Plenary talks

P-1 Interacting quantum spin chains

A. Zheludev
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For two decades the development of our understanding of quantum magnetism was primarily driven by inelastic neutron scattering studies. It is fair to say that basic one-dimensional systems are, by now, rather well understood. Ironically, Landaus criticism of the 2-sublattice model for antiferromagnetism introduced by Neel, a debate dating back to the early 30s, is well justified for 1D magnets. The magnetic ground state and excitation spectrum in 1D compounds are nothing like those in semi-classical spin wave theory, known to work well for 3D systems. The new challenge is to bridge the gap between the strikingly different and apparently incompatible behavior observed in 1D-quantum and 3D-”classical” magnets. Experiments on weakly-coupled quantum spin chains reveal a unique duality of the excitation spectrum in such systems: ”classical” spin waves compete for spectral weight with quantum multi-particle continua and bizarre ”soft-spin” excitations. High-field experiments provide an alternative way to suppress quantum fluctuations in 1D magnets and drive them towards more ”classical” behavior. It is gratifying to see that the progress made is driven not only by the discovery of new model materials, but also by the development of advance instrumentation and data analysis techniques. Several examples of recent neutron scattering studies of quasi-1D quantum magnets will be reviewed.

P-2 Neutrons in the Post-Genome Sequencing Era

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The methods of neutron scattering in biology were developed essentially in the 1970’s and 1980’s, taking advantage of the special properties of the neutron’s interaction with matter, and especially the large isotope effect for hydrogen. Neutron crystallography localised important H atoms in enzyme active sites. Contrast variation applications to protein-nucleic acid complexes provided essential structural information on the organisation of complexes such as ribosomes, chromatin, viruses and on kinetic interactions between transfer RNA, enzymes and elongation factors involved in translation. The triangulation experiments, placing all the proteins in the small ribosomal subunit, and solving polymerase quaternary structure, represented a major feat, both in their biochemical and scattering analysis aspects. In the biological membrane field, neutron diffraction provided unique information on the conformation of lipid molecules in bilayers and on protein-lipid-water structure in n! atural membranes, as well as contributing in a complementary fashion to the resolution of membrane protein structures. Studies of the important role played by hydration and solvation in biological macromolecules were initiated. The large number of high resolution structures that are becoming available following Synchrotron Radiation crystallography and NMR now emphasise even more that such knowledge is a starting point in understanding a biological system and not an end in itself. The special advantages of neutrons combined with the progress in biochemistry and molecular biology are powerful reasons to stimulate a rebirth of neutron scattering experiments in biology in the post genoime sequencing era. When the structures of the components of a system are known, the questions are: how do they interact with each other? what is the role of the environment, through hydration and solvation? what is the dynamics underlying the structures? how do they move? All questions that can be addressed by neutron scattering. In the dynamics field in particular, neutrons are unique in being able to provide simultaneously the amplitudes and frequencies of molecular thermal motions – motions that have already been shown to be involved in biological function and activity. Key experiments on proteins, membranes, and protein-nucleic acid complexes will be presented and the perspectives of the methods will be discussed.

P-3 Neutron Scattering Studies of Hierarchy Structure and ”Interphase Scattering” in Phase-Separating Binary Mixtures

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We overview time-evolution of phase-separating structure in binary mixtures for a wide range of wave number q by using time-resolved small-angle neutron scattering (SANS), light scattering and laser-scanning confocal microscopy. By taking an advantage of using polymers we could elucidate evolution of hierarchy structures comprised of global structure, interface structure, and local composition fluctuations within two phases. The global structure is highlighted to have a sponge-like structure with a hyperbolic interface. The sponge-like structure is found to be a structure universal to ”symmetric” polymer mixtures and simple liquids and to be predicable by using a time-dependent Ginzburg-Landau theory. SANS studies unveiled ”interphase scattering” that originates from composition fluctuations within interfacial region with a finite interfacial thickness. This interphase scattering gives the scattering excess to the scattering arising from the local composition fluctuations within the two phases and becomes remarkable as the Porod scattering from the interface becomes negligibly small in the q-range of the observation.

P-4 Novel Magnetic Excitations in Metals and Superconductors

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Recent years have seen the rapid development of instrumentation, both at reactor and spallation neutron sources, for the investigation of coherent magnetic excitations in single crystals. There has also been a concomitant supply of new materials with novel magnetic excitations. In this talk I will show how new techniques, particularly those involving the use of position sensitive detectors on chopper spectrometers, have been used to address novel magnetic excitations. I will draw examples from high-temperature superconductor, transition metals, and transition metal oxides.

P-5 The Spallation Neutron Source: A Powerful Tool for Materials Research

T.E. Mason
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The wavelengths and energies of thermal and cold neutrons are ideally matched to the length and energy scales in the materials that underpin technologies of the present and future: ranging from semiconductors to magnetic devices, composites to biomaterials and polymers. The Spallation Neutron Source (SNS) will use an accelerator to produce the most intense beams of pulsed neutrons in the world when it begins operation in 2006. The project is being built by a collaboration of six U.S. Department of Energy laboratories. It will serve a diverse community of users drawn from academia, industry, and government labs with interests in condensed matter physics, chemistry, engineering materials, biology, and beyond.

P-6 Japanese Spallation Neutron Source

S. Ikeda
High Energy Accelerator Research Organization, Ibaraki, Japan

The Japanese ”Joint Project” is a new project to pursue frontiers in particle physics, nuclear physics, materials science, life science, and nuclear technology, using a new proton accelerator complex at the highest beam power in the world. This project had been jointly proposed by the High Energy Accelerator Research Organization (KEK) and the Japan Atomic Energy Research Institution (JAERI), and was approved at the end of 2000. This accelerator complex allows production of a variety of intense secondary particle beams. It also offer the exciting prospect for measurements of neutrino oscillations and CP violation, materials and life sciences with neutron and muon beams, and accelerator-driven nuclear transmutation of long-lived nuclides in nuclear waste. As one of the major facilities in this project, the next generation of pulsed spallation neutron source with 1 MW will be constructed by the end of 2006. It is comparable to the new pulsed sources which will be realized in US and Europe. In this paper, the details of the new neutron facility in ’Joint Project’ are summarized.

P-7 The European Spallation Source Project

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The European Spallation Source (ESS) will be a third generation neutron source driven by a proton accelerator with a beam power in the 5 MW range. Such a neutron source offers news perspectives for experiments beyond today’s high flux reactors. In my presentation, I will present the status of the ESS project, I will discuss the different accelerator options and in particular relate to the option of a multi purpose facility (CONCERT project). On the basis of the scientific opportunities, offered by different target options, in June 2001 the Council of the ESS will have defined the target specifications. I will report on the scientific evaluation and the conclusions leading to this decision.

P-8 The New Neutron Source FRM-II

W. Gläser
Technische Universität München, Germany

The FRM-II is a new beam tube research reactor at the Technische Universität München to replace the research reactor FRM at Garching after 43 years of successful operation. The concept of the FRM-II as a future national neutron source and basis for our international cooperation was strongly recommended by the German Science Council. High intensities of thermal neutrons are provided by a particular densely packed core of highly enriched uranium and are extracted by 12 beam apertures. The low thermal power of 20 MW allows the positioning of a D_2 cold source at a maximum of the thermal neutron flux in the D_2O moderator. This cold source is seen by 3 beam tubes, one of which feeds a neutron guide hall. A graphite hot source shifts the thermal spectrum to shorter wavelenghts with a maximum of the Maxwellian distribution at $\approx$0.5 Å. Construction started in 1996 and was completed at the beginning of 2001. Several research groups at universities, research centers and the Max-Planck society are actively participating in the scientific instrumentation of the facility. Concept and status of the facility and its first generation of instrumentation will be presented.

P-9 From zero to three dimensions: Neutron spectroscopy of polymeric fullerides

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Fullerenes form crystalline structures with the molecules spinning nearly unhindered at high temperatures. Compared to the stiffness of the cages the inter-molecular bonding is weak making fullerenes close-to-ideal representatives of molecular crystals. Fullerenes have a strong tendency to undergo solid state chemical reactions provided these are catalyzed by appropriate conditions - like exposure to light, high pressure at elevated temperatures or doping. The reactions lead to a variety of polymer topologies with varying dimensionality. Upon network formation the molecular crystal character breaks down leaving text book signatures in the spectra. These signatures allow to monitor the network formation process in real time via inelastic neutron scattering (INS). Combined with lattice dynamical calculations the INS experiments yield valuable information on the bond types and bond topologies in the networks. While many systems show a simple activated behavior upon bond formation or bond break-up some systems pass through a stage of phase separation featuring coexistence of monomer and polymer regions.

P-10 Advancing Neutron Diffraction as a Tool for the Engineer

T. M. Holden
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The first stress measurements on engineering components by neutron diffraction appeared about fifteen years ago and there has been a steady demand to solve industrial problems since then. Recently, there have been major efforts to measure and model the in-situ strain response to applied stress in industrial alloys in the elastic regime and above the yield point in the plastic regime. The results reveal the fundamental modes of deformation, such as slip and twinning, and give the magnitudes of the critical resolved shear stresses. Of equal importance, the results show how to account for the intergranular strain contributions to the different reflections and thus to interpret measured strains correctly in terms of the macrosopic stress fields of interest to the engineer. Round-robin experiments conducted worldwide on test samples have lead to standardized procedures for strain measurement with neutrons.

Walter Hälg Prize

Polarised Neutrons: An ideal tool for magnetic crystallography

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The magnetic properties of crystals which have been revealed by many different kinds of experiment in the past 60 years are many and varied. Those which pertain to their ordered structures form only a small part of the whole, yet the wealth of different spin configurations which have been found in nature challenges the imagination. At the electronic level the phenomena contributing to the magnetisation are yet more varied. The prime tool which has allowed access to the spatial distribution of magnetisation is neutron scattering, and since this is a space full of vectors, what better than to use the neutron’s own vector property, its spin, to study it. In the ideal neutron scattering experiment the energy, momentum and spin direction of the incident neutron beam would be defined, and the scattered energy, momentum and spin direction determined. Unfortunately ”ideal” experiments are seldom practical. However less than ”ideal” experiments can yield rich information when they exploit the vector properties of the dipole interaction as well as the phase sensitivity implicit in diffraction.

Oral Presentations

- **T** Low Dimensional and Quantum Spin Systems
- **T** Methods and Instrumentation I
- **T** Materials in Motion
- **T** Complex Fluids
- **MS** Magnetic Thin Films and Multilayers
- **MS** Neutrons and High-Energy X-Rays in Materials
- **MS** Hydrogen Atoms in Biological Function
- **T** Bulk Polymers
- **T** Magnetic Structure and Dynamics I
- **T** Methods and Instrumentation II
- **T** Hydrogen in Materials
- **T** Molecules under Restraint
- **MS** Spin, Charge and Orbital Degrees of Freedom in Perovskites and Related Compounds
- **MS** Optimization of Neutron Devices by Simulation
- **MS** Industrial Applications of Neutron Scattering
- **T** Biological Systems I
- **T** Biological Systems II
- **MS** Charge, Lattice and Isotope Effects in High-Tc Superconductors
- **MS** Instrumentation at Advanced Pulsed Neutron Sources
- **T** Frustrated Magnets
- **T** Polymer Solutions
- **T** Organic Molecules
- **T** Interfaces and Confined Systems
- **T** Magnetic Structure and Dynamics II
- **T** Unusual Material States
- **T** Glasses and Liquids

T-1 Polarimetric neutron-scattering study of the optic mode in the spin-peierls compound CuGeO$_3$

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The spin dynamics associated with the acoustic and optic modes in the inorganic spin-Peierls system CuGeO$_3$ have been studied by means of unpolarized inelastic neutron scattering under field and polarized inelastic neutron scattering in zero field. In a magnetic field applied along the **a** axis, the acoustic and optic modes split into three distinct modes with quite different relative spectral weights. The longitudinal polarimetry on the optic mode for a polarisation set parallel to Q (defined as x) shows that much more conventional. Our experimental results can be qualitatively understood by assuming that the excitations are mixed (sructural and magnetic) objects.

T-2 Structural and magnetic properties of the quasi-1D and 2D molecular magnets Cu(NCS)2pyz and Fe(NCS)2pyz2

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The structure of Cu(NCS)2pyz determined by powder neutron diffraction consists of Cu chains linked by pyrazine while the Fe(NCS)2pyz2 structure is formed by Fe 2D sheets linked by pyrazine with a almost perfect square lattice. In both cases, inter-chain and inter-sheet interactions provided by the NCS ligand are very weak leading to quasi-1D and 2D systems. This picture is confirmed by powder neutron diffraction although the magnetic susceptibilities show maxima respectively at 7 and 8.5 K being characteristic of antiferromagnetic interactions. No long range 3D magnetic ordering was observed down to 4K. However, we do find structural changes that correlate with maxima in the susceptibilities. We also discuss zero-field splitting excitations for the Fe sample determined by INS.

T-3 Neutron Scattering Studies of the One-Dimensional Quantum Spin Magnetism in Yb$_4$As$_3$

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Yb$_4$As$_3$ is a unique lanthanide compound which exhibits typical behaviors of a one-dimensional S=1/2 Heisenberg antiferromagnet. The 1D properties are due to the formation of 1D chains of Yb^{3+} ions by the charge ordering from the mixed valence state, and the interrelation between the 1D magnetism and the charge ordering as well as the heavy-Fermion-like anomaly of electrical resistivity attracts much attention. We present recent polarized neutron diffraction and inelastic neutron scattering works which played important roles to reveal the 1D quantum spin magnetism of this material. We will also discuss the recent finding of the evidence for the staggered field effect on the 1D spin system under magnetic field.

T-4 Spin dynamics in the high-field phase of quantum critical S=1/2 TlCuCl$_3$

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An external magnetic field suppresses the spin energy gap in singlet ground state S=1/2 TlCuCl$_3$. The system becomes quantum critical at H$_c \approx 5.5$ T, where the energy gap between the lowest Zeeman split triplet level and the nonmagnetic ground state vanishes. Antiferromagnetic ordering is reported above H$_c$, which underlines the collective nature of the observed quantum phase transition. The intrinsic parameters of the title compound allow to access the critical region microscopically by neutron scattering. A substantial study of the spin dynamics in the high-field phase of TlCuCl$_3$ at T=2 K up to H=12 T was performed for the first time. The results indicate two dynamical regimes, which can be understood within characteristically renormalized triplet modes and a low-lying dynamics of possibly collective origin.

T-5 Excitations of a 2D frustrated quantum magnet in the high-field ferromagnetic phase

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We have recently discovered a new fractional quantum spin liquid state in the 2D frustrated quantum magnet Cs$_2$CuCl$_4$ [1]. We use high magnetic fields to manipulate the ground state fluctuations and neutron scattering to determine the nature of the excitations. The saturated high-field ferromagnetic phase provides a reference phase where the Hamiltonian can be determined exactly as ground state fluctuations are quenched out and excitations are magnons with dispersion equal to the Fourier transform of the couplings. Measurements reveal a 2D triangular antiferromagnet with partially-released frustration. Comparison with the zero-field spin-liquid phase gives large quantum renormalizations for the incommensuration and the excitation energies. [1] R. Coldea et al, Phys. Rev. Lett. 86, 1335 (2001)

T-6 Spin Excitations in the 2D orthogonal-dimer system $SrCu_2(BO_3)_2$

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We report high energy resolution inelastic neutron scattering results on the strongly frustrated 2D orthogonal-dimer system $SrCu_2(BO_3)_2$[1]. It was pointed out by Miyahara and Ueda[2], that this system can be mapped on the Shastry-Sutherland model close to the quantum phase transition from a Neel to a singlet dimer state. Strongly localized first triplet excitations at around 3meV with a small dispersion due to the DM interaction in zero and applied magnetic field perpendicular to the 2D plane are studied. Higher energy excitations around 5meV, probably due to the triplet bound states, will be also discussed. [1] H. Kageyama et al. Phys. Rev. Lett. 82 (1999) 3168. [2] S. Miyahara and K. Ueda, Phys. Rev. Lett. 82 (1999) 3701.

T-7 Overview New Larmor Precession Techniques

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Larmor precession has been used in the past in neutron spin-echo and neutron depolarisation. In the last decade, the inclined front and end faces of the precession regions combined with the resonant Larmor precession spin-echo technique, underwent a revived interest. Various techniques based on these inclined faces have been developed, such as spin-echo small angle neutron scattering (SESANS), high-resolution diffraction using Larmor precession and off-specular neutron reflectometry using SESANS. An overview will be given of the state of the art of the developments of the various techniques.

