of that of sound, can be related to the screening of the ionic potential due to the electron gas. In light alkali and low density polyvalent metals, the observed anomalous dispersion can be reproduced by the simple Bohm-Staver model from the ion plasma, while in more complex systems such as $Li(ND_3)_4$ and high density metals an approximation beyond Random Phase is needed in order to take into account the ion-core contributions. This interpretation of the dynamics of liquid metals emphasizes the electron-related features in the ion dynamics and suggests that the role of the long-range potential against the repulsive ion contribution is predominant.

New results on disparate-mass binary alloys, liquid metals under pressure, and undercooled liquid metals inspiring new trends in the field of neutron studies of liquid metals will also be discussed.

11:40

A MICROSCOPIC VIEW ON MASS TRANSPORT IN SILICATE MELTS

A. Meyer [1]
[1]*Physik Department E13, Technische Universität München, Germany*

We use inelastic neutron scattering to study the mechanisms of mass transport in silicates melts at temperatures up to 1600 K. Binary alkali silicates exhibit alkali diffusion channels that become visible through emerging prepeaks in the elastic structure factors on intermediate length scales as well as through a characteristic q dependence of amplitude and time scale of the quasielastic signal. The non-homogeneous distribution of the alkali ions in the disrupted tetrahedral Si-O network strongly influences the structural relaxation, i.e. the viscosity, of the network. By replacing Na_2O by Al_2O_3 the channel structure gets disrupted causing a decrease in the sodium mobility and a drastic increase in the viscosity. Neutron scattering on water-bearing silicate glasses reveals, that although dissolved water has a drastic impact on the melt viscosity, the structure is barely affected by the presence of OH groups. Vibrational spectra, that are dominated by the scattering of the hydrogen atoms, strongly depend on the anhydrous silicate composition, whereas the vibrational densities of states do not exhibit systematic changes in the concentration range of the dissolved water between 1 to 5 wt%. A neutron time-of-flight experiment on water-bearing silicate melts at high pressures is under preparation.

11:55

EXPLORING NOVEL QUANTUM MAGNETS - THE ADVENT OF IN8C AND PROSPECTS FOR MULTIPLEXING

H. M. Rønnow [1]
[1]*Laboratory for Neutron Scattering, Paul Scherrer Institute and ETH-Zurich, Switzerland*

The exploration of novel quantum magnets is a significant challenge for inelastic neutron scattering: intensity from spin 1/2 is weak; the excitation spectra are distributed over large ranges of (q,w) space; and novel materials are often only available as small crystals. Presenting several recent experiments on IN8c we demonstrate a new range of possibilities on the frontier of quantum magnetism. In particular we report on the results and prospects of multiplexing triple-axis techniques for mapping (q,w) space in small samples.

PARALLEL SESSION G. NEUTRON METHODS
Friday 28 April, 10:30 - 12:45

10:40

THE LIFE EXPECTATION OF NEUTRON GUIDES *OR* DO NEUTRON GUIDES LIVE FOREVER?

J. Beaucour, D Bazzoli, L Didier, R Gaehler, M Kreuz, C Mounier, A Perillo Marcone, P Thomas
Institut Laue- Langevin, Grenoble, France

Neutron guides are usually considered as fairly robust. 30 (or even more) years old neutron guides are still working reliably and with good transmission in various neutron facilities. In some cases, however, transmission degrades rapidly and evacuated guides may even cause safety issues.

We review recent observations of guide degradation and discuss possible failure modes. Based on this, simulations are presented with the aim to predict lifetimes of neutron guides made of Borofloat and Borkron glass. Conclusions for the future neutron guide system at ILL will be given as well.

10:55

NEW AREAS AND LIMITS OF SAMPLE ENVIRONMENT: MAGNETIC FIELD AND TEMPERATURE

M. Meißner [1]
[1]*BENSC, Hahn-Meitner Institut Berlin, Germany*

Superconducting split-pair cryomagnets have widely been used in neutron scattering experiments. Designs with horizontal or vertical magnetic field aligned parallel or perpendicular to the beam have allowed to study samples of dia.~15 mm with field strength between 4 T and 17 T. Due to limits in superconducting technology, at present, 15 T to 18 T in a vertical split-pair and 20 T to 22 T in a solenoid magnet can not be exceeded. New horizons came up with the serial hybrid magnet technique where an inner resistive coil field is boosted by an outer superconducting solenoid, running in series at ~20kA current. In the new Neutron Guide Hall at BENSC the Extreme Sample Environment Diffractometer (EXED) will consist of such a horizontal high-field magnet with tapered bores on both ends. Facing high magnetic field gradients inside and outside the magnet warm bore, new wide-range temperature devices have to be designed.

Present thinking is that liquid-helium-free, gas-cooling devices (like CCR and PTR) might be an appropriate technology, providing moderate cooling power and easy temperature control. Extending the limiting temperature of a CCR below ~3 K, at BENSC we developed a Joule-Thomson (J/T) helium gas expansion stage which operates as a 3rd stage attached to the 2nd stage of the CCR. By external injection of pressurized helium gas into the J/T-unit and subsequently pumping the vapour-liquid we achieved base temperatures of 1.3 K and 0.6 K with ^{4}He and ^{3}He, respectively. As sample changes are frequent in neutron and x-ray scattering experiments, the cooling time from 300 K and variable positioning are important issues, the J/T-unit and heat exchangers have therefore been designed to a small size. Due to these construction details our present design can be operated in a HUBER 6-circle-cradle – and may work in the horizontal warm bore (dia.~40 mm) of a 30 T magnet.

11:10

MILAND (MILLIMETER LARGE AREA NEUTRON DETECTOR) - DEVELOPMENTS AND STATUS

F. Fraga [1]
[1]*LIP Coimbra, Departamento di Fisica, Portugal*

The European MILAND project, a partnership of seven laboratories aiming to develop a high-performance detector designed for neutron diffraction instruments is a JRA of NMI3 - Integrated Infrastructure Initiative for Neutron Scattering and Muon Spectroscopy, sponsored by the EU 6th Framework Programme (FP6).

The aim of MILAND is the development of a gas detector that will improve the spatial resolution by a factor of 2, when compared with current detectors of equivalent size, and having a global counting rate capability increased by a factor of 5, keeping all the other relevant parameters (gamma discrimination, counting stability and uniformity, efficiency) at the same performance level.

Several approaches were considered for this project (MWPC, MSGC and GSPC), we will report on their results, the collaboration choice for the final detector and the current status of the detector building.

11:25

BEYOND 15 TESLA

M. Enderle [1]
[1]*Institut Laue-Langevin, Grenoble, France*

Neutron scattering is unique in its sensitivity to structure and dynamics of magnetic phenomena at a microscopic level. Combining this with the ability to modify the ground state of a system in a continuous and homogeneous way by controlling the magnitude of an applied magnetic field makes it possible to reveal the nature of a system's Hamiltonian in a clear and unambiguous way.

Magnetic field is an important thermodynamic parameter. The application of a magnetic field can control quantum criticality and destroy or induce superconductivity. It produces new exotic phases, such as field-induced Bose-Einstein condensation or Luttinger liquid phases in quantum magnets. Although such transformations may be revealed by macroscopic or local probes, only neutron scattering is capable to determine precise magnetic structures, to study directly the energy and momentum dependence of magnetic excitations even in the absence of long-range order, as well as to reveal the surface and interface roughness of heterostructures.

The energy scale of typical magnetic interactions and anisotropies lies beyond 15 Tesla. A world of exciting phenomena becomes accessible for neutron scattering, if this field strength is doubled. Such a perspective is opened by recent breakthroughs in conceptual magnet designs. The talk aims to demonstrate the unique scientific potential of combining magnetic fields beyond 15 Tesla with high-flux neutron scattering instrumentation for elastic and inelastic work.

11:40

UPDATE ON POLARISED ^{3}He

E. Lelièvre-Berna [1]
[1]*Institut Laue-Langevin, Grenoble, France*

Neutron spin filters are being actively developed by several neutron facilities within the framework of a Joint Research Activity funded by the European Commission. Both the spin-exchange (SEOP) and metastability-exchange (MEOP) optical pumping techniques are concerned. As of today, they reach similar effective ^{3}He polarizations while the MEOP technique remains faster and more reliable. We explain why both techniques are complementary and will certainly be necessary at neutron facilities. We also present new widgets that minimize the depolarization of the gas during the storage, transport and spin-flip of ^{3}He cells.

11:55

THE EUROPEAN SCENE OF HIGH-QUALITY NEUTRON IMAGING FACILITIES

B. Schillinger [1]
[1]*Forschungsreaktor FRM-II, TU Muenchen, Germany*

With the advent of electronic imaging detectors, Neutron Imaging has seen a major revival in Europe during the past decade. Neutron Computed Tomography has been developed as a routine industrial inspection tool at NEUTRA and ICON (PSI), at ANTARES (FRM-II), NEUTROGRAPH (ILL) and CONRAD (HMI). With the advance of detector technology, high-speed imaging has become feasible at the stronger beamlines. Stroboscopic imaging of repetitive motion has been jointly developed by the aforementioned institutes, and the most recently developed detectors allow for continuous imaging with several thousand frames per second.

NEUTROGRAPH is unique among the European neutron imaging facilities, offering the highest flux worldwide on a large beam cross section. The second strongest facility ANTARES offers a flux 30 times lower than NEUTROGRAPH. (CONRAD uses a neutron guide with a very strong but small-area beam.). NEUTROGRAPH is therefore the best facility to pursue continuous high-speed imaging with time resolution in the order of ten microseconds and high-speed tomography with total data collection time in the order of one second. Furthermore, the intense beam serves in detecting small contrast variations with very good counting statistics. These properties make the investigation of e.g. boiling processes in 2D and the diffusion of liquids in 3D possible. Furthermore, the intense beam serves in detecting small contrast variations with very good counting statistics, which is very useful for the examination of metal welds and bonds or samples from the geosciences.

The properties of NEUTROGRAPH are due to its position at the beamline H9 behind the LOHENGRIN experiment for fission products. Neutrograph has replaced the beam dump of Lohengrin, which makes use of only 3% of the available neutron flux. The geometrical setup of Lohengrin has a strong influence on the beam formation of Neutrograph. Due to the inserts of Lohengrin, the beam cannot be collimated with small circular diaphragms, as is common in other radiography facilities, where even higher spatial resolution can be achieved. Therefore it was an ideal solution to optimize for the high flux, which fits very well into the concept of European facilities complementing each other. Examples of fast imaging will be given both from NEUTROGRAPH and ANTARES, at the latter limited by the lower flux, but illustrating the potential at NEUTROGRAPH.

Friday 28 April, 14:00 - 16:00

14:00

ENABLING THE MILLENNIUM PROGRAMME: ADVANCES IN INSTRUMENTATION

K.H. Andersen [1]

[1] *Institut Laue-Langevin, Grenoble, France*

As an introduction to the poster session, advances in some of the key components in neutron scattering instrumentation are presented. These come from areas in which the ILL has a world-leading technological edge: detectors, polarization devices and monochromators. Highlights from the poster session are introduced, making the link to the instrumentation technologies, which have enabled them.

PLENARY SESSION – SCIENTIFIC ADVANCES 2

Friday April 28, 16:30 - 18:00

16:30

MAGNETIC CORRELATIONS IN METALLIC Na_XCoO_2

A.T. Boothroyd[1], L.M. Helme[1], D. Prabhakaran[1], R. Coldea[2], D.A. Tennant[3], A. Hiess[4], J. Kulda[4], A. Stunault[4], G.J. McIntyre[4], N. Kernavanois[4], C.D. Frost[5]

[1] Department of Physics, Oxford University, U.K., [2] H.H. Wills Physics Laboratory, University of Bristol, U.K., [3] Hahn-Meitner Institut, Berlin, Germany, [4] Insitut Laue-Langevin, Grenoble, France, [5] ISIS Facility, Rutherford Appleton Laborator, U.K.

The recent discovery of superconductivity in water-intercalated Na_xCoO_2 has been greeted with great excitement and has raised speculation about a new unconventional mechanism of superconductivity. What is interesting is that both the magnetic transition-metal (cobalt) and the geometry of the layers (triangular) are different from other known transition-metal oxide superconductors. I will report neutron scattering measurements of the magnetic fluctuations in Na_xCoO_2 (x = 0.75), which is a precursor to the superconducting phase and which exhibits magnetic order below 22 K. The data reveal ferromagnetic correlations within the triangular layers, and show that the spin correlations are three-dimensional despite the layered structure of the material. I will discuss some of the implications for the superconducting phase of hydrated Na_xCoO_2, and point out a number of remaining puzzles.

[References for this work: A.T. Boothroyd et al., Phys. Rev. Lett. 92 (2004) 197201, L.M. Helme et al., Phys. Rev. Lett. 94 (2005) 157206; L.M. Helme et al., Phys. Rev B 73 (2006) 054405.]

17:00

NUCLEAR PHYSICS AT ILL

J. L. Durell [1]

[1]School of Physics and Astronomy, The University of Manchester, UK

An overview will be presented of current research in Nuclear Physics at ILL. The activity at ILL contains two unique strands:

* precision spectroscopy to test nuclear models, and to investigate the role of underlying symmetries in nuclei;
* the study of neutron-rich nuclei produced as fission fragments.

