Poster Session B

B-1 Lamor precession neutron diffraction technique for high precision determination of strain in eutechtic single crystal composite $Al_2O_3/Y_3Al_5O_{12}$ (YAG)

M. Ono[1,4], K. Habicht[2], T. Keller[3],
[1] Research Reactor Institute, Kyoto University, Osaka-fu 590-0495, Japan
[2] Hahn-Meitner-Institute, D 14109 Berlin
[3] MPI for Solid State Research, D 70569 Stuttgart
[4] Advanced Institute of Materials Research, Sendai-shi 982-0252, Japan

Using a neutron spin echo instrument with tilted coils, summing up the Lamor precession phases in two arms of spectrometer 1), we demonstrate a high precision strain measurement in a two-phase single crystal composite $Al_2O_3/Y_3Al_5O_{12}$ (YAG) by means of the novel Lamor diffraction technique. The results show a sensitivity increased by an order of magnitude compared to conventional techniques like Bragg angle analysis and time-of-flight analysis [2-4]. The methodological points of the present method is discussed with respect to the previous ones. [1] M.T.Rekveldt, T. Keller and R.Golub, Europhys.Lett.(2001) (in press). [2] M.Ono et al., Mater.Sci.Forum, Vol.347-349, 530 (2000). [3] M.Ono et al., Residual Stresses-ICRS-6, 49 (2000). [4] M.Ono et al., MECA-SENS 2000, J.Neutron Research (in press).

B-2 Apocrypha of Standard Scattering Theory

V. Ignatovich[1],
[1] Frank laboratory of neutron physics of Joint Institute for Nuclear Research

It is shown that description of scattering with spherical waves contradicts to the principles of standard quantum mechanics, because an outgoing spherical wave is not an eigen state and even is not a solution of the homogenious Schroedinger equation. Since we accept a plane wave as an eigen state of an incident particle, the scattered wave function should be expanded over plane waves, and scattering event should be described as a transition with dimensionless probabilities determined by dimensionless coefficients in this expansion. It is important to note, that with such a description the scattering process becomes a nonstationary one even in elastic case. I calculated total scattering probability on a monatomic gas (4He) and found that its dependence on temperature and energy differs considerably from the one presented in all text books, and which had never been checked. Further investigation in that direction reveals an important fact that with dimensionless probabilities one cannot describe such a simple thing as transmission exponent for a sample with given density of scatterers and given thickness. To construct the transmission exponent one is compelled to introduce a parameter with dimension of area. This parameter is a characteristics not of a scatterer, but of a scattering radiation. Thus scattering events contain information not only about scatterer, but also about scattered radiation. I discuss all these fundamental questions and possibilities to extract information about scattering radiation.

B-3 Effect of cold neutron spin rotation at passage through a noncentrosymmetric crystal

V. V. Voronin[1], V. V. Fedorov[1], E. G. Lapin[1], S. Yu. Semenikhin[1],
[1] Petersburg Nuclear Physics Institute RAS

Effect of cold neutron spin rotation at passage through a noncentrosymmetric crystal was experimentally observed. The effect is caused by Schwinger interaction of moving neutron with an interplanar electric field of the noncentrosymmetric crystal and depends on a direction and energy of neutron. For α-quartz crystal it was shown, that the mean value of effect is $\sim 1 \cdot 10^{-4}$ rad/cm in a broad band of wavelength of neutron (from 2.8 up to 5.5 Å) and is restricted by energy resolution (for our case $\Delta\lambda/\lambda \sim 5 \cdot 10^{-2}$). The measured effect has well coincidence with the theoretical one.

B-4 The Accuracy of Diffraction Peak Location

M. R. Daymond[1], P. J. Withers[2], M. W. Johnson[1],
[1] ISIS Facility, RAL, Chilton, Didcot, Oxon. OX11 0QX, UK
[2] Dept. of Materials Science, Manchester University, Grosvenor St, M1 7HS, UK

Many research areas require accurate determination of Bragg diffraction peak location and shape. It is important to know how long one must measure on a given instrument for a required level of precision; dependent on incident flux and instrument geometry, which in turn determine peak shape and background. One can proceed by acquiring continuously and repeatedly fitting until a required accuracy is achieved. However, it is useful to determine a priori the expected level of precision; to plan experiments, to compare instrument capabilities, or to check performance and reliability of peak fitting routines. We present a method for predicting precision of peak location, width and intensity in terms of the diffracted signal, peak width and signal to noise ratio. The formulation is derived for Gaussian peaks, but is broadly applicable to other peak shapes. Our primary interest is the location of peak position for strain measurement, but the methods have a much wider range of applicability. The analysis allows a quantitative analysis of the effect of depth on required measurement time.