T-8 Advances in Specular Neutron Reflectometry

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Specular neutron reflectometry provides a depth profile of the scattering length density (SLD) and, ultimately, of the chemical and magnetic composition of a layered material. To date, numerous productive applications of neutron reflectometry have been demonstrated. With the new development of methods for phase determination, the problem of deducing unambiguous SLD profiles from reflectivity data has been solved in principle and, largely, in practice as we briefly review. Nonetheless, the fact that reflectivities can only be measured up to a finite maximum wavevector transfer Q still limits the spatial resolution attainable. Lately, neutron reflectivities as low as 10^{-8} out to values of Q approaching 0.7 $Å^{-1}$ have been measured, yielding spatial resolutions of a fraction of a nanometer. We discuss the results of recent experiments which illustrate the current sensitivity of neutron reflectometry and present some approaches, both instrumental and analytical, for effectively extending the Q range.

T-9 Simultaneous Polarization Analysis of Zeeman Splitting in Polarized Neutron Reflectometry using a Polarized ^{3}He Neutron Spin Filter

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A polarized ^{3}He neutron spin filter was used to analyze polarized neutrons reflected from a 1000Åthick Fe thin film immersed in a magnetic field. Using the large solid angle of the polarized ^{3}He spin filter, we were able to simultaneously analyze both the specularly-reflected component and the off-specular component caused by the phenomenon of Zeeman splitting of surface scattered neutrons observed by Felcher et al. [G. P. Felcher, S. Adenwalla, V. O. de Haan, A. A. Van Well, Nature, 377, 409 (1995)]. The sample of polarized ^{3}He was polarized by metastability-exchange optical pumping and compressed into a glass cell at Indiana University, and transported to POSY I at IPNS. Results are in agreement with theory. To our knowledge this work represents the second experiment to employ a polarized ^{3}He neutron spin filter in neutron reflectometry.

T-10 First realization of Bonse-Hart angular profiles for multiple Bragg reflections

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We have produced a monochromatic neutron beam with the sharpest yet angular profile. We evolved an optimal design for the geometry of a channel-cut perfect crystal effecting a multiple Bragg reflection. Using a pair of such channel-cut silicon crystals, we recorded rocking curves for a triple-triple symmetric 111 Bragg reflection of 5.229 Åneutrons at the V12b Double Crystal Diffractometer in BENSC. The data agrees with the theoretical Darwin reflection curves over an intensity range spanning 5 orders of magnitude. This constitutes the first realization of the proposal made by Bonse and Hart 35 years ago. Our results mark an order of magnitude improvement over the previous best USANS profiles.

T-11 The Low Frequency Density of States for Amorphous and Crystalline Ice Phases

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Incoherent inelastic neutron scattering measurements have been carried out on high-density amorphous (hda) ice, low-density amorphous (lda) ice, and crystalline ice Ic and Ih. Data was collected at temperatures from 5 to 80 K for hda and from 5 to 120 K for the other phases. The low-frequency (n $<$ 1 THz) densities of states, g(n), of the four phases are compared. The data show clearly an excess number of modes in g(n) for hda ice at 5 K, centered at 0.65 THz . The excess g(n) is considerably reduced on heating to 20 K, but the excess modes are still observed up to about 60 K. Above 60 K, g(n) for hda ice exhibits predominately Debye behavior, g(n) An2, as n 0. No such excess modes are observed in lda or in the two crystalline phases, although in all three there is a slight but significant kink in g(n) between 0.60 and 0.83 THz. By means of lattice dynamics calculations on an experimental structure derived from reverse Monte Carlo analysis of neutron diffraction data for hda ice, we identify the excess modes in hda ice as localized excitations of short chains and isolated molecules. This study has given the best insights to date on the microscopic origin of the excess low-frequency modes that are a characteristic feature of amorphous materials.

T-12 Static and Dynamic Studies of the Fast Silver Ion Conductor Ag_7GeSe_5I by Neutron Scattering

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The phase Ag_7GeSe_5I belongs to the argyrodite family of super-ionic conductors and its high conducting form still exists at very low temperature. Neutron scattering experiments have been performed in order to fully characterise the static and dynamic behaviour of this compound. Thermal evolution of the normalised elastic intensity deduced from quasielastic data and using the fixed window method suggests a freezing of the diffusion process below 100 K. Thermodiffractometry results show a classical behaviour for cell parameter and Debye-Waller factor, and only a slight anomaly is observed above 300 K. A cristallographic model based on non-harmonic development of the atomic displacement parameters is refined for single crystal neutron diffraction data collected at 20 and 300 K.

T-13 Anomalous Phonon Damping in the High Temperature Shape Memory Alloy $Ti_{50}Pd_{42}Cr_8$

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Neutron scattering measurements of the high temperature shape memory alloy $Ti_{50}Pd_{50-x}Cr_x$ were performed to probe the phonon precursors to the Martensitic transformation. For $x = 0$, the transformation temperature, T_M ∼800 K [1] and for the composition studied, $x = 8\%$, it is reduced to ∼400 K. Above this temperature the crystal possesses a simple CsCl-type cubic structure. Transverse acoustic phonons propagating along the $[\zeta\zeta 0]$ direction with atomic displacements along $[-\zeta\zeta 0]$ were studied at temperatures up to 675 K. The phonons are well defined near the zone center, but for $\zeta > 0.15$, they remain strongly overdamped at all temperatures studied. An elastic peak develops in the cubic phase at $\zeta = 0.22$ and increases in intensity as T_M is approached. However, the phonons do not show any characteristic anomaly at this particular ζ. *Work at Brookhaven supported by DOE under contract No. DE-AC02-98CH10886 [1] K. Enami and Y.Nakagawa in Proceedings of ICOMAT-92, ed. by C. M. Wayman and J. Perkins (Monterey Institute for Advanced Studies, Monterey, CA 1993) p. 521.

T-14 Inelastic Neutron Scattering Selection Rules for Phonons: Application to Leucite Phase Transition

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Recently, it has been proven the existence of phonon symmetry selection rules in inelastic neutron scattering experiments [1]: the resulting extinctions depend only on the mode symmetry and the Brillouin zone. The simplicity and importance of the selection rules in the analysis of phonon scattering data is shown by its application to the leucite case [2]. The straightforward extension of the procedure for problems of thermal diffuse scattering widens the applicability of the result. [1] J.M. Perez-Mato, M.I. Aroyo, J. Hlinka, M. Quilichini, R. Currat. Phys.Rev.Lett. **81**, 2462-2465(1998). [2] H. Boysen. In emphPhase Transitions in Ferroelastic and Co-elastic Crystals, E.K.H. Salje, pp.335-349, CUP, Cambridge, 1990.

T-15 Amphiphilic Block Copolymers as Efficiency Boosters in Microemulsions: A Two Dimensional Contrast Variation SANS Investigation of The Role of Polymers

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Amphiphilic PEP-PEO block copolymers increase the emulsification power of surfactants in microemulsions dramatically [1]. We investigated the role of the block copolymers by SANS. A highly precise contrast variation method around the matching point of oil, water and surfactant allows to extract the polymer scattering. It was found that the polymer decorates the surfactant membrane and not aggregates forming micellar structures. In addition, this method could be used to extract the partial scattering functions of the different components. We derived theoretical expressions for the functions and interpreted corresponding data [2]. Theoretically it is explained that the decoration of polymers changes the bending rigidity of the membrane, which is confirmed by the phase behavior and our scattering results. [1] B. Jakobs, et al., Langmuir 15 (1999) 6707 [2] H. Endo, et al., Phys. Rev. Lett. 85 (2000) 102

T-16 Neutron Spin-Echo Investigation of the membrane dynamics in bicontinuous microemulsions

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Bicontinuous microemulsions of equal amounts of water and decane with the non-ionic surfactant C10E4 in the vicinity of the fish-tail or optimal point of the phase diagram have been investigated by NSE. The effect of added PEP-PEO blockcopolymers that are long-chain analoga of C10E4 has been studied. These polymers strongly enhance the emulsification efficiency of the surfactant, i.e. they shift the optimal point towards lower surfactant concentration. Systematic series of samples have been investigated by NSE to separate concentration effects (structural lengthscale) and temperature effects from genuine influences of the polymer on the membrane dynamics. The spectra at high Q (0.1-0.2 $Å^{-1}$) follow qualitatively the model of Zilman and Granek that predicts a streched exponential decay (β=2/3) and a rate proportional to Q^3. The validity of this model and the influence of the bending moduli on the dynamics are discussed.

T-17 Additives of Intermediate Polarity - Their Location in Amphiphilic Aggregates and Their Influence on the Corresponding Structures

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Additives of intermediate polarity (esters, aromatic hydrocarbons, long-chain alcohols)in nonionic surfactant systems have been studied by SANS with respect to their influence on micellar structures and on the solubilization capacity of these systems for hydrocarbons. Already the ternary systems of these additives show a behavior that is quite different from that of typical cosurfactants. In general for low concentration of the additive one finds that they promote growth of rodlike micelles. However, at higher concentrations the structures formed depend subtly on polarity and structure of the additive. External contrast variation allowed to determine the location of the different additives in the amphiphilic film. There exists a close relation between the location in the film, the structures of the aggregates and the solubilization capacity of the systems.

T-18 Influence of Carbonate Ions on the Micellization and Phase Separation in Triblock Coploymer Solutions

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SANS was used to investigate the micellization and phase separation in aqueous solutions of triblock copolymers (F38, F68, F98 and F108) as functions of carbonate ion concentration and temperature. SANS data were fitted to determine the sizes of the core and corona, inter-micelle distance, aggregation number and the volume fraction of the micelles. As the polymer molecular weight increases the radii of the core, corona and the inter-micelle distance increase. The carbonate ion concentration and polymer molecular weight have dramatic influence on the temperatures at which the micellization, spherical-to-cylindrical micelle transformation and the phase separation occur. The mechanism by which all these phenomena occur in the triblock copolymer solutions is through gradual dehydration of polymers with either increasing carbonate ion concentration and/or temperature.

T-19 Sequence-Dependent Hydration Properties of Ionic ABA and BAB Triblock Copolymer Micelles from SANS.

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SANS patterns from solutions of ABA- and BAB triblock copolymer micelles formed from poly(methyl methacrylate) and poly(sodium acrylate) blocks were interpreted by choosing Gaussian-type functions for representing the core- and shell profiles. Intermicellar interactions were described in terms of the DLVO potential. A reasonable fit could be achieved only if the molecular volumes were considered free fitting parameters. The volume of the hydrophobic units in both types of micelle was the same; that of the hydrophilic ones was significantly greater in BAB micelles; this property is confirmed by the concentration dependence of the Porod-invariant. The work was supported by BMfBF, BASF AG, Germany and by OTKA, Hungary, contract No. T029958.

T-20 Tuning of exchange coupling in Ho/Y superlattices with deuterium

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Ho/Y superlattices have been studied extensively concerning their phase transition and magnetic spiral propagating through the Y spacer layers. The exchange coupling (EC) between Ho layers is mediated by the RKKY interaction, supported by the nesting feature of the Y Fermi surface in the c-direction. We have investigated the magnetism of a [Ho(77Å)/Y(52Å)]30 superlattice before and after deuterium uptake. Neutron reflectivity at RT confirms that D preferentially occupies the Y spacer layers. LT reciprocal space maps of the pristine Ho/Y superlattice exhibit a magnetic satellite peak τ, convoluted with the satellite peaks of the chemical period, indicative for EC between the Ho layers. After D uptake the splitting of the τ peak vanishes, showing that the individual Ho layers scatter independently. Before and after D loading T_N remains 118 K due to scaling effects. Thus, D in the Y spacer layers magnetically decouples the Ho layers, ascribed to a depletion of the Y electron DOS at E_F, by opening a new hydrogen derived band below the 4d5s Y-band.

T-21 Polarized neutron reflectometry studies of GaMnAs/GaAs superlattices

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Currently a great deal of attention is being focused on spintronics, a novel version of electronics that utilizes not only the electron charge but also its spin. Spin valves and spin injectors are examples of first successful applications of spintronics. GaMnAs is a prototype spintronics material: it is semiconductor ferromagnet which can readily be integrated into GaAs based heterostructures and devices. To gain more insight into the magnetic properties of thin epitaxial GaMnAs layers, polarized and unpolarized neutron reflectivity measurements have been carried out on a number of GaMnAs/GaAs superlattices with different compositions. The data have been collected on the NG-1 reflectometer at Center for Neutron Research, National Institute of Standards and Technology, in Gaithersburg (USA). The samples were prepared by low temperature MBE technique. The Mn content in GaMnAs was 6%. The thicknesses of magnetic layers varied from 10 to 50 monolayers (mnls), and the thickness of the nonmagnetic spacers from 4 to 8 mnls. All four spin-flip and non-spin-flip cross sections have bean measured in zero and applied (100 G) magnetic fields, below and above the Curie temperature (T_C $\sim$45-60K). The occurrence of magnetic superlattice Bragg peaks at the same positions as a nuclear ones clearly indicates that the GaMnAs layers are ferromagnetically coupled across the intervening non-magnetic GaAs spacers. Full polarization analysis of the observed reflectivity profiles reveals that the FM spin order forming in the samples upon cooling in zero external field consists – in most cases – of a single magnetic domain only. The experimental results are compared with theoretical calculations of the reflectivity profiles, based on dynamical approach; both sets of data are found to be in excellent agreement.

T-22 Observing a frozen ferromagnetic moment in the antiferromagnet of an exchange bias system

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Exchange coupling between ferromagnetic (F) and antiferromagnetic (AF) layers can give rise to exchange bias – a shift of the ferromagnetic hysteresis. Several theories suggest that the exchange bias is caused by a net ferromagnetic moment induced in the AF close to the AF/F interface as the sample is cooled in a saturating field. We observe a significant asymmetry in the polarized neutron reflectometry of a Co/$LaFeO_3$ bilayer in positive and negative saturation. This asymmetry is consistent with a net ferromagnetic moment in the AF layer remaining unchanged during the magnetization reversal of the F layer, giving rise to exchange bias.

T-23 Magnetic profiles and coupling in Fe/Cr (110) superlattices

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Epitaxial Fe/Cr superlattices, grown with (211) and (100) orientation, are known to exhibit a magnetic behavior that is a function of the Cr layer thickness t_{cr}. The coupling between the Fe layers oscillates between antiferromagnetic (AFM) and ferromagnetic (FM) by varying t_{cr} with the same period for both growth directions. We present results on Fe/Cr (110) superlattices, with three identical Fe layers of magnetization M. For the FM samples, the hysteresis curve is characterized by two levels (-3M and +3M), whilst for the AFM samples the curve has four levels: $-3M$, $-M$, $+M$, $+3M$. Polarized neutron reflectivity measurements, identified the orientation of the layers magnetizations at different stages of the hysteresis curves. It was found that in spite the structural symmetry, the bottom Fe layer had a different coupling strength from the top Fe layer, a feature that could have caused ambiguities of interpretation if magnetic measurements only were available. Work at Argonne was supported by US DOE, Office of Science contract # W-31-109-ENG-38. Work at UCSD supported by DOE.

T-24 Off-specular polarized neutron scattering from magnetic fluctuations in films and multilayers

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Polarized neutron off-specular scattering from magnetic domains, interfacial rougness and dynamical fluctuations in thin films and multilayers is theoretically considered within and beyond the Distorted Wave Born Approximation (DWBA). The criteria for the DWBA validity range are explicitly formulated and alternative approach is suggested if DWBA fails. It is shown that 3D polarization analysis can be employed not only to deduce parameters of the domain structure, but also for separation of inelastic sygnal from elastic scatering. Theoretical consideration is illustrated by a number of examples typical for the experiments on polarized neutron reflectometry.

T-25 3DXRD: a new tool for bridging the length scales in materials science.

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Initially the 3-Dimensional X-Ray Diffraction (3DXRD) technique for characterisation of the individual grains within millimetre - centimetre thick specimens is presented. Based on diffraction with hard x-rays (E>40 keV), the position, volume, morphology, orientation and elastic strain of 10-1000 grains are determined simultaneously, typically within a few minutes. The detection limit is $(0.3\mu m)^3$. As examples of results, we mention new insight on the dynamics of the three fundamental processing steps in metallurgy: deformation, nucleation and grain growth. In the second part, it is discussed how 3DXRD can complement conventional neutron or x-ray based methods such as powder diffraction (stress, texture and lineprofile analysis), small angle scattering and tomography. Unique dynamic data is provided on several length scales, enabling tests of unified models.