Examples of current research will be presented. The importance of future plans involving new instrumentation and a new external beam line in strengthening further nuclear physics research will be illustrated.

17:30

TIME-RESOLVED POWDER DIFFRACTION EXPERIMENTS

W.F. Kuhs [1]

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Time-resolved neutron powder diffraction is a powerful tool to study transformation processes in a variety of materials of importance in material science, physical chemistry and geoscience. The choice of neutrons rather than X-rays for such time-resolved studies is due to their specific advantages like e.g. the sensitivity to light elements, the detection of volume rather than surface phenomena or the low absorption in case of bulky sample environments. In recent years it has become increasingly evident that neutron diffraction often forms an essential complement of in-house kinetic work in providing a quantitative time-space averaged picture of the processes studied.

Besides ongoing developments at the upcoming spallation neutron sources, constant wavelength diffraction at steady-state sources needs to be pushed further, the park of instruments available at ILL and other institutes, sometimes historically grown over three decades, needs major upgrading to overcome remaining limits in reciprocal space coverage, resolution and intensity. The existing instruments should be upgraded with large two dimensional detector arrays, additional types of monochromator such as bent crystal monochromators, advanced neutron optics components such as radial or honeycomb collimators, focussing guides and ^{3}He polarization, and the possibility of changing the take-off angle continuously. One should consider an optimised position of the existing instruments (closer to the source for intensity, end-of-guide position for flexibility in take-off angles). New instruments, such as DRACULA at ILL (focussed on very high intensity and very small samples) need to be constructed in order to let each instrument concentrate more on a smaller range of configurations thus becoming more efficient. Constant-wavelength diffraction does not stand in direct competition to time-of-flight techniques, both techniques are complementary, and one particular advantage for time-resolved work of reactor-based diffraction is the reliability of source. Yet, to profit fully from the advantages of neutron scattering one has not only to improve the performance of the instruments. Equally important is also the sample environment. Some devices are available at neutron scattering centres, others need to be built or adapted by the user. Support for these adaptations is essential for the success of experiments.

PLENARY SESSION – SCIENTIFIC ADVANCES 3

Saturday April 29, 08:30 - 10:30

08:30

COLLECTIVE DYNAMICS OF MULTILAMELLAR LIPID MEMBRANES: INELASTIC NEUTRON AND X-RAY SCATTERING

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Membranes are the most important biological interface, and are subject to a range of functionally important dynamic modes. As model systems for biological membranes, we investigate the structure and the collective dynamics of planar lipid membranes on the molecular and the mesoscopic length scale. For the experiments, we deposit highly oriented multilamellar stacks on a solid support. Multi-component lipid mixtures and lipid membranes with membrane active molecules such as stereols, peptides, and membrane proteins can be prepared with controlled concentration. In the past, our main emphasis was on the molecular structure, elasticity properties and interaction potentials. More recently, collective dynamics such as bending fluctuations, compressional modes, or density waves in the plane of the bilayer, have been addressed to achieve a more complete understanding of these soft and highly dynamic state biomolecular systems.

Here we report on X-ray and neutron studies on the collective dynamics of multilamellar membranes. On the molecular scale, density fluctuations and oscillatory motion of the acyl chains were probed by three-axis spectrometry. On the mesoscopic scale, we have investigated the dynamics associated with bending and compressional elasticity of the lipid bilayers. We compare the approach of inelastic neutron scattering (spin echo, three-axis spectrometry [1], backscattering [2]) to results of diffuse X-ray scattering [3], coherent x-ray scattering, and in particular also to first XPCS experiments on these systems. The undulation modes of solid-supported lipid membranes could only be assessed by spin echo measurements. Note that typical bending rigidities of lipid membranes are an order of magnitude higher than the surfactant systems, and the resulting time scales are to short for XPCS [5]. Finally, we give an outlook on where inelastic neutron scattering can contribute to membrane biophysics in the future.

References

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09:00

PARTICLE PHYSICS WITH ULTRA-COLD NEUTRONS

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Ultra-cold neutrons are a unique tool to address important questions about the basis of our existence. How were the chemical elements formed in the big bang? Why there seems to be so much matter and virtually no antimatter in the Universe? Do we really well understand the fundamental interactions governing our world or did we not miss some tiny effects with strong impact on our view of life? Answering these questions in most cases requires to gain "the next order of magnitude" in accuracy of particular observables measured in a handful of key experiments. Progress will be due to new experimental strategies and new sources of ultra-cold neutrons being prepared in several laboratories around the world.

09:30

SOLVING SIGNAL TRANSDUCTION IN BIOLOGY: A QUANTITATIVE MODEL FOR AN ARCHAEAL SIGNAL

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Archaea, the third kingdom of life, offer some attractive modules for a systems biology approach. One example is halobacterial phototaxis in which the input of photons of different quality and intensity is integrated via a two-component system and results is an output at the flagellar motor of the cell as a modulated response time for a stop. The archaeal flagellar motor although not known for its molecular components, which could not even be unrevealed by genomic analysis, nevertheless can be very exactly described in its unstimulated and stimulated behaviour. Coupled as a module to two photoreceptors mediating three light responses of the cell a first quantitative model of signal transduction could be established, which covers all aspects of phototaxis in these archaeal cells and explains the experimental results of the past 20 years. The model further unifies and includes also very different models proposed over the years from various labs, none of which cover all experimental results. An introduction into the system and a detailed description of the model of the signal transduction cascade will be presented.

10:00

SPIN DYNAMICS IN THE HIGH-T_C CUPRATES

Ph. Bourges[1], B. Fauqué[1], Y. Sidis[1], S. Pailhès[1], B. Keimer[2], V. Hinkov[2], C. Ulrich[2], L. Capogna[2], L.P. Regnault[3] , A.S. Ivanov[4]

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The spin dynamics of high-T_c superconductors measured by inelastic neutron scattering will be reviewed. Over the years, these measurements have evidenced a magnetic resonance peak in various cuprates with crystal structures comprised of CuO_2 monolayer units ($Tl_2Ba_2CuO_{6+\delta}$) and bilayer units ($YBa_2Cu_3O_7$ (YBCO) and $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi2212)). This novel excitation must hence be considered as a generic excitation of the superconducting state at least of those cuprates with a high maximum T_c. Detailed momentum dependencies reveal a downward and an upward dispersion of the resonant excitation from the antiferromagnetic wave-vector, yielding incommensurate-like excitations at a fixed energy transfer. Measurements in detwinned YBCO samples show that the characteristic geometry of these incommensurate excitations is basically two-dimensional. These findings point towards Fermi-liquid-based theoretical scenarios rather than rigid one-dimensional stripe arrays.

Further, we also reported a second distinct magnetic resonant mode (with an even symmetry with respect to exchange between adjacent copper oxide layers). From the relative spectral weight of both resonant modes, one can infer the manifestation of the Stoner electronic continuum of d-wave superconductors. The presentation will focus on recent advances essentially obtained on the ILL triple-axis spectrometer IN8 (See e.g. S. Pailhès et al, cond-mat/0512634).

FINAL PLENARY SESSION

Saturday April 29, 11:00 - 12:30

11:00

PARTNERSHIPS ON THE ILL SITE

P.A. Timmins[1]

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For some years the ILL has promoted a policy of "not only neutrons". In this way the added value of using other techniques in parallel with neutron scattering has been recognized. An ideal way in which to implement this policy is through the creation of partnerships with other institutions who are expert in these complementary techniques. Established examples of this are FAME38, the Facility for Materials Engineering and the PSB, the Partnership for Structural Biology. In this talk I will describe the setting up and operation of these partnerships, in particular the PSB, and discuss how far they may be used as models for the establishment of new initiatives such as the putative Partnership for Soft Matter… and beyond.

Poster Abstracts

POSTER SESSION

Friday April 28, 14:15 - 16:00

PA1

THE PROTON SPECTRUM IN FREE NEUTRON DECAY: FIRST RESULTS WITH THE aSPECT SPECTROMETER

S. Baeßler[1], F. Ayala Guardia[1], M. Borg[1], K. Eberhardt[2], F. Glück[1], W. Heil[1], I. Konorov[2], G. Konrad[1], N. Luquero Llopis[1], R. Muñoz Horta[1], G. Petzoldt[3], D. Rich[4], M. Simson[3], Y. Sobolev[1], H.F. Wirth[3], O. Zimmer[3]

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The purpose of our project is a precision measurement of the proton spectrum in free neutron decay. Its shape depends on the angular correlation between the momenta of the antineutrino and electron for kinematic reasons. The angular correlation coefficient a is quite generally given by

$$dw \alpha (1 + a\beta \cos \theta_{e\upsilon})$$

where dw is the decay probability, β the electron velocity in units of the velocity of light, and $\theta_{e\upsilon}$ the angle between electron and antineutrino. Nowadays, an improved measurement of the coefficient a is of great interest in order to test the Unitarity of the CKM matrix. A non-unitarity CKM matrix would signal new physics beyond the Standard Model of Particle Physics.

The design of the spectrometer aSPECT [1] is based on Magnetic Adiabatic Collimation followed by an Electrostatic Filter (MAC-E-Filter). With this system, one measures the integrated energy spectrum of the protons, simply by counting the protons that reach the detector as a function of the Electrostatic Filter potential. First measurements with the aSPECT spectrometer have been performed during the last few months at the new beamline MEPHISTO at the FRM-II in Garching, Germany. A description of the system as well as results of the test beamtime will be given.

[1] F. Glück, S. Baeßler, J. Byrne et al., Europhys. Journ. A 23, 135 (2005)

PA2
ROTATION OF NUCLEI IN FISSION INDUCED BY COLD POLARIZED NEUTRONS

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[1] *Univ. Tübingen,* [2] *PNPI Gatchina,* [3]*TU Darmstadt ,* [4] *ILL*

Experiments on ternary fission conducted in the summer of 2005 at the beam position PF1B of the ILL have revealed unexpected phenomena. The interpretation of the asymmetries in the angular distributions of ternary particles for fission of ^{235}U induced by polarized neutrons have unequivocally led to the conclusion that the particles were ejected from a rotating mother nucleus. A collective rotation of the nucleus at scission is from the point of view of theory not surprising but has never been observed in experiment. The experimental findings have been corroborated by trajectory calculations of the 3-body decay. Since, owing to the strong Coulomb repulsive forces, the reaction partners are flying apart after scission, the moment of inertia of the system increases and for given angular momentum the rotation comes very fast to a stop. The time scale of the rotation is only a few 10^{-21} s and the integrated angle of rotation is well below 1°. The sense of the rotation depends on the polarization of the neutrons and allows to deduce the capture spin of the compound nucleus ^{236}U leading to fission. Ternary fission has thus become a startling method to determine capture spins for fissile nuclei. The new effect is proposed to be called the ROT effect. It has to be distinguished from other P-even, P-odd and T-odd asymmetries of particle emission in binary and ternary fission having been studied in the past. It will be a challenge for future work to disentangle these latter effects and the ROT effect in the evaluation of fission experiments with polarized neutrons.

PA3
SPIN-PATH ENTANGLEMENT IN NEUTRON INTERFEROMETER EXPERIMENTS

Y. Hasegawa[1], G. Badurek[1], M. Baron[1], S. Filipp[1,2], J. Klepp[1], R. Loidl[1], H. Rauch[1]
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Non-local correlations between subsystems sufficiently separated in space-time have been extensively discussed in the light of the Einstein, Podolsky, and Rosen (EPR) paradox, together with the Bell's inequality. Within quantum terminology, such a non-locality can be interpreted as a consequence of the entanglement of subsystems as well as commuting observables due to the different position. Thus, a more general concept, i.e., contextuality, compared to non-locality can be introduced to describe other striking phenomena predicted by quantum theory. As an example of quantum contextuality, we report a neutron interferometer experiment, which clearly demonstrates the violation of a Bell-like inequality. Entanglement is achieved not between particles, but between the degrees of freedom i.e., spin and path, in this case, for a single-particle. Appropriate combinations of the direction of spin analysis and the position of the phase shifter allow an experimental verification of the violation of a Bell-like inequality. Our experiments exhibit the fact that manipulation of the wavefunction in one Hilbert space influences the result of the measurement in the other Hilbert space: manipulation without touch! In addition, experimental results of so-called state tomography, tomographic analysis of the density matrix of a quantum system, are presented to characterize neutrons' entangled states. These experiments manifest high fidelities, up to 91%, of the entangled neutrons' states. We are planning to utilize these highly entangled neutrons' states for investigations of non-unitary dissipative evolutions of a quantum system, i.e. neutron's decoherence, depolarization, etc., in near future.

PA4
CONFINEMENT-INDUCED NEUTRON PHASE

H. Lemmel[1], R. Loidl[2,] H. Rauch[1]
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When neutrons pass through narrow channels a quantization of the transverse momentum occurs which also changes the longitudinal momentum because of energy conservation [1,2]. In neutron interferometry this effect results in a phase shift. It is a purely quantum mechanical phenomenon as it arises most distinctively for neutrons which classically do not touch the walls. First measurements at the S18 instrument at the ILL have given promising results [3]. Additional effects due to the wavefield interaction between the slit system and the interferometer crystal are subject of recent investigations.