B-5 The Neutron Diagnostics of Small-Size Plasma Systems

A. S. Tsybin[1], A. E. Shikanov[2], A. Yu. Kuznetsov[1], A. V. Ilínsky[2],
[1] Moscow State Engineering Phyisics Institute (technical university), Russia
[2] State Unitary Enterprise for Nuclear Geophysics and Geochemistry, Moscow region, Russia

The radiation method to evaluate deuterium concentration and its gradients in small-size (1-100 cm^3) plasma systems, irradiating neutrons, is considered. The algorithm, allowing to realize such evaluation by means of neutron fluence F measuremements in different points of space arround the plasma volume, is offered. This algorithm is based on integral correlation between F (R) and the function f(R)= A(R)n(R)+ B(R)n(R)n(R), where A and B are factors, connected with a distribution of electrical field in plasma, n is a deuteron concentration and R - radius-vector. The data array of neutron fluence measurements are placed in the integral relation, connecting F (R) values with f(R). After substitution of the integral expression by the approximate sum the linear system of algebraic equations for f(R) values in nodal points of the integral is obtained. The solution of this system for n(R) may be realized by the least squares method. Presented diagnostics can provide an important information about a plasma behaviour in neutron generating devices.

B-6 Direct measurement of $\Delta d/d$ by neutron Larmor diffraction

T. Keller[1], K. Habicht[2], M. Th. Rekveldt[3],
[1] Max-Planck-Institute for Solid State Research, Heisenbergstr. 1, D70569 Stuttgart
[2] Hahn-Meitner-Institut, Glienickerstr. 1, D14109 Berlin
[3] Interfaculty Reactor Institute, University of technology Delft, 2629 JB, Delft, The Netherlands

Two essential properties of neutron monochromators are the mosaicity β and the distribution of the lattice spacing $\Delta d/d$. The novel *Larmor diffraction technique* (Rekveldt 1999) allows for the first time the direct measurement of $\Delta d/d$ independent of the sample mosaicity with resolutions up to $\Delta d/d \leq 10^{-5}$ The method was demonstrated at the Neutron Resonance Spin Echo setup at Bensc Berlin. We show the basic principles and present results of an $\Delta d/d$ measurement of a pyrolytic graphite crystal.

B-7 The comparative analysis of the diffraction standards of VNIIMS and NIST

V.A. Sarin[1], A.M. Balagurov[2], B.N. Kodess[3], A.D. Perekrestenko[1], A.V. Rakseev[1],
[1] Institute for Nuclear Research RAS, 117312 Moscow, Russia
[2] Frank Laboratory of Neutron Physics, 141980 Dubna, Moscow region, Russia
[3] Russia Research Institute for Metrological Service,119361 Moscow, Russia

The results of comparison of resolution function R of high resolution neutron time of flight fourier diffractometer (HRFD), measured with the help of Si and Al_2O_3 diffraction standards of VNIIMS (Gosstandard of Russia)and NIST (USA) are presented. The R values are practically coincided for Al_2O_3 samples, smoothly decreasing from 0.0017 up to 0.0015 in a working interval of interplanar distances 0.5-2.5 Å. Closed R values on a sample of Si of VNIIMS are obtained. For a sample of Si of NIST the values of R are in interval of 0.0014-0.0012. Is shown that the basic contribution to half-width of diffraction lines of HRFD is given by tool component. Samples of VNIIMS could be utilized as reference samples in measuring of diffraction lines broadening in high resolution experiments. The measuring of Russia state reference sample of lattice constant V_3Si and sample of $SrFeO_3$ have shown a possibility to study changing in diffraction line width caused by defects of different type.

B-8 Measurement of the lateral coherence of a neutron beam.