T-26 Diffuse Scattering Experiments Using High-Energy X-rays and Neutrons

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Diffuse x-ray scattering has been an important tool for understanding the atomic structure of multicomponent systems for nearly fifty years. For practical applications x-rays and neutrons differ mostly in the available flux and the penetration power in materials. In the case of x-rays the absorption length in materials can be increased by orders of magnitude using high energy x-rays. This intensity gain combined with the ability to measure the intensity from an entire plane in reciprocal space using two-dimensional x-ray detectors permit extensions of diffuse scattering studies to time resolved measurements. The specific merits of both neutrons and high energy x-rays for diffuse scattering experiments will be discussed for the model spin glass system Cu-17at%Mn and the binary alloy TiV.

T-27 Complementary x-ray and neutron measurements on contained and levitated liquids

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The recent availability of high-energy x-ray beams at third generation sources, together with beams of short-wavelength neutrons produced by spallation sources and hot sources at reactors, make it possible to carry out complementary diffraction experiments on contained liquids, exploiting the different contrasts for the two types of radiation. This talk will review some recent results obtained in this way: $FeCl_3$, KPb and H_2O/D_2O will be chosen as representative of three different classes of liquid. Recent experience with complementary x-ray and neutron measurements on levitated liquid samples will also be discussed. This work was supported by the Office of Science, US Department of Energy under Contract W-31-109-ENG-38.

T-28 Magnetic moment determination by the complementary methods of high-energy magnetic x-ray and magnetic neutron diffraction

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A comparison of high-energy non-resonant magnetic x-ray diffraction and magnetic neutron diffraction will be given. Especially the direct determination of the pure spin magnetic moment will be discussed which is possible due to the very simple scattering cross-section at high photon energies. These results, obtained first on chromium and then on FeF_2 and CoF_2, are compared with measurements of the total magnetic moment by magnetic neutron diffraction and can thus reveal spin and orbital magnetic moment separately. For FeF_2 a magnetic spin moment equal to the moment of the free Fe^{2+} ion is determined whereas CoF_2 shows a spin moment considerably lower than the free ion value.

T-29 Capabilities of neutrons and high energy X-rays for material science

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Both thermal neutrons and high energy X-rays exhibit a comparable penetration depth into materials and hence allow to grain subsurface information e.g. about phase composition, texture and residual stresses. However, the marked differences in the radiation characteristics between neutrons and high energy X-rays, e.g. wavelength,divergence, intensity lead to different capabilities of the methods for the analysis of materials and components. The special advantages and limitations of both radiations and their complementarity will be discussed by presenting examples which represent typical challenges for materials science.

T-30 Scattering of Neutrons and Photons - Complementary Methods for Diffusion Studies

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Quasielastic neutron scattering (QNS) and nuclear resonant scattering of synchrotron radiation (NRS) have been successfully used to study the microscopic details of self diffusion in ordered alloys [1,2]. The basic questions are: Between which sites do the diffusing atoms jump? What are the jump frequencies? What is the correlation of subsequent jumps? How are defects involved in the diffusion mechanism? The two methods, QNS and NRS, give access to different types of samples, but also provide complementary information on different scales in time and reciprocal space. This will be discussed on the example of the B2 alloys (CsCl-structure) NiGa, CoGa and FeAl. [1] M. Kaisermayr, J. Combet, B. Sepiol, H. Ipser, H. Schicketanz and G. Vogl, Phys. Rev. 61, 12038 (2000); Phys. Rev. B 63, 054303 (2001). [2] B. Sepiol, A. Meyer, G. Vogl, H. Franz, R. Rüffer, Phys. Rev. B. 57 (1998).

T-31 Collective dynamics of liquid Hg investigated by inelastic x-ray scattering

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Hg is the only element that is a liquid metal at room temperature, and one of the few metals whose liquid-vapor critical points occur at temperatures and pressures accessible in the laboratory. Therefore it is an important substance for structural, thermodynamic, and electronic investigations including those in the low-density limit. Despite a number of intensive studies on liquid (l-) Hg, its microscopic dynamic properties were never experimentally investigated, not even at room temperature. This is due to extremely high absorption cross section of Hg for thermal neutrons. In this paper, we present the first results on the dynamic structure factor $S(Q,\omega)$ for l-Hg at room temperature obtained from a high-resolution inelastic x-ray scattering experiment carried out at APS/ANL. Distinct excitations resulting from propagating modes can be identified. The slope of the phonon dispersion at low Q is about 15% larger than that expected by the hydrodynamic sound velocity. This effect is about 50% larger than in liquid alkali metals. For a further understanding of the underlying microscopic mechanism, comparison with theory is now in progress.

T-32 Protein Crystallography with Spallation Neutrons

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Neutrons are ideal to probe the details of a proteins complex structure. Neutrons reveal protonation states, water of hydration and the functional and structural important hydrogen bonds. With the development of genetic cloning techniques it became possible to produce fully deuterated proteins with nearly identical function. The use of perdeuterated protein crystals improved data collection rates by greatly reducing the incoherent background caused by hydrogen atoms reducing thus the impact of the inherent low flux of neutron sources. In parallel to these genetic 'crystal improvements', improvements in diffraction techniques and instrumentation, particularly the development of better and larger detectors makes neutron protein crystallography a much improved tool to study the details of a protein's function and structure.The availability of spallation neutrons for structural biology promises a further major improvement in data collection rates. Spallation neutrons with their time dependant wavelength distribution have all the advantages of the Laue process without any of its disadvantage. Initial results obtained with a partially decoupled moderator collected with an 8 segment position sensitive detector at the LANSCE spallation neutron source will be be presented.

T-33 The Structure of Aldose Reductase at 0.66ÅResolution Shows the H-Aoms Relevant for Inhibitor Binding and the Catalytic Mechanism

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The structure of Aldose Reductase (ALR2; EC 1.1.1.21) complexed with the inhibitor IDD594 was obtained and refined from X-ray crystallographic data at 0.66Å, the highest resolution ever recorded for an enzyme of this size. It shows many details, such as H-atom positions, deviations from standard stereochemistry, exact determination of atomic species, bond electron density, multiple conformations and detailed solvent structure. This accuracy enables the unambiguous assigning of the orientation of His110 ring around the Ca-Cb bond and the positioning of hydrogen atoms involved in catalysis. The inhibitor binds to the active site, with strong contacts involving the carboxylate head and a Br atom which are shown by an unusually short Br-O distance.

T-34 A combined neutron crystallography/IQNS study of water around lysozyme

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This seminar reports a structural and dynamical study of water around proteins. For the first time, both experiments were done on the same type of sample, triclinic crystal of hen-egg white lysozyme. It allowed us to directly compare the results and to propose a model of the dynamics of water around proteins, at 300 K, with atomic resolution, and under about a few hundreds ps. Neutron diffraction data were collected with a resolution of 1.7 Å[1]. About 80 % of water molecules theoretically present in the unit cell were constructed, and it gives interesting information, especially concerning the dynamical disorder, the arrangement around apolar parts of the protein. Water molecules could be divided into two groups acoording to their single-particle diffusive dynamics [2]. As protein crystals have a highly crowded arrangement close to the packing of macromolecules in cells, this model can be discussed in the light of solvent behaviour in intracellular media. [1] Bon, C. et al. 1999. Acta Cryst. D 55(5):978-87. [2] Bon, C. et al. Submitted.

T-35 Hydrogen in Proteins: Recent Results from the Single Crystal Neutron Diffractometer BIX-3

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A high resolution neutron diffractometer, BIX-3, dedicated to protein crystallography has been successfully constructed at the reactor JRR-3M at the JAERI and is now in routinely operation. The combination of a large cylindrical neutron sensitive image plate and the usage of monochromatic neutrons provides the possibility to collect high resolution data sets of biological macromolecules to a resolution of $d<1.5$Å. This resolution makes it possible to investigate deviations from stereochemical predicted hydrogen bond angles in proteins. In addition the analysis of protonation states and the extent of exchange of hydrogen atoms by deuterium within the protein can be investigated. Recent results from BIX-3 will be presented.

T-36 Biological applications of monochromatic neutron diffraction

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Neutron scattering experiments provide important information in structural biology that is not accessible by x-ray scattering alone. In neutron protein crystallography, the Laue method used on the LADI instrument at the ILL has started to produce extremely useful information on location of hydrogen atoms and of water molecules. However in certain situations monochromatic instruments offer important advantages. In fibre diffraction the advantages of using neutron diffraction for the investigation of solvent structure around molecules such as DNA [2,3] and the location of hydrogen atoms in cellulose [4] are very clear - no comparable information on solvent structure has been obtained from X-ray diffraction, and instrument D19 at the ILL has a steadily growing portfolio of activity in this area. Major developments are planned for D19. This will involve a massive increase in the detecting solid angle and open up new areas of science for the study of fibrous structures and small proteins. [1]Myles et al., Physica B, Vol. 241-243,1122-1130 (1998) [2]Shotton, Pope, Forsyth, Langan, Denny, Giesen, Dauvergne, Fuller, Biophysical Chemistry 69 (1), 85-96 (1998) [3]Shotton, Pope, Forsyth, Denny, Archer, Langan, Ye, Boote, J. Appl. Cryst. 31 (5), 758-766 (1998) [4]Langan, Nishiyama and Chanzy, J. Am. Chem Soc. 121 (43), 9940-9946 (1999)

T-37 Neutron Diffraction Studies on the Thermostability of Rubredoxin

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Single-crystal neutron diffraction data up to a resolution of 1.5 Åhave been collected at room temperature on two forms of rubredoxin using the new BIX-3 diffractometer at the JRR-3 reactor of JAERI. Rubredoxin is a small iron-sulfur redox protein with 53 amino acid residues, and the source of this particular protein is the hyperthermophile Pyrococcus furiosus, a microorganism that normally lives at temperatures near that of boiling water. Data were collected on crystals of the wild-type protein and a mutant in which three of the residues have been replaced. We were interested to see if the results of the neutron analysis would provide some reasons to explain the remarkable thermal stability of the wild-type protein from this intriguing microorganism. For the wild-type rubredoxin, data were collected on a single crystal having dimensions of $2.5 \times 2.5 \times 0.8mm$ up to a resolution of 1.5 Å. Exposure times ranged from 60 to 77 minutes per frame, and the net time required to collect the total of 717 data frames was 35 days. Refinement of the structure was carried out in the resolution range 5-1.5 Å. Included in the refinement were 301 hydrogen atoms and 40 deuterium atoms, and 29 water molecules were also identified. The second sample in this structural analysis is a ”triple mutant” in which three residues in the core of the molecule were mutated to resemble the rubredoxin of Clostridium pasteurianum, a mesophilic (room-temperature) bacterium. This mutant is known to have a lower thermal stability than the wild-type protein at low pH. Data collection was carried out at room temperature on a crystal with dimensions $3 \times 2 \times 1mm$, also to a resolution of 1.5 Å. The current model in the least-squares refinement includes 292 H atoms, 78 D atoms and 83 solvent molecules. In these structural analyses, it was found that the H/D exchange pattern was quite revealing. Most of the N-H bonds of the main polypeptide backbone had been exchanged by deuterium except those clustered around the N-terminus of the molecule. This implied that the hydrogen bonds near the N-terminus are ”protected” from the solvent, and suggested that this section of the molecule is especially resistant to unfolding. The extra stability of this region may provide an explanation for the unusual thermal stability of this protein.

T-38 The Gaussian behavior of the alpha-relaxation in glass-forming polymers revisited. MD-simulations & QENS results

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Neutron scattering results of many different polymers show that in the time and Q-range where the alpha-relaxation is observed by these techniques (typically: t between 5ps and 2ns; Q between 0.2 Å^{-1} and 1.8 Å^{-1}) the incoherent intermediate scattering function Fs(Q,t) shows an approximate Gaussian behavior. This behavior suggests a homogeneous character for the alpha-relaxation in glass-forming polymers in contradiction with recent results from relaxation techniques. Recent fully atomistic MD-simulation results suggest a crossover from homogeneous/Gaussian to heterogeneous/non Gaussian behavior, taking place in the Q-range (about 1.5 Å^{-1}) of the first maximum of the static structure factor S(Q). The existence of such a crossover in real samples would allow to rationalize the apparent contradiction between neutron scattering and relaxation techniques. However, the experimental observation of this crossover is a difficult task due to the Q-range covered by the most common backscattering instruments. We have investigated this crossover in several glass-forming polymers by means of NSE and IN13 instruments extending the Q-range up to about 5 Å^{-1}.

T-39 On the pressure, temperature and molecular weight dependence of the local polymer dynamics in the glass and the melt

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Inelastic neutron scattering experiments on polybutadiene (PB), Mw=7600, and polyisobutylene (PIB), Mw=680, were carried out as a function of pressure and temperature on IN6 and IN16, ILL Grenoble. Increasing pressure induces changes in $S(Q,\omega)$, mainly on the low frequency side of the Boson peak, which are similar, but much weaker than caused by decreasing temperature at P$_{atm}$. High energy resolution experiments on PB gave relaxation isochrones on the ns-time scale along which the fast ps-relaxation process changes. The relaxation along microscopic isochores, determined on D7, turns out to be strongly temperature dependent. From elastic scans on IN16 as a function of P and T we find that PIB behaves more complex than PB, revealing a strong pressure dependent dynamic process. A possible influence of molecular weight (Mw between 390 and 73000) was investigated for PIB as a function of temperature. Both, changes in the ns-relaxation on IN16 and in the Boson peak region (ps) are observed for molecular weights lower than Mw = 4040.

T-40 Constraints of motion in polymer melts: coherent and incoherent scattering analyzed by neutron-spin-echo spectroscopy

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A series of new extended time range neutron-spin-echo (NSE)-data of coherent scattering from polyethylene(PE)-melts with different molecular weights allows a systematic investigation of the reptation dynamics. The results show an increase of the tube diameter, the remaining free parameter in deGennes form of S(Q,t) in the reptation model, with decreasing molecular weight M$_w$. For M$_w$ lower than 14 000 g/mol a sudden failure of the reptation expression to fit the data was found in accordance with a theory of entanglement formation as postulated by Kavassalis et al predicting a failure of the tube conception at $M_c \approx 7M_e$. For the first time also the incoherent structure factor of purely protonated high-M$_w$-PE was measured at the NSE spectrometer in Jülich. The data corroborate the crossover from Rouse to local reptation dynamics at the entanglement time τ_e. However, there is a discrepancy between the tube diameter determined by coherent and incoherent scattering.

T-41 Frozen Concentration Fluctuations of a Poly(N-isopropyl acrylamide) Gel Decomposed by Neutron Spin Echo and Small-angle Neutron Scattering

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Although the frozen concentration fluctuations in a polymer gel have been observed as the excess small-angle scattering, there is no direct observation of their fraction or q-behavior. By employing neutron spin echo (NSE) and small-angle neutron scattering (SANS), we first determined q-behaviors of the frozen concentration fluctuations in a poly (N-isopropyl acrlyamide) (NIPA) gel. For a NIPA gel, we observed a crossover from collective diffusion to single chain Zimm dynamics as q increases, which is well established for a semidilute polymer solution including a NIPA solution. We further observed a significant retardation of decay for a NIPA gel. If we compare the two decay curves of a gel and a solution, it is turned out that the frozen concentration fluctuations decreases obeying q^{-4} at high q. We further obtained a fraction of the frozen component for a NIPA gel at low q, occupying the scattering of 35% at 28°C or 55% at 33.3°C. All measurements were performed at Jülich Forschungszentrum in Germany or at Institute Laue-Langevin in France.

T-42 Phase Behavior of Binary Polybutadiene Copolymer Mixtures as an Example of Weakly Interacting Polymers

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Binary blends of statistical copolymers of different vinyl content and molar volume were explored by SANS. These samples represent the most simple class of statistical copolymer mixtures. In spite of this simplicity changes in vinyl content, molar volume, deuterium and hydrogen content of the chains give rise to strong changes; phase separation occurs between minus 230°C to more than plus 200°C and can even reverse from an enthalpy driven one at low temperatures (UCST) to an entropically driven one at high temperatures (LCST). The entropic and enthalpic terms of the Flory-Huggins (FH-)parameter as determined from experiment are in excellent agreement with Lattice Cluster Theory calculations. The enthalpic term is a small number and determined from van der Waals nearest neighbor interactions; the corresponding interaction of the PB(1,4) monomers is largest and their deuteration leads to a negative enthalpic FH-parameter and thereby to a change from an UCST to a LCST behavior.