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[2] D. M. Greenberger, A new non-local effect in quantum mechanics. Physica B 151, 374-377 (1988);
[3] H. Rauch, H. Lemmel, Measurement of a confinement induced neutron phase. Nature 417, 630-632 (2002)

PA5
INTERFEROMETER AND USANS INSTRUMENT S18

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[1]*Atominstitut der Österreichischen Universitäten,Wien, Austria;* [2]*Institut Laue-Langevin, Grenoble, France*

The S18 neutron interferometer and ultra small-angle scattering instrument is worldwide the most powerful instrument in this field. Many fundamental quantum experiments have been performed with this instrument, which contributed to the advent of matter-wave quantum optics. Recently, entanglement induced quantum phenomena has been verified and quantum tomographical measurements to determine the state of the neutron ensembles have been carried out. Phase-contrast tomography, which is particularly sensitive to phase shifts instead of beam-attenuation (radiography), was realized. A confinement-induced phase due to the transverse quantization of the neutron momentum in narrow slits has been investigated. Dynamical and topological phases of matter-waves became measurable. In an alternative mode the instrument can be used as an ultra-small-angle scattering camera for the momentum transfer range 10^{-5} Å^{-1} ≤ Q ≤ 10^{-3} Å^{-1}. Under optimal conditions a peak-to-background ratios of 2×10^5 has been achieved. Recent experiments dealt with sediments, hydration of concrete and magnetic materials. Both options - interferometry and USANS - can be adapted for the use of polarized neutrons and a third axis can be installed for postselection experiments. Up to ten differently shaped interferometer crystals and two sets of multi-channel USANS crystals are available to fulfil the requirements of different experiments.

PB1
KEY NOTES FROM VIVALDI

G.J. McIntyre[1], M.-H. Lemée-Cailleau[1], C. Wilkinson[2]
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Neutron Laue diffraction with image-plate detection on a thermal beam is now a high-performance technique especially well suited to small crystals, rapid chemical crystallography, reciprocal-space surveys and studies of structural and magnetic phase transitions. The first years of operation of ILL, VIVALDI (**V**ery-**I**ntense **V**ertical-**A**xis **L**aue **Di**ffractometer) [1] have been a resounding success, producing spectacular diffraction patterns and exciting new science at a furious pace, with gains in data collection rate over conventional diffractometers of up to 100 fold.

In just a few hours VIVALDI has yielded detailed atomic structural information on large organic molecules [2], shown 2-D magnetic ordering in astounding clarity [3], revealed new magnetic structures [4], allowed full data collection from small crystals inside anvil pressure cells [5], and followed variations of bond lengths with temperature in fine detail [6].

We describe the unique technical aspects of VIVALDI, and through review of the experiments and scientific highlights of the first years of operation, we draw some general conclusions as to the applicability of the Laue technique. The Laue experiment is becoming as easy as a powder diffraction experiment, and often just as fast, with the additional qualities of single-crystal diffraction.

[1] C. Wilkinson et al, Neutron News **13** (2002) 37-41; M.-H. Lemée-Cailleau et al. J. Phys. IV France **131** (2005) 335-341.
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PB2
STRUCTURE AND DYNAMICS OF VITREOUS B_2O_3 AND ALKALI BORATES: NEUTRON SCATTERING AND MD SIMULATIONS

C. Mondelli[1], M. A. Gonzalez[2], M. Johnson[3]
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The structure of vitreous boron trioxide (v-B_2O_3) has been extensively studied and nowadays it is generally accepted that the molecular building block of v-B_2O_3 is the planar BO_3 group. However, the manner in which those triangles are connected remains a matter of controversy and there are contradictory results about the presence in the structure of the glass of a large fraction of planar boroxol rings. Likewise the structural changes brought forward by the addition of network modifiers are not well understood. In an effort to better understand such questions we have started a systematic research of the structure and dynamics of a series of alkali borates combining neutron scattering and

DFT and classical molecular dynamics simulations. By varying the alkaline modifier cation from Li^+ to Cs^+ it is expected that voids of different increasing size are created, bringing forward also very different dynamic properties. We have studied the structure and dynamics of a series of borates with different alkali concentrations by means of the neutron powder diffractometer D1B and the time-of-flight spectrometer IN4, both at the ILL (Grenoble, France). We have also performed numerical simulations (using both DFT and classical MD simulations) in order to interpret the experimental results and obtain a more complete view of the microscopic structure of pure boron oxide and its alkali borates.

PB3
THE TEMPERATURE DEPENDENT STRUCTURAL PHASE TRANSITION IN MULTINARY CHALCOPYRITY TYPE SEMICONDUCTOR ALLOYS: A STUDY USING NEUTRONS AND SYNCHROTRON X-RAYS

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Solid solution series of I-III-VI_2 ternary chalcopyrites with their isoelectronic analogs of II-VI binaries allow a systematic variation of structural and physical properties with composition. The multinary semiconductor alloys 2(ZnX) – $CuInX_2$ (X=S, Se, Te) show a non-linear variation of the optical band gap with composition and thus give the possibility to create tailor-made photovoltaic materials.

Comparable to the ternary end member $CuInX_2$ structural phase transition from the tetragonal chalcopyrite structure to the cubic sphalerite structure occur in dependence of temperature in $(ZnX)_{2x}(CuInX_2)_{1-x}$ alloys with chalcopyrite structure ($x<0.1$) too. This transition in $CuInX_2$ was studied by *in-situ* high temperature synchrotron X-ray diffraction. The cation site occupancies, determined by Rietveld analysis of the data, revealed the Cu-In anti site occupancy as driving force of the structural phase transition.

The distribution of the cation *Zn*, *Cu* and *In* on the two cation sites of the chalcopyrite structure would be a crucial key for the understanding of the phase transition in the alloys. A precise differentiation between *Zn* and *Cu* on different structural sites is not possible using X-ray diffraction because of their similar scattering power (only one electron difference), thus only site changes of (*Zn*+*Cu*) and *In* can be derived from the synchrotron X-ray experiments. Neutron diffraction is the only possibility to solve the differentiation problem, and experiments were performed at the high-intensity diffractometer D20.

For the first time the order parameter of the transition in $CuInX_2$ and in multinary alloys as well as the static critical exponent β were determined.

PC1
DESTRUCTION OF THE SUPER-FERROMAGNETIC ORDER BY ZERO-POINT QUANTUM FLUCTUATIONS IN A CRYSTAL OF NANOMAGNETS.

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We use thermal neutron diffraction to probe the magnetization of a single crystal of molecular clusters. Each of these contains 12 manganese atoms and behaves, at low temperatures, as a nanomagnet with spin S=10 and strong anisotropy along the crystallographic c axis. Application of a magnetic field $B_\perp$ perpendicular to the c-axis enhances quantum tunneling between opposite spin orientations, enabling the spins to attain thermal equilibrium. Below T_c = 0.9(1) K magnetic dipolar intermolecular interactions turn this equilibrium state into a ferromagnetically ordered phase. However, if $B_\perp \geq 5.5$ T the magnetic state of each molecule becomes a superposition of states with spin pointing up and down along c, which destroys the long-range ferromagnetic correlations. For the first time in these molecular systems, the existence of quantum superpositions of up and down states has been shown by directly measuring the vanishing magnetization along the anisotropy axis

PC2
SPIN REORIENTATION AND CRYSTAL STRUCTURE DISTORTION IN $HoCO_{4.5}Si_{0.5}$

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In this paper we present the effect of substituting Si for Co in the $HoCo_5$ compound. Both the magnetic and crystal structure phase diagrams are found to be dramatically modified. Neutron powder diffraction investigation has confirmed that $HoCo_{4.5}Si_{0.5}$ retains the $CaCu_5$ crystal structure at room temperature. The Si atoms are located preferentially on the Co 3g atomic position. This limited substitution induces serious modifications of the magnetic features. The ordering temperature is significantly reduced comparison with the $HoCo_5$ parent compound. A spin reorientation is observed at low temperature. This spin reorientation corresponds to a change of the easy magnetization direction from the c-axis of the hexagonal $CaCu_5$-type structure (at high temperature) towards the basal plane at below the spin reorientation temperature. A detailed structural investigation has been undertaken between 4 and 300K on the D1B powder diffractometer. This analysis has shown that the spin reorientation induces a significant lattice distortion thus leading to a lowering of the crystal symmetry. The $HoCo_{4.5}Si_{0.5}$ crystal symmetry is changed from P6/mmm at room temperature to Cmmm at 4K. The magnetic phase diagram has been obtained in the whole temperature range and the thermal evolution of the magnetic moments determined.

PC3
MAGNETIC STRUCTURES OF THE THREE CRYSTALLOGRAPHIC PHASES IN THE NUCLEARLY CHIRAL MOLECULAR MAGNET $[Cr(CN)_6][Mn(S)\text{-}pnH(H_2O)](H_2O)$

C. González[1,2], J. Campo[1], G. J. McIntyre[2], F. Palacio[1], Y. Numata[3], Y. Yoshida[4], K. Kikuchi[4], K Inoue[3]

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Molecular materials are ideally suited to combine several functional properties. An exciting but as yet unrealized possibility is the discovery of magnetic chirality in a nuclearly chiral molecular compound. We report here on the magnetic structure of the three phases of the nuclearly chiral ferrimagnet $[Cr(CN)_6][Mn(S)\text{-}pnH(H_2O)](H_2O)$ with Tc = 38 K, 39 K and 73 K for, respectively, phases I, II and III. The three nuclear phases, which differ on the position of the chiral carbon and some in the water content, are reversible and accessible in a single experiment. Measurements were carried out on two single-crystal diffractometers, D10 and VIVALDI. The three different magnetic structures show four canted interpenetrating magnetic sublattices where competing Dzyaloshinskii-Moriya interactions play a crucial role and help to understand the likely mechanisms for magnetic chirality in molecular magnets.

PC4
FERRIMAGNETIC CORRELATIONS IN PARAMAGNETIC $ErCO_2$

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$ErCo_2$ is a ferrimagnet with a first-order transition at T_c =32K. When a magnetic field is applied, the Er moment is parallel to the field at all temperatures. As expected for a ferrimagnet, Co is ordered antiparallel to Er below T_c and, at sufficiently high temperatures, the Co sublattice is polarized parallel to the applied field. However, contrary to some previous hypotheses, our X-ray Magnetic Circular Dichroism experiments at the $L_{2,3}$ Co and $M_{4,5}$ Er absorption edges in $ErCo_2$ have revealed that the temperature, T_f , at which the Co changes its orientation relative to the field is substantially higher than the critical temperature ($T_f > T_c$), well within the paramagnetic regime. This result evidences a ferrimagnetic coupling between the Er and Co sublattices in a wider temperature range than expected. We have measured Small Angle Neutron Scattering (SANS) in order to demonstrate the formation of "ferrimagnetic clusters" in this region of the magnetic phase diagram and to determine its correlation length ξ. We observe the expected divergence of ξ right above T_c and a wide region, in the vicinity of T_f, where the correlation length has an almost constant value of about 7Å.

PC5
NEUTRON LARMOR PSEUDO-PRECESSION AT REFLECTION SEEN BY SPIN-ECHO

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Polarized neutrons perform Larmor Pseudo-Precession at reflection from magnetic films [1]. Larmor Pseudo-Precession occurs when a magnetic film is magnetized at an angle with respect to the incident polarization vector direction and is a result of quantum interference between the different spin components of the neutron wave reflected from the back and the front face of a magnetic film. This interference manifests as an effective rotation of the neutron polarization vector around the film magnetization direction. The angle of effective rotation or Larmor Pseudo-Precession as a function of the incoming angle depends on the parameter set of the film, e.g. the layer magnetization distribution. In this work we show the first direct experimental evidence of Larmor Pseudo-Precession. The magnetization of a ~100 nm thick ^{57}Fe film on a sapphire substrate was determined by these spin-rotations in the total reflecting region. The polarization rotations are verified using the thermal neutron triple-axis spectrometer IN3 at ILL (Grenoble) combined with the ZETA Spin-Echo installation.

[1] B.P. Toperverg, H. J. Lauter, V. Lauter-Pasyuk, Physica B **356** (2005) 1

PC6
$Pr_5Co_{19}B_6$ MAGNETIC STRUCTURE: LOCAL ENVIRONMENT INFLUENCE

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The magnetic structure of the $Pr_5Co_{19}B_6$ phase has been investigated using the D1A and D2B high-resolution diffractometers. Besides a measurements at 2K in order to specify the magnetic structure, two measurements at 300K and 463K have been also carried out. $Pr_5Co_{19}B_6$ presents a ferromagnetic behaviour with a Curie temperature of about 440K. Like the other existing $R_{n+m}Co_{3n+5m}B_{2n}$ phases (R= rare earth), this compound (for which n=3 and m=2) presents a structure deriving from the RCo_5 one by an ordered B for Co substitution. All these structures can be built up from only two structural blocks: RCo_5 and RCo_3B_2. They are hexagonal P6/mmm and present several unequivalent sites for R and Co. Their structural feature allows studying the evolutions of the atomic magnetic moment with respect to local atomic environment. For the $Pr_5Co_{19}B_6$ compound, the magnetic moments of the 3 Pr sites and the 4 Co sites have been determined. They are discussed in the light of the chemical bonds and in particular the 3d-2p hybridization between cobalt and boron.

