Friday 17 September
Morning session

Time		Session/Subject Area	Speaker
09:00	AUDITORIUM	Feedback from science sessions	***Andrew Harrison*** Institut Laue-Langevin
09:45		The importance of data analysis	***Mark Johnson*** Institut Laue-Langevin
10:30		Interface laboratories at the European Photon and Neutron site (EPN): perspectives and practicalities	***Trevor Forsyth*** Institut Laue-Langevin
11:15		Coffee break	
11:45		The wider environment	***Richard Wagner*** Institut Laue-Langevin
12:15		Summary and actions	***Andrew Harrison*** Institut Laue-Langevin
12:30		Farewell	***Richard Wagner*** Institut Laue-Langevin

NEUTRONS FOR SCIENCE®

Posters index

ILL 2020 Vision - 15-17 September 2010 - Grenoble - France

Zero dimensional systems probed in four dimensions: single crystal study of an add-electron nine-metal ring by inelastic neutron scattering.

Michael L. Baker (1,2), Stefano Carretta (3), Paulo Santini (3), Tatiana Guidi (4), Floriana Tuna (2), Grigore A. Timco (2), Hannu Mutka (1), Eric J. L. McInnes (2), David Collison (2), Hans U. Güdel (5), and Richard E. P. Winpenny(6).

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The study of magnetic based molecules by inelastic neutron scattering (INS) has played a crucial role in characterization [1] and investigation of novel physical phenomena [2,3]. INS provides a direct probe of quantum spin eigenvalues, while neutron momentum transfers (Q) reveal wavefunction spatial properties. Instrumental development has enabled for the first time, a broad coverage survey of S(Q,ω) on a $\{Cr_8Mn\}$ ring, which is an odd-numbered odd-electron ring. Calculated response has shown excellent agreement with experimental data showing direct measurement of correlation functions and energies which could not be obtained by other techniques.

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Gas loading apparatus for Paris-Edinburgh cells

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The Paris-Edinburgh cell [1] is a widely used large-volume opposed-anvil pressure cell for neutron scattering. Up until now it has been successfully used with a number of solid and liquid samples and pressure media. However, so far there is no reliable technique developed for loading gases into sample volume. The only known method is a cryogenic loading of liquid gases. However this technique cannot be used with some gases such as helium or hydrogen. The ability to load gases at room temperature would bring several benefits. It would allow us to study any gas or gas mixture under high pressure. It would also make it possible to replace liquid pressure transmitting media with gases in order to achieve more hydrostatic compression conditions. Here, we will present a gas loading device for Paris-Edinburgh cell. A special clamp holding Paris-Edinburgh cell anvils and a pressure vessel have been designed. The clamp with anvils and gasket are placed into the vessel, which allows us to introduce gas under pressure of up to 150 MPa into the sample volume and compress the anvils to seal the gas enclosed within the gasket. The anvils with the sealed gasket are then placed into Paris-Edinburgh press for further compression and neutron scattering measurements.

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Dynamics of carbon-based molecular crystals using Time Of Flight spectrometers

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We present two different examples of studies involving Time Of Flight (TOF) spectrometers – IN4 and IN5 – coupled with molecular dynamics calculations to resolve the dynamics of carbon-based molecular crystals. The first example concerns the co-molecular crystal C_{60}•C_8H_8, which has the particularity of being a rotor-stator molecular system at ambient temperature. TOF data allowed us to directly witness the phase transition from the disordered rotor-stator phase, in which the cubanes remain static whereas the fullerenes rotate freely, to an ordered phase in which the fullerenes rotations are reduced to librations [1]. The second example is the so-called "nano-peapods" guest-host system in which C_{60} fullerenes are encapsulated in single-walled carbon nanotubes. By orienting the peapods in a plane, we are able to witness the longitudinal motion of the fullerenes along the nanotubes axis and follow this dynamics as a function of temperature.

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Frustrated magnetic structure of Y-substituted CePdAl studied by powder neutron diffraction

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CePdAl is a heavy-fermion antiferromagnet with T_N = 2.7 K, crystallizing in the ZrNiAl-type structure. The magnetic structure is described by the propagation vector k = (1/2, 0, x), x = 0.35, with the cerium magnetic moments aligned along the c-axis [1]. One third of magnetic moments remains disordered due to the geometrical frustration. Specific heat measurements on substituted $Ce_{1-x}Y_xPdAl$ compounds revealed strong reduction of T_N with Y substitution and the antiferromagnetic order vanishes around x = 0.2. To investigate the microscopic details of the changes in the magnetic structure evoked by nonmagnetic ion substitution, we have performed an experiment on the powder neutron diffractometer E6 at HZB on the samples with x = 0.02, 0.06, 0.1. Measurements showed the magnitude reduction of the ordered cerium moments with Y substitution while the propagation vector and other magnetic structure characteristics remain unchanged.

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Probing magnetism in electrodeposited thin films of $Co_xNi_yCu_z$ using polarised neutron reflectivity

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Electrodeposition is one of the oldest thin film deposition techniques and has enjoyed something of a renaissance in recent years, matching MBE and sputtering in many test of quality, being able to grow epitaxial [1] and very thick films with low roughness's [2]. In this study we use polarised neutron reflectometry, on the CRISP beamline at ISIS, to study the magnetic and interface properties of simple $Co_xNi_yCu_z$ / Cu bilayers and multilayers. The composition of the layers was controlled during growth by a simple potentiostatic method which allows for a wide range of compositions, including pure copper, to be grown from a single electrolyte solution without removal of the sample. This simple ternary alloy system allows for useful magnetic properties with improved corrosion resistance and roughness compared to a binary cobalt and copper system.

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Measuring gravitationally induced quantum phaseshifts with Ramsey's method of separated oscillating fields

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We propose to apply Ramsey's method of separated oscillating fields to the spectroscopy of the quantum states in the gravity potential above a horizontal mirror. This method allows a precise measurement of quantum mechanical phaseshifts of a Schrödinger wave packet bouncing off a hard surface in the gravitational field of the Earth. Measurements with ultracold neutrons will offer a sensitivity to Newton's law or hypothetical short-ranged interactions, which is about 21 orders of magnitude below the energy scale of electromagnetism.

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Temperature induced proton migration and phase transition in deuterated 3,5 pyridinedicarboxylic acid

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Hydrogen bonds are ubiquitous in materials across the chemical spectrum, from inorganic to biological. They influence the structure, the functionality, and therefore the potential applications of materials in which they are present. [1] Of particular interest are short strong hydrogen bonds which, contrary to the primarily electrostatic nature of their weaker counterparts, possess a quasi-covalent character. Their presence can lead to interesting phenomena, such as proton migration [2] and proton order-disorder transitions. 3,5-pyridinedicarboxylic acid (35PDCA) contains one of the shortest N-H…O hydrogen bonds reported in the literature, with an N…O separation of 2.51 Å. [3] A two-temperature single crystal neutron diffraction study on the fully protonated compound has shown that temperature dependent proton migration occurs in this hydrogen bond. [4] At 15K, the proton is closer to the nitrogen atom, with a N-H distance of 1.213(4) Å and O…H distance of 1.311(5) Å; at 296K it has moved significantly towards the oxygen atom, resulting in an N…H distance of 1.308(6) Å and an O-H distance of 1.218(6) Å. The same effect, but more pronounced, has been found in crystals in which the carboxylic hydrogen atom positions involved in hydrogen bonding have been deuterated. In this case, the N-D distance changes from 1.161(9) Å at 15 K to 1.471 (6) Å at 300 K. Variable temperature powder diffraction experiments on both the fully protonated and fully deuterated 35PDCA between 15 and 300 K, using both laboratory X-ray diffraction and high resolution neutron diffraction, [5] were carried out. It was shown that in the protonated phase, the unit cell volume varied smoothly with temperature in the range observed. However, the unit cell volume variation for deuterated 35PDCA shows a change of curvature between 150 and 200 K. This effect is reversible, reproducible and it is observed both in the powder X-ray and neutron diffraction data. Also, using variable temperature single crystal neutron diffraction experiments, it was found that the deuteron position in the hydrogen bond changes gradually over the temperature range employed. This shows that unlike in its protonated analogue, the proton migration in fully deuterated 35PDCA is facilitated by a structural change.