T-43 Magnetic correlations in heavy fermion CeMIn$_5$ (M=Rh, Ir and Co)

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Antiferromagnetism and superconductivity, with very high transition temperatures for heavy fermion compounds, exist in close proximity in the heavy fermion materials with chemical formula CeMIn$_5$ (M=Rh,Ir,Co). These tetragonal materials consist of alternating layers of the cubic heavy fermion antiferromagnet CeIn$_3$ and the intervening MIn$_2$. Magnetic structures of the heavy fermion antiferromagnets CeRhIn$_5$, Ce$_2$RhIn$_8$, Ce(Rh,Ir)In$_5$, and (Ce,La)RhIn$_5$ are determined using neutron diffraction. Dynamic magnetic correlations of CeRhIn$_5$, CeIrIn$_5$ and CeCoIn$_5$ are investigated with inelastic neutron scattering. Effects of hydrostatic pressure and magnetic field on the antiferromagnetic orders are also investigated. Insight on relation between the quasi-two-dimensional crystal structure, antiferromagnetism and superconductivity in these new heavy fermion materials, obtained through systematic study of the family with various M, changing ratio of the CeIn$_3$ and MIn$_2$ layers, doping on the Ce site, and external fields, will be discussed.

T-44 Pressure and temperature dependence of the ordered magnetic U moment of USe

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In the U monochalcogenides, the magnetic properties are characterised by an interplay between localised, rare earth like magnetic moments and itinerant, electron band like magnetism due to hybridisation effects. By neutron powder diffraction, we have measured the temperature dependence of the U moments, which was found to be accompanied by a strong trigonal distortion of the NaCl type lattice. The application of pressures below 1 GPa leads to a drastic reduction of the U moments from 2.5 μ_B to 1.3 μ_B, which is presumably caused by a domain reorientation associated with the trigonal distortion. Up to pressures of 7.5 GPa, no further significant change of the ordered U moment was observed.

T-45 Pressure-induced magnetic structures in UNiGa

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UNiGa below T_N (= 39 K) exhibits 4 AF phases formed by ferromagnetic planes of U moments μ_U with various stacking along the hexagonal c-axis. The ground state has the $++-+--$ sequence ($\mu_U = 1.4\mu_B$/U aligned along c). Thermal-expansion data indicate that at hydrostatic pressures above 1.8 GPa a new magnetic phase may appear. In a neutron diffraction experiment using a 2.3 GPa clamp cell and carried out on D9 at ILL below 38 K we have observed only magnetic peaks corresponding to $\mathbf{q} = (001/2)$. These point to a simple AF stacking of μ_U along the c-axis, not observed in UNiGa at ambient pressure. The $p - T$ magnetic phase diagram will be discussed within the ANNNI model.

T-46 New dispersive magnetic mode in neutron spectra of unstable valence Sm$_{1-x}$Y$_x$S

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The magnetic response function of powder and single-crystal ^{154}Sm$_{1-x}$Y$_x$S in the intermediate-valence state has been determined by inelastic neutron scattering experiments. Changes in the intermultiplet transitions for both Sm^{2+-} and Sm^{3+-} configurations due to the valence instability have been detected. In particular, two magnetic modes were observed in the energy range of the Sm^{2+-} spin-orbit transition (25-40 meV) . The energy dispersions and intensities of these modes were studied along the main symmetry directions. The peak at higher energy can be regarded as reminiscent of the Sm^{2+-} spin-orbit transition. As suggested previously for SmB$_6$, the extra component may result from the formation of a new quantum-mechanically mixed ground-state wave function containing a partially delocalized 4f component.

T-47 Spin-fluctuations and the spin-liquid to spin-glass transition in β-MnAl

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Substitution of Al into non-magnetic β-Mn results in the stabilisation of short-range magnetic order at low temperatures. While Al substitution has been found to promote local magnetic moment formation, strong zero-point spin fluctuations are observed. We have recently performed inelastic neutron scattering studies of pure β-Mn and β-Mn$_{1-x}$Al$_x$ on the HET and IN6 spectrometers. All alloys studied showed a broad response, peaking at Q$\sim$1.5Å^{-1} persisting to 4K. While the inelastic linewidth shows only weak temperature dependence, the quasi-elastic intensity is found to fall off sharply at low temperatures while the ”elastic” intensity increases. The most striking feature of S(Q,ω) for β-Mn is its temperature dependence - the energy loss side being completely temperature independent. This behaviour implies non-Fermi-liquid scaling in a system displaying critical scattering associated with a T=0K phase transition, and leads to a scaling of the dynamical susceptibility as a power of ω/T.

T-48 The design and simulation of a curved-guide plus flight tube setup for neutron radiography and tomography at the new research reactor FRM-II at Technical University Munich

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The new reactor FRM-II of Technical University Munich will offer a professional radiography and tomography facility for industrial use. In a first stage, the facility will consist of a classical flight tube setup. In about five years, the second external experimental hall will be finished, and neutron tomography will move into that hall in order to enable for a triple beam port on SR-4 housing the ultracold source and two guide systems. The new hall will allow easier access for very large samples and will have the possibility of installing cooling systems and exhaust ducts for a test stand for live combustion engines. The new experimental position will be 42 meters away from the reactor core, so a flight tube only would deliver unsufficient flux. In order to achieve large beam cross section and high flux at the experimental position as well as a very parallel and homogenous beam, a combination of a supermirror guide and an additional flight tube will be used. The guide will transport the reactor flux distribution far away from the reactor itself, feeding again a system of circular diaphragm and consecutive flight tube. The geometry will again be only determined by the diaphragm and the flight tube if the distance between the end of the guide and the sample is sufficiently high; the acceptance angle of the guide determines the size of the illuminated field at the sample position. The illuminated area can be determined for each single wavelength; for a whole neutron spectrum, the spectral and intensity distribution becomes dependent on the radius from the midpoint of the guide, giving a conical intensity distribution. Apart from difficulties with the detector dynamics and in normalizing the images, quantitative neutron radiography becomes very difficult with such a setup with the full reactor spectrum because the spectrum at the sample position is inhomogeneous and a homogeneous sample would show different position-dependent attenuation coefficients.

T-49 Development of Neutron Optical Devices

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An integrated research and development of neutron optical devices is in progress in Japan. We present an overview of the research activities which covers the development of magnetic optics, refractive optics on material surface, flat and/or round surface supermirrors and neutron imaging device for the evaluation of the optical devices. We also report the recent results on adiabatic neutron spin control for realizing a magnetic doublet, neutron prism on the basis of the refractive effect on the surface of MgF_2 and wavelength shifting fiber readout neutron scintillator.

T-50 The NRSE-TAS Spectrometer at the FRM-II

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The combination of zero-field spin echo and triple axis spectroscopy at a high-flux spectrometer under construction at the FRM-II will allow the determination of the energies and lifetimes of dispersing excitations, including both phonons and magnons, over the entire Brillouin zone. We discuss the technical design of the instrument and give examples of the envisioned scientific applications. We will also present the results of pilot experiments carried out at the FLEX spectrometer at the HMI.

T-51 Neutron wave resonator as a spin-echo spectrometer element

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The peculiarities of the reflection and transmission of neutron waves through a layered structure in an inclined magnetic field are discussed. It is shown that the magnetized layer can be used as an effective turner of polarization by 90 and 180 degress and that a three-layer magnetic structure can act effectively as a phase shifter of the neutron wave. The conclussion is that the discussed magnetic structures can be used as elements of the spin-echo spectrometer in the study of low-frequency excitations in near-surface layers.

T-52 Quasielastic neutron scattering studies of H motion in Laves-phase compounds

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Our quasielastic neutron scattering (QENS) studies of hydrogen diffusion in cubic Laves-phase compounds $\mathrm{AB_2H}_x$ ($x < 1.5$) have revealed a coexistence of two frequency scales of H hopping. The faster jump process corresponds to the localized H motion within the hexagons formed by tetrahedral g-sites (A_2B_2), and the slower process is associated with H jumps from one g-site hexagon to another. We have also found a relation between the hydrogen hopping rates and the positional parameters of hydrogen atoms in g-sites (determined from the accompanying neutron diffraction measurements). Furthermore, the positional parameters of H atoms in g-sites are shown to be related to the ratio of the metallic radii of the elements A and B. Thus, our results give a key to understanding the systematics of H motion in cubic Laves phases.

T-53 Measurement of the Momentum Distribution in Hydrogen Bonded Systems

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Measurement of the momentum distribution of hydrogen in a hydrogen bond can provide detailed information on the dynamics and environment of the bond. Recent measurements made using eVS at ISIS on KDP and oxalic acid will be presented as example. The proton in the high temperature phase of KDP does indeed delocalize over the two equivalent sites identified from neutron crystallography. Knowing the momentum distribution for a symmetric bond allows the direct measurement of a Born-Oppenheimer potential. We will present the potential for KDP.

T-54 Proton Conduction Based on Intracrystalline Chemical Reaction

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Proton Conductivity in $M_3H(SeO_4)_2$ crystals (M=K, Rb, Cs) is shown to be due to a dynamic disorder in the form of an intracrystalline chemical equilibrium reaction : alternation between the association of the monomers $[HSeO_4]^{1-}$ und $[SeO_4]^{2-}$ resulting in the dimer $[H(SeO_4)_2]^{3-}$ (H-bond formation) and the dissociation of the latter into the two monomers (H-bond breaking). By a combination of neutron diffraction, quasielastic and inelastic neutron scattering, as well as FTIR-spectroscopic experiments, covering the time scales from 0.1 ps to 10 ns, reaction rates, life times of monomers and dimers, and potential wells for H-bond formation and breaking, respectively, were obtained, as well as rates of proton exchange between selenate ions, leading to diffusion. The results demonstrate, that this reaction plays a central role in the mechanism of proton transport in these solid state protonic conductors.

T-55 Studies of new metal hydrides

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A major unsolved problem for the introduction of the ”Hydrogen Economy” is efficient and safe storage of hydrogen. Metal hydrides are promising materials for hydrogen storage. This presentation focuses on recent structural studies of new metal hydrides. The results are based on high resolution powder neutron diffraction data (JEEP II reactor, Kjeller) and X-ray diffraction (conventional and synchrotron radiation, ESRF). An example is RENiIn-hydrides, RE=Nd, Ce, La with extraordinary short H-H distances, ranging from 0.1570(8) (Nd) to 0.1635(8) nm (La). This is significant shorter than the established empirical ”0.20 nm criterion” for metal hydrides. Another example is TbNiAl-deuterides with interesting properties depending on the deuterium content, e.g. change of lattice symmetry, H-ordering, change of type of magnetic ordering and magnetic ordering temperature.

T-56 Diffraction study of CD_4 and D_2 adsorbed carbon nanotubes

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We report neutron diffraction data from bare and methane (CD_4) or hydrogen (D_2) covered single-walled carbon nanotube powder samples together with model calculations of the diffraction profiles. We find, that the ”grooves” at the outer surface of bundles formed by individual carbon nanotubes are likely candidates for the preferred adsorption sites but that a certain fraction of the available interstitial channels can also be filled by nearly one-dimensional CD_4 or D_2 chains. Upon further adsorption the chains in the grooves grow to form increasingly broader stripes until the outer surface of the bundles becomes completely covered by a hexagonally ordered CD_4 or D_2 layer.

T-57 Structure and Dynamics of gas hydrates

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We report the results of experiments with inelastic and elastic neutron scattering [1][2] on both natural hydrates sampled from the pacific sea floor and laboratory synthesized gas hydrates. Gas hydrates are inclusion compound in which small guest molecules or atoms like e.g. CH_4 or Xe are trapped in cages formed by an ice-like hydrogen bonded network of water molecules. Of special interest are the natural hydrates (methane hydrate) as large accumulations have been found on the sea floors which may serve as a future energy resource. The INS experiments of CH_4 hydrate focused on the low temperature rotational dynamics of the trapped guest molecules. Precise crystallographic parameters on both the host network and the guest molecules have been obtained from a high-resolution diffraction experiment on a fully deuterated methane hydrate. The vibrational dynamics of the host network has been studied by means of an INS experiment of xenon hydrate, showing a strong guest-host coupling at low frequencies. References : [1] C. Gutt, B. Asmussen, W. Press, M.R. Johnson, Y.P.Handa and J.S. Tse, J.Chem.Phys. 113, 4713 (2000), [2] C. Gutt, W. Press, A. Hueller, H. Casalta and J.S Tse, J.Chem.Phys, 114, 4160 (2001)

T-58 The isomorphous transition between $Co(NH_3)_6(PF_6)_2$ and $Ni(NH_3)_6(PF_6)_2$

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$Co(NH_3)_6(PF_6)_2$ and $Ni(NH_3)_6(PF_6)_2$ are isostructural at low temperatures, other than a $\pi/4$ rotation of the NH_3 groups. These groups are octahedrally coordinated around the metal ion and undergo almost free quantum rotation which is also coupled to a centre of mass movement of the NH_3 groups. In order to study the transition between the Co and Ni structures we have studied the tunnelling spectra of mixed crystal Co/Ni salts across the whole composition range (this transition cannot be induced by pressures up to at least 5Kbar). At Ni:Co ratios below 60:40 we find the structure to be that of the cobalt salt for both types of ion. There is then an abrupt transition above 60:40 to the structure of the nickel salt for both types of ion. This is in stark contrast with the expected smooth transition over a range of compositions that was expected on the basis of a range of possible NH_3 orientations with almost the same energy. No abrupt change in the magnetic characteristics arises over the entire composition range.

T-59 Solid Monolayers of Simple Alkyl Molecules Adsorbed from their Liquid to Graphite

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Incoherent elastic neutron scattering has been used to show the formation of solid monolayers adsorbed from liquid alk-1-enes, phenyl-alkanes and fluoro-alkanes on to graphite as a means of investigating the influence of different chemical groups on solid monolayer formation.

T-60 Superstructures in Manganites and other Doped Oxides

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In many doped transition metal oxides there occur with decreasing temperature different superstructures: charge, orbital ordering, stripes etc. The mechanisms leading to their formation are not always clear: they may be caused by the purely electronic effects (Coulomb interaction, superexchange), may be connected with the magnetic structure, or caused by the electron-lattice interaction. In this talk I will discuss one particular, rather general mechanism which can give these superstructures, at least in insulating systems: the elastic interaction caused by the distortion of the lattice by ions with different valence and different electronic configurations. This interaction is long-range ($1/R^3$) and is anisotropic, having different signs in different directions. This quite naturally can lead to many types of superstructures, including stripes and 2d ”sheets” in manganites. Several typical examples will be considered from this point of view. This talk is largely based on the work with K.I.Kugel (cond-mat/0103317 and to be published).

T-61 Charge and Stripe order in $La_{2-x}Sr_xNiO_4$

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Stripe order in $La_{2-x}Sr_xNiO_4$ with $0.289 \leq x \leq 1/2$ was studied with neutron scattering technique. The stripe order of holes and spins at low temperatures are observed in all samples. Incommensurability ϵ of the stripe order is approximately linear to the hole concentration up to $x = 1/2$. The stripe order at $x = 1/3$ is unusually stable and affects the stripe order of the both side of the hole concentration with $x < 1/3$ as well as $x > 1/3$. On the other hand, the behavior at $x = 1/2$ is drastically different. The checkerboard-type charge ordering is formed at high temperatures above 400K, but it is taken over by the charge and spin stripe order at low temperatures. Our preliminary studies established that the stripe ordering is surprisingly robust against hole doping, surviving up to very high hole concentration as much as $x \sim 0.7$.

T-62 Heavily Doped Bilayer Manganites: Links Among Structure, Charge, and Spin

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Bilayer manganites $La_{2-2x}Sr_{1+2x}Mn_2O_7$ offer an exceptional opportunity to explore the connections among crystal structure, magnetic structure, and charge order. We have recently succeeded in synthesis of the phase diagram x ¿ 0.5, and have used both neutron and x-ray diffraction to explore both the broad features and subtle details of this highly Mn^{4+}-rich system. In particular, we find a progression of magnetic structures in concert with theoretical predictions, and which can be connected to structural response to orbital ordering. We also find an unexpected region in which no long-range magnetic order is found and discuss possible explanations based on short-range order measured by neutron pair distribution function analysis. We also address the evolution of charge order in these materials and discuss its stability as a function of dopant ion concentration and competition with incompatible magnetic ground states. Finally, we propose a chemical method for interrogating the role of dimensionality in the bilayer manganites.