PC7
INCOMMENSURATE MAGNETISM IN THE SPIN-TETRAHEDRAL SYSTEM $Cu_2Te_2O_5X_2$ (X=Cl, Br)

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$Cu_2Te_2O_5X_2$ (X=Cl, Br) compounds are built of interacting frustrated tetrahedral magnetic Cu S=1/2 clusters. They belong to an interesting class of entangled materials with properties lying between those of quantum spin systems and classical magnets.

Our neutron scattering experiments on single crystals reveal very complex incommensurate antiferromagnetic order with the propagation vectors k_{Cl}=[0.150,0.422,1/2], k'_{Cl}=[-0.150,0.422,1/2], and k'_{Br}=[-0.172,0.356,1/2] below T_N=18 K for X=Cl and 11 K for X=Br. In some crystals we observe a coexistence of two symmetrically independent wave vectors, k' and k associated with two different magnetic structures. Models of these structures are determined based on polarized and unpolarized neutron diffraction studies performed at ILL.

A feature of the k'-model, common to both the bromide and chloride, is a canted coplanar motif for the 4 Cu^{+2} spins on each tetrahedron which rotates on a helix from cell to cell following the propagation vector. The model proposed for the k-structure implies the presence of two canted pairs within the tetrahedra.

The ground-state spin arrangement and spin dynamics are determined by competition between the geometrically frustrated intra-tetrahedral coupling, the exchange between tetrahedra and the antisymmetric Dzyaloshinski-Moriya interactions. The exact Hamiltonian of the system, which enables its theoretical description, remains to be determined.

PD1
NEUTRON AND CALORIMETRIC STUDIES OF AN ANTIMICROBIAL PEPTIDE

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The evolution of the energy landscape of proteins from the harmonic regime to complex hydration-dominated interactions above ~200 K has been studied extensively. Parallel work on systems intermediate in size between small peptides and proteins is less developed. We studied the dynamics of an antimicrobial 15-residue peptide (CA(1-7)M(2-9)), a hybrid from Cecropin A and Melittin. We have performed neutron spectroscopy (using MIBEMOL at LLB) and low-temperature adiabatic calorimetry for the lyophilised "dry" peptide (6.8% residual hydration as structural water) and a 49% H_2O hydrated sample.

The mean-square proton mobilities determined from integrated quasielastic intensities show that in this peptide two dynamic transitions occur. A first one at ~145 K, probably due to the structural water, and another at higher temperature (~230 K), closer to that observed in the tripeptide glutathione. In inelastic spectra, up to 200 K, we observe a region of excess intensity over Debye

behaviour at around 3 meV. Well-defined spectra up to 50 meV quantify the temperature and Q dependent evolution of bands of damped vibrational modes, suitable for comparison with our current heat capacity measurements. The calculated mobilities as a function of temperature for the dry and 49 % hydrated samples will be presented, as well as the heat capacities calculated from the proton-weighted vibrational density of states. Results of the measured heat capacities of the three samples ("dry", 49%, and 451% H_2O) will be shown for the temperature range 6 – 300 K.

PD2
THE SUBUNIT ARRANGEMENT OF TYPE I RESTRICTION MODIFICATION ENZYMES

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Type I restriction-modification (R-M) systems encode multisubunit/multidomain enzymes. Two genes (M & S) are required to form the tetrameric 160kDa methyltransferase that methylates a specific base within the recognition sequence and protects DNA from cleavage by the endonuclease. SAXS revealed an unusually large structural change in the methyltransferase following DNA binding; this involves a major repositioning of the subunits of the enzyme, resulting in a 60Å reduction in the dimensions of the enzyme on forming a complex with DNA.

Type I R-M enzymes have been prepared in varying protonated/deuterated states (S and M subunits protonated, S deuterated and M protonated) for which SANS data has been collected in a number of H:D solvent contrasts in the presence and absence of DNA. Ab initio shape determination of this contrast matched data has allowed us to determine the change in subunit positioning that occurs on DNA binding and how this results in the 60Å reduction in the dimensions of the enzyme.

PD3
LIPID/PROTEIN INTERACTION STUDIES ON D17

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Recent results on model biomembrane systems and planar bilayers/protein interactions obtained from neutron reflectivity studies will be presented.

PD4
A DOUBLE MAP OF THE INTRACELLULAR MATRIX

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Due to the large variety of the interactions between solvent and macromolecules, and between macromolecules inside the cell, in vivo neutron studies can enrich considerably the characterization of the crowded cellular environment. In the present work, we drew a double map of the intracellular matrix, by measuring the rigidity of the cell interior in vivo, what we call 'dynamical mapping', and by characterizing the crowding inside intact E.coli, what we call 'non dynamical' mapping. On the one hand, RNA and protein dynamics were investigated using selective deuteration and incoherent elastic neutron scattering, allowing a resilience value to be extracted for both types of macromolecules. On the other hand, the in vivo contribution due to the membrane inside the cell was extracted through the contrast variation technique and SANS measurements.

PD5
THE DEVELOPMENT OF NEW FACILITIES FOR X-RAY AND NEUTRON DIFFRACTION IN THE PSB AND THEIR APPLICATION TO THE STUDY OF COMPLEXES BETWEEN DNA AND ANTI-CANCER DRUGS.

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Our work concerns the development of instrumentation and software for X-ray and Neutron beamlines of common interest to Grenoble's Partnership for Structural Biology (PSB), and to apply these developments for the study of novel DNA complexes with intercalating acridine and/or phenazine drugs. Both types of beamlines involved are the subjects of major investments. In the case of the ESRF as part of the PSB beamline ID23, and in the case of the ILL as part of the UK EPSRC-funded upgrade of the D19 diffractometer. The X-ray and neutron beamlines will benefit from a strong computational approach for data-collection strategy and sample alignment. In particular the Neutron beamline will require the development of efficient data collection strategies, and the Microfocus X-ray beamline will need precise sample centering and 3-D visualization of the sample. This will benefit data scaling and maximize any anomalous signal. The scientific target itself is one that will benefit considerably from a combined X-ray/Neutron approach.

PD6
SELECTIVE DEUTERATION STUDIES OF DNA: RESULTS FROM D19 AND THE DEUTERATION LABORATORY

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DNA structure is highly dependent on sequence, water, and ionic environment. This variability is likely to be exploited in biological function. X-rays provide very important information on DNA structure itself. However they are less effective for study of location of water in polymers. Neutron fibre diffraction provides a powerful way of investigating hydration patterns in DNA. The ability to deuterate the biopolymers either throughout the entire molecule or in a more specific way adds a powerful dimension to work aimed at investigating hydration patterns or hydrogen positions and changes that occur during water-driven transitions. This poster describes neutron fibre diffraction experiments that have been carried out on the instrument D19 at the ILL using samples of selectively deuterated DNA made in the Deuteration Laboratory. This type of experiment offers a completely different approach in structure determination and validation.

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2. Arnott, S., Chandrasekaran, R., Puigjaner, L.C., Walker, J.K., Hall, I.H. and Birdsall, D.L. Nucleic Acids Research, 1983, 11, 1457-1474
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PD7
NANOFIBRILLAR STRUCTURE AND MOLECULAR MOBILITY IN SPIDER DRAGLINE SILK

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Spider dragline silk is a biopolymer with outstanding mechanical properties. It has been in the focus of intense research using a wide variety of experimental techniques and theoretical modelling. However, its macroscopic properties are still not well linked to its microscopic structure and dynamics. Synchrotron radiation scattering experiments have in recent years particularly contributed to the development of microscopic structural models.

In a recent thesis project, neutron scattering techniques have been used for the first time for the study of spider silk. The high scattering contribution of hydrogen and the scattering length difference of hydrogen and deuterium have allowed a fresh look at structural and dynamical properties of spider silks. Thus the results support a hierarchical, three-phase model of nanofibrils composed of crystalline and short-range order domains embedded in an amorphous matrix. Complementary X-ray experiments suggest that water absorbed by the amorphous matrix forms an amorphous ice at low temperatures. Wide-angle neutron scattering (WANS) experiments showed a meridional superlattice peak not observed by X-ray experiments, which is assigned to a smectic beta-sheet structure in the short-range order domains. The exchange of H_2O against D_2O in small-angle neutron scattering (SANS) experiments allowed changing the neutron scattering length density contrast in the nanofibrils and the contrast of the nanofibrils against the amorphous matrix. The molecular mobility was probed by inelastic and quasielastic neutron-scattering techniques. A hierarchy of relaxation processes seems to describe hydrated silk, while native silk behaves like a glass at room temperature.

References: D.Sapede et al., Macromolecules **38**, 8447 **(2005)**; D.Sapede, PhD Thesis, University Joseph Fourier, Grenoble (2006).

PD8
STRUCTURAL STUDIES ON IMPase, THE TARGET OF LITHIUM AS A MOOD-STABILISING DRUG.

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IMPase (Myo-Inositol Monophosphatase) is the target of lithium therapy for Bipolar Disorder, a disease that affects 1% of the population worldwide. Lithium has a small therapeutic range of concentrations before it becomes toxic and is known to cause severe side effects. Bipolar patients show high levels of inositol presumably due to overactivity of IMPase.

The aim of this project is to determine the precise binding site(s) for lithium ions and thereby detail the mechanism by which IMPase is inhibited. The studies will involve determination of the neutron structure of bovine IMPase with lithium bound, to define the protonation states of active site groups and to identify the physiological metal-binding sites. Since lithium ions do not scatter x-rays strongly, the neutron studies will allow us a much-improved definition of the lithium binding sites than could be achieved by x-ray analysis. Structural information from neutron studies aims to facilitate the design and development of better therapeutic agents for bipolar disorder.

PD9
DYNAMICS OF THE PURPLE MEMBRANE AND ITS HYDRATION WATER

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Neutron scattering is a spectroscopic technique unique in the energies and momentum values accessible, values that correspond to those of functional dynamics in biological molecules.
Here we have performed experiments on the Purple Membrane (PM), a naturally occurring biological membrane, made up of 25% lipids and 75% of a single retinal binding protein called Bacteriorhodopsin, which functions as a light-driven proton pump. We are studying individual amino acids to discover if different amino acids display different dynamics and correlating these results to their environment in the membrane. For this we have also studied the hydration water to see to what extent the membrane's dynamics are coupled to the water.

We produced a completely deuterated PM and hydrated it in H_2O to study hydration water dynamics and compared to a native membrane hydrated in D_2O (where the scattering comes from the membrane). We observed a transition in the water at 200K, which does not trigger one in the membrane.

We produced specifically deuterated PM samples in which one amino acid is hydrogenated in a completely deuterated membrane, to focus on the dynamics of specific amino acids. We studied the dynamics of lysines, isoleucines and leucines. The lysine residues are mostly found at the surface of the protein and appear to follow closely the dynamics of the hydration water. The isoleucines and leucines, hydrophobic residues that are mostly in the lipid environment, appear protected from the water and display dynamics similar to that of the mean membrane.

PE1
FLUX LATTICE PHASE TRANSITIONS IN NIOBIUM

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Using small-angle neutron scattering, we have investigated spontaneous symmetry-breaking flux lattice phase transitions in niobium - supposedly a 'conventional' superconductor. Also, using very high temperature resolution, we have also searched for signs of flux lattice melting (analogous to the 1^{st}-order melting transition seen in High-T_c materials) by SANS and heat capacity measurements.

PE2
INFLUENCE OF THE NATURE OF SALT ON THE SIZE AND GROWTH OF ANIONIC VESICLES: A SMALL ANGLE NEUTRON SCATTERING STUDY

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Scattering experiments provide powerful method to explore colloidal structures from the scale of a few Ångströms to thousands of Ångströms. The new generation of SANS diffractometers like D22 at the ILL (Institut Laue Langevin, Grenoble) with very high flux at the sample position (up to 10^8 neutrons/s/cm^2) and a large dynamic q-range allows very short acquisition times, of the order of a few hundreds of ms with a reasonable signal-over-background ratio.

A stopped-flow apparatus has been adapted to fulfil the geometrical requirements of scattering experiments on D22. The interest of this equipment is to control the mixing of several solutions within a short time window (10-90 ms) and to control precisely the delay between the time of mixing and the beginning of observation.

We have studied the formation and growth of spontaneous vesicles after addition of salts (NaCl, NaBr, KCl, KBr) in a micellar solution of AOT in D_2O from 500 ms to 5 hours after mixing with a time resolution increasing from 500 ms to 3 minutes.

The driving force of the transition is the screening of the electrostatic repulsion between adjacent surfactant head groups that favour formation of a locally plane bilayer. Assuming that the aggregation is controlled by micelle diffusion, a simple kinetic approach predicts that the average radius increases with the power law $R \propto t^{1/6}$ in close agreement with the experimental data.