P. Humbert[1], F. Ott[2], C. Fermon[1,2],
[1] SPEC, CEA Ormes des merisiers, 91191 Gif sur Yvette, France
[2] Laboratoire Léon Brillouin CEA/CNRS, 91191 Gif sur Yvette, France

We have estimated the lateral coherence of a neutron beam by doing reflectivity measurements on grated samples. A metallic grating (Al, Au or Cu) was deposited on glass or silicon substrates with periods ranging from 2 to 50 microns. Reflectivity measurements were performed on these samples with the grating lines parallel to the incident neutron beam. Depending on the grating periodicity, the specular reflectivity curves can be adjusted either with an incoherent sum (A[metal]^2 + A[substrate]^2) of the reflectivity on both materials or with an mean optical index between the metal and the substrate (A[metal+substrate])^2. We attribute the critical grating periodicity for which this change occurs to a neutron lateral coherence bigger or smaller than the grating periodicity. These measurements have been performed on the PRISM reflectometer at the LLB.

B-9 The total neutron scattering cross section of ^{3}He

W. Nistler[1], R. Scherm[1], M. Weyrauch[1],
[1] Physikalisch-Technische Bundesanstalt, Bundesallee 100, D38116 Braunschweig, Germany

The scattering cross sections of ^{3}He are of great interest for the theory of the four-nucleon system. The coherent scattering cross section is well known, whereas the two existing measurements of the total scattering cross section of ^{3}He are discrepant up to now. We report recent measurements at the FRG-1 research reactor in the GKSS research centre at Geesthacht, Germany. A new improved apparatus is used. The total scattering cross section of ^{3}He is determined relative to the well-known scattering cross section of ^{4}He. Neutron scattering intensities of a ^{3}He gas are compared with those of a ^{3}He-^{4}He mixture, which contains exactly the same amount of ^{3}He. Thus normalisation problems of intensities and solid angles as well as the huge neutron absorption effects essentially cancel out. A remaining small correction factor is evaluated by a Monte Carlo calculation. By variation of the critical parameters of the measurement the consistency of the measuring results is tested.

B-10 Atomic Resolution Neutron Holography

L. Cser[1], G. Krexner[2], Gy. Török[1],
[1] Research Institute for Solid State Phys. and Optics, POB-49, H-1525, Budapest, Hungary
[2] Institut für Experimentalphysik, Universität Wien, Boltzmanngasse 5, A-1090, Austria

Various approaches to the feasibility of atomic resolution neutron holography is discussed. For this there are two different schemes. In the frame of the first approach a point-like source of slow neutrons should be produced inside of the investigated crystal. Due to the extremely large value of the incoherent scattering cross section of the proton, hydrogen atoms imbedded in a metal single crystal lattice may serve as point-like sources as the sample irradiated by a monochromatic beam of slow neutrons. The second approach utilizes the registration of the interference between the incident and scattered beams by means of a point-like detector inserted in the lattice of the crystal under investigation. In addition, neutron-induced electron holography is considered.

B-11 D17, The New Reflectometer at the ILL

R. Cubitt[1]
[1] Institut Laue Langevin, 6 rue Jules Horowitz, B.P. 156, 38042 Grenoble Cedex 9

D17 has been operational for a year and has already proved to be an excellent tool for investigating surfaces and interfaces in the realms of Physics, Biology and Chemistry. The instrument has two modes of operation, Time-of-Flight (TOF) and monochromatic which incorporates the polarised neutron option. Both modes are flexible in the wavevector transfer (q) resolution. The loosest resolution required to resolve the sample structure can be chosen (hence the highest flux) enabling the lowest reflectivities and hence the widest q-range to be measured.

B-12 Representation of the Image Formation in Applied Neutron Radiography in Terms of a Point Spread Function Superposition

N Kardjilov[1], E Lehmann[2], P Vontobel[2], G Kühne[2],

[1] Technische Universität München, D-85748 Garching, Faculty for Physics E21

[2] Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland

The process of a neutron radiography image formation can be described in terms of a Point Spread Function (PSF) superposition. This way all distortions in the radiography picture obtained under different experimental conditions can be described as alterations in the corresponding PSF. Monte Carlo simulations were performed for the calculations of PSF for different materials, thickness and distances between sample and detector. A set of radiography experiments was performed to confirm the PSF superposition procedure. The good agreement between the superposition method and experimental data allows to use the Monte Carlo simulations as a base for corrections in the neutron radiography images.