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Neutron backscattering and spin-echo experiments on globular proteins in aqueous solution

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Proteins in solution form highly monodisperse colloidal suspensions. In addition to their biological role, proteins in solution are therefore of fundamental interest in a context of soft matter science. Proteins, however, differ in one important aspect from many simple colloidal systems: The distribution of charges on the surface of a protein is in general inhomogeneous. This inhomogeneous surface charge distribution can in turn be assumed to have a fundamental biological relevance in controlling for instance aggregation phenomena and biological activity such as docking processes. Characteristic of proteins in their native environment is the molecular crowding – i.e. relatively large volume fractions being occupied by proteins – and the aqueous solvent containing salt ions. These salt ions are crucial for the understanding of the effective interactions of proteins and the resulting structures as well as indeed the dynamics [1]. We study protein dynamics in aqueous solutions with different salt concentrations by quasi- elastic neutron scattering [2] performed at selected temperatures and protein concentrations. Spin-echo spectroscopy was used to further investigate the center-of-mass diffusion of the proteins. It was found that the addition of salt has a significant effect on the relaxation rates on length scales commensurate with protein center-to-center distances. By interpreting both backscattering and spin-echo spectra, we address the internal self-diffusion as well as the collective diffusion [3].

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Interesting proton behaviour in molecular complexes of urea and its derivatives

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Systems showing proton disorder, transfer and migration are an area of increased interest in recent times and can be probed using variable temperature diffraction experiments. These often subtle processes can affect the molecular properties of systems and are often observed in materials containing short strong hydrogen bonds. Our aim here is to be able to characterise systems that show such effects, and then in turn be able to predict and control this potentially "tunable" behaviour. These processes have already been observed in complexes of urea [1]. Single crystal X-ray and neutron diffraction (on VIVALDI at ILL) have been used to study molecular complexes of urea and its derivatives with a particular focus on characterising the hydrogen atom behaviour. The proton behaviour is monitored over variable temperatures to show the movement of the proton with changing temperature.

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The role of myelin proteins in degenerative diseases – a neutron investigation

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Myelin is the multi-lamellar tightly packed membrane which is wrapped around the nerve axons in the central nervous system (CNS) and the peripheral nervous system (PNS). Besides the fast transfer of nerve impulses, electrical insulation of the axons and mechanical protection, it is essential for the proper functioning of the vertebrate nervous system. Myelin is destroyed by autoimmune processes in inflammatory demyelinating diseases such as multiple sclerosis (MS) in the CNS and the Guillan-Barré syndrome in the PNS. Biochemically the main components of myelin are lipids (75-80%) and proteins (20-25%) [1]. In spite of a well-defined subset of the myelin-specific proteins [2], relatively little is still known about their influence on the membrane dynamics, i.e. the myelin stability.While the CNS contains only the myelin basic protein (MBP) and the proteolipid protein (PLP), the constituents of the PNS are the MBP, the protein P0, the basic protein P2 and the PMP-22 proteins. While MBP-C1 cornnsponds to the least modified form of MBP, MBP-C8 mimics the form seen, e.g. in multiple sclerosis [3].During our study the components of the membrane, the lipids and proteins, and their interactions are investigated to understand better the structure and dynamics of healthy and affected myelin. The research profits by the unique advantages of neutron scattering techniques, a method to probe biological matter. Experiments on reconstituted membranes made of mixed DOPS+DOPC lipids (1:1 ratio) with and without the myelin proteins P2 and MBP-C1, the least modified form of MBP, were recently performed on IN5, IN13 and D16 at the ILL and are presented here. The results suggest a stabilization effect induced by the myelin proteins on the membrane dynamics.To understand better the structure and dynamics of affected and healthy myelin, experiments with the MBP-isomers MBP-C1 and MBP-C8 bound to a reconstituted membrane are planned as an investigation of the role of the mutant C8 on the membrane stability.

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SUN-2: A high-intensity and versatile source of ultra-cold neutrons

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Ultra-cold neutrons (energy<250 neV) play an important role in fundamental investigations in particle physics, such as, in the search for the neutron electric dipole moment and precision measurements of the neutron lifetime. Currently the most intense source in the world is the PF2 turbine at the ILL which provides densities of around 50 cm^3. The new SUN-2 source currently in development under the ESFRI ILL20/20 project is based on conversion of a cold neutron beam to the ultra-cold energy range via single phonon (8.9 Å) or multi-phonon (3 - 8 Å) excitations in a He-II converter. SUN-2 will demonstrate a density of more than 1000 cm^3 during an experiment on PF1b this year. The potential of the source in a magnetic UCN storage application will also be demonstrated in a prototype version of the HOPE magnetic trap [2]. SUN-2 will have a 4 L volume of ultra-pure He-II (via superleak filtration) with highly reflective walls cooled to below 0.8 K. UCN will be accumulated and extracted vertically out of the source with a mechanical cold-valve (demonstrated by the prototype SUN-1 [3] to be used as a source for the Granit experiment).

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Neutron scattering and the square-lattice Heisenberg antiferromagnet

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The square-lattice Heisenberg antiferromagnet is an important model system in quantum magnetism. Experimental and theoretical studies of this model have provided deep insights into the role of low-dimensionality and quantum effects in the static and dynamical properties of the many-body spin systems. Inelastic neutron scattering on well-chosen compounds is of crucial importance, allowing a direct benchmarking of theoretical concepts and often revealing unexpected phenomena.The poster will present recent neutron scattering results, obtained on the ILL triple-axis instruments IN20 and IN14, from two different S = ½ square-lattice materials. We will show the strength of polarization analysis to disentangle weak magnetic continua from strong sharp magnon peaks and thus leading to the first observation of a 3-magnon continuum in such system. Then, we will discuss the exciting possibilities offered by the combination of strong vertical magnetic field and high resolution spectroscopy to explore the rich spin dynamics of square-lattice antiferromagnets in applied field.

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Magneto-structural correlations in $[Mn_3O]^{7+}$ core single-molecule magnets

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Since the discovery of Mn_{12} and the characterization of its magnetic properties synthetic chemists have put a lot of effort into the search of new single molecule magnets (SMMs). This has been accompanied by the work of spectroscopists and theoreticians who try to identify the magneto-structural correlations that lead to strong SMM behavior. Recently a series of Mn_6 SMMs, including the former record barrier magnet (U_{eff} = 86.4K) was published [1]. The Mn_6 clusters consist of two off-set stacked $[Mn_3O]^{7+}$ subunits, whose metal ions are bridged with a μ_3-oxygen and three oximate bridges. We present the results of DFT calculations on the dependence of the exchange coupling within the Mn_3 subunits on the out-of-plane shift of the μ_3-oxygen and on the oximate twisting angle. Furthermore different $[Mn_3O]^{7+}$ core SMMs were synthesized and their electronic structures were characterized by SQUID measurements, high-field high-frequency EPR and inelastic neutron scattering. These experimental results display the effect of the local ion easy axis tilting in respect to the global zero-field-splitting axis on the relaxation barrier.