I. Grillo, E.I. Kats, A.R. Muratov Langmuir (2003), 19 (11) 4573-4581

PE3
NEUTRON SPECULAR REFLECTION AND OFF-SPECULAR SCATTERING FROM FREE-STANDING LIQUID FOAM FILMS

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A foam film is formed by two monolayers of surfactant molecules with the hydrophobic parts facing air and the hydrophilic head groups in contact with a central water core. The thickness of such foam films depends on the interactions between the film surfaces. This makes them a suitable model to study the forces in colloidal systems which is a central problem in basic studies in colloidal and interfacial sciences. The most widespread experimental technique in foam film studies is the interferometric measurement of the film thickness. This technique hardly can give any information about the internal film structure as usually the method provides only the total film thickness. X-ray reflectometry studies provide more detailed information as they can visualize the hydrophobic part of the surfactant molecules. Because of the different origin of the contrast neutron reflectometry can supply information about the orientation of the whole surfactant molecule – its hydrophilic and hydrophobic part, and such might help to find the position of the planes of interaction between the film interfaces. In our present study we used tetraethylammonium perflurooctane sulfonate (TAPOS) for the formation of free-standing liquid foam films which were examined by neutron specular and off-specular reflectometry to receive detailed internal structural information of such systems.

PE4
SELF-ORGANIZED COMPLEX NANO-COMPOSITES STUDIED AT THE NANO-SCALE

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How to organize complex materials at the nano-scale is investigated with neutron grazing incidence techniques (specular reflection, off-specular scattering and grazing incidence small angle scattering, GISANS). A “smart” method based on the principle of self-organization is employed to construct new nano-composite materials containing high density of magnetic nano-particles arranged into the well ordered regular block-copolymer lamellar structures. We investigate how the particle concentration and size affect the architecture of the composite film. New morphologies predicted theoretically (R.B. Thompson et al. Science **292**, 2469 (2001)) are obtained and explored in our studies. We show that the details of the internal structure of composite films are encoded in the two-dimensional map of the intensity scattered by the film and can be extracted via the quantitative data analysis. A dedicated theoretical approach based on the distorted-wave Born approximation (DWBA) is developed for analysis of the full two-dimensional intensity map including the dynamical range close to the total reflection region and depth-dependent GISANS intensity maps. This approach will be applied to a wide range of technologically important systems and can be used to design novel composite architectures.

PE5
COMPLETE REFLECTOMETRY FOR NANO-STRUCTURES

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Complete reflectometry fulfils the requirement of nano-science to determine functional structures embedded in host matrices over a wide range of length scales and to provide lateral and depth sensitivity of layered nano-structures. The most complete and detailed three-dimensional information of layered nano-structures is gained from a complete reflectometry study consisting of specular reflection and off-specular scattering together with GISANS. The averaged structures are obtained in the depth profile, whereas the nano-structure dimensions and arrangements are probed along the two lateral directions. A variation of the grazing incident angle provides focusing of the neutron wave field onto different structural elements across a multilayer and the extracted SANS signal carries a signature of the lateral nano-structure dimensions of these highlighted elements. Due to specifics of off-specular and GISANS kinematics it accesses lateral scales over an enormous range from nano- up to sub-millimetres. This allows in the present study probing the roughness spectrum in the model of capillary waves at the interfaces of a polymer multilayer.

PE6
SPIN-ECHO RESOLVED GRAZING-INCIDENCE SCATTERING (SERGIS)

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The encoding of neutron momentum transfer by spin-echo makes possible the detection of objects of lateral dimensions ranging from a few nanometers to some microns, either in the bulk or at interfaces, with features that are novel and distinct from those of conventional scattering. Spin-echo resolves the scattering vector rather than the wave vector of the incoming or of the scattered neutrons: no collimation is needed. Further, spin-echo provides directly the correlation in real space of the scattering objects, without operating a mathematical Fourier transform on the recorded intensities. The combined effect of these characteristics was evident in a recent experiment on anodic porous alumina, which yielded an exceptionally clean pair-density function of the two-dimensional pore assembly. The lower statistics of objects confined to the surface or an interface (rather than filling an entire volume) means that their scattering is inherently weak. Since they require only relaxed resolution, neutron spin-echo grazing-incidence scattering experiments are considerably more feasible than conventional scattering. This point is proven in an experiment aimed at finding the correlations existing in an assembly of polymer droplets dewetted on a silicon surface. The type and number of scientific problems that can profitably be addressed with this technique is still under scrutiny, but includes the study of surface and interface landscapes such as islands, facets, and capillary waves in inorganic and biological membranes.

PE7
USING NEUTRONS TO INVESTIGATE THE MORPHOLOGY OF DIBLOCK COPOLYMER MEMBRANES

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In this structural study we use diblock copolymer as a model system to investigate the correlation between morphology and transport properties in ionomer materials. Diblock copolymers with a fluorinated block and a sulfonated polystyrene block synthesized at Simon Fraser University allow control of the ionic exchange capacity (IEC) by adjusting either the length of the sulfonated polystyrene chains or their degree of sulfonation. We have studied the structure of membranes made from various polymer configurations by Small Angle Neutron Scattering (SANS) using contrast variation. The analysis shows that there is phase separation at length scales of the order of a few tenths of nanometers due to the non-miscibility of the two polymer blocks; and that there is a substructure within the sulfonated polystyrene domains due to the segregation between the hydrated ionic groups and the hydrophobic polystyrene. These results will be reported and compared to images from Transmission Electron Microscopy (TEM) and with proton conductivity measurements.

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PE8
TIME-RESOLVED SANS STUDIES (TISANE) OF FIELD-INDUCED ORDERING IN FERROFLUIDS.

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We report on real-time stroboscopic investigations of the kinetics of field-induced ordering processes in concentrated Co-ferrofluids by means of SANS. Ordering of the magnetic particles was forced by an alternating magnetic field of frequency ν_s with a maximum amplitude of $H_{max}=\pm 200$ Gs. We applied for the first time the TISANE method [1] where a fast chopper of frequency ν_e was synchronized to ν_s and adjusted to a data acquisition frequency ν_d of the detector. A considerable gain in intensity and resolution was obtained by this technique where a large frame overlap and high repetition rates could be achieved. Up to about $\nu_s=1300$ Hz the SANS scattering patterns oscillated as a function of time from isotropic at H=0 to strongly anisotropic at H_{max} The observed threshold frequency is far below the resolution limit of the TISANE technique which must therefore result from the characteristic time needed for re-orientation of the magnetic particle moments. In a conventional stroboscopic SANS experiment when the data acquisition was triggered by a signal from the ac-field the periodic response was detected only up to about $\nu_s=600$ Hz. With increasing frequency the oscillations are smeared out by the different flight times corresponding to the wavelength resolution of the velocity selector $\Delta\lambda/\lambda=0.1$.

[1] R. Gähler, R. Golub ILL Scientific council April (1999) SC 99-1, page 73

PF1
THALES - TOWARDS THE NEXT GENERATION COLD NEUTRON THREE-AXIS SPECTROMETER

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The cold neutron three-axis spectrometer IN14 at the ILL looks back on more than two decades of world-leading scientific achievements by investigating the low-energy excitations in condensed matter. IN14 combines a high cold-neutron flux with good energy and momentum resolution, key for high-quality quantitative results. With an incident neutron energy range of 2 to 15 meV the instrument is well adapted for exploring the magnetization dynamics in e.g. strongly correlated electron systems as well as low-dimensional or frustrated magnets.

Building on the strength of the present instrument, but using state-of-the-art neutron optics, we intend to create the next-generation cold-neutron three-axis spectrometer ThALES with the following aims: (i) An overall increase of data collection rate provided by the combination of optimised super-mirror guides, a double-focusing monochromator and a multiplexed secondary spectrometer, (ii) unique measurements using an efficient and easy-to-use polarized neutron option, (iii) extending the incident neutron range to higher energies to bridge the gap with thermal instruments, and (iv) non-magnetic materials allowing for high-field magnets under optimised conditions.

The vast range of experimental possibilities and the increased instrumental flexibility will permit using smaller samples under challenging conditions such as high magnetic fields and high pressure to meet the requirements of our user community.

PF2
SUPERCONDUCTIVITY AND ANTIFERROMAGNETISM IN $CeCu_2Si_2$

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The prototypical heavy-fermion compound $CeCu_2Si_2$ orders antiferromagnetically and shows superconductivity at low temperatures. We performed single-crystal neutron scattering experiments and simultaneous measurements of the ac susceptibility at temperatures below 1 K and in magnetic fields up to 2 T to study the interplay between superconductivity and antiferromagnetism in $CeCu_2Si_2$. Measurements on different single crystals give clear evidence that superconductivity expels antiferromagnetic order at low temperatures and that both phenomena do not coexist on a microscopic scale.

PF3
MAGNETIC EXCITATION FROM CHARGE-STRIPE ORDERED ELECTRONS

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The low-energy magnetic excitations of $La_{(2-x)}Sr_{(x)}NiO_{(4)}$ with x = 1/3, 0.275 were studied using polarized- and unpolarized-neutron scattering with thermal and cold triple-axis spectrometers. Excitations from the carriers in the charge stripes in both materials were observed to be nearly equivalent and hence doping independent. The excitations were observed to be gapped with a gap energy of 1.3 meV and the exchange interaction strength was estimated to be 3.2 meV. The excitations are not successfully modelled as excitations from an independent spin system, indicating that interactions with the ordered spins need to be taken into account.

PF4
EXCITATIONS OF LIQUID HELIUM CONFINED TO NANOSCALES

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The excitations of quantum liquids confined in porous media as revealed by neutron scattering show surprises and new physics. Even when confined to nanoscales, superfluid ^{4}He supports a well-defined phonon-roton mode. In fully-filled porous media and at saturated vapor pressure, the energy and lifetime of the mode is the same as in bulk superfluid ^{4}He. The temperature dependence of the weight of the mode, however, is different and suggests that there remains a Bose-Einstein condensate above the superfluid to normal (S-N) transition temperature T_c in the "normal" liquid phase [1]. This "normal" phase BEC above Tc is localized by the disorder. Indeed the S-N transition in porous media is apparently associated with an extended to localized BEC crossover. We have also observed the P-R modes in superfluid ^{4}He held at negative pressure [2] and at high-pressure [3] above the bulk liquid-solid transition pressure where a quantum phase (S-N) transition is possible. One-dimensional solid helium on nanotubes has also been created [4]. Directions for exciting new measurements and the challenges they offer to instrumentation and sample environment facilities will be discussed.

[1] F. Albergamo, H. R. Glyde, et al. Phys. Rev. B69, 014514 (2004).
[2] F. Albergamo, H. Schober, et al., Phys. Rev. Lett. 92, 235301 (2004).
[3] J. V. Pearce, J. Bossy, et al., Phys. Rev. Lett. 93, 145303 (2004).
[4] J. V. Pearce, M. A. Adams, et al. Phys. Rev. Lett. 95, 185302 (2005).

PF5
ELEMENTARY EXCITATIONS IN LIQUID D_2 CONFINED IN MCM-41

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We present a comparative study of the excitations in bulk and liquid D_2 confined within the uniform pores of MCM-41. The assessment of the precise location of the sample within the pores is carried out by means of pressure isotherms. The study was conducted at pore fillings well below completion. Within the range of wavevectors where collective excitations can be followed up ($0.3 \leq Q \leq 3.0$ Å^{-1}), we found that confinement brings forward a large shortening of the excitation lifetimes that shifts the characteristic frequencies to higher energies. In addition, coherent quasielastic scattering shows signatures of reduced diffussivity.

PF6
ILL'S RENEWED THERMAL THREE-AXIS SPECTROMETER IN8: A REVIEW OF ITS FIRST THREE YEARS ON DUTY

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The primary spectrometer of ILL's thermal three-axis spectrometer IN8 has undergone a major rebuild during the last few years. We here summarize the characteristics of the new instrument and highlight its enhanced performance in terms of flexibility and luminosity. Flux measurements indicate an increase of monochromatic flux at the sample position of x3 to x5 depending on monochromator and wavelength as compared to the previous instrument IN8B. We also highlight the scientific impact of the instrument as well as further instrumental developments envisaged.

PF7
ATOMIC AND MOLECULAR DYNAMICS STUDIES WITH HOT NEUTRON SPECTROMETER IN1: STATE-OF-ART AND PERSPECTIVES

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In the past decade the user demand in the field of atomic and molecular dynamics with high neutron energies has experienced a sensible re-orientation to the high-resolution experimental set-up. The presently available IN1-TAS spectrometer components were pushed to their limit in order to ensure Brillouin scattering experiments on atomic dynamics in liquids. A similar high-resolution trend is in the agenda for the filter-analyzer type of experiments performed with the IN1-BeF spectrometer. This secondary spectrometer option presently offers uniquely high luminosity for phonon density of states measurements. The current and pending development of IN1 spectrometer units is presented.

PF8
STRUCTURE AND DYNAMICS OF WATER IN PLANT CELL WALLS

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Many unique features of water in plant cell walls have been reported over the last decades. Water adsorbed in the disordered regions of cellulose, the main constituent of plant cell walls, exhibits liquid dynamics below the freezing point and is therefore termed “non-freezing”. However, neither the structural properties of water in cellulose nor the nature of the freezing transition are fully understood. Neutron scattering techniques might provide the missing clues for a structural and dynamic model of water in plant cell walls below 0 °C. Upon cooling, an increasing part of the water molecules freezes in a gradual, heterogeneous glass transition to a new type of amorphous ice. The remainder is supercooled and is liquid down to 200 K with its dynamics being strongly retarded. In models for water adsorption to cellulose, the water molecules are thought to be inserted between individual hydrogen-bonded cellulose chains. The investigation of oriented cellulose fibres with inelastic neutron scattering recently revealed that the dynamical properties of the water molecules are anisotropic as are their surroundings. This finding could explain why no extended crystalline ice networks are formed in plant cell walls.