B-13 How to Produce Spatially Defined Protons Domains in Matter: A Novel Tool for Small-Angle Polarized Neutron Scattering Structure Studies

B. van den Brandt[1], S.F.J. Cox[2], H. Glättli[3], P. Hautle[1], H. Jouve[4], J. Kohlbrecher[1], J.A. Konter[1], E. Leymarie[3], S. Mango[1], R. May[5], H. Stuhrmann[4], O. Zimmer[6],

[1] Paul Scherrer Insitute, CH - 5232 Villigen PSI, Switzerland

[2] ISIS Facility, Rutherford Appleton Lab, Chilton, Oxon, OX11 0QX, UK

[3] CEA Saclay, SPEC, F - 91191 Gif-sur-Yvette, France

[4] Institut de Biologie Structurale Jean-Pierre Ebel, F - 38027 Grenoble Cedex 1, France

[5] Institut Laue Langevin, BP 156, F - 38042 Grenoble Cedex 9, France

[6] Technische Universität München, James-Franck-Strasse, D - 85748 Garching, Germany

An apparatus has been devised and implemented to establish by dynamic nuclear polarization (DNP) and rf irradiation proton polarization gradients around a paramagnetic center in a dielectric solid. The aim is to develop techniques of local contrast enhancement for small-angle neutron scattering studies of macromolecules. The apparatus consists of a cryostat with an integrated 3,5 Tesla split pair magnet, a continuous flow 4He insert with top loading capability, a 98 GHz microwave system for DNP, and a NMR as well as a rf irradiation system to measure and manipulate the proton spin polarization. It has been successfully operated in several experimental runs.

B-14 Applied energy-selective neutron radiography and tomography

N. Kardjilov[1], S Baechler[2], E Lehmann[2],

[1] Technische Universität München, D-85748 Garching, Faculty for Physics E21

[2] Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland

The attenuation coefficient for monoenergetic thermal neutrons changes quite drastically at the Bragg cut-offs for many solid materials due to the coherent neutron scattering by the crystal lattice. In many cases the alteration in the total cross section for the corresponding element is significant and this fact can be used for achieving a material discrimination in radiography and tomography images by changing the spectrum of the applied neutron beam. Such energy-selective neutron radiography and tomography experiments were performed at the spallation source SINQ at the Paul Scherrer Institute in Switzerland. For this purpose a velocity selector was installed at the PGA beam position at SINQ to obtain a defined neutron energy distribution.

B-15 Towards 0.1 mm spatial resolution

A. D. Stoica[1], X.-L. Wang[1],

[1] Spallation Neutron Source, 701 Scarboro Road, Oak Ridge National Laboratory, Oak Ridge, TN 37830, USA

One of the design goals for VULCAN, the SNS engineering diffractometer, is the ability to measure spatial changes with 0.1 mm resolution (in one-dimension). The major challenge here is to define 0.1 mm wide incident and diffracted beams. Because the targeted applications often involve the use of large samples or special environment, slits cannot be used for this purpose. In this paper, methods to achieve 0.1 mm spatial resolution are outlined. For the incident beam, a new compact focusing device is proposed. The device is made of a stack of bent silicon wafers, each having a reflective multilayer (supermirror) deposited on one side and a neutron absorbing layer on the other side. The optimal design to minimize the optical spatial aberrations is discussed and Monte-Carlo simulation results are presented. The present design for the diffracted beam focuses on imaging. Preliminary testing results with Bragg Mirror imaging will be presented.

B-16 Neutron quantum state reconstruction

M. Baron[1,2], H. Rauch[1], M. Suda[3],

[1] Atominstitut der Österreichischen Universitäten, A-1020 Wien, Austria

[2] Institut Laue-Langevin, F-38042 Grenoble, France

[3] Austrian Research Center, A-2444 Seibersdorf, Austria

The neutron interferometer set-up S18 at the ILL-reactor has been used for the first neutron quantum state reconstruction experiment. By a simultaneous measurement of the coherence function and of the modulated momentum distribution behind the interferometer the Wigner function of various quantum states can be reconstructed, which is equivalent to the knowledge of the particle wave function. The spatial dimension follows from the measurement of the coherence function which is the auto-correlation function of the wave function and the shape in momentum space follows from momentum post-selection experiments. Non-orthogonal cuts through the (x,k)- phase space have to be measured for an unambiguous reconstruction. Nearly classical (coherent) and non-classical states in form of Schrödinger cat-like states have been identified. Comparisons of calculated and measured Wigner funtions will be shown. The work has been supported by the EU-TMR-Network on *Perfect Crystal Neutron Optics - PECNO* (ERB-EMRX-CT96-0057).