T-63 Orbital and Spin Dynamics in Titanates and Vanadates

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Three-dimensional magnetic insulators, a hot subject in the 1960’s, have faded into obscurity in recent years. This situation has recently changed with a renewed focus on orbital degrees of freedom and their interplay with the lattice and spin dynamics in manganese oxides. We will present inelastic neutron scattering experiments providing evidence of interesting quantum dynamics in the orbital sector of insulating titanate and vanadate perovskites. While the spin excitation spectra of these systems are qualitatively different from what would be expected if the t_{2g} orbitals were purely static, theoretical models that take orbital quantum fluctuations into account provide a quantitative description of the neutron scattering data. In some members of the titanate family, this orbital zero-point motion is particularly pronounced and appears to stabilize an ”orbital liquid” phase.

T-64 Theory of Colossal Magnetoresistant Materials

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Recent studies of manganites have revealed intrinsically inhomogeneous ground-states. The effect involves ferromagnetic metallic and antiferromagnetic charge and orbital ordered insulating phases. This tendency could originate in phase separation with percolative characteristics, driven by disorder near first-order transitions. Implications for Cu-oxides are also discussed [1]. [1] A. Moreo et al. Science **283**, 2034 (1999); E. Dagotto et al., Physics Reports **344**, 1 (2001); M. Mayr et al., PRL **86**, 135 (2001); J. Burgy et al., preprint.

T-65 Resistivity Rise and Short-Range Charge Ordering in CMR Manganites

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We use neutron scattering to demonstrate that the resistivity rise and insulating behavior in CMR manganites are intimately related to the presence of lattice polarons and their short-range correlations. We establish the orientation, commensuration, and coherence length of the polaron correlations in $La_{1-x}Ca_xMnO_3$ as a function of x and in $A_{0.7}B_{0.3}MnO_3$ manganites as a function of Tc. We show that the low temperature transport properties in these materials are determined by the competition between the polaron correlations and the ferromagnetic double-exchange interaction.

T-66 The Tertiary Spectrometer: the role of software in the design and performance of instruments and experiments.

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Software plays a central role in neutron scattering - in the design of sources and instruments, in the control of instruments and sample environment and in the visualisation and analysis of data. However these are normally viewed as a set of separate activities, and not as integral parts of a single process. I will give an overview of how the combination of different software might be used to maximise the most important variable, which is the scientific information output per unit of beam time.

T-67 A model instrument for Monte Carlo code comparisons

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In the same manner that standard samples are used to cross check the measurement precision of neutron instruments, štandard modelsčan be used to compare the various Monte Carlo codes currently in use to simulate the instruments. For the first such intercomparison, we have chosen to model a 14.7 meV vanadium calibration measurement on a triple-axis spectrometer (TAS), using as a basis the H8-TAS (formerly located at the High-Flux Beam Reactor at Brookhaven National Laboratory) for which dimensional and count rate documentation is conveniently available. Our instrument model contains as elements a fixed source, apertures, Soller collimators, monochromator and analyzer crystals (mosaic, curved, vertical focusing), an incoherent scattering vanadium sample, and a 3He detector. Initial comparisons will be made in terms of neutrons counted per source neutron at specified positions along the beam path. Should a need for more details arise, the program could be expanded to include acceptance diagrams and/or 2D distributions. The authors represent the five Monte Carlo groups currently involved in the study.

T-68 A comparison of Monte-Carlo simulations using RESTRAX and McSTAS with experiment on IN14: the effects of using a focusing guide on resolution

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The effects of using a focusing guide between monochromator and sample have been simulated using the two Monte-Carlo programs RESTRAX and McSTAS. The simulations were compared with experiment. The flux gains and the energy spreads of the resultant beam at the sample position have been previously documented [1]. This paper presents simulations of the divergence of the beam in real space, and the angular distribution of the wavevectors at the sample position. The simulation results for both programs compare extremely well on a quantitative level with the experimental findings, giving confidence in the accuracy of both the simulation programs and highlighting the dangers of using focusing optics on high resolution instruments. [1] A. R. Wildes et al., Physica B 276-278 (2000) 177

T-69 Measurement and Simulation of the Inelastic Resolution Function of a Time-Of-Flight Spectrometer

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The deconvolution of inelastic neutron scattering data requires the knowledge of the inelastic resolution function. The inelastic resolution function of the time-of-flight spectrometer IN5 /ILL has been measured by exploiting the sharp resonances of the roton and maxon excitations in superfluid Helium for the two respective (q, ω)-values. The results of detailed Monte-Carlo simulations at three wavelengths and chopper speeds are compared to the experimental data. The agreement between simulation and experimental data is excellent, allowing to extrapolate the simulations and thus determine the resolution function in the whole accessible dynamic range of IN5.

T-70 Design of a TOF-SANS instrument for the proposed Long Wavelength Target Station at the Spallation Neutron Source

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We have designed a versatile high-throughput SANS instrument [Broad Range Intense Multipurpose SANS (BRIMS)] for the proposed Long Wavelength Target Station at the SNS using the Los Alamos NISP Monte Carlo simulation package. This instrument is optimized to take advantage of the 10 Hz source frequency and the cold neutron spectrum from a tall coupled solid methane moderator (12 cm x 20 cm). A supermirror guide and bender assembly is employed to separate and redirect the useful portion of the neutron spectrum (wavelength ¿ 1 Å) away from the direct beam for background suppression. BRIMS is designed to produce data in a Q range spanning from 0.0025 to 0.7 Å^{-1} in a single measurement by simultaneously using neutrons with wavelengths from 1 to 14.5 Åin a time-of-flight mode. In the high resolution mode it can produce data in a Q range of 0.0018 to 0.35 Å^{-1} by using neutrons from 1 to 12.75 Å. The effects of various collimation choices including puliple confocal pinhole apertures on count rate, resolution and Qmin have been characterized using spherical particle and delta function scatterers. The anticipated performance of BRIMS is compared with that of the best existing reactor-based SANS instrument D22 at ILL. This work has benefited from the use of IPNS, supported by the U.S. Department of Energy, BES-Materials Science, under contract W-31-109-ENG-38 to the University of Chicago and NSF grant # DMR-0073038.

T-71 Simulations of the Neutron Spin Precession Inside a TOF Spin Resonance Energy Filter

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A computer package for the calculation of neutron trajectories including spin precession in arbitrary magnetic fields is presented. The method is applied to the spin precession of neutrons traveling inside a Drabkin type spin resonance flipper. This device is very promising to be used for dynamic energy filtering of polarized neutrons at pulsed neutron sources. To calculate the spin precession in spatial inhomogeneous magnetic fields for given initial conditions, coupled equations of motion for the neutron position and spin vectors have to be solved. For the computation of the relevant magnetic field gradients generated by permanent and soft magnets as well as electromagnets, current sheets etc., a modified boundary element field calculation program has been developed.

T-72 New features in McStas, version 1.5

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The neutron simulation package McStas has attracted numerous users, and the development of the package continues with version 1.5 to be released at the ICNS conference. New features include: support for neutron polarisation, tracking of neutron histories, realistic source and sample components, and interface to the Risø instrument control software TASCOM. At the conference we give a general introduction to McStas and present the latest developments. In particular, we give an example of how the neutron history option has been used to locate the origin of a spurious side-peak, observed in an experiment with RITA-1 on Risø.

T-73 Algorithms for the Simulation of Inelastic Neutron Scattering Experiments

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A number of computer programmes exist for the simulation of neutron scattering instruments by Monte Carlo ray tracing techniques. The sample kernels included in these programmes have, to date, predominantly been for elastic scattering (Bragg peak, powder, small angle scattering). In this paper some algorithms for the inclusion of inelastic scattering kernels (for dispersion relations and dynamic critical phenomena) in the PRMON programme are described and compared with experimental results.

T-74 Use of the Rietveld refinement with the generalized spherical-harmonic model for describing crystallographic texture in polycrystalline NiTi shape memory alloys with neutron powder diffraction data

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The NiTi shape memory alloys (SMA) properties are based on a martensitic transformation from a cubic high-temperature to a monoclinic low-temperature. The monoclinic texture is formed by a crystallographically oriented phase transformation from the cubic hot-rolling texture. The GSAS multiple-data-set capabilities with the *generalized spherical-harmonic* model was used to extract the quantitative texture description (QTD) directly from a refinement with several tens of time-of-flight neutron diffraction patterns taken from a SMA sample held in a variety of orientations in the diffractometer. The crystal structure data obtained from the present refinements are essentially identical to the single crystal results. Moreover, the recalculated pole figures derived from the ODF using the popLA software agreed well with the corresponding pole figures computed by Rietveld analysis. Therefore, it can be concluded that this work provides the QTD simultaneously with the SMA crystal structure.

T-75 Characterisation of Creep Cavitation Damage in a Pressure Vessel Stainless Steel using Small Angle Neutron Scattering

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Grain boundary cavitation is the dominant failure mode associated with initiation of reheat cracking, that has been widely observed in austenitic stainless steel pressure vessels operating at temperatures within the creep range (¿ 450°C). Small angle neutron scattering (SANS) experiments at the LLB PAXE instrument (Saclay) and the V12 double crystal diffractometer of the HMI-BENSC facility (Berlin) are used to characterise cavitation damage (in the size range 10nm - 2000nm) in a variety of creep specimens extracted from ex-service plant. Factors that affect the evolution of cavities and cavity size distribution are discussed. The results demonstrate that SANS techniques have the potential to quantify the development of creep damage in type 316H stainless steel, and thereby link microstructural damage with ductility exhaustion models of reheat cracking. The work described in this paper has been carried out as part of the EC co-funded collaborative project VORSAC (Variation of Residual Stresses in Aged Components).

T-76 High-temperature stress evolution in brazed samples for plasma-facing components in fusion reactors

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Near term fusion reactors, such as the International Thermonuclear Experimental Reactor (ITER), will require structural plasma-facing components consisting of an assembly of Copper alloy cooling pipes, coated by sacrificial armour of temperature stable material, such as Tungsten. Clearly, the determination of the internal stress field is essential to define the engineering parameters necessary to design real-scale components. This study has been carried out on mock-ups obtained by brazing Glidcop onto a Tungsten platelet using different procedures. The internal stress field was determined by means of neutron strain scanning at different temperatures between room temperature and 500°C under vacuum. The results are discussed with reference to the adopted brazing procedures and to the expected consequences of such stress evolution on the mechanical behaviour in service conditions.

T-77 Neutron Diffraction Measurement of the Evolution of Strain for Non-Uniform Plastic Deformation

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Neutrons are particularly adept for the validation of modeling predictions of stress and strain. In recent years, there has been a significant effort to model the evolution of both the macroscopic stresses and the intergranular stress during plastic deformation. These have had broad implications with regards to understanding the evolution of residual stress and to diffraction-based measurements of strain. Generally the modeling and associated measurements have been for simple uniaxial tension, leaving questions with regards plastic deformation under multi-axial stress and non-uniform stress. Extensive measurements of the strain profile across a plastic hinge for each of a series of loading and unloading cycles to progressively higher degrees of plastic deformation will be presented. These measurements will be used to validate multiple-scale Finite Element Modeling (FEM) of the plastic hinge in which the elements will range in dimension from singlecrystallites (as used in successful simulations of uniaxial tension) to macroscopic elements (as is typically used in FEM simulations).

T-78 Residual Stress in Sprayed Ni+5%Al Coatings Determined by Neutron Diffraction

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Coatings from nickel-based alloys are used in numerous high-performance applications. Their properties and lifetime are influenced by factors such as residual stress. Neutron diffraction is a powerful tool for nondestructive residual stress determination. In this study, through-thickness residual stress profiles in Ni+5%Al coatings on steel substrates were determined. Two examples of significantly different spraying techniques - plasma spraying and cold spraying - are highlighted. Different stress generation mechanisms are discussed with respect to process parameters and material properties.

T-79 A Tomography System at Neutron Thermal Column of ENEA Casaccia TRIGA Reactor

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The developed system is intended for use of a collimated thermal neutron beam with a flux of about 10^6 n/cm^{2}s. The system works with a cooled CCD (192x165 pxls) and an intensifier for a light from NE426 scintillator with traditional optical coupling. A fine mechanical regulation system allows an accurate positioning of the tomographer, ensuring also the alignment of CCD array with the rotation and translation axis. The acquisition of 200 projections is carried out in about 30 min with a reconstruction time (40 min max) depending on reconstruction matrix order. Radiography and tomography of significant objects are illustrated. The reconstruction algorithm, including spatial and temporal unhomogeneity corrections and filters, was tested, with good results, by projections until to 512x512 pxls.

T-80 Measurement of very small hydrogen content in materials by measuring the incoherent neutron scattering

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In the neutron scattering experiments, the incoherent scattering contributes to the background signals which is an unwelcoming property of matter. Among the nuclei of nature, hydrogen nucleus (proton) has remarkably large value of incoherent neutron scattering crossection which is mainly due to the spin incoherence. Therefore very small amount of hydrogen in a material could be analysed by measuring the incoherent scattering of the material. The hydrogen content of a metal or semiconductor is a matter of concern and interest because it can affect significantly to the physical or chemical properties of materials though the amount of hydrogen is very small. In this study, the incoherent neutron scattering (INS) were measured from the neutron diffraction patterns obtained using the high resolution powder diffractometer installed in HANARO research reactor. The sensity and accuracy of the measurement were 2 ppm and 0.5 %, respectively for the 1 hour measurement. From the calibration curve which was obtained by measuring the INS of artificial samples (zircaloy + polyprophylene films), the relative amounts of hydrogen in a few zircaloy samples were estimated and compared with the result from the chemical analysis.

T-81 Living polynucleotides formed by the spontaneous aggregation of dilauroylphosphonucleosides.

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The aggregational properties of phosphatidylnucleosides, lipids bearing a nucleoside moiety on their polar head, with various acyl chain lengths, are a current subject of study in our group. We have found that self-aggregation of phospholiponucleosides triggers molecular recognition properties similar to those observed in nucleic acids between complementary bases. This contribution concerns a structural and dynamic investigation of dilauroylphosphonucleoside aggregates in aqueous solutions as a function of ionic strength and surfactant concentration. A micellar growth in the axial direction to form wormlike aggregates is observed as the surfactant concentration is increased, until the system show a distinct viscoelastic behavior, that suggests the presence of a polymerlike network. SANS and static light scattering allow inferring the structural properties of such micellar networks below and above the threshold concentration of entanglement. The wormlike aggregates are characterized in terms of persistence length and overall molar mass, while the micellar network can be described by its mesh size.

T-82 Hindered protein dynamics in the presence of a cryoprotecting agent

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The disaccharide trehalose is a widely spread bioprotecting molecule with a remarkably high efficiency. It is found in a number of cells, organisms and biomolecules who can survive conditions of extreme drought or low temperature. Even if the protective effect is already used in food and pharmaceutical industry, the protective mechanisms on a molecular length scale still remain unclear. The C-Phycocyanin is a small protein, extracted from cyanobacteria. Its structure is known at a good resolution. Recently dynamics of this protein in hydrated powders as well as in solution has been studied by quasielastic neutron scattering and MD Simulations. We study the influence of trehalose on the internal dynamics of this protein. Using different neutron scattering techniques we cover a time range from few pico- up to several nanoseconds. Evidence for a slowing down of protein movements has been found.