PF9
SPIN EXCITATIONS IN THE ANISOTROPIC BOND-ALTERNATING QUANTUM *S*=1 CHAIN SYSTEM NTENP IN A MAGNETIC FIELD

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Inelastic neutron scattering experiments on the S=1 quasi-one-dimensional bond-alternating antiferromagnet $Ni(C_9D_{24}N_4)(NO_2)ClO_4$ (alias NTENP) have been performed under magnetic fields below and above the critical field H_c at which the energy gap closes ($H_c \approx 11.4$ T). Normal field dependence of Zeeman splitting of the excited triplet modes below H_c has been observed, but the highest mode at about 2 meV is unusually small in intensity and smears out with increasing field well below the critical field. This behavior can be explained by an interaction with a low-lying two-magnon continuum at $q_{//}=\pi$ that is present in the dimerized chains but absent in the uniform ones like, e.g., the Haldane chains. The field dependence of magnetic excitations in the antiferromagnetically long-range ordered high-field phase has been investigated. Above H_c, we find only one excited mode, in strong contrast with the three massive excitations previously observed in the structurally similar Haldane-gap materials NENP and NDMAP. In addition to the previously observed coherent long-lived gap excitation around 1.2 meV [M. Hagiwara et al., Phys. Rev. Lett. **94**, 177202 (2005)], a broad continuum is clearly detected at lower energies in the range 0.3-1.2 meV. This observation is consistent with recent numerical studies, and helps explain the suppression of the lowest-energy gap mode in the magnetized state of NTENP. Yet another new feature of the excitation spectrum is found at slightly higher energies ("re-entrant" 2 meV mode), and appears to be some kind of two-magnon state.

PF10
USING NEUTRON SPECTROSCOPY TO STUDY COLLECTIVE DYNAMICS OF BIOLOGICAL AND MODEL MEMBRANE SYSTEM

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While most spectroscopic techniques, as, e.g., nuclear magnetic resonance or dielectric spectroscopy probe macroscopic responses, neutron and within some restrictions also x-ray scattering experiments give the unique access to microscopic dynamics at length scales of intermolecular or atomic distances. Only recently, it has become possible to study collective dynamics of planar lipid bilayers using neutron spectroscopy techniques [1]. We determined the dispersion relation of the coherent fast picosecond density fluctuations on nearest-neighbor distances of the phospholipid acyl chains in the gel and in the fluid phases of a DMPC bilayer. By combining different neutron scattering techniques, namely three-axis, backscattering and spin-echo spectroscopy, we present measurements of short and long wavelength collective fluctuations in biomimetic and biological membranes in a large range in momentum and energy transfer, covering time scales from about 0.1ps to almost 1μs and length scales from 3Å to about 0.1μm.

Because of optimized setups and sample preparation, inelastic neutron scattering experiments supply for the first time sufficiently strong coherent inelastic signals for quantitative analysis. The measurements offer a large window of length and time scales to test and refine theoretical models of dynamics of biomimetic and biological membranes. From an advanced theory the long wavelength dispersion relations give then direct access to the elasticity parameters of the membranes.

[1] M.C. Rheinstädter, C. Ollinger, G. Fragneto, F. Demmel, T. Salditt, Phys. Rev. Lett. 93, 108107 (2004).
[2] M.C. Rheinstädter, T. Seydel, F. Demmel, T. Salditt, Phys. Rev. E 71, 061908 (2005).

PF11
HIGH FREQUENCY COLLECTIVE EXCITATIONS IN LIQUID TELLURIUM

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The spectra of collective excitations of liquid Tellurium have been measured by means of inelastic neutron scattering. The dynamics of this liquid metal have been studied at two different temperatures, just above melting (T_m = 723 K) and at ~ 1000 K. Estimates for the velocity of propagating excitations for both temperatures have been obtained from the experimental data and a contrasting behaviour is found with respect to anomalies shown by the adiabatic sound velocity measured by ultrasound methods.

PF12
MAGNETIC EXCITATIONS IN NON-FERMI LIQUID $YbRh_2Si_2$

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Inelastic neutron scattering on $YbRh_2Si_2$ powder has been performed to investigate the magnetic response in this compound close to quantum criticality. The high-energy response is dominated by crystalline electric-field excitations, found at 17, 25, and 43 meV. In contrast, the low energy response is quasielastic and shows a critical slowing down as the temperature is reduced. However, the quasielastic response seems to be non-Lorentzian like, but can be described by a distribution of relaxation rates. The observed behavior might arise from the vicinity of the system to a quantum phase transition.

PG1
SIMULATION RESULTS ON THE BACKSCATTERING SPECTROMETER IN16B

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With the Millenium project the new Backscattering Spectrometer IN16B at the ILL is designed to keep it extremely high energy resolution, in the region of sub- μeV at the elastic peak, while the use of a Phase Space Transformer, PST will allow, by increasing the divergence of the incoming beam, a significant increase of the flux at the sample position.

It is clear that to profit from the PST gain, IN16 has to be re-located at the end of a cold neutron guide. In order to optimize the layout of individual components and to estimate the instrument performance, the Monte-Carlo simulation programs McStas and VITESS (Virtual Instrumentation Tool for ESS), developed respectively at Risø National Laboratory and Hahn-Meitner-Institute, have been used. McStas and VITESS offer a general framework to compose virtual neutron scattering instruments and supports both reactors and spallation sources. Comparing the simulations results obtained using both packages allows to take advantage of the strength of each program separately and also check for any possible inaccuracy of the final results. Moreover, with the idea of validating the results, the actual IN16 and the cold triple axis IN14 were simulated as well. Afterwards, the simulations of IN16B were performed for three different guide-end positions, H53 and H52 looking at the Horizontal Cold Source (HCS) and H112 looking at the Vertical Cold Source (VCS). Here we discuss the benchmarking calculations and the performance of IN16B at each possible location at the ILL.

PG2
REFRACTION AS A MEANS OF ENCODING WAVELENGTH FOR NEUTRON REFLECTOMETRY

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Neutron reflectometry is a well-established technique used to analyze the structure of interfaces as a function of depth normal to the surface. On a continuous source of neutrons, such as a reactor, the measurement can be done at a fixed incident angle and a white beam with the neutron wavelength encoded by the use of choppers to measure the time of flight. Although providing a certain flexibility in wavelength resolution, choppers have low transmission. This paper explores the possibility of using refraction to encode neutron wavelength opening the possibility of reactor sources to use almost the full-time-averaged neutron flux available and hence, increase the performance of neutron reflectometers by orders of magnitude.

PG3
GEOMETRIC PHASE ARISING FROM PATH-DEGREES OF FREEDOM IN A NEUTRON INTERFEROMETER

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Foucault's pendulum is an example where the underlying geometry affects the state of the pendulum: due to the spherical shape of the earth the oscillating plane does not, in general, return to its initial position after 24 hours. In a similar manner in quantum mechanics the geometry of the state space is responsible for an additional phase factor as discovered by Berry [1]. In a neutron interferometer the two path possibilities give rise to a spatial geometric phase due to the subjacent spherical state space. We have verified its occurrence experimentally using a double-loop perfect-crystal silicon interferometer at the S18-instrument at the ILL [2]. The experiment exhibits a shift of the interference pattern in accordance to theoretical predictions.

[1] M. V. Berry, Proc. R. Soc. London 392, 45 (1984)
[2] S. Filipp et al., Phys. Rev. A 72, 021602(R) (2005)

PG4
DRACULA: AN EXTREMELY FAST MEDIUM-RESOLUTION DIFFRACTOMETER

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The Dracula project[1] responds to an under-exploited advantage of reactor sources as compared to pulsed sources: high time-averaged flux on the sample. Historically, resolution considerations have limited the use of very large solid-angle detectors for 2-axis diffractometers on reactor sources. However, by using moderately high monochromator take-off angles and q-space focussing, coupled with 2D detection, very large solid angles (1.5 sr) can be used without much sacrifice in resolution. The ILL's detector group has developed very large 2D gas detectors that meet the needs of the Dracula diffractometer, as well as very fast detector electronics, first used on D2B and D22. This combination, together with large doubly focussing monochromators reflecting a wide band of wavelengths, will result in a machine ideally suited to the study of small samples (e.g. at high pressure) or very fast chemical kinetics.

[1]DRACULA Proposal for a new ILL instrument. A.W. Hewat et al. (2004) Millennium Project detailed draft proposal, ILL Instrument Committee 17 Oct 2003

PG5
RECENT DEVELOPMENTS AT THE D20 INSTRUMENT

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During the ILL's UFI programme of 1995-2000, the D20 diffractometer[1] acquired a microstrip detector with 12 times the solid angle of the previous multiwire detector. Monochromator improvements since 2000 have led to another 1.5 times increase in incident flux, resulting in an overall counting-rate gain factor of 18. The important qualitative gains since 2000 are the high resolution mode (thanks to a 120 degree takeoff angle and a variable vertically-focussing Ge monochromator), an improved very fast (several ms) data acquisition system, and a new radial oscillating collimator (ROC) that has undergone successful preliminary tests. Other upgrades over the past 2 years include a top-loading furnace with higher maximum temperature, a larger diameter cryostat tail, a new multiwire beam monitor, and an improved secondary beam shutter (OS2). Taken in their ensemble, these developments have increased D20's versatility and established its place as the world's highest-intensity (constant-wavelength) neutron diffractometer.

[1]P. Convert, T. Hansen, A. Oed and J. Torregrossa, Physica **B** 241-243 (1998) 195—197.

PG6
THE WIDE-ANGLE SPIN-ECHO SPECTROMETER PROJECT WASP AT ILL

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This presentation will give an overview of design and projected performance of the new ILL spin-echo spectrometer WASP (Wide-Angle Spin-echo spectrometer). At present, ILL offers two spin-echo only spectrometers to the user community specialized in high signal (IN11) and high resolution (IN15), respectively. The aim of the project is to increase the detection and acceptance angle of the high-signal spectrometer IN11 by changing the design of the magnetic coils.

The design of WASP profits from the experience gained with the novel spectrometer SPAN, which has recently been commissioned at the Hahn-Meitner Institute in Berlin, Germany [1]. In the SPAN/WASP design nearly perfect 360º field symmetry is achieved by replacing the conventional collinear NSE field solenoids by a pair of "anti-Helmholtz" solenoids placed above and below the neutron beam plane. Furthermore, careful field analysis revealed that within this design a near perfect $\cos^2$ field shape [2] can be created along the neutron trajectories, so that field correction can be minimized.

We will present improvements on field-optimization calculations using Biot-Savart field calculations and Monte Carlo ray-tracing calculations. Very recently we have incorporated genetic algorithms into our design package. Using this tool we have been able to accelerate the rather complex coil design with typically more than 10 free parameters. The design of WASP also includes a TOF option, using a set of disk choppers, which will allow for the *in-situ* tracing of dynamics into shorter times than the ones that can be reached with NSE.

[1] C. Pappas, R. Kischnik and F. Mezei, Physica B 297 (2001) 14.
[2] C.M.E. Zeyen, P.C. Rem, R.A. Hartmann and L.J.N. Klundert, IEEE Trans. Magn. 24 (1988) 1540.
[3] P.M. Bentley, C. Pappas. K. Habicht and E. Lelièvre-Berna, accepted for publication in Physica B.

PG7
FIGARO: PROGRESS ON THE PROJECT FOR THE NEW ILL REFLECTOMETER

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FIGARO will be a vertical-reflection-plane time-of-flight reflectometer to be used mainly for the study of fluid interfaces. The scientific case and progress in the design of the instrument will be presented.

PG8
THE ILL MILLENIUM PROJECT FOR THE NEUTRON BACKSCATTERING SPECTROMETER IN16B

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The ILL was leading for years the research in high-energy resolution neutron backscattering spectrometry and IN16 is still one of the most demanded instruments at the ILL. New neutron backscattering spectrometers with high flux were built elsewhere having a higher flux compared to IN16. With the Millenium project IN16B the ILL aims to gain its leading position back in terms of flux and to maintain its excellent signal-to-noise ratio.

Higher neutron flux is achieved by more efficient neutron optics and a major technical challenge, a phase-space-transformation (PST-) chopper at a guide end position. The latter goes at the expense of beam divergence. We have developed a new design for the disc and crystal cassettes of the phase space transformation chopper, which according to finite-element calculations will allow reaching a crystal speed of 300m/s at a relative small disc radius, using two reflecting segments. The most critical point, whether the graphite crystals will stand the high centrifugal forces is being tested now. The dynamic range will increase with a new linear motor Doppler drive to ±32 μeV and requires the data acquisition to be changed. Finally, in order to reduce the background - an intrinsic problem with the PST-backscattering design - a background-suppression chopper is proposed as well as a large vacuum chamber. The analyzer surface of IN16B should be doubled with respect to IN16. The large $30m^3$ evacuated analyzer housing must be mobile to allow for several analyzer configurations and for a possible later extension towards an optional 3X-mode.