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Quasielastic and elastic scattering studies of aligned DMPC multilayers at different hydrations

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Lipid model membranes such as 1,2-Dimyristoyl-sn-Glycero-3-Phosphocholine (DMPC) serve as role models for their more complex counterparts in biological systems. Quasielastic neutron scattering (QENS) [1,2], inelastic neutron scattering (INS) [3] and neutron spin echo spectroscopy (NSE) [4] have been employed to study local as well as collective dynamics of these membranes on a ps-ns time scale. Most of these studies lack a systematic investigation of the behaviour of the model membranes in dependence on their hydration. We now started a detailed investigation of hydration effect on model membrane systems. In the here presented work we have used chain deuterated DMPC-d54 to study the dynamics of the lipid head group. The hydration for the samples was adjusted by hydrating them for pure D2O and from a saturated salt solution respectively, resulting in two different states of hydration (repeat distance d=62.5 Å with 15 water molecules per lipid and d = 54.9 Å with 9 water molecules per lipid, respectively). The alignment and mosaicity were checked prior to the measurements for all samples. QENS experiments were performed at the time-of-flight spectrometer TOFTOF at the Munich research reactor FRMII , elastic incoherent neutron scattering (EINS) measurements were performed at the backscattering spectrometers IN13 and IN16 both at the Institut Laue-Langevin. To cover the main phase transition from the gel phase to the liquid phase of DMPC around 23°C experiments were performed in a temperature range from 5°C to 30°C. For the QENS experiment elastic incoherent structure factors (EISF) and diffusion constants were extracted, which indicate that hydration has a clear influence on the mobility of this system [5]. The integrated intensities from the EINS experiments showed a shift of the main phase transition as a function of hydration which coincides with a change of the slopes of the mean square displacements [6]. In addition to earlier QENS [1,2] and backscattering [7] investigations, these experiments extend our knowledge of model membrane systems.

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Pressure cell for inelastic neutron scattering

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Compared to neutron diffraction, inelastic scattering experiments typically require an order of magnitude longer data collection times for the same sample size and sample environment [1]. We present the design of the piston-cylinder pressure cell optimised by the means of finite element analysis in order to minimize the attenuation. The plug with electric feed-through and manganin pressure sensor enables the accurate monitoring of pressure in the whole range of temperatures. The novel design of the pressure seal eliminates the need in the teflon capsule providing more space for the sample. The cell is made of non-magnetic materials and is capable of reaching the pressure of 2 GPa.

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4. Presenting authors’ abstracts

NEUTRONS FOR SCIENCE®

4.1 Afternoon session
Wednesday 15 September

Millennium update

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The ILL Millennium Programme was approved at the end of 2000 and the initial financial commitments were included in the 2001 budget. The aim of the Millennium Programme is to maintain and develop the ILL's instrument suite as the world reference, as well as to upgrade our support facilities and basic neutron technologies so that they continue to satisfy changing demands from the user community. In the first stage of the Programme covering the period 2001-2009, six new instruments were delivered and a further eight were extensively upgraded. Significant developments were also made in detectors, spin polarisers and monochromators, and 350 meters of new high-performance neutron guides were installed. At the end of this stage, the detection rate for all the ILL instruments has increased by an average factor of 19. The total budget for this period was 42 M€, i.e. 4.6 M€ per year. We are currently working on the second stage of the Millennium Programme for the period 2009-2014. Our goals are to deliver 4 new instruments, to upgrade a further 4, to redesign and install 600 metres of new neutron guides, to enhance our sample environment suite, and to improve some of our basic infrastructures, including the neutron guide halls. In parallel, seven new or upgraded Collaborating Research Group (CRG) instruments will be added to our suite. By the end of 2010, three of the upgraded instruments will be completed, as will the installation of two new cold guides. The modernisation programme is moving forward at a rapid pace, motivation within the various teams is high, and plenty new of ideas are emerging to fuel the next stage of our Millennium Programme for the period 2013-2017.

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Neutron scattering studies of model magnets

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In recent years systematic studies of model magnets have revealed novel magnetic states of matter, quantum phase transitions between them, new types of order, exotic elementary excitations and other unconventional phenomena triggered by quantum many-body effects, frustration, or strong correlations. Neutron scattering experiments in these areas have often provided crucial input for the fundamental understanding of these systems, and they have been enabled by the availability of state-of-the-art instrumentation, high-quality single-crystal samples, and sample environment providing extreme conditions (temperature, magnetic field, and pressure). I will review our experimental work on a number of model magnetic materials, ranging from the discovery and control of novel elementary excitations in low-dimensional systems [1,2] to unconventional ordering phenomena [3-5]. The results will be discussed in the context of past ILL Millennium-Programme developments and future perspectives in neutron spectroscopy, especially on small samples and in high magnetic fields (proposed instruments exTAS and HIFI).

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Physics of magnetic charges in spin ice

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Several recent papers have revealed the emergence of nearly point-like magnetic charges or "monopoles" in spin ice materials like $Dy_2Ti_2O_7$. Spin ice is named after water ice, H_2O, in which the protons (H^+) can become free to carry electricity. The emergent magnetic monopoles of spin ice are, in principal, equivalent to the electrical charge carriers of water ice: protons and proton-holes. In this talk I will show how this picture was derived by neutron scattering experiments, but how "slower" techniques like μSR and bulk magnetic relaxation were necessary to fully visualize the monopole motion. I will conclude by highlighting recent experimental work that has demonstrated the magnetic equivalent of electricity ("magnetricity") in spin ice, including measurement of the "elementary" magnetic charge, and the experimental distinction of free and bound magnetic monopole currents.

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Structures under high pressure: what D20 can do for you

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High pressure is a window to observe matter in unusual and sometimes exotic states. In this talk I will review results of high pressure powder neutron diffraction experiments carried out at D20 by my group and collaborators [1,2]. These measurements were made possible through our commitment over the last five years to install and further develop at the ILL one of the most advanced high pressure technologies currently available. I will talk about the magnetic structures we discovered in solid oxygen at 6-8 GPa (60-80 kbar), and temperatures of 4-300 K [1]. A second example covers the discovery of "salty" ice VII, a high-pressure ice structure which is alloyed with LiCl, and which we identified by in-situ diffraction experiments at D20 [2]

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Membranes and Interfaces

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Biological systems near interfaces represent one of the most dynamic and expanding fields in science and technology and have been at the centre of recent major scientific and technological advances [1]. Biological interfaces include the surfaces of cells and organelles within cells where many biological mechanisms happen, as well as artificial mimics of biological surfaces. Current research in membrane protein biophysics highlights the emerging role of lipids in shaping membrane protein function. Cells and organisms have developed sophisticated mechanisms for controlling the lipid composition and many diseases are related to the failure of these homeostatic regulatory mechanisms. One of the recent advances in the field is the discovery of the existence of coexisting micro-domains within a single membrane, important for regulating some signaling pathways. Many important properties of these domains remain poorly characterized. The characterization and analysis of bio-interfaces represent a challenge. Performing measurements on these few nanometer thick, soft, visco-elastic and dynamic systems is close to the limits of the available tools and methods. Neutron and x-ray reflectometry are rapidly developing techniques for these studies and are attracting an increasing number of biologists and biophysicists at large facilities. As the deuteration of proteins is becoming an active field of research, the use of fully deuterated or partially deuterated proteins has opened up new possibilities in the study of lipid protein interactions or protein structures at lipid surfaces. Examples of recent reflectivity studies on the structure and fluctuations of model membranes at interfaces and the interaction these with proteins will be presented. The need for future developments particularly in off-specular measurements for the study of domains and fluctuations will be highlighted.