B-17 Comparative study of the use of a *white* and a *monochromatic* beam in Small Angle Neutron Scattering, for some soft matter samples.

G. Pépy[1], M. Jerjini[2],
[1] Laboratoire Léon Brillouin, 91191 Gif sur Yvette, France
[2] CNESTEN, 65 rue de Tansift, Agdal, Rabat, Maroc.

When Small Angle Neutron Scattering (SANS) appeared it was commonplace to use a *white beam* (i.e. all the neutrons coming out of a neutron guide). However this archaic method was very fast abandoned for monochromatic scattering (i.e. a 10% wavelength bandwidth). Meanwhile, even when they are working at powerful neutron sources, SANS experimentalists are often frustrated by the poor intensity from some very interesting samples ; at less powerful sources it would be of greatest interest to use improved scattering methods. Thence we have made an experimental comparison of both methods at the SANS spectrometer PAXE, in LLB, for some soft matter samples (polymer in bulk or in solution, proteins.For the data treatment discussion we consider 2 cases according to the available information about the scattering law. If the scattering law type is known, the data treatment task typically consists in determining a prefactor and a width. The comparative study will asses what is the uncertainty degradation due to the white beam. When the scattering law type is not known the data treatment includes a deconvolution (scattering reconstruction) which may imply some analytical extension assumption. This paper shall discuss when the *white beam* technique may give valuable information.

B-18 New method of absorption coefficient determination of various materials by neutrography with fast neutrons

S. J. Mourad,
[1] Bureau of System Engineering International Ltd., Winzerer Str. 50, 80797 München

The neutrography (radiography with neutrons) is a method to determine the absorption coefficient of known and unknown materials dependent on the site. In this study the procedure is performed with fast neutrons. The result are darkening patterns on a film or a monitor screen revealing other informations than the well-known slow neutron scattering because of the different absorption cross-sections. By calibration of the neutron exposures with an experimental darkening curve it is possible to determine the absorption coefficients of various homogenous and heterogenous materials specimen very precisely. Site-dependent structures (mixed materials) can be displayed with high resolution. The method was tested by evaluation of 150 samples with micro-densitometry and image analysis. The basic results are summarized in the study presented here. The experimental absorption coefficients are in agreement with theoretical results from the pertinent literature to a high extent. The construction of the film cassettes is very sophisticated in order to separate the different contributions from neutrons of variable energy; the different materials and their sheet assembly is also evaluated in our study. Possible practical applications for the method are wide-spread and include many fields of modern science: medicine, biology, mineralogy, military research, material testing and others.

B-19 The first results on observing new effects at the setup for a neutron EDM search by the new crystal-diffraction method.

V. V. Fedorov[1], E. G. Lapin[1], S. Yu. Semenikhin[1], V. V. Voronin[1],
[1] Petersburg Nuclear Physics Institute

Recently a new diffraction method of a search for a neutron electric dipole moment (EDM) was proposed, using some new effects for neutrons diffracted by the crystal without center of symmetry.The first experimental results were obtained at the pilot setup, mounted at VVR-M reactor in Gatchina, which allowed to study a dynamical diffraction of polarized neutrons in thick crystals, using a direct diffraction beam for Bragg angles close to 90°. The considerable delay of the diffracting neutron in the crystal for Bragg angles close to 90° was experimentally proved. The velocity of a neutron in the crystal measured by TOF method turned out to be 46 m/s for Bragg angle of 87° (the velocity of the incident neutrons was 810 m/s). The depolarization effect for diffracting neutron was first observed. It corresponds to an invariable (up to 87°) electric field of 2.20×10^8V/cm, acting on a neutron in the crystal. This value coincides with the theoretical one and our earlier experimental value for Bragg angles $\sim 25^\circ$ obtained by the other way. These results confirm the predicted opportunity to increase essentially the setup sensitivity to neutron EDM, using the diffraction angles close to 90°. So in our case the value Et, determining the sensitivity, turned out to be comparable with that of the most sensitive now magnetic resonance method, using ultra cold neutrons.