PG9
FUTURE DEVELOPMENTS AT THE D20 INSTRUMENT

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As a result of the upgrades over the last 5-10 years, detailed on the recent upgrades poster, D20 is the most versatile high-intensity (constant-wavelength) diffractometer in the world today. However, projects are underway to improve D20 further in order to bring an ever-wider user and science base to the instrument and to the ILL in general. First, we describe the plans to offer the possibility of polarized neutrons at D20 with CRYOPOL and redesigned pre-sample optics. Secondly, the implementation of smart programs for data manipulation, visualization and treatment are outlined. Third, ongoing work towards providing a simple basic sample-environment module is presented, where users would be able to insert their own lab-built sample-environment modules, e.g. chemical, electrochemical or pressure cells, flow apparatus and furnaces. Finally, upgrading the current 1D position-sensitive detector (PSD) to a large area 2D PSD is discussed.

PG10
CYCLOPS, A HIGH-FLUX REAL-TIME LATTICE EXPLORER USING CCD DETECTORS AT ILL

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New single-crystal diffractometers on spallation sources, with ultra-large area detectors, such as TOPAZ at SNS and SXD-II at ISIS, will allow real-time exploration of reciprocal space and rapid structure refinement. ILL pioneered similar techniques with image-plate machines[1,2], and retains a potential advantage because of the high flux on the sample from a continuous white neutron source. Yet neutron image plates are not real-time, are presently only ~20% efficient, and the image decays even as the data is collected. These differences have been made startlingly clear by recent in-situ comparisons of LADI with electronic PSD's. We propose to build a new machine, the **CY**lindrical **C**cd **L**aue **O**ctagonal **P**hoto **S**cintillator, using methods similar to those used for SXD, but with much higher flux. A small prototype machine at ILL, OrientExpress[3] has already proved the principle. Apart from its much larger 2π sterad detector, the new CYCLOPS machine would be constructed on a supermirror thermal guide with a flux on the sample unequalled in the world.

[1]Neutron Laue diffraction in macromolecular crystallography D.A.A.Myles et al. (1997) Physica B, **241-243**, 1122.
[2]VIVALDI – A Thermal-Neutron Laue Diffractometer for Physics, Chemistry and Materials Science C. Wilkinson, et al. (2002) Neutron News **13,** 37-41.
[3]A new Laue diffraction facility for single-crystal characterization B.Ouladdiaf et al. (2006) ILL Annual report 2005.

PG11
IMPS: A MULTI-ANALYSER DETECTOR SYSTEM FOR THE THERMAL THREE-AXIS SPECTROMETER IN8

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The primary spectrometer of the ILL's thermal-beam three-axis spectrometer IN8 has been recently rebuilt to increase the flexibility of the instrument and the monochromatic flux at the sample position [1]. The new instrument is now fully operational [2]. The next step forward to improve the instrument further will be performed by installing a multi-analyzer detector system to multiplex the instrument that will allow us to perform an imaging of selected regions in (Q,ω) space. In order to optimize the performance of such a multiplexed secondary spectrometer, computer simulations have been performed using the neutron ray-tracing package McStas [3]. Based on the simulation results we have determined the characteristics of the new secondary spectrometer of IN8C: the size of the multi-analyzer system, the crystals to be installed and the spatial detector resolution. Finally, the gain in flexibility with its performance will be discussed [4].

[1] A. Hiess et al., Physica B 276-278, 91-92 (2000)
[2] A. Hiess et al., Proceedings of SCNS workshop, ILL, Grenoble 2002
[3] K. Nielsen et al., Physica B 283, 426-432 (2000)
[4] M. Jiménez-Ruiz et al., Proceedings of ICNS 2005

PG12
PROPOSAL FOR A NOVEL STRUCTURED-PULSE ENGINEERING SPECTROMETER (SPES)

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A novel ToF-system has been developed for the new structured-pulse engineering spectrometer (SPES) proposed by the GKSS-Research Centre for measuring both textures and residual stresses. The chopper device of SPES is distinguished by two features: On the one hand it allows for very high transmission of typically more than 5% due to the low resolution of its base pulses and on the other hand for very high resolution ($\Delta d/d \leq 2\ 10^{-3}$) resulting from a novel pulse-structuring technique. The transmission of this chopper device is thus comparable to multi-burst techniques such as realized in the pulse-overlap ToF diffractometer (POLDI) at PSI and in Reverse-ToF instruments at GKSS or in Gatchina/St. Petersburg which are designed for the analysis of residual stresses. In contrast to these instruments, however, the SPES-chopper will allow for measurements without pulse overlap and will, thus, offer excellent conditions for the determination of position, shape and absolute intensity of peaks in highly symmetric materials. Due to this chopper performance and the integration of a large and high-resolution 2D-detector system SPES will offer new perspectives for the combined analysis of textures and strain fields. Finally, complex sample environments will be made available for very different engineering applications.

PG13
FIRST TESTS OF THE *FLATCONE* TAS MULTIANALYZER SETUP

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We report on the design, construction and first tests of a new secondary spectrometer module [1] for ILL's three-axis spectrometers (TAS). It consists of 31 discrete channels, each containing two elastically bent Si 111 analyzers and an individual ^{3}He detector tube. The channels are separated by absorbing partition walls to minimize their crosstalk. The overall angular range covered is 75º with the possibility to choose between final neutron wave numbers of $k_f = 1.5$ Å^{-1} and 3 Å^{-1}. The flat-cone geometry with tilt angles between –10º and +20º permits to cover the range of about one Brillouin zone in the direction perpendicular to the equatorial plane. The results of first test experiments - mapping inelastic response in relaxor ferroelectrics - confirm a data collection rate increased by an order of magnitude as compared to the up-to-date TAS with doubly focusing optics and competitive with the direct-geometry inelastic spectrometers at next-generation pulsed source.

[1] M. Kempa, B. Janousova, J. Saroun, P. Flores, M. Boehm, F. Demmel and J. Kulda, Physica B (2006) accepted.
Proceedings ICNS 2005, Sydney, Australia.

PG14
IN20 - THE HIGH-FLUX POLARIZED-NEUTRON TAS

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The upgrade of IN20 [1] has been one of the highest priorities among the first generation of the ILL Millennium projects. It resulted in a spectacular gain factor of about 50 times in the data collection rate as compared to the configuration in use till 1999. As a consequence, the sensitivity of the upgraded IN20 in polarized mode is now comparable to that of a non-polarized thermal TAS at the ILL in the 80's, which means that single crystal volumes of 0.1 – 1 cm^3 became sufficient for successful investigations of most systems of current interest in magnetism and in the physics of highly-correlated electron systems. Moreover, its increased luminosity opened access to an efficient use of sophisticated experimental techniques like 1D and 3D polarimetry of the magnetic response anisotropy and high-resolution spin-echo spectrometry for excitation life-time studies.

[1] J. Kulda, J. Saroun, P. Courtois, M. Enderle, M. Thomas, P. Flores, Appl. Phys. A74 [Suppl.] (2002) S246-S248.

PG15
INSTRUMENT SIMULATIONS FOR THE ILL MILLENNIUM PROJECT USING MCSTAS

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The McStas software package has been used to simulate different instruments, which are going to be built or improved in the framework of the ILL Millenium project (D2b, D11, IN16b, D7...). The diffractometer D2b was simulated in detail and options to improve the resolution were checked. The planned guide renewal of D11 was simulated extensively; ideas to increase the flux at sample could be verified.

Furthermore, the performance of SANS instruments at ILL has been determined in comparison to SANS instruments at spallation sources. This comparison is going to be extended to diffractometers and reflectometers.

PG16
A NEW HIGH-Q DIFFRACTOMETER AT ILL

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The Rietveld refinement of high-resolution powder diffraction data revolutionised materials science. However, this method uses only the Bragg peaks and not the diffuse scattering and therefore gives information only on the time- and spatially averaged structure. In recent years development of electronic materials, like high-T_c superconducting and colossal-magnetoresistive materials, made it necessary to investigate the local structure of these materials. This is because the electronic properties of these materials are sensitive to the nanoscale rather than to the average structure. The local instantaneous structure of these materials is often different from the average structure due to the formation of time-dependent local distortions, such as polarons. Such deviations from the average structure are by no means restricted to the above-mentioned electronic materials but are typical of almost every important functional material. In order to elucidate the nanoscale structure of these materials, we need to use the total scattering data including the diffuse background. Egami and co-workers have recently developed the technique of atomic pair-distribution-function (PDF) analysis [1] of the total scattering data from crystalline materials. This method is of course well known to the scientific community that investigates liquids and amorphous materials, and probes the local instantaneous structure. To get complete structural information one needs to perform a joint Rietveld and PDF analysis of the total scattering data up to a high value of momentum transfer Q. At the present time ILL has no diffractometer which is suitable for such investigations. The diffractometer D4 has a large Q-range but its Q-resolution is not quite good enough for such analysis. We discuss the design parameters of a high-Q powder diffractometer, which ideally might have a Q-resolution $\Delta Q/Q \approx 10^{-3} - 10^{-2}$ for $Q_{max} \approx 25 - 30$ Å^{-1}. The diffractometer must be placed on a beamline with high-flux hot neutrons and will use neutron wavelengths in the range from 0.3 to 0.9 Å. The inclined beam-tube for hot neutrons IH2 at ILL might be used for such a diffractometer, although the inclination of 35 degrees does not easily allow a horizontal scattering plane. However, state-of-the-art mechanics and control should be able to cope with such a geometry.

1. T. Egami and S.J.L. Billinge, Underneath the Bragg Peaks: Structural Analysis of Complex Materials, Pergamon Press (2003).

PG17
NEUTRON OPTICAL BENCH USING DISPERSIVE MULTIPLE REFLECTION MONOCHROMATOR

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As we have already reported [1-3], using bent prefect crystals we have determined several strong multiple-reflection (MR) processes realized on two sets of lattice planes mutually in the dispersive setting. They provide doubly reflected beams with a narrow band-width $\Delta\lambda/\lambda$ of 10^{-4} - 10^{-3} and collimation of 10^{-4} - 10^{-3} rad. Such strong MR-processes realized in the cylindrically bent perfect crystal (often called as Renninger or *Umweganregung* effect) proved their possibility for using for ultra high-resolution monochromatization. In NPI Rez we are building a neutron optical bench employing such multiple-reflection dispersive monochromator which will operate at the neutron wavelength of λ=0.16 nm. The bench could be used e.g. for some neutron optics testing and for investigation of structure quality of real single crystals. First preliminary results will be presented.

[1] P. Mikula, M. Vrana and V. Wagner, Physica B, **350** (2004) e667-e670.
[2] P. Mikula, M. Vrana, V. Wagner and K. Inoue, Zeitschrift für Kristallographie, in print.
[3] P. Mikula, M. Vrana, V. Wagner and D. Lott, Proc. of the ICANS-XVII-17th Meeting, April 25-29, 2005, Santa Fe, New Mexico.

PG18
A CHOPPER TIME-OF-FLIGHT SPECTROMETER ON THE HOT SOURCE OF A NEUTRON REACTOR

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Present-day mechanical choppers permit us to design a chopper spectrometer on the hot source with physical dimensions very similar to those of a spectrometer on the cold neutron source (for example, IN5 at ILL). Such a spectrometer would operate over the energy range from ~ 20 meV to ~ 1000 meV with energy resolution in the range 3 to 5 %. Given the high luminosity of the hot source at ILL, the performance of such a spectrometer is estimated to be an order of magnitude superior to that of a comparable spectrometer, such as MARI, at the pulsed neutron source ISIS, well up to a relatively high incident energy of 500 meV.

PG19
A STEP TOWARDS THE LARGE-AREA PIXELATED-DETECTORS TIME-OF-FLIGHT INSTRUMENT

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The upgrade of the IN5 cold-neutrons Time-of-Flight (ToF) instrument has begun almost 10 years ago on the ground of the technological jump that was possible for the instrument components while the principle of the technique remains the same. While improving its flexibility as well as its reliability, the main goal of the upgrade was to bring this 30-years-old instrument to a best level of performance while other attractive instruments of the same type were put online in other places.

The first part of the upgrade was carried out on the primary spectrometer: from the reactor guide to the sample environment, including the disk-chopper monochromator. The 4 choppers have been changed for a more reliable 6-disk counter-rotating magnetic-bearing chopper system. The guide has been converted to a focusing guide, thanks to the possibility of obtaining reliable super-mirror neutron guides with high index (up to 3 in this case). A gain factor in flux at sample of 10 (or more) has been obtained while the sample area was reduced in size, allowing routine experiments on smaller samples.

The upgrade of the secondary spectrometer (from the sample to the detectors) will open up the possibilities of the instrument. The single detectors will be replaced by an array of 3m-long position-sensitive detectors (PSDs) in a cylindrical arrangement. In addition to a net gain of 6 in effective solid angle, the pixelated area will allow single crystal experiments complementary to those made on three-axes spectrometers. With this new type of detector, a massive data collection during measurement, not exploitable directly, will be necessarily coupled to a powerful data-processing analysis to format the results.