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Surface diffusion studies using neutron spectroscopy

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Neutron spin-echo (NSE) spectroscopy [1] is not a technique that comes to mind immediately for surface science studies as most neutron spectrometers need quite large sample quantities due to the limited beam intensity. In this presentation we will show, however, that NSE can give a wealth of new information that is not accessible with more standard techniques and that it can help to understand surface diffusion – especially if it is used in combination with other neutron and helium scattering techniques [2,3]. Molecular dynamics simulations are used to verify the interpretation of our data and give deep insights into the microscopic surface diffusion [4]. We will present a range of data from aromatic hydrocarbons adsorbed on graphite and we will show how spectroscopy can be used for a "perfect" friction experiment.

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Neutron reflectometry and gravitational states

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The "whispering gallery" effect has been known since ancient times for sound waves in air, later in water, more recently for electromagnetic waves of a broad range: radio, optics, Roentgen etc. It consists of wave localization near a curved reflecting surface. For matter waves it would include a new feature: a massive particle would be settled in quantum states with parameters depending on its mass. Here we present the first observation of the quantum whispering gallery effect for matter waves, namely for cold neutrons [1], measured at D17 [2] and PF1B [3] instruments at the ILL. This problem provides an example of an exactly solvable problem analogous to the "quantum bouncer"; it is complementary to the recently discovered gravitationally bound quantum states of neutrons [4]. These two phenomena provide the first direct demonstration of the weak equivalence principle for a massive particle in a pure quantum state. Deeply bound whispering gallery states are long-lived and weakly-sensitive to surface potential; highly excited states are short-living and very sensitive to the wall potential shape. Therefore they are a promising tool for studying fundamental short-range interactions [5], quantum neutron optics and surface physics effects. Studies of/with the gravitational and centrifugal quantum states of slow neutrons will be continued using the GRANIT spectrometer that has been constructed recently at the ILL. The scientific program to be studied using the GRANIT spectrometer was discussed at the dedicated GRANIT-2010 Workshop [6] in Les Houches, France, 14-19 February 2010. The topics covered applications of these phenomena (this spectrometer) to various domains of physics, ranging from studies of fundamental short-range interactions and symmetries to neutron quantum optics and surface investigations, as well as related instrumental and methodical developments.

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Preparing ILL for the future

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The Millennium Programme has made a tremendous difference to ILL's performance, with the average detection rate across the instrument suite rising by a factor of almost 20, and a marked increase in the scope of science that can be done here. Plans are in place and funding approved to maintain the momentum of the Programme through to 2014. However, it is not too early for us to plan developments yet further into the future, working with the user community on a strategy to deliver the best science through neutron methods throughout the next decade. An outline of the main components of this strategy will be given: specific new or upgraded instruments; improved neutron delivery systems; better infrastructure such as sample environment, support laboratories or software. Several of these projects benefit from recent technical developments that promise leaps in performance. Some of the key principles for assessing the various strands of this strategy, and establishing priorities will be presented, starting with the scientific opportunities, and the size and strength of the user community in various fields – now and in the future.

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4.2 Morning session

Thursday 16 September

Overview of guides, sources and guidehalls

Ken Andersen (1)

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An overview of the current neutron delivery system will be presented. In addition we will present the options for the location of new instruments, which may imply the need to build new guides, sources or a new guidehall.

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List of proposals in the clip session

HIQ: Total-scattering diffractometer to high Q for PDF determination;
Michaela Brunelli, Institut Laue-Langevin, France

OCTOPUS: multimodal diffractometer for neutron macromolecular crystallography;
Matthew Blakeley, Institut Laue-Langevin, France

Neutron-CSI: Integrated platform for non-destructive Composition and Stress Imaging with Neutrons;
Thomas Materna, Institut Laue-Langevin, France

RAINBOWS: Refractive Analysis of Interfaces with Neutron Beams Optimised for a White Spectrum;
Bob Cubitt, Institut Laue-Langevin, France

D44: Multiple beam SANS for dynamic studies on small sample volumes;
Albrecht Wiedenmann, Institut Laue-Langevin, France

VCN-SANS: Compact High Resolution SANS using very cold neutrons;
Shane Kennedy, ANSTO, Australia

S18B: High precision neutro interferometer;
Yuji Hasegawa, Atom Institut, Austria

HIFI: HIgh magnetic Field Instrument for spectroscopy and diffraction;
Mechthild Enderle, Institut Laue-Langevin, France

BATS: Backscattering And Time-of-flight Spectrometer;
Bernhard Frick, Institut Laue-Langevin, France

PANTHER: Polarisation ANalysis with THERmal neutrons;
Pascale Deen, Institut Laue-Langevin, France

RAMSES: RApid Measurement and Special Environment time-of-flight Spectrometer;
Helmut Schober, Institut Laue-Langevin, France

FIPPS: FIssion Product Prompt gamma-ray Spectrometer;
Herbert Faust, Institut Laue-Langevin, France

SANS-SESSANS: Combined SANS-SESSANS: From 1 nm to 100 micrometre in one instrument;
Wim Bouwman, Institut Laue-Langevin, France

exTAS: Next-generation, TAS for small samples and extreme conditions;
Jiri Kulda, Institut Laue-Langevin, France

TOFLAR: Time OF Flight with LArmor Precessions;
Ad Van Well, Delft University of technology , The Netherlands

SuperSUN: Small Volume, high-density ultra-cold neutron source;
Oliver Zimmer, Institut Laue-Langevin, France

PST: Phase space transformer: source of high intensity monochromatic pulsed beams of ultra-cold neutron;
Helmut Rauch, TU, Vienna

NANODIAMOND: Diamond Nano-powder reflectors for very cold neutrons;
Valery Nesvizhevsky, Institut Laue-Langevin, France

ALADIN: Advanced Laue Diffraction Instruments using Neutrons: move VIVALDI and/or CYCLOPS;
Marie-Hélène Lemée-Cailleau, Institut Laue-Langevin, France

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New standards in sample environment

Eddy Lelièvre-Berna, (1) **Helmut Schober** (1)

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The actual sample environment equipments suite has been designed for instruments built a few decades ago. Since then, we have considerably improved the ILL instruments and the experiments are now slowed down by the performance of the sample environment. There are also many scientific challenges that cannot be investigated without specific equipment presently unavailable at ILL. We present the work performed during the past few years for modernizing the equipments and building the foundation for the next-generation sample environments. We then propose to establish a new standard that will permit to exploit the new instruments and to develop the environments not presently available for investigating novel scientific challenges.