T-83 Supercooled water in plant cell walls – Structure and dynamics of water adsorbed to cellulose

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Plants can survive at temperatures below 0°C if they can prevent ice crystal formation in cells and cell walls. We could show that the suppression of crystalline ice is an inherent property of cellulose as the main constituent of plant cell walls: In inelastic neutron scattering (INS) experiments it was proven that artificial amorphous cellulose is a model system for disordered and, therefore, water–accessible regions of plant cell walls [1]. A combined quasielastic neutron scattering (QNS) and neutron diffraction study of water adsorbed to amorphous cellulose [2] revealed a fast (picosecond) dynamics of water molecules far below the melting point of bulk water. At lower temperatures, this supercooled adsorbed water gradually freezes to an amorphous polymorph of ice with resemblance to low–density amorphous ice. [1] M. Müller et al., Macromolecules 33, 1834-1840 (2000) [2] C. Czihak et al., Journal de Physique IV – Proceedings 10, 199-202 (2000)

T-84 The Role of Picosecond Fluctuations for Activity and Stability in Proteins

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The importance of equilibrium fluctuations in proteins is evident from very basic principles: at low temperatures or in a very dry state, thermal equilibrium fluctuations are strongly reduced. Under these conditions proteins are not operative or the reactions are slowed down drastically. On the other hand, in nature biomolecules have shown to be very successful in adapting to extreme environmental conditions, like high temperatures (thermophilic organisms). Therefore, for proteins thermal equilibrium fluctuations play a crucial role for the balanced interplay between structural flexibility (required for a proper function) and rigidity (preserving the specific and unique fold) of protein structures. We have received insights in the function-dynamics and the stability-dynamics relations by applying incoherent neutron scattering to the light-driven proton pump bacteriorhodopsin and to two alpha-amylases coming from mesophilic and thermophilic organisms.

T-85 Determination of Structural Parameters and Hydration of Unilamellar Vesicles by Neutron Scattering Using a Novel Method

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A novel method of evaluating SANS curves is presented which allows for the first time to determine in a straightforward manner simultaneously the internal geometry and hydration of single bilayers in unilamellar vesicles at high water excess. Three independent structural parameters are directly obtained by fitting the scattering curve in the q-range from 0.06 nm^{-1} to 3.82 nm^{-1}. The potentialities of the method are demonstrated by elucidating structural and hydrational parameters of mixed unilamellar POPC/C12E4 and POPC/C12E3Glyc vesicles.

T-86 Structure and Reactions of Proteins at Interfaces

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Proteins behave as surfactants and therefore adsorb at the air water and other interfaces. This paper describes the use of x-ray and neutron reflectometry together to determine structure and follow the reactivity of proteins at interfaces. Because of the different contrasts involved, the two techniques are quite complementary and should always be used together where possible. In addition the x-ray method has the possibility of a time resolution which may extend to milliseconds. We are currently developing a ”millisecond reflectometer” with this capability at a synchrotron source. The lecture will describe the properties of myoglobin at the air/water interface and also of a short highly surface active peptide derived from myoglobin. In this case there is ”incipient denaturation” due to the unbalancing forces at the interface. Complementary experiments where this tendency is greatly reduced in b lactoglobulin in of its genetic variants will be described as well as preliminary experiments on the reactivity of b lactoglobulin and k casein at interfaces.

T-87 The Interaction of the synthetic Peptide NK2 with Modell Membranes

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Antibacterial peptides are widely abundant in nature. They can be found in insects (cecropines), amphibians (magainins) and also in mammals (defensins). Those peptides are relatively small and build up by 20 - 35 amino acid residues. Usually they are amphipathic molecules. Contrary to classical antibiotics which effect is based upon the interaction with bacterial enzymes, peptide antibiotics destroy the bacterial membrane purely by physical interaction. Enzymes are not needed in this case. This physical mechanism of destruction makes peptide antibiotics especially interesting for drug design. In this work we present first results of the interaction of a synthetic peptide (NK2), derived from NK-lysin, a antibacterial peptide found in porcine NK-cells, with modell membrane systems.

T-88 Interaction of Water with Protein Resistent Self-Assembling Monolayers: Neutron Reflectivity Measurements of Water Density in the Interphase Region

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Poly- and oligo(ethylene glycol) (PEG and OEG) derivatives are known to exhibit outstanding protein resistance. While the inertness of PEG has been explained by steric repulsion, the protein resistance of OEG has been related to its molecular conformation: whereas the helical and amorphous conformers are inert, the planar all-trans conformer does adsorb protein. It has been supposed that the protein resistance of OEG stems from its ability to form an interphase water layer which prevents the surface from direct contact with protein. Neutron reflectivity measurements on amorphous, protein resistant methoxy tri(ethylene glycol) undecanthiolate self-assembled monolayers (SAMs) in contact with deuterated water in fact reveal the presence of an extended ($\sim$5 nm thick) water interphase with a noticeably reduced density ($\sim$ 85-90% bulk water density). This experimental result is in agreement with Grand canonical Monte Carlo simulations of water next to the SAM surface.

T-89 Results and Relations in Cuprate Superconductors

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Recent experiments and theories have advanced the fundamental understanding of the copperoxide superconductors considerably. As an introduction, results from a number of groups will be reviewed. Data from inelastic neutron scattering and photoemission underline the basic vibronic character of the CuO_2 planar system. Furthermore inelastic neutron scattering has revealed huge oxygen- and copper-isotope effects at the stripe formation temperature T*, which are understood by the same vibronic concept. A model for Jahn-Teller bipolarons properly reflects the phonon anomalies observed by inelastic neutron scattering, EXAFS, electron paramagnetic resonance (EPR), and other important experimental findings regarding the superconducting transition temperature T_c. Another quantitative model in which the planar and out of plane electronic bands are coupled via rotational tilting modes, yields the isotope effects on T* and its doping dependence, and is supported by the quantitative understanding of the fast EPR relaxation observed.

T-90 Lattice and Charge Effects in High-Temperature Superconductors

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Phonons are generally considered to be irrelevant, or even harmful, to high-temperature superconductivity (HTSC). However, there are a number of indications that phonons are playing some active role in the HTSC phenomenon. Our inelastic neutron scattering measurements on single crystals of $YBa_2Cu_3O_{6+x}$ (YBCO) support this view. The measurements were made using the triple-axis-spectrometer at the HFIR of the Oak Ridge NL, as well as the TOF spectrometer the ISIS of the Rutherford-Appleton Lab. We found that the Cu-O bond-stretching LO mode shows anomalous dependence on composition and temperature. Since the change in the Cu-O distance induces charge transfer between Cu and O, the electron-phonon interaction is strong for this mode. The results suggest that the short-range dynamic cell-doubling, perhaps by CDW, exists in the HTSC phase. If the e-p coupling is highly directional the phonon mechanism may not be in conflict with the spin mechanism for the d-wave superconductivity. It is likely that the phonons play a critical role in the HTSC phenomenon.

T-91 Search for charge fluctuation effects in the phonons of $YBa_2Cu_3O_x$

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Extensive inelastic neutron scattering experiments have been performed on the high-T_c compound $YBa_2Cu_3O_{6.6}$ (O6.6) and the insulating reference compound $YBa_2Cu_3O_{6.2}$ to look for phonon anomalies possibly related to dynamic charge stripe order. Pronounced anomalies have been observed in the bond stretching vibrations of O6.6 but it seems difficult to reconcile these anomalies with the current picture of charge stripe order. On the other hand, no anomalous features have been found in the bond bending vibrations of O6.6 in contrast to what has been advocated by Mook and co-workers (Nature 401, 145 (1999) and Nature 404, 729 (2000)).

T-92 Spin fluctuations of in high-T_c cuprates; cross over from static charge stripes to dynamical spin density waves

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I present a brief review on the spatial spin/charge fluctuations in high-T_c cuprates. In the hole-doped 2-1-4 compounds the fluctuations are incommensurate at low frequencies or temperatures unless the doped carriers are tightly trapped near the dopant sites as in the case of Li-doped $La_2Cu(Li)O_4$. The q-vector of the spin modulation depends on both the crystal structure and electron transfer. In the insulating phase of Sr-doped La_2CuO_4(LSCO) the q-vector is along the diagonal direction to the Cu-O square lattice. One dimensional spin modulation on the CuO_2 planes strongly suggests an existence of static charge stripes stabilized by a particular buckling of CuO_2 planes. On entering into the superconducting phase a dramatic change in the q-vector occurs from the diagonal to parallel direction. However, even in the superconducting phase another type of CuO_2 buckling plays an important role for the stability of charge stripes. Such incommensurate spin fluctuations depend on both the frequency and temperature. In underdoped $YBa_2Cu_3O_{6+x}$ compounds incommensurate spin fluctuations at low energies merge into commensurate ones at the so-called resonance energy with increasing the frequency. On the other hand, a different type of incommensurate-commensurate crossover is observed in LSCO system where no well-defined resonance energy is so far defined. In the Conference I would like to discuss a simple interpretation of spin fluctuations revealing such strong system dependence.

T-93 Isotope effects on the pseudogap in high-temperature superconductors studied by inelastic neutron scattering

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Isotope effects, i.e. ^{18}O vs ^{16}O and ^{65}O vs ^{63}Cu, on the relaxation rate of crystal-field transitions in the slightly underdoped high-temperature superconductor $HoBa_2Cu_4O_8$ have been studied by means of neutron crystal-field spectroscopy. Both substitutions give rise to relatively large shifts in the pseudogap temperature T*, being $\Delta T^* \approx 25$ and 50 K for copper and oxygen substitution, respectively. Possible explanations of such effects as well as their relation with the pairing mechanism will be discussed. Additional isotope effect experiments, which are being performed in both the $YBa_2Cu_3O_x$ and $La_{2-x}Sr_xCuO_4$ families and from which relevant information is expected, will also be presented.

T-94 Doping Dependence of the Tetragonal-Orthorhombic Phase Transition in the Superconducting $La_{2-x}Sr_xCuO_{4\pm d}$ Compound

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The phase transition from tetragonal to orthorhombic structure in $La_{2-x}Sr_xCuO_{4\pm d}$ (La214) has been studied by means of elastic and inelastic neutron scattering. Both underdoped (x=0.09) and overdoped (x=0.17) compounds have been investigated. From the temperature dependence of the superstructure peaks, we are able to estimate the critical exponent beta, which is found to increase with increasing x. We also observe that the temperature interval over which the critical behavior appears to be valid is unusually large and strongly doping dependent. The temperature dependence of the soft phonons associated to the phase transition has also been measured.

T-95 Anharmonic Lattice Dynamics and Nonlinear Electron-Phonon Coupling in new 40 K Superconductor MgB_2

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We report first-principles calculations of the electronic structure and lattice dynamics of MgB_2[1]. We found an excellent agreement between the calculated phonon density of states with the inelastic neutron scattering measurements[1]. Frozen phonon calculations indicate that the in-plane boron phonons are very anharmonic, increasing the harmonic mode energy by about 25%. We also calculated the deformation energy within frozen phonon approach and found that the anharmonic boron modes strongly and non-linearly couples to the partially occupied planar boron sigma bands near the Fermi level. The very anharmonic in-plane B modes and their strong non-linear electron-phonon couplings are essential to explain the high Tc in MgB_2 [1].([1]T. Yildirim et al, submitted to Science).

T-96 Powder diffraction at advanced pulsed neutron sources: past, present and future

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The outlook for powder diffraction at the new high-power sources (SNS, ESS and HIPAF-TOKAI) is extraordinarily bright. Powder diffractometers at present pulsed sources are already competitive with steady-state machines, and one can expect further gains of 1-2 orders of magnitude at the new facilities. Nevertheless, one can already identify a few challenges. First of all, there is a general desire to broaden the scope of time-of-flight powder diffraction towards traditional reactor techniques. Secondly, we will have to adapt to a new target-moderator landscape, in which truly sharp cold moderators are notably absent. Thirdly, we will have to complete the evolution from the original suite of instrument designs developed in the late seventies to a new generation of machines matching the technology of the new millennium. The characteristics of the new sources and new technology seem to favor instruments with relatively narrow single-frame bandwidth and very large detector coverage. In this respect, newly built instruments such as GEM at ISIS represent a very important stepping stone towards future machines, as well as delivering now unprecedented data collection speed and accuracy. We will describe the successes and challenges we encountered in commissioning GEM, and how this experience may be of help in shaping the future of neutron powder diffraction.

T-97 High-position resolution scintillation neutron imaging detector by crossed-fiber readout with novel centroid finding method

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Aiming to high-position resolution neutron imaging, a novel centroid finding method was proposed for a scintillation neutron imaging detector with the crossed-fiber readout. Crossed wavelength shifting fibers are arranged on and under the detector. Luminescences generated in the detector are emitted and detected by several fibers surrounding to the incident point. In the novel method, the X and Y position of incident neutron are decided by coincidence of the center signal and both neighboring signals, respectively. By preliminary experiments using a ZnS:Ag/^{6}LiF scintillation sheet of 0.5mm thickness and crossed wavelength shifting fibers of 0.5 mm diameter, it was confirmed that the position resolution is about 0.5mm.

T-98 A novel large-area, low-pressure detector with high position and time-of-flight resolution for thermal neutron imaging

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The pulsed high-flux neutron source ESS, in synergy with advanced focusing neutron optics and spectrometers, will require novel imaging detectors with better resolutions and faster response, necessary for exploiting the improved beam emittancy, flux density and time structure. As a first generation of very high resolution and fast gas detectors utilising composite ^{157}Gd/CsI foil converters, at HMI novel robust large-area multilayer micro-strip gas chamber (MSGC) detectors are being developed which are optimised for a low-pressure two-stage gas amplification mode. In the present contribution the read-out and data acquisition system is discussed in conjunction with the signal properties of the hybrid MSGC detector. All signals are fed into 8-channel multihit TDC chips (120 ps LSB) of the F1 type, located on the PCI boards of the DAQ system. By means of the DSP the data of the four registered coordinates X/Y/TOF/PH are calibrated and transformed online into 2D spectra which can be accumulated in the HM and monitored via the PC. Furthermore the optimisation of the composite foil converter will be presented. The number of secondary electrons emitted by fast electrons from columnar CsI layers is measured by means of an electron spectrometer.

T-99 Possibilities for Novel Polarized Pulsed Neutron Instrumentation Based on the TOF Spin Resonance Energy Filter

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We present a new approach for dynamic energy filtering of neutrons suitable for time-of-flight experiments at spallation neutron sources. The method utilizes polarized neutrons and is based on a Drabkin-type spin resonance energy filter. The device consists of a polarizer/analyzer system, an energy-selective spin flipper and fast electronic controls. The latter allow rapid tuning of the selected neutron energy and bandwidth, which overcomes limitations in other energy filtering devices like choppers or monochromating crystals. In our contribution we will discuss possibilities for using the spin resonator i) as a general resolution tuning device, ii) as a p̈ulse tailoringd̈evice for cold coupled moderators, iii) as $\pi/2$ flipper and dynamic phase shifter in TOF spin echo instruments and iv) as a dynamic energy selector/analyzer in a novel inelastic spectrometer.

T-100 New multiplexing concepts to enhance the efficiency of use of pulsed sources.

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Pulsed spallation sources offer high peak fluxes and are well adapted for time-of-flight techniques. However, the efficient use of these advantages is often hampered in specific applications by not optimal source pulse repetition rate and by contradictory requirements on wavelength band width and resolution. We will discuss the new instrument design concepts Repetition Rate Multiplication (RRM) and Wavelength Frame Multiplication (WFM), which allow us to largely overcome these disadvantages. In RRM time-of-flight spectroscopy several pulses with several wavelengths impinge on the sample within each source frame. WFM offers a possibility to extend the wavelength band of data collection beyond usual limits. RRM is being implemented in the IN500 time-of-flight spectrometer project at LANSCE and it has been experimentally emulated on spectrometer NEAT at HMI. We will also discuss the application of WFM in small angle scattering and powder diffraction and the design approach we have developed for the complex chopper systems needed for methods.

T-101 Anticipated Performance of the SNS Liquids Reflectometer

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Barring a monumental failure of design execution or of performance estimation, the liquids reflectometer at the SNS will provide unprecedented capabilities for the study of liquid and solid surfaces. Design of the instrument is well underway and procurement of components has begun. Neutrons from a coupled 20-K supercritical hydrogen moderator will be delivered via a multi-channel supermirror bender and tapered guide onto either a horizontal or tilted sample surface. Collimating slits select the beam incident angle from a 0-7° vertical intensity distribution provided by the optics. Bandwidth choppers and frame-overlap mirrors define a user-selected 3.75-Å-wide wavelength band out of a 1.75Å-13.5Åusable wavelength range. The user can collect data using either a 1-mm^2-resolution two-dimensional position-sensitive detector or a single ^{3}He tube. With the SNS running at 2 MW, the instrument will be able to accumulate a complete specular reflectivity scan from D_2O ($R<10^{-7}$, $Q>0.5$ Å^{-1}) in less than 10 minutes. By tilting a solid surface, a user will be able to measure specular reflectivities R 2×10^{-10} ($Q>1.5$ Å^{-1}) from large samples in less than three hours. Rapid data-collection times may also be expected for off specular and grazing-incident SANS measurements. We will describe the calculations underlying our design choices and performance estimates and report on construction progress.