PG20
THE NEW TIME-OF-FLIGHT POWDER DIFFRACTOMETER FOR EXTREME SAMPLE ENVIRONMENTS AT THE HAHN-MEITNER-INSTITUT BERLIN

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The Extreme Environment Diffractometer (EXED), actually under construction at the HMI in Berlin, is based on the time-of-flight principle and will thus benefit from variable resolution to achieve either ultra-high resolution or very high intensities at conventional resolutions. EXED is devoted to studies under extreme sample conditions, for instance the TOF technique permits the access of a broad range of Q-values or d-spacing domains under scattering angle access strongly restricted to forward and backward directions by the use of highest-field magnets (25T and possibly later on 40T). Both cold and thermal neutrons are delivered to the instrument by a new multispectral extraction system and a ballistic guide and give rise to a very broad wavelength spectrum of 0.7 Å $< \lambda <$ 20 Å The neutron pulses are produced by a very complex chopper system. Depending on the speed and phases of the choppers the wavelength bandwidth can be adapted to the demand of the experimenter. The neutron beam commissioning is planned for summer 2006.

PG21
PHOTOSTIMULABLE STORAGE PHOSPHORS AND IMAGE-PLATE DEVELOPMENT FOR NEUTRON IMAGING

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Storage-phosphor imaging plates (IP) are widely used as position-sensitive detectors based on the effect of photostimulated luminescence (PSL). They consist of a film of finely dispersed storage phosphors (e.g. $BaFBr:Eu^{2+}$) in an organic binder on a thin plastic support. On irradiation, metastable color centers are created, which can then be excited by visible light to emit luminescence. Scanning the IP with a focused laser allows simultaneous excitation and detection of luminescence from the colour centers so that stored information is read out spot-by-spot. These storage phosphors can be made sensitive to thermal neutrons by adding a neutron converter. Commercial neutron IP's use a Gd_2O_3/BaFBr phosphor mixture and are also highly sensitive to γ and X-ray radiation. Neutron sensitive IP's in combination with a suitable scanner exhibit excellent characteristics of high spatial resolution (about 150 μm), large linear dynamic range (up to 7 decades), unlimited detector size, and high DQE (30 - 40 %).

Currently, there are two ILL instruments, equipped with neutron IP's, VIVALDI, the first completed instrument of the Millennium Programme, and its sister Laue Diffractometer LADI. At this presentation we will:

1. Summarize the current status of research in the field of X-ray and neutron storage phosphors with emphasis on the specific requirements for both storage phosphor and neutron converter.

2. Report the luminescence properties - emission and stimulation characteristics - and the temperature dependence, of current NIP's.

3. Report new results of comparative measurements of PSL recorded after neutron irradiation of a number of new combinations of converter/storage phosphors, namely Eu-doped BaSrFBr, CsBr etc, containing varying quantities of Gd_2O_3 or $Li_2B_4O_7$ powder.

4. Demonstrate the preparation of large uniform prototype IP's by layering $BaSrFBr:Eu^{2+}$ phosphor alternately with Gd_2O_3 converter.

PG22
IN12-UFO: A NEW CONCEPT FOR MULTIPLEXING A TRIPLE-AXIS SPECTROMETER

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The IN12 instrument is operated by the Research Centre at Jülich in collaboration with CEA Grenoble as a CRG-B instrument at the Institute Laue Langevin in Grenoble. As a triple-axis spectrometer for cold neutrons it is dedicated for high-resolution studies of low-energy excitations. To meet further challenges as a state-of-the-art instrument IN12 is currently being upgraded with a multi-analyzer option. IN12 will then be equipped with a large 2-dimensional position-sensitive detector and an array of fifteen individual analyzer blades which can be rotated and positioned separately in order to map the scattered beam on a user-chosen path in Q-ω space. We refer to this set-up as IN12-UFO (Universal Focusing Option). The innovative flexibility of the analyzer array is realized by completely non-magnetic drive mechanisms where all relevant parameters are controlled by an optical absolute encoding system. The mechanics allow to position the individual analyzers so that a) there are no gaps or overlaps as seen from the sample (optimum coverage) and b) all reflected beams from the analyzers meet at one single focus point on their way to different spots on the detector surface. The focus point is controlled by a movable diaphragm and provides the only opening between analyzer and detector shielding to prevent cross talk and to keep the background low. We will present further details of this set-up and demonstrate its flexibility and multiplex advantages for specific physical applications.

PG23
PHASE-SPACE TRANSFORMATION USING MOVING MOSAIC CRYSTALS

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The new IN16B backscattering spectrometer will feature a so-called phase-space transformation chopper disk as a device to enhance the neutron flux at the sample at the expense of beam divergence. Although the principle of phase-space transformation (PST) using a Bragg reflection from a moving mosaic crystal is known since long in neutron scattering and has been verified experimentally, some aspects of its theoretical implementation are not yet sufficiently elaborated for accurate predictions. This holds in particular for a 3-dimensional description of the PST using non-isotropic mosaic crystals. We will present our recent and ongoing work to obtain more detailed knowledge on the gain factors in terms of signal-to-noise ratios that may be anticipated.

PG24
POLARIZED NEUTRON SCATTERING AND PROTON POLARISATION *IN STATU NASCENDI*

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Time-resolved polarized neutron scattering and simultaneous NMR measurements from various small radical molecules in solvents with different deuteration have shown that a strong proton polarization gradient is established within a few seconds of dynamic nuclear spin polarization (DNP) [1]. While in these cases the polarization gradient appears to be outside the radical molecule (r=0.5 nm), an intramolecular polarization gradient has been observed with a larger biradical molecule with radical sites at 4 nm distance.

The direct proton polarization by the solid effect is known to occur preferentially at an angle of 45° with respect to the external magnetic field. In our experiments at D22 of the ILL, the deviation of the direction of the magnetic field from that of the incident neutron beam happened to be 7° in the horizontal plane. The proton-polarization-dependent intensity distribution on the area detector then would have a half-width slightly smaller in the horizontal direction than in the vertical direction. The difference is of the order 1/1000 with a radical molecule having a dumb-bell proton distribution, which is hardly more than the experimental error. A future experiment aiming at the detection and use of the angular dependence of the electron-spin proton-spin interaction in structural studies will do better by at least an order of magnitude with a larger angle between the magnetic field and the neutron beam.

[1] B. van den Brandt, H. Glättli, I. Grillo, P. Hautle, H. Jouve, J. Kohlbrecher, J.A. Konter, E. Leymarie, S. Mango, R.P. May, A. Michels, H.B. Stuhrmann, and O. Zimmer, Time-resolved nuclear spin dependent small-angle neutron scattering from polarized proton domains in deuterated solutions, Eur. Phys. J. B 49, 157-165 (2006)

PG25
NEUTRON IMAGING FOR MODERN ENGINEERING APPLICATIONS AND EARTH SCIENCES

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The unique properties of neutrons make them very powerful tools in material and earth sciences, where the probing beam has to penetrate metals and rock material. The high intensity beam of Neutrograph, ILL's neutron tomography facility, allows to visualize even small contrasts and to make investigations in real-time. We present typical experiments from materials and earth sciences as well as engineering applications.

In material sciences, the high mechanical requirements for metal joints led to the development of a multitude of new welding and bonding techniques. Preliminary experiments at Neutrograph show internal structures in a friction stir weld and a diffusion profile in a transient liquid phase bond. A non-destructive testing method is urgently needed also in archaeology for the investigation of rare and

precious specimens. X-rays are suitable to only a limited extent. Neutrons offer the capability of penetrating even bulky materials and providing enough contrast between the fossil and the rock material. We present results from 50-million-years-old plant fossils.

The high intensity of our neutron beam makes Neutrograph the neutron imaging facility with the highest time resolution. In cyclic processes a time resolution of down to 100 μs is available, for tomography it is a few seconds. Two-phase flows in channel systems and diffusion processes in porous media can be investigated in real-time.

PG26
THE REFLECTOMETER ADAM AT THE ILL

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The angle-dispersive neutron reflectometer ADAM at the ILL, operated by the Ruhr-University Bochum as a CRG-B instrument, offers high flux combined with an excellent Q resolution and full polarization analysis. Since the inauguration ceremony ten years ago nearly all the important components of the instrument have been modified to remain a state-of-the-art instrument. To supplement the zero-dimensional detector a two-dimensional area detector was installed. A new detector electronics allows to follow the evolution of the detector image in real time and the possibility of GISANS measurements on ADAM was demonstrated. The 7-crystal HOPG monochromator was replaced by a 21-crystal monochromator increasing the accepted wavelength band by approximately a factor of 2 and wide-angle polarization analyzers have been mounted. A contact-free flipper reducing the small-angle scattering will be available for the start of the next cycle and we envisage to replace the Beryllium filter used for λ/2 suppression by a fundamental monochromator, reflecting only one wavelength, in the near future. A large electromagnet for fields up to 0.8 Tesla is available fitting on the sample position together with a closed cycle refrigerator (temperature range 10 to 400 K). For the restart of the reactor an additional liquid Helium cryostat will allow temperatures down to 1.5 K. For more sophisticated sample environments the ILL equipment can be used. Different types of shear cells have been developed recently and a new flow cell will arrive in this summer. The dedicated and continuing effort to improve and optimize the characteristics of ADAM has resulted in a large number of scientific highlights covering all areas of neutron reflectivity. A brief overview on already published results from our external users will be given.

PG27
ADAM2 - RECONSTRUCTION OF THE REFLECTOMETER ADAM AT ILL

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It is now ten years since the construction of the reflectometer ADAM started at ILL. About one and a half years later the first users arrived and since then ADAM offers unique possibilities for the investigation of interfaces and thin films. To maintain the present outstanding position in the area of neutron reflectivity and remain competitive with recently built instruments we plan to reconstruct the reflectometer ADAM with the main focus on magnetic scattering for the analysis of perpendicular and lateral magnetic nanostructures. ADAM2 will again be an angle-dispersive reflectometer. The flux will be increased by roughly a factor of 50 due to a new beam position (anticipated present IN16 position), new neutron guide (H53), fundamental monochromator, reflecting only one wavelength, and longer collimation. For the incident beam the instrument will offer variable wavelengths (to reduce aluminum scattering) and monochromators with different wavelength resolution between 0.5 and 2 %. Optional neutron optic devices to focus the beam will push the limit with respect to the samples size needed for a reflectivity experiment aiming at 1x1 mm^2 samples. The polarization analysis will be improved by use of contact-free flippers and an efficient area analyzer. The shielding for the large, fast and efficient area detector will be optimized. Magnetic fields up to 7 Tesla will be available at the sample position by use of a super-conducting magnet. We expect unique possibilities for the investigation of magnetic thin films due to the high flux (10^8 without collimation), the low background (10 orders of magnitude dynamic range) and excellent polarization analysis.

PG28
RESULTS OBTAINED ON ADAM

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As ADAM is a CRG-B instrument a fraction of the beam time is reserved for the University of Bochum operating the instrument. The focus of our research is the area of magnetic interfaces and thin films. Several examples, obtained during the last years, will be presented: 1. Finite size effect: It has been shown that the thickness dependence of the helical antiferromagnetic ordering temperature T_N for a Ho film decreases characteristically with the film thickness. 2. Exchange coupling: By introduction of hydrogen in the V layers of a Fe/V superlattice it is possible to tune the magnetic coupling strength between the Fe layers and to switch them from ferromagnetic to antiferromagnetic coupling. 3. Exchange bias: The asymmetry in the first and second magnetization reversal of CoO/Co bilayers has been related to nucleation or domain-wall movement and magnetization rotation, respectively. 4. Domain walls: Banana shape off-specular scattering has been explained by a simple optical model including refraction at domain walls. 5. Quantum spin states of neutrons: From the intensity at the total reflection edges of a magnetic film the quantum spin state of neutrons inside magnetic samples has been proven. 6. Heusler alloys: In $[Co_2MnGe/V]_N$ multilayers an antiferromagnetic dipolar ordering was found stabilized by magnetic roughness. 7. Lateral structures: Correlated magnetic reversal in magnetic stripe arrays was resolved by specular and off-specular neutron reflectivity. In addition, we have recently started activities in soft-condensed-matter physics. In particular we could extract first results on the influence of the solid-liquid interface on the structure and dynamics in liquids under shear. Additionally the crystallization of polymer micelles close to attractive and repulsive walls was investigated in detail.

PG29
PRESSURE/FLOW CELL FOR THE INVESTIGATION OF LIQUID SAMPLES

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For flow experiments the pressure necessary to pump a sample through a narrow slit or tube increases with viscosity and flow rate. The problem with high pressures in neutron experiments is the bad signal to background ratio. To overcome this problem we have developed new pressure cells for the investigation of liquids and gases using a bunch of narrow capillary tubes. Parallel tubes (inner diameter down to 0.2 mm, outer diameter below 1 mm) allow covering a large neutron beam of several square centimetres. All the equipment fits into a standard ILL orange cryostat. Heated capillaries leading down the cryostat allow an *in situ* change of pressure. The equipment was tested for pressures up to 2 kbar.

Two types of cells have been constructed. The first one consists of one capillary tube passing the area of the neutron beam several time and is suited for pressure experiments. The second one consists of several capillary tubes connected to a reservoir and allows flow experiments. To account for the long times needed for a neutron experiment the sample is pumped forth and back. The data acquisition is triggered by the change of flow directions.

Data from a pressure experiment made on IN16 with samples of glycerol, a pure and a block copolymer solved in D2O will be presented. The samples show a slowing down of the translational diffusion with pressure. Additional information is extracted from an elastic scan. In addition we will present a flow experiment performed with a decanol sample. The inelastic scattering from the flowing liquid is clearly visible.