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High steady magnetic fields for neutron and X-ray scattering

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Fabrice Wilhem (3)

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Research in high magnetic fields applies to a large range of topics in contemporary science. Steady magnetic fields up to 45 T are available for macroscopic and local probes and create numerous open questions that can only be answered by the knowledge of the crystalline or magnetic structure as well as the microscopic static and dynamic correlation functions, directly probed by the neutron scattering cross section. However, only up to 17.5 T are available for neutron scattering today. Steady magnetic fields of 30 T and more require resistive technology, either alone or together with hybrid technologies. This implies an infrastructure of considerable complexity. Grenoble is the only place in the world where such an infrastructure can be shared by world-class X-ray (ESRF) and neutron sources (ILL), and favourably located between two rivers. ESRF, ILL, LNCMI, HFML Nijmegen, HLD Dresden have completed a design study financed by the European commission (FP7) to evaluate the feasibility of 30 T - 40 T magnets at the Grenoble site in combination either with X-ray or neutron diffraction. 30 T in the most versatile vertical split-coil geometry have been shown to be feasible in a compact resistive magnet with 34 mm bore and 180° open scattering angle. Such an installation should allow neutron and X-ray experiments in a range of fields completely unexplored to date.

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4.3 Parallel sessions

Thursday 16 September

Spectacular effects observed by neutron scattering in nanoporous materials

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Interesting results have been recently observed concerning molecular diffusion in nanopores, e.g. quantum effect, blowgun effect, levitation effect, explanation for the discrepancies between various techniques, non ideal behaviour of adsorbates in MOFs, etc. Most of these effects can only be observed at the microscopic level by neutron scattering. Following molecular diffusion in porous networks requires a wide range of time scales, a limitation towards long times being still problematic with neutron techniques. Other desired improvements will be discussed. At very short times, where vibrational modes are observed, the IN1 LAGRANGE project will extend considerably the range of applications of vibrational spectroscopy with neutrons.

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High throughput neutron diffraction in chemistry – new opportunities in hydrogen location in molecular and materials structure

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Many structural studies of small molecule materials now rely on the ability to study structures on a shorter timescale, to examine a series of samples or a single sample under a range of conditions. This "high throughput" approach has only recently become feasible for neutron diffraction in chemistry by the provision of instrumentation with massive detector arrays and very high count rates. This allows neutron chemical crystallography to respond to modern trends in structural molecular science, extending the applications of neutron diffraction in the area of molecular materials. Many of these exploit the power of neutron diffraction in determining accurately the hydrogen atom parameters in materials. The potential of this new capability will be illustrated by a range of recent studies on hydrogen atom disorder and transfer, polymorphism in molecular complexes, water location in materials and in the location and full description of hydrogen in inorganic materials. To continue enhancing this impact of neutron diffraction in important contemporary areas of chemistry, it is vital that instrumentation and associated capabilities at major facilities such as the ILL are developed to respond to the evolving requirements of users for rapid data collection and access times, and for experiments under more dynamic regimes. The potential of neutrons in this area will be examined, and something of a wish-list presented for developments to allow full exploitation of neutrons in structural chemistry on the timescale of the 2020 vision.

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Prompt gamma activation analysis in chemical research

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Prompt gamma activation analysis (PGAA) is a rapidly developing chemical analytical method utilizing nuclear techniques. It is based on the radiative neutron capture of nuclei, in other words, the (n,γ) reaction. Each isotope of every chemical element (with the exception of ^{4}He) is capable of absorbing a neutron, followed by relaxation in the form of γ radiation. The emitted prompt γ radiation is characteristic, that is, the detected energies identify the nuclides, and the intensities are proportional to their amounts in the analyzed sample. The method is also capable of resolving isotopic composition. We have combined PGAA with heterogeneous catalytic chemical reactors to investigate catalytic materials under their operational condition and thus unravel mechanistic details of heterogeneous catalytic processes [1,2]. In my presentation I will provide with examples from our research and discuss possible future applications.

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Novel magnetic order and excitations in high-T_C copper oxides superconductors

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One of the leading issues in high-T_c superconductors is the origin of the pseudogap phase in underdoped cuprates. Many theories attribute the pseudogap origin to the proximity of a competing state, but there is a wide disagreement about the nature of this state. Using polarized elastic neutron diffraction on the triple axis spectrometer 4F1 at Orphée Reactor (CEA-Saclay), we identify a novel magnetic order in the $YBa_2Cu_3O_{6+x}$ system only in the underdoped regime [1,2]. The observed magnetic order can be described as Q=0 anti-ferromagnetic (AFM) order with two opposite magnetic moments per unit cell. It preserves translational symmetry as proposed for orbital moments in the circulating current theory of the pseudogap state. Similar observation of the same magnetic order in $HgBa_2CuO_{4+\delta}$ [3] suggests that the phenomenon is general for all cuprates (with bi-planes or single plane structures). The temperature of the transition is that expected for the pseudogap suggesting that the pseudogap is directly connected with the magnetic order. To date, it is the first direct evidence of a hidden order parameter characterizing the pseudogap phase of high-Tc cuprates. Recent measurements in $La_{2-x}Sr_xCuO_4$ [4] reveal that a similar ordering occurs in that system for x=0.085 but is short range and bi-dimensional. That difference might be related to the existence of stripes phase exclusively in this last cuprate family. Recently, using polarized neutrons triple axis spectrometer IN20 at ILL, we have additionally observed magnetic excitations in $HgBa_2CuO_{4+\delta}$ around 55 meV [5], likely related to this novel magnetic order. These excitations could be described as Ising like excitations as they exhibit only a weak dispersion through the Brillouin zone.

Collaborators: Victor Balédent, Yvan Sidis (LLB-Orphée), Yuan Li (Stanford University), Guichuan Yu, Martin Greven (Minnesota University), Benoit fauqué (ESPCI Paris), Vladimir Hinkov (MPI Stuttgart), Paul Steffens (ILL Grenoble), Louis-Pierre regnault (CEA Grenoble), Ekaterina Pomjakushina, Joel Mesot (PSI Villigen) Xavier Chaud (CRETA Grenoble).

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Coupling of spin and electronic degrees of freedom intransition-metal oxides

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The coupling of electronic and magnetic degrees of freedom causes hybridized ordering phenomena which play the key role at least in the colossal magnetoresistance in manganates. Comparably to the well-studied nickelate and cuprate stripe phases, $La_{2-x}Sr_xMeO_4$ with Me = Co or Mn exhibits incommensurate ordering schemes yielding a common relation between the amount of charge doping and the electronic and magnetic incommensurabilities [1]. In manganates, the orbital degree of freedom also participates in the ordering leading to an incommensurate entanglement of four different order parameters. Detailed structure analyses can be performed by analysing the weak superstructure reflections associated with the electronic ordering. The combination of these structural studies with density functional theory calculations yields the nature of the electronic order in the manganates and points to a low-spin state of Co^{3+} in $La_{2-x}Sr_xCoO_4$. Finally we discuss the magnetic excitations, which give another direct view on the underlying electronic order. In spite of distinct energy scales, the $La_{2-x}Sr_xMeO_4$ series exhibit surprising analogies: Only the magnetic correlations at the lowest energies reflect the incommensurate ordering, whereas the high-energy part of the spectrum is almost indistinguishable from that of the associated commensurate parent phase.