T-102 Comparison of Bragg-Edge Neutron Spectroscopy at ISIS and LANSCE

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The Bragg edges appearing in the neutron transmission spectra of a polycrystalline material represent its coherent-scattering response at $2\Theta = 180$. Structural information such as texture, phase content or strain may be derived from the intensity and position of these edges. Transmission diffractometers have been recently developed at both LANSCE and ISIS and used for studying the dynamics of phase transformations and strain imaging respectively. The incident neutron spectra vary due to the different neutron moderators and flight paths used in the two instruments. Complimentary approaches have also been taken to data analysis (c.f. Rietveld vs. Pawley). This paper reports a comparative study of the two instruments and their software obtained using a portable loading rig to measure strain in the same well characterised steel sample. The relative advantages of each instrument and its software are analysed and described.

T-103 Degeneracy Breaking In The Frustrated Pyrochlore Antiferromagnet

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What is the ground state of the pyrochlore lattice antiferromagnet? In 1979 Villain argued that it should be a highly frustrated ”spin liquid” state but suggested that dipolar interactions or thermal fluctuations might break this degeneracy and restore magnetic order. Our neutron scattering experiments on the almost ideal model materials ^{160}Gd$_2$Ti$_2$O$_7$ (a Heisenberg system) and Er$_2$Ti$_2$O$_7$ (an XY system) have now provided a clear answer to this thirty year old question. For Gd$_2$Ti$_2$O$_7$ the dipolar coupling induces partial order that is selected from an almost degenerate manifold of states. For Er$_2$Ti$_2$O$_7$, on the other hand, one finds magnetic order stabilised by spin fluctuations that drive the system close to a quantum critical point, These results provide an interesting contrast to the reported behaviour of the pyrochlore lattice materials Cs(NiCr)F$_6$ and (Y,Sc)Mn$_2$ which both show spin freezing in the presence of quenched chemical disorder.

T-104 Magnetic correlations in the Neel and spin liquid phase of a geometrically frustrated magnet ZnCr$_2$O$_4$

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A spin-Peierls-like phase transition has recently been reported in the geometrically frustrated magnet, ZnCr$_2$O$_4$, in which magnetic Cr^{3+} ions form a network of corner-sharing tetrahedra [1]. ZnCr$_2$O$_4$ undergoes a first order phase transition at $T_c = 12.5$ K from cubic and paramagnetic into a tetragonal and Neel phase. A local spin resonance at around 4.5 meV develops abruptly in the Neel phase. We report inelastic neutron scattering measurements on single crystals of ZnCr$_2$O$_4$. Both the Neel and the spin liquid phase have strong dynamical spin fluctuations at the Brillouin zone boundaries. Even though their characteristic energies are different, the structure factor associated with spin fluctuations in the two phases have the same wave vector dependence. Such local spin fluctuations may be generic in geometrically frustrated magnets and key to understanding the physics of geometrical frustration. The measurements were performed on single crystals with a total weight of only 200 mg. They were made possible by the intense cold neutron at NIST, and the horizontally focusing multicrystal analyzer and the position-sensitive detector on the cold neutron triple axis spectrometer SPINS. [1] S.-H. Lee, C. Broholm, T.H. Kim, W. Ratcliff II, and S-W. Cheong, Phys. Rev. Lett. 84, 3718 (2000).

T-105 Direct evidence of spin frustration in fcc antiferromagnet NiS$_2$

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NiS$_2$ is well known Mott insulator with anomalous antiferromagnet (AF) long-range order (LRO); which is coexistence of type I ($\mathbf{Q}_M$=(1,0,0), $T_{N1} = 40$ K) and type II ($\mathbf{Q}_M$=($\frac{1}{2}$,$\frac{1}{2}$,$\frac{1}{2}$), $T_{N2} = 30$ K). Extensive neutron scattering studies revealed that paramagnetism in NiS$_2$ is governed by a geometrical spin frustration effect that creates the magnetic diffuse scattering extends on the fcc zone boundary continuously. The diffuse scattering exists even at 300 K (7.5 T_{N1}). Then the diffuse scattering disappears rapidly below T_{N2} associated with a tiny crystal distortion. We also observed a clear energy gap besides the low energy spin-wave excitation well below 30 K.

T-106 Non-classical spin configurations in a kagome based frustrated antiferromagnet: analysis of dynamic disorder by the Reverse Monte-Carlo method

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Local configurations with null total moment are expected to be the hallmark of geometrically frustrated antiferromagnets. We have attempted an experimental verification of such ideas in the SrCr$_{9x}$Ga$_{12-9x}$O$_{19}$ (SCGO) compound, using the reverse Monte-Carlo (RMC) analysis, recently adapted to the investigation of the magnetic correlations starting from total scattering powder data. The microscopic spin configurations obtained by RMC were used for calculation of the spin nematic correlation function proposed to be of importance for classical spins on the kagome lattice. In the low temperature range our analysis shows a strong deviation from the behaviour of classical spins on the SCGO lattice obtained with our standard Monte-Carlo simulations. Moreover, in this temperature range the spin dynamics shows scaling typical of a disorder controlled quantum critical regime.

T-107 Dynamic scaling in spin glasses : NSE results and theory

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Dynamics is the key to the understanding of glassy transitions. For spin glasses an early NSE measurement in 1979 [1] showed that the relaxation is very non-exponential in the spin glass phase but also well above the glass temperature T$_g$. These results strongly influenced subsequent thinking and experiments on glassy dynamics but spin glasses have been neglected. A detailed analysis of s(Q,t) in the spin glass system AuFe 14% and a revisited analysis of the early NSE data on CuMn 5% [1] show that at T$_g$ the autocorrelation function decays as t^{-x}, with x$\sim$0.12, in excellent agreement with the predictions of dynamic scaling. Above T$_g$, s(Q,t) is then described by the Ogielski form t^{-x}exp(-(t/t$_o$)$^{\beta}$). These results compare directly with the predictions of large scale numerical simulations in spin glasses [2] and are the first direct confirmation of dynamic scaling in spin glasses. [1] F. Mezei, JAP **53** 7654 (1982) [2] A.T. Ogielski, PRB extbf32 (1985) 7384

T-108 Dynamics of frustrated magnetic moments in TbNiAl

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We have studied the dynamics of Tb spins in the intermetallic compound mboxTbNiAl in the paramagnetic (pm) and ordered antiferromagnetic (afm) phases by means of neutron time-of-flight and spin-echo spectroscopy. TbNiAl is a frustrated antiferromagnet ($T_N = 47$ K). In the afm phase both regular long-range ordered Tb spins as well as frustrated Tb spins exist (the latter have a reduced moment). The quasielastic measurements show that in the ordered phase the frustrated moments relax on a time scale of 0.01 ns to 0.1 ns. Their auto-correlation function $I(q,t)$ is q-independent and exponential in time. Below T_N, in the spin-echo time window $I(q,t)$ reaches a plateau above zero, while above T_N the relaxation is complete (the correlation function converges to zero).

T-109 Structure and dynamics of giant wormlike micelles and their reversion to globular micelles at high salt concentrations

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Micellar morphology in aqueous micellar solutions of cationic surfactants such as cetyltrimethylammonium (CTAX) can be manipulated by changing the counterions, X-. Some counterions that penetrate the micellar interface, especially substituted chloro- and hydroxybenzoates (salicylates) and tosylate, produce very large, semi-flexible wormlike micelles. Furthermore, adding high concentrations of the counterions sodium salt (NaX) to the solution causes reversion to a globular micellar shape; this occurs at an NaX concentration that is counterion-specific. The alternative, the production of a highly branched micellar system rather than discrete globules, is not consistent with our scattering data. We have determined by SANS the contour lengths, persistence lengths (flexibility) and cross-sectional radii of the worm-like micelles. Some aromatic counterions increase micellar flexibility; others decrease it. In addition, for the case of CTA 2,6-dichlorobenzoate, we have used micelles prepared with deuterated counterions and used SANS with external contrast variation to determine the role of counterion binding in the reversion to globular micelles. We have also used neutron spin echo (NSE) spectroscopy to study the dynamics of these discrete globular micelles.

T-110 Non-equilibrium studies of polymers under flow

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Recognition that polymers may exhibit liquid crystalline properties dates back only 25 years. The first tailored side chain liquid crystalline polymers (SCLCPs) were then discovered by inserting a spacer in between the main-chain and lateral mesogens graftings. Much of the subsequent research has sought to control the properties of these tailored systems and to understand the coupling between the polymer main-chain and the mesogen. These materials are also technologically interesting because of their ease of processing. However, their flow behaviour was almost not explored. They are expected to show original rheological behaviours reflecting a mixture of their polymeric and mesomorphic characters. For example, it was commonly believed that the main-chain/mesogen coupling is a constant potential entirely defined by the molecular parameters [1]. We will here prove experimentally that the shear flow acts on this coupling potential. This property is emphasised in the nematic phase: the polymer main-chain executes under flow a reorientation from perpendicular to parallel to the mesogen orientation. Finally, in the isotropic phase, we have discovered that the flow induces the appearance of a non-equilibrium nematic phase [2]. These shear induced behaviours will be presented in the frame of an experimental approach coupling rheology and SANS techniques. [1] Wang X.J., Warner M., J. Phys. A, 20, 713 (1987). [2] Pujolle-Robic, C., Noirez, L., Nature 409 (2001) 167.

T-111 Time-resolved SANS investigation of a shear induced lamellar-to-vesicle transition

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The influence of shear on structure and orientation complex fluids has attracted a great deal of attention in recent years. Particular attention [1] has been given to lyotropic lamellar phases which exhibit two interesting features under shear. One is the flipping of aligned parallel lamellae and the second concerns the formation of multi-lamellar vesicles (MLVs). In this study [2] the mechanism and kinetics of a shear induced formation of multi-lamellar vesicles in a lyotropic lamellar phase of C10E3 (Triethyleneglycol-decylether) was investigated by rheology and time resolved small angle neutron and light scattering (SANS, SALS). Starting from a well defined, macroscopically oriented lamellar phase, the transition occurs in two steps. First, there is the formation of an intermediate structure oriented in the flow direction which scatters only perpendicular to the flow. This is compatible with long, multi-lamellar tubuli. As shear is continued, multilamellar, spherical vesicles are formed. [1] Diat O., Nallet F. and Roux D., J. Phys. II, 3 (1993), 1427. [2] J. Zipfel, F. Nettesheim, P. Lindner, T. Le, U. Olsson, W. Richtering, Europhys. Lett. 53 (2001), 335.

T-112 Partial structure factors in star polymer/colloid mixtures

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Addition of polymer to colloidal suspensions induces an attractive part to the colloid pair potential, which is of purely entropic origin (”depletion interaction”). We investigated the influence of polymer branching by studying mixtures of hard sphere colloids and star polymers with increasing arm number $f = 2 - 32$, but constant R_g. We found a pronounced effect of branching on the position of the gas/liquid demixing transition. Using SANS we were able to measure partial structure factors in star polymer/colloid mixtures. The relative distance to the demixing transition is reflected in our scattering. All experimental results are in good aggreement with recent theoretical calculations.

T-113 Investigating Self-Assembly and Metal Nanocluster Formation in Aqueous Di-Block Copolymers Solutions

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Self-assembling properties of di-block copolymers in aqueous solution can be exploited to obtain metal nanoparticles stable dispersion. The formation of metal nanoparticles is obtained by using a metal precursor compound that is adsorbed to the hydrophobic micelles core. The nanosized metal particles obtained by means of a fast reducing homogenous agent, are therefore stabilized in the micelle core. The reduction rate of the metal precursor, size, shape and the center-center distance of the nanoparticles is controlled either by the chemical nature of the the solvent and of the block copolymers along with concentration and thermodynamic conditions. Results will be here presented for block copolymers dissolved in water. The SANS structural investigation has been performed over different molecular weights of both hydrophilic and hydrophobic block, by varying temperature and concentration of the copolymer, going from random coil chains to aggregates. We report structural characterization of Platinum nanoparticles dispersed in different block copolymer systems.

T-114 Neutron spectroscopy and QC modeling low frequency internal vibrations m-xylene molecules with deuterated subunits

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Neutron inelastic scattering (INS) investigations of solid 1,3-methyl benzene, i.e. m-xylene-D_4, m-$(CH_3)_2C_6D_4$, and m-xylene-D_6, m-$(CD_3)_2C_6H_4$, were performed on the NERA spectrometer at the IBR-2 pulsed reactor of JINR in Dubna in the temperature range from 10 to 100 K. The influence of temperature and the H-D isotopic exchange on the INS spectra, make it possible to do experimental assignments some the low frequency internal modes of the investigated molecule. Thus, the INS spectra can be used as a test of quantum chemistry (QC) modeling vibration spectra of these molecules. The molecular geometry was optimized for an isolated molecule on the AM1 and PM3 semi-empirical levels, and the restricted Hartree-Fock level with the 6-31G* basis set. As a result, three sets of vibrational frequencies and their intensities in the INS spectra have been calculated and compared with the experimental data. In principle, a proper assignment of the low frequency internal modes of m-xylene molecule can be done using any of these three methods, however a proper frequencies of these modes in solid m-xylene need the individual scaling factors or additional fitting of the force field obtained from QC methods to the experimental frequencies.

T-115 The effects of confinement on rotational tunneling

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We have measured the effects of confinement on rotational tunnel splitting using neutron backscattering spectroscopy for two different organic molecular solids at low temperature: methyl iodide and 4-fluorotoluene. Most of our work has focused on methyl iodide confined to porous glass disks with pore diameters ranging from 2.5 nm up to 20 nm. In bulk methyl iodide at low temperature, the tunnel peaks appear at ± 2.4 μeV. In the largest pores, the tunnel peaks shift to slightly higher energy transfer and broaden. In addition to these tunnel peaks, there is an additional broad spectral component which we attribute to disordered methyl groups located close to the pore walls. As the pore size decreases, the tunnel peaks shift to higher energy and broaden. At the smallest confinement length scales, in pores that are 2.5 nm in diameter, there are no well-defined peaks and only the diffuse disordered spectral feature remains. Our preliminary measurements on 4-fluorotoluene confined in 5.8 nm pores show that only a broadened tunneling component exists at the bulk tunneling energy (± 18 μeV) within the dynamic range of the instrument.

T-116 Lattice dynamics and methyl group rotation of dimethylacetylene (DMA)

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On the basis of the recently determined low temperature crystal structure [1] the lattice dynamics of DMA (2-butyne) and a single particle methyl rotational potential are calculated using Williams74 pair potential parameters [2] within the model of semirigid molecules.The agreement of ab-initio calculations with neutron spectra of the internal modes shows the validity of this approach. In the regime of lattice modes the existence of three methyl librational bands with significant dispersion can explain the measured density of states [3]. The single particle librational energy obtained for the rotational potential from the Schrödinger equation of the methyl rotor coincides well with the mean librational band energy. The calculated single particle tunnelling frequency is only 33% lower than observed in experiment. [1] R. M. Ibberson, M. Prager, Acta Cryst. B51, 71-76 (1995) [2] K. J. Tilly, B. Alefeld, Mol. Phys. 36, 387 (1978) [3] D. Williams, Acta Cryst. A30, 71 (1974)

T-117 Symmetry breaking, pretansitional phenomena and molecular disorder in an aperiodic molecular composite crystal

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Incommensurate composite are made of at least two interpenetrating lattices with irrational periodicity in at least one direction. These crystals show similarities with the well-known incommensurately modulated crystals but also with quasicrystals (essentially they are aperiodic by construction and do not have any mean basic lattice). All these properties are encountered in the molecular series of inclusion alkane in urea. The structural instabilities present in these compounds are described in term of symmetry breaking in a superspace, and are accompanied by very strong pretansitonal phenomena. Coherent neutron scattering together with single crystal deuterium NMR allows the analysis of the associated static and dynamic susceptibility. Incidence of these pretransitional phenomena on the molecular alkane disorder will be discussed considering both inelastic coherent neutron scattering study of the molecular diffuse scattering and incoherent neutron scattering. Results concerning phonons in these aperiodic crystals will also be presented.

T-118 Interfacial Characteristics of Block Copolymers with Various Architectures Studied by Neutron Reflectometry.