References

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Quantum criticality and the emergence of novel states of matter

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Many of the outstanding problems in condensed matter physics are related to understanding how strongly correlated electron systems evolve in the vicinity of quantum critical points. Examples include understanding the mechanism of high-Tc superconductivity, the anomalous behaviour of certain types of metals at low temperatures (so-called non-Fermi liquids), and the statistical mechanics of low-dimensional quantum magnets. In this talk, a review will be presented of recent experiments selected to highlight the various ways in which neutron scattering has provided unique insights into the emergence of novel states of matter at quantum critical points. Consideration will also be given to the exciting opportunities arising from new generations of neutron instrumentation, most especially those being developed as part of the Millennium Programme.

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Interaction between amyloidogenic proteins and lipid membranes

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The proteins Aβ and α-synuclein are found in the protein aggregates characteristic for Alzheimer and Parkinson disease. In the literature there are many parallel findings between Aβ and α-synuclein on aggregation and membrane interactions. For both proteins, we have identified conditions leading to reproducible kinetic experiments, which is a major achievement in this field [1,2]. In recent studies of Aβ, we have demonstrated that the aggregation rate is retarded in the presence of lipid bilayers [3]. This effect is larger for less fluid lipid systems. Interestingly, we did not observe any significant effect on the aggregation kinetics by varying lipid charge. However, for both proteins there are many indications from the literature and our own studies that membrane charge changes the protein binding properties. One conclusion from this is that the amyloid aggregation process cannot be directly predicted from membrane association only, and require more detailed structural studies of the penetration of α-synuclein and Aβ in the bilayer membrane. This clearly motivates the use of neutron reflectivity to understand link between membrane association and protein aggregation, and our first set of experiments indicate clear roles of both lipid composition and protein aggregation status.

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Perdeuteration allows neutron diffraction studies with "tiny" crystals: the cases of Aldose Reductase and antifreeze protein.

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Recent advances in instrumentation and preparation of perdeuterated crystals for neutron diffraction have permitted the study of biological systems at medium to high resolution (2.5 – 1.5Å) with crystal volumes of only 0.1-0.2 mm^3, as illustrated by our studies of human Aldose Reductase (h-AR, 36 kDa) and type III antifreeze protein (AFP, 7 kDa). Neutron diffraction studies of h-AR were performed to study the enzymatic mechanism, which includes a hydride donation from the coenzyme NADPH and a proton donation from the enzyme. Using a perdeuterated crystal of h-AR (volume = 0.15 mm^3) neutron Laue diffraction data were collected to 2.2 Å resolution on LADI-1, and these were combined with X-ray data to 1.8 Å resolution, for use in a joint X+N refinement. The structural analysis of the resulting maps suggested the mobility of catalytic protons in the system Asp43-Lys77-Tyr48. These complementary observations led to an energetically favourable MD-QM model of the proton donation mechanism, which identified the proton donating residue (Tyr 48), activated by the movement of neutral Lys 77. The homologous AFP sub-family shares the capability to inhibit ice growth that would otherwise be fatal to organisms that live in subzero environments. AFPs work by binding to ice crystal nuclei through a flat 'ice-binding surface'. Despite extensive X-ray studies, the fine structural features underlying the antifreeze mechanism remain unclear; therefore neutron studies have been performed in order to provide information on the protonation states of the residues at the ice-binding surface, and the solvent structure surrounding the protein. Using a perdeuterated crystal of AFP (volume = 0.13 mm^3) neutron Laue diffraction data were collected on LADI-III to 1.85 Å resolution, and these were combined with X-ray data to 1.05 Å resolution, for use in a joint X+N refinement. Experimental details and current status of the project, including a model of the AFP-ice interaction, will be described. Both examples highlight the capability of neutron macromolecular crystallography to study biological systems at the protonation level with "tiny" perdeuterated crystals. This overcomes the major bottleneck of the large crystal volume requirements for neutron diffraction, allowing more diverse and challenging biological questions to be addressed. As LADI-III is already a heavily sought-after instrument (typically oversubscribed by a factor of 2 – 3), the development of new instrumentation for neutron macromolecular crystallography, such as the proposed OCTOPUS diffractometer, is necessary in order to keep up with the increasing demand from the structural biology community.

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Structural systems biology

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Structural biology techniques have developed into powerful, well established tools for elucidating the structures of isolated biological molecules. But molecules work in teams and their interactions with partners determine biological function. Studying complexes is now the norm; and often one complex is just one component of a multifaceted and intricate pathway. We have used a combination of structural methods to investigate how a jumping gene is cut from one place in a genome and inserted at another. The pathway of DNA transposition shuffles genetic information and facilitates genome evolution. A combination of X-ray crystallography (ESRF) [1] and contrast variation SANS experiments (ILL) have revealed how transposon DNA is manipulated at various stages in the pathway.The future will see a broader, systems approach to biology. The aim will be to understand dynamic biological processes at scales ranging from molecular to cellular up to whole organisms. The challenge that faces structural biology is to bring physical reality to molecular interactions on these scales: what are the interactions between molecular pathways? How do molecular machines communicate? An integrated and high throughput approach that utilises a range of structural methods will be essential to meet these challenges.

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Using neutron scattering to gain insight into particle aggregation and phase separation

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Colloidal gels and glasses represent classes of non-equilibrium solids that are not only interesting topics in fundamental soft matter physics, but also play an important role in various food and materials science applications. Colloids or proteins with short-range attractions, possibly combined with a soft long-range repulsion, can exhibit different liquid-solid transitions as a function of the strength of the attraction and the volume fraction. The possibility to modify the suspension properties by playing with interparticle interaction strength and range leads to interesting phenomena and provides a tool kit to produce cluster phases, gels and glasses with tailored structural and mechanical properties. However, the resulting systems often pose enormous problems to experimentalists and theoreticians due to the existing very large range of length and time scales. Here I will demonstrate how we can use small-angle neutron scattering and neutron spin echo experiments combined with complementary techniques such as video microscopy and small-angle light scattering to obtain a wealth of data on these interesting systems.

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Where dynamics is heading for in soft matter

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Here again the usual disclaimer applies, you have to be really brave to predict the future orientation in science for the next ten years. There is only one thing for sure, you can’t stand still. In this talk I will focus on the one hand upon trends observed in the last few years and extrapolate from these trends; on the other hand I will try to illustrate what we plan to face these challenges. I will primarily deal with the dynamical aspects, and more specifically in which direction we think Neutron Spin Echo will evolve hopefully in the nearest possible future.

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Studying atmospheric aerosol with neutron reflectometry

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Neutron reflectometry was recently applied to atmospheric chemistry problems [1,2]. The technique allows monitoring the gas-phase destruction of organic monolayers and provides insight into the nature of the reaction products. Latest experiments [3] pushed for high time resolution for investigation of fast kinetics of the reaction of ozone with d-methyl oleate. We also started to study reactions of night-time oxidants, in particular nitrate radicals, with proxies for organic films on atmospheric aerosol. In the talk I will present recent results and outline development routes for ILL-based experiments and synergistic on-going research in collaboration with the Max Planck Institute for Chemistry [4,5].

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Future nuclear structure studies of neutron-rich nuclei at the ILL

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One of the current aims of nuclear-structure studies is to test the interactions used in shell-model calculations far from stability, where current predictions for the shell structure of heavier nuclei, such as those beyond ^{132}Sn are divergent. Worldwide, an intense effort is underway to construct powerful new radioactive-beam facilities to study neutron-rich nuclei. The ILL has a rich history in contributing to such studies. Fission is one of the best mechanisms to produce very neutron-rich, medium-heavy nuclei and thermal neutron-induced fission is a particularly good reaction due to its huge cross section (~1000 b). The ILL will continue to contribute to this field in the future and ideas for experimental programs with existing and upgraded instruments will be presented in this talk. The Lohengrin fission-fragment spectrometer currently has excellent production intensities for neutron-rich nuclei however its resolution is not as good as those found at other facilities. Improvements in resolving power, possibly by the addition of extra ion-optical elements, combined with an implantation detector, would allow this instrument to remain world class. An emerging field at the ILL is the prompt X-ray spectroscopy of fission fragments produced using neutrons from a neutron guide. Ideas for further studies in this field will be presented.

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New infrastructures for the next decades of neutron particle physics

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Ultracold neutrons (UCN) play a key role for very precise investigations of particle physics at the low-energy frontier. Prominent examples are the search for the electric dipole moment, an electric charge, neutron – mirror neutron transitions, the neutron lifetime and quantum mechanics of the neutron in the earth's gravitational field. ILL has for long possessed the world's leading UCN facility, a position currently challenged by various institutes around the world. Therefore a new facility for UCN operating with liquid helium as converter material shall be implemented at an intense cold neutron beam at the ILL, providing much higher UCN densities then presently available and competitive with numbers projected for other future sources. Storage experiments with UCN will greatly benefit from this development. Complementary to work with UCN, cold neutrons offer advantages for some observables, such as angular correlations in neutron decay and parity violating asymmetries in nuclear few-body systems. Implementation of an adaptive neutron optics in front of the user experiment would provide a significant gain in intensity and versatility of the cold neutron beam facility PF1B.

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Future reactors for research – science, technology and policy

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The world is experiencing a renaissance in civil nuclear power production. It is reported that worldwide 57 nuclear energy reactors were under construction in June 2010 with 439 such reactors already in operation [1]. Thirty countries generate electricity using nuclear energy, but 56 operate a total of approximately 250 civil research reactors [2]. Research reactors of diverse types provide various services:

- Materials test capability and irradiation studies
- Medical isotope production
- Neutron beams
- Technology demonstration
- Training

The technology and policy issues facing a renaissance in research reactors differ from those shaping the renaissance in civil nuclear power generation and these aspects will be considered. Key issues for future research reactors include: safety, cost, performance, and proliferation resistance. These issues combine considerations of scientific utility (for public and private users) with aspects of international security and even conceptions of national sovereignty. In the United Kingdom capacity to explore such technology and policy issues has recently been enhanced via the creation of the National Nuclear Centre of Excellence [3]. It is also noteworthy that some functions historically provided by critical civil research reactors may now be provided by other means. To what extent, if any, does this signal the decline of the research reactor? In Europe the current reality indicates an opposite future of expansionary ambition with noteworthy projects including: the ILL Millennium Programme, the Pallas Research Reactor NRG Netherlands, and the Jules Horowitz Reactor Cadarache France among others.

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The key role of neutron scattering in multiferroics research

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The discovery of new ‘‘multiferroic’’ systems, in particular spin-driven ferroelectrics has triggered a huge interest in condensed-matter physics over the last few years. Research has progressed rapidly from the initial measurements, for example of giant magnetoelectric effects or abrupt polarization flops under magnetic field, to an in-depth understanding of the coupling mechanisms involved. Neutron scattering has played a central role in the study of these systems, in particular providing quantitative information about the usually complex magnetic states (incommensurate phases, complex exchange topology), and their couplings to structural parameters and electric field. I will review the work recently conducted in this area, the impact of ILL instruments in this field and I will outline benefits from future neutron instrument/software developments.

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Neutron spectroscopy and powder averaged lattice dynamics calculations as key techniques to understand the low-thermal conductivity, thermodynamics and elastic properties of open-framework materials

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Minimizing the lattice thermal conductivity k is one promising way of improving the figure of merit of thermoelectric materials [1]. The principle mechanism of efficiently reducing k is known to be the scattering of heat carrying acoustic phonons. Phonon scattering can be accomplished in many ways. Imperfection of materials in the form of structural and site disorder, the presence of voids, interfaces, surfaces and dislocations opens up temperature independent scattering channels for acoustic phonons. In perfectly ordered, crystalline matter umklapp–scattering and multi–phonon events establish efficient scattering mechanisms at sufficiently high temperatures. Open–framework crystals like filled skutterudites MFe_4Sb_{12} (M = Ca, Sr, Ba, La, Yb, ...and clathrate structures are particular materials whose of the host-lattice (Fe_4Sb_{12}), of the intercalated guest atoms (M) and the complex interplay between them is made responsible for the strong suppression of k [2]. Apart from conjectures upon the interaction of collective host-lattice modes with localized 'rattling' vibrations of the guests as possible decay channels for heat carrying acoustic phonons, only limited information on the vibrational dynamics has been gained on quantitative grounds. As so often with functional materials of complex structure they rather form in a polycrystalline state making the detailed study of the inelastic response a difficult venture. We will discuss how to overcome, to a certain degree, the disadvantage of working with polycrystalline materials by combining high-resolution time-of-flight spectroscopy and ab initio powder averaged lattice dynamics (PALD) calculations [3,4]. We will demonstrate as well how both techniques can be combined to gain reliable information on thermodynamic and elastic properties of materials. Inelastic neutron scattering proves to be the key experimental technique to study the complex dynamics of open-framework structures, since the modes made responsible for the reduction of k are predominantly inactive to Raman and Infra Red techniques.

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Getting smart; engineering tomorrows materials and devices

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Tomorrows materials and devices will exploit phase transformations to control residual stresses; to empower microelectronic machines and to respond intelligently to changes in environmental conditions. At the heart of all these materials are phase transformations triggered to respond on demand. Achieving this requires an understanding of how chemistry and processing can be exploited to deliver the right response under the right conditions. In this talk I will outline a range of examples where neutrons can provide the necessary insight to help develop the next generation of such materials. Examples will include smart weld fillers for manipulating weld stresses, piezo electric actuators, shape memory devices and superelastic materials. In each case neutron diffraction provides a means to follow the extent and nature of the controlling phase transformation under processing or in-service conditions. Future developments in neutron instrumentation will radically extend the range of environments that will be accessible as well as shorter transformation timescales. Such advances will rapidly accelerate the development of these engineering materials and devices.

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Neutron reflectivity: visions for 2020 and beyond

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Neutron reflectivity has in the past played an essential role for the exploration of thin films and interfaces in soft and hard condensed matter. Polymer and liquid films, magnetic and superconducting heterostructures, as well as hydrogen containing materials have been analyzed with much success for unravelling their unique physical and chemical properties confined to lower dimensions and affected by interfaces. Furthermore neutron reflectivity has expanded into the off-specular regime probing domain structures and lateral magnetic patterns on the micrometer scale. The power of neutron reflectivity for the analysis of films and multilayers will remain and will always be essential when x-ray reflectivity by various reasons will not deliver the proper answer, either because of weak scattering contrast or because of radiation damage. All aforementioned studies are taken on a time scale of hours to minutes. Fast neutron reflectivity can be envisioned with TOF techniques at spallation sources on the scale of seconds. However, many reversible phenomena occur on much shorter time scales. Time dependent studies can be performed either in real time by pump-probe techniques, or in the frequency domain by applying an ac signal. In either case, time dependent neutron reflectivity experiments can be envisioned which go far beyond the present limits into the micro- to nanosecond regime. We will outline some recent experimental developments [1,2] which will break the quasi static barrier and which will lead to new opportunities in the future by studying time dependent phenomena. Applied to polarized neutron reflectivity for studying magnetism, we prefer to term this new technique ac-PNR. This work is supported by BMBF 05KN10PC1.