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Microphase-separated interfaces of I)styrene-d8-2-vinylpyridine(DP)diblock, II)PDP triblock, III)DPD triblock copolymers and IV) a DP_2 graft copolymer, were investigated by neutron refrectivity measurements and were compared. The thin-film specimens for reflectivity measurements were prepared by spin-coating on silicon wafers, and then were sufficiently annealed at 433 K. NR measurements were performed on CRISP of ISIS Facility, UK and ARISA reflectometer newly installed at KENS. It was found by specular refrection analysis that all the copolymers have quite similar narrow interfacial thicknesses in the strong segregation regime irrespective of the chain connectivity.

T-119 Neutron reflection from foam films

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The structure and stability of thin liquid films determine the macroscopic properties of foams, and such films are also convenient one-dimensional model systems for colloidal interactions. In this presentation a thin-film balance for simultaneous measurement of pressure/thickness isotherms and neutron reflectivity of single foam lamellae is described. The combination of these two techniques permits determination of the structural properties of thin liquid films in various states of drainage and/or under applied pressure, and used in conjunction with isotopic substitution to change the contrast of the film components, the method can provide previously inaccessible details about the internal structure of foam films. Results from studies of surfactant and surfactant-polyelectrolyte systems are presented, and the merits of the method in various situations will be discussed.

T-120 Temperature Induced Changes in Polyelectrolyte Films at the Solid-Liquid Interface

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Polyelectrolyte multilayers (film thickness 20-50 nm) were built on top of silicon substrates by layer-by-layer deposition from aqueous solutions (A) from a charged homo-polymer, PDADMAC, and a diblock-copolymer with a thermosensitive PNIPAM block and (B) from two co-polymers of opposite charge both containing NIPAM units. X-ray and neutron reflectivity experiments revealed that type A systems formed thick and smooth films while type B systems, prepared under identical conditions, showed reduced film thickness and increased roughness. Thermal behavior and subsequent structural changes of the functionalized films against D_2O were investigated by neutron reflectometry. The thermosensitive films showed a decrease in thickness at elevated temperature ($> 30^\circ$C) while the reference samples, composed of thermo-insensitive polyelectrolytes only, did not.

T-121 Interface and Surface Formation in Self-Assembled Polymer Multilayers by Off-Specular Neutron Scattering

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Three - dimensional treatment of neutron specular reflection and off-specular scattering was developed and employed to study the interface and surface formation of symmetric polystyrene-polybutylmethacrylate P(dS-b-nBMA) diblock copolymer multilayers. Investigations have been performed for polymers with different molecular weight of the constituent blocks with attention focusing on the lateral structure of the interface and the surface of the film. The major features observed in off-specular neutron scattering arise from randomly distributed islands or holes on lamellar films and the interfacial structure. Both are quantitatively described in terms of distorted wave Born approximation (DWBA) - based theory. Parameters of the islands or holes and interfacial fluctuations are obtained. The distribution of intensity between Yoneda scattering and conformal roughness scattering is an important tool in the data evaluation.

T-122 Phase separation of weakly incompatible polymer blends confined into isolated droplets

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Phase separation of the weakly incompatible blend system polystyrene and polyparamethylstyrene confined into isolated droplets is investigated. The droplet geometry imposes a two-dimensional spatial restriction. With specular, diffuse and grazing incidence small angle neutron scattering the surface topography as well as the chemical morphology inside the drops is determined. Due to the differences in surface tension a core-shell like structure characterized by a most prominent length scale inside the droplets is installed.

T-123 Polarised neutrons and chiral criticality

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Polarised neutrons give direct information on the critical phenomena in chiral magnets. The chirality, $\mathbf{C} = [\mathbf{S}_1 \times \mathbf{S}_2]$, is shown to be a critical variable that orders at T_{N}. The critical exponents $\beta_{\mathbf{C}} = 0.44(2)$ of the chirality, and $\gamma_{\mathbf{C}} = 0.84(7)$ of the chiral susceptibility in a triangular antiferromagnet CsMnBr$_3$ are consistent with the Monte Carlo values, and the scaling relation $\alpha + 2\beta_{\mathbf{C}} + \gamma_{\mathbf{C}} = 2$ is fulfilled, which indicates that the transition belongs to a new chiral universality class, apparanrly as in the XY phase of CsNiCl$_3$. In Ho, $\beta_{\mathbf{C}} = 0.90(3)$ is twice as large, while $\gamma_{\mathbf{C}} = 0.68(5)$ is close to the chiral scenario value. It is shown that $\beta_{\mathbf{C}} \leq 2\beta$, which indicates that the chirality is an independent component of the order parameter.

T-124 Spontaneous Weak-Ferromagnetism in the Superconductor ErNi$_2$B$_2$C

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The coexistence of weak-ferromagnetism and superconductivity in ErNi$_2$B$_2$C (T$_C$=11K)has been of great interest recently. Here we report a detailed study of the magnetic structure in a single crystal ErNi$_2$B$_2$C using the polarized and unpolarized neutron diffraction, performed at zero applied magnetic field. Cooling through T$_N$ = 6.0K, the compound enters a square-wave modulated incommensurate antiferromagnetic state, indicated by a fundamental satellite peak at (0.553a*,0,0) with the accompanying odd high order harmonics. Below T$_{WFM}$ = 2.3K, we have observed even order harmonics which originate from the existence of weak ferromagnetism. Our polarized neutron measurements show that both the odd and even order peaks are purely magnetic, clearly confirming the spontaneous weak-ferromagnetism below T$_{WFM}$ = 2.3K. Work by SCM and JWL supported by NSF DMR-9986442 and DMR 97-01339 and work by PCC and SLB by contract W-7405-Eng-82 and the Office of Basic Energy Sci.

T-125 Inducing antiferromagnetism with pressure in TbPt and TbPt$_{0.6}$Cu$_{0.4}$: a neutron diffraction study

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We present the evolution of the magnetic structures under pressure up to 65 Kbar of TbPt and TbPt$_{0.6}$Cu$_{0.4}$. The first compound is ferromagnetic non-collinear -CxFz, while in the Cu-diluted one an almost AF behaviour appears corresponding to a complex structure in which the -CxFz phase coexists with an incommensurate one. We have found that pressure favours a general antiferromagnetic behaviour, which manifests as a clear increasing of the AF component in the non-collinear phase, and in the evolution to a pure AF structure for the incommensurate one. It appears that pressure favours the x direction as an easy magnetisation axe.

T-126 Observation of Spinwaves in a Magnetic Superlattice by Inelastic Neutron Scattering

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So far only light scattering and ferromagnetic resonance techniques have been used to extract information on magnetic excitations in magnetic layered systems. However, only inelastic neutron scattering (INS) can access wide portions of the Brillouin zone allowing the determination of spin wave dispersion curves. We present the first successful INS measurements on a magnetic superlattice, yielding a bulk-like acoustic magnon dispersion curve in a folded Brillouin zone. The latter effect is due to the superlattice periodicity which is not present in bulk. The existence of a helimagnetic Bragg peak in the small angle reflectivity regime, where the magnetic form factor approaches its maximum, provides a unique opportunity for a very strong spin wave signal. The first inelastic data from this regime will be presented. Limitations as well as future perspectives and applications of INS measurements on superlattices will be discussed.

T-127 Low energy nuclear spin excitations in Nd and NdCu$_2$

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We have investigated the low energy inelastic neutron scattering from the Nd nuclear spin systems in Nd and NdCu$_2$ which become polarised below the ordering temperature of the Nd electronic spin by the hyperfine interaction. The nuclear spin system are coupled by Shul-Nakamura interaction and therefore can give rise to nuclear magnetic excitations including cooperative nuclear spin waves. We have neasured the low energy inelatic scattering from Nd as a function of temperature down to T = 0.06 K. At T = 0.06 K we observe inelastic peak with energy transfer of about 2.5 μeV on the both energy loss and energy gain sides. As the temperature is raised the energy of the inelastic peaks decreases continuously and finally the inelastic peak disappears in the elestic peak above $T_N \approx$ 20 K. Close to the magnetic phase transition T$_2 \approx$ 8.2 K we observe two peak structure. We interprete these inelastic scattering due to the nuclear spin excitations. The two peak structure arises due to the perticipation of Nd nuclear spin on both hexagonal and cubic sites of the dhcp structure. NCu$_2$ also shows similar inelatic peaks below $T_N \approx$ 6.3 K.

T-128 Neutron diffuse scattering study of disordered quasicrystal $Al_{72}Ni_{12}Co_{16}$ up to 1000°C

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Disordered decagonal quasicrystals $Al_{72}Ni_{12}Co_{16}$ were investigated by recording diffuse neutron scattering at instruments D10 and IN8 of the ILL up to 1000°C. Neutron data supplement and contrast x-ray diffuse data in order to learn about the relative influence of almost isoelectronic Co/Ni and to get rid off TDS by using an analyzer. A 1D superorder along the periodic direction reflected by diffuse layers perpendicular to it, dissolves at 950°C. Short-range-order maxima, which remain still obervable at 980°C, might be due to fluctuations. Prominent diffuse streaks within the quasiperiodic plane, which vanish between 800°C and 900°C, may be interpreted by fluctuations of phason strain values and the occurrence of lamellar domains. In general, the disordered structure of the decagonal phase is governed by complex intermixed transient ordering states: twinned lamellar domains of true 2D quasicrystalline sequences, 1D quasicrystalline sequences, and periodic domains accompanied by phason straining.

T-129 Martensitic and Magnetic Transformations of Ni_2MnGa-based Shape Memory Alloys

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As we had observed a shape memory effect of a single crystal of Heusler-type $Ni_{2.18}Mn_{0.82}Ga$ alloy, we carried out the powder neutron diffraction of this alloy. Rietveld analysis revealed that the martensitic transformation temperature is reasonable to explain the shape memory effect. We also discovered the coexistence of an orthorhombic structure and a monoclinic structure with a shuffling of a six-layer period of the (220) plane in the martensitic phase. In the case of powder neutron diffraction of $Ni_{2.19}Mn_{0.81}Ga$ alloy under magnetic field, we found that a magnetic field causes the martensitic transformation near the martensitic transformation temperature that is coincident with the Curie temperature. This fact suggests a possibility of controlling the shape memory effect by external magnetic field.

T-130 Lattice Dynamic of PbMg1/3Nb2/3O3 Relaxor Ferroelectric

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The dynamical properties of PMN at low temperatures were studied by triple axis technique in a broad energy range. Using the IN20 and IN1 spectrometers the main high-symmetry directions were studied at T∼10 K. In extreme contrast to the usual simplification of spectra of crystals at lower temperatures only the low-energy part of the INS spectrum of PMN can be considered as due to typical perfect-lattice phonons with well-defined energies and polarization vectors, while at intermediate to higher energies we have observed broad bands without a definite eigenvector polarization and dispersion curves can be followed only as the "streams" in the 2-dimensional intensity maps. Shall model calculations have been performed and satisfactory agreement for the low and medium energy part was obtained. This work was supported by RFBR grants 99-02-18074, 99-02-18316

T-131 Origin of negative thermal expansion in cubic ZrW_2O_8

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Large isotropic negative thermal expansion (NTE) has been known in cubic ZrW_2O_8 upto 1050 K. High pressure neutron inelastic scattering measurements have been carried out at ILL using the IN6 spectrometer at several pressures upto 1.7 Kbar, which show a pronounced softening of the phonon spectrum compared to that at ambient pressure by about 0.1-0.2 meV for phonons of energy below 8 meV. This unusual phonon softening is able to account for the observed NTE over the entire range of temperature. These observations are in agreement with the prediction of our lattice dynamical calculations (Phys. Rev. B 61, 7234 (1999)).

T-132 Non-Brownian Diffusion in a simple Liquid

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In a series of quasielastic neutron scattering experiments on liquid sodium the density dependence of the single particle motion was investigated for a variety of states along the liquid vapor coexistence curve. The results are in excellent agreement with computer simulation studies on hard sphere systems and can -on a quantitative basis- be discussed in the light of Mode-Coupling-Theory. A distinct universal deviation for the density dependence of the diffusion constant is found which can be understood on a purely microscopic basis: At high density, the particle's motion is hindered by a coupling to longitudinal density fluctuations, while at elevated temperatures and intermediate densities a coupling to transverse shear modes sets in promoting single particle dynamics relative to Brownian Diffusion. At even higher temperatures and low liquid densities mode coupling effects die out and a gradual approach to simple binary collision dynamics is observed.

T-133 Dynamical properties of the molecular glassforming Toluene : a complementary study by inelastic neutron scattering and realistic Molecular Dynamics simulations.

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Toluene has proved to be one of the most simple and promising model system for detailed studies of the normal and supercooled liquid state down to the glass transition. Recent coherent and incoherent neutron scattering experiments are presented over a wide temperature range from the glass transition temperature Tg to well above the melting point Tm. For a better understanding of the specific behavior of the correlation functions in glassforming liquids, realistic Molecular Dynamics simulations are developped in a temperature region close to and above a so-called dynamical critical temperature Tc introduced by the mode coupling theory.Owing to the rigid character of the molecule, the remarkable agreement of the simulations with the experiments allows their extension and the analysis of the interplay of the translational and rotational motions in the relaxation processes, as well as the crucial question of the existence of dynamical heterogeneities in the supercooled regime.

T-134 On the structure of red amorphous phosphorus

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The structure factor of a fine powder sample of red amorphous phosphorus has been determined by using the SLAD liquids and amorphous diffractometer at Studsvik NFL (Sweden). By comparing these data to earlier results serious discrepancies have been found at lower scattering vector values (up to about 5 Å^{-1}). Using the method of Reverse Monte Carlo modelling, the new data could easily be reproduced by a structural model whereas difficulties have been encountered concerning the earlier data set.

T-135 Structure of lithium borate glass and melt using neutron diffraction with isotopic substitution

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Alkali borate melts are considered as fragile liquids and should thus undergo rapid changes of the intermediate range order with increasing temperature, contrary to strong glass former such as B2O3. The possibility of a boron coordination change with temperature is still controversial. For example, a coordination change from [3]B to [4]B is difficult to observe by 11B NMR since, above Tg, a single narrow peak prevents an exact determination of the [4]B/[3]B ratio [1,2]. Raman spectroscopic studies at high temperature show some rearrangement of the borate groups which could be induced by a change in the [4]B/[3]B ratio [3,4]. Moreover, the detailed determination of the cation environment at high temperature is not well understood, and especially the possible site distortions or coordination changes, the connectivity with the polymerized network or the cation distribution. The study of oxide glasses, particularly at ISIS, has shown that the method of isotopic substitution is very well suited to the observation of the structural organization around the cations, even if this cationic arrangement is not apparent in the total correlation function [5]. To our knowledge, no such study has been reported on the corresponding liquids of oxide glasses. We measured the structure of a Li2B4O7 glass and melt using neutron diffraction with isotopic substitution of Li. Three glasses, synthesized by standard melt quenching technique, are enriched in 11B isotope and contain different Li isotopic content (pure 6Li, pure 7Li, and an equal mixture of 6Li and 7Li). The neutron diffraction experiments were carried out at the neutron spallation source ISIS (U.K.) on the SANDALS diffractometer using a standard vandium furnace and a vandium container. Temperatures up to 1400K can be obtained, allowing to probe the liquid state for borate samples. We obtained the diffracted intensity for the glass at ambient temperature, the supercooled liquid and the liquid. Using the first difference method, the Li site can be determined precisely in the glass and the melt and in particular the distortion of its site. Due to the access to high Q values, the two different B-O nearest-neighbor distances can be partially resolve and the question of the variation of the [4]B/[3]B ratio with the temperature will be addressed. Using the difference technique, it is possible to obtain a function containing the B-a pairs, only, which give information on the borate network and on the borate groups present in the glass structure. These results allow to achieve a better understanding of the structure of supercooled liquids and melts and the structural differences between the glass and the liquid. [1] J.F. Stebbins, In Structure dynamics and properties of silicate melts, eds. J.F. Stebbins, McMillan, P.F., Dingwell, D.B., Mineralogical Society of America, 32 (1995) 317. [2] Y. Inagaki, H. Maekawa, T. Yokokawa, Phys. Rev. B, 47 (1993) 674. [3] A.K Hassan, L.M. Torell, L. Börjesson, Phys. Rev. B, 45 (1992) 12797. [4] R.A. Condrate, A.K. Jillavenkatesa, In Borate glasses, crystals and melts, Eds A.C Wright, S.A. Feller, A.C. Hannon, (1997) 164. [5] L. Cormier, G. Calas, P.H. Gaskell, Chemical Geology, 174 (2001) 349.