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Structure and dynamics in membranes for fuel cells

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The extremely high proton conductivity of some polymers containing functional acidic groups in the hydrated state make them interesting candidates as separator materials in high drain electrochemical cells, such as PEM fuel cells. Such polymers combine in one macromolecule the hydrophilic character of terminal acidic functional groups (usually $-SO_3H$) and the hydrophobicity of the polymer backbone (mostly perfluorinated, but aromatic high-performance polymers are also currently being used). Especially in the presence of water, this leads to some hydrophilic/hydrophobic nanoseparation. The transport properties are determined by the confinement of water within the hydrophilic interconnected nanodomains and the interaction with the acidic functional groups. The neutron scattering techniques are perfectly suited to approach the complexity of these materials: structural organization, sorption properties, dynamical behaviour of protons. We will show examples of SANS investigations of different membranes at equilibrium and in a running fuel cell specially designed for neutron experiments[1]. We also present a QENS study of the molecular motions of water and protons in perfluorinated systems [2].

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Understanding liquids in nanomaterials and devices: limits and opportunities for neutron science

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The emergence of nanotechnologies has brought new excitement for basic research, as it implies that some entire areas of the physics of condensed matter should be revisited. For instance, the manipulation of fluids at the nanometer scale modifies profoundly the phase behavior, self-assembling tendency, molecular dynamics, and flow conditions in an intricate way. These phenomena are scientific bottlenecks for the future control of infinitesimal volumes of materials in devices. Stimulating unresolved issues concern systems with a higher degree of complexity, which is relevant for rapidly growing sectors of application, such as nanofluidics, molecular electronics, biotechnologies or nanomaterials design. Neutron possesses unique space and time-scale resolutions to address some of these questions. Based on illustrations extracted from the recent literature on the subject, we will try to underline what are the current limits for neutron sciences, and which challenges and opportunities are raised for the future.

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New frontiers for liquids and glasses

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The structural disorder of liquids and glasses confer them with unique physico-chemical and opto-electronic properties that make them an essential part of our daily lives. Applications range from optical fibres for use in telecommunications to polymer electrolytes for making small and flexible batteries and it should not be overlooked that the liquid state is a prerequisite for many chemical and biological processes. The main theme of this talk is on the recent inroads that have been made on the structure of liquids and glasses at the ILL. Examples include the study of materials under extreme conditions of temperature and pressure, the use of isotopes having a small scattering length contrast to obtain information at the partial structure factor level for new materials, and the development of a deconvolution procedure to account for the asymmetric broadening of peaks caused by the resolution function of a diffractometer. The discussion will focus on development of the instrumentation and sample environments required to study systems of increasing complexity that are relevant e.g. to energy and the environment.

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4.4 Morning session

Friday 17 September

The importance of data analysis

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The ILL2020 vision user meeting is about defining new projects to take ILL in to the future. Typically projects involve new sources, guide systems and instruments that collectively bring more neutrons to the detectors. But funding partners look elsewhere (publications, impact factors, societal impact, etc) when they evaluate how well the money has been spent. If any phase in the production of scientific results fails, the return on investment and the delivery of scientific discovery and solutions are diminished. Software for data reduction, analysis and interpretation probably constitutes the least visible phase in the production of scientific results but it is the phase closest to the scientific outcome in which neutron scatterers from many fields interact with their data. Traditionally, writing software has been the job of instrument scientists and their input is essential. But computing skills that go beyond those to be expected from scientists are now required to integrate scientific algorithms in robust, user-friendly, software that allow large volumes of data to be treated efficiently and advantage to be taken of modern computing hardware. The value of good software is now being recognised and the inclusion of this talk in the programme is a measure of that. The talk will address the current situation and future directions.

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Interface laboratories at the European Photon and Neutron site (EPN): perspectives and practicalities

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The way in which science is being carried out at central facilities such as the ILL and ESRF has been changing steadily over the past decade or so. The reasons for this are in many ways obvious: neutron beam and synchrotron X-ray sources are valuable resources and it is widely accepted that all efforts should be made to maximise the efficiency of the instruments available and the quality of the results obtained. Whereas central facilities were originally developed along rather classical lines within mainstream areas (eg physics, chemistry, biology), key developments in the recent past have generated intense interest at the interfaces between these subject areas. This has important practical consequences for the future. Firstly, needs for sample preparation have changed substantially - there are growing areas of science where the best possible results require advanced sample production, manipulation, or characterisation in close proximity to the relevant instruments. Secondly there are now compelling needs for interdisciplinary approaches. This is true for most areas of modern research but is easily demonstrable in the life sciences. There is increasing recognition of the fact that biological systems have to be studied in a far more integrated way, using methods that span resolution boundaries from atomic to cellular levels, and employing a wide range of techniques for sample preparation and in vitro and in vivo biophysical and structural characterisation. High on the list of priorities is the joint exploitation of neutron and X-ray data; beyond this, techniques such as NMR spectroscopy, electron microscopy, and a wide range of other biophysical techniques are playing a crucial role in maximising the value and scope of neutron and X-ray studies. Thirdly, it has become clear that the additional capabilities needed to fulfil the vision of genuinely integrated approaches are not always easily accessible to members of the user communities. Hence there is a strong economic argument to maximise cost effectiveness by co-locating these capabilities in a way that maximises access for the widest possible range of users. On the European Photon and Neutron (EPN) site in Grenoble, the first interface laboratory to be built was the Partnership for Structural Biology (PSB). The PSB has had a huge impact for biological neutron scattering both in terms of sample preparation (in particular through the availability of the D-LAB as a user facility) and interdisciplinarity. A number of other interface laboratories are now planned, including a Partnership for Soft Condensed Matter (PSCM), and a Materials Science Support Laboratory. A new science building is being built to accommodate these initiatives. This presentation aims to stimulate discussion on the needs of these laboratories, and the operating model(s) that should be deployed to maximise benefit to ILL's users.

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The wider environment

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Over the last four decades of operation of the ILL High-Flux Reactor, research on scientific and technological problems relating to the structure and dynamics of matter, whose investigation depends crucially on neutron scattering, has grown tremendously in both complexity and range of application. The ILL, which still offers its ever-growing user community the world's premiere neutron source, has responded to these challenges with the completion of the first phase (in 2008) and the successful launch of the second phase (2007-2014) of its instrument and infrastructure modernisation programme (the "Millennium Programme"). As discussed at this ILL user meeting, as part of our constant efforts to structure the future of neutron science, we have already begun to prepare our plans for further development beyond 2014. These plans will not be made in isolation, but rather will recognise that the major neutron facilities across Europe each have their different strengths and that the user community as a whole will benefit if a co-operative and complementary approach is adopted to both planning and development. The possible creation of a future European Spallation Source (ESS) will be part of our deliberations. In the framework of a European-funded project (ESFRI ILL20/20), we have already performed a benchmarking of present and future ILL instruments against possible instruments at a 5MW long-pulse ESS. We will present reasons why the high-flux neutron source will continue to play a crucial role in supporting Europe's user community as the ESS comes up to full operating power and why the Institute's stakeholders consider the ILL as the focal point among European neutron facilities, a veritable hub to be maintained until at least 2030.

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5. Taking ILL further into the Millennium

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