B-20 A new neutron interferometry approach to the determination of the n-e interaction amplitude

A. Ioffe[1], M. Vrana[2],
[1] Forschungszentrum Jülich GmbH, Institut für Festkörperforschung, IFF-8: Streumethoden, 52425 Jülich, Germany
[2] Nuclear Physics Institute of CAS, 20568 Rez near Prague, Czech Republic

A new experimental approach to the determination of the neutron-electron interaction amplitude is proposed. The main idea of this approach is to use a perfect crystal neutron interferometer both as a sample and a device for the measurement of the extra phase shift caused be the neutron interaction with atoms of Si. Indeed, such sample (an interferometer blade) has the well known atomic density and is á priori perfectly aligned with respect to the crystal lattice of the interferometer crystal. This results in the minimization of systematic errors caused by the sample alignment and increases the overall experimental accuracy. Some theoretic estimations and details of an experimental set up will be discussed.

B-21 Performance of the new pyrolytic graphite analyser bank on the IRIS spectrometer at ISIS

M. T. F. Telling[1], S. I. Campbell[1], D. D. Abbley[1], D. A. Cragg[1], J. J. P. Balchin[1], C. J. Carlile[2],
[1] ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, OXON, OX11 OQX
[2] ILL, 6 Jules Horowitz, BP156, 38042, Grenoble, France

The pyrolytic graphite (PG) analyser bank on the IRIS high-resolution inelastic spectrometer at the ISIS facility, RAL, UK has been upgraded. While the original design utilised a 6 row by 225-column array of 2mm thick (1 cm^2) graphite crystals cooled to 25K, the new design is comprised of 4212 crystal pieces (1mm thick, 18 rows by 234 columns). In addition, the graphite is now cooled close to liquid helium temperature to further improve the sensitivity of the spectrometer. In this paper we compare the performance of the newly upgraded instrument to resolution and intensity measurements collected prior to the modifications.

B-22 Development of a doubly focused silicon monochromator and a new neutron 4-circle diffractometer for studies of structural phase transition

Y. Noda[1], H. Kimura[1], R. Kiyanagi[1], S. Komiyama[1], A. Kojima[2], I. Yamada[2], Y. Morii[3], N. Minakawa[3], N. Takesue[4],
[1] Research Institute for Scientific Measurements, Tohoku University 2-1-1 Katahira, Aoba-ku, Sendai 980-8577 Japan
[2] Graduate School of Science and Technology, Faculty of Science, Chiba University, Yayoi, Chiba 263-8522 Japan
[3] Advanced Science Research Center, Japan Atomic Energy Research Institute, Tokai-mura, Naka-Gun, Ibaraki 319-1195 Japan
[4] The Institute for Solid State Physics, The University of Tokyo, 106-1 Shirakata, Tokai, Naka-gun Ibaraki 319-1106 Japan

We have developed a 4-circle diffractometer for a single crystal experiment at the guide-hall of the reactor JRR3M-JAERI(Japanese Research Reactor) at Tokai. The name of the diffractometer was adapted as FONDER (Four-Circle Off-center Type Neutron Diffractometer). We also developed a horizontally and vertically bend monochromatore with silicon plates. We could succeed to get well-focused neutron beam as a size of 1cm times 2cm at the sample position by using nine Si422 plates. Wavelength of the neutron is 1.54Åat the moment and the maximum scattering angle of a sample is 156 degree. We investigated several hydrogen bond materials like squaric acid and MeHPLN, oxide materials such as $CuGeO_3$, an oxide ferroelecric and antiferromagnetic compound YMn_2O_5, and obtained their structure and the phase transition scheme. We also studied structure and magnetic structure of manganese fluoride MnF_2. Very good R-factor was obtained, and electron density which is carrying spins was obtained. Maximum entropy method and Fourier synthesis methods were applied to btain nuclear density with great success.

B-23 Neutron Monochromatization in Reflectometry by Means of Thin Film Multilayers

D. Clemens, M. Horisberger,
[1] Laboratorium für Neutronenstreuung, ETH Zürich & Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland

Thin film mutlilayers are suitable devices to tailor the wavelength bandwidth to the needs in particular instruments. Their Bragg peak can be placed to $q > 1$ nm^{-1} by preparing a multilayer with correspondingly small d-spacing by the penalty of high repetition numbers and reflectivities that are decreased by the influence of interface roughness. Additionally, unwanted long wavelength neutrons may be present in the beam path due to total reflection from the mirror. Thus, the artificial structure is the reason for inherent natural limits. Nevertheless, installations working with a relatively large bandwidth or in a geometrically constrained set up can profit from their application. We report on the performance of a multilayer monochromator at AMOR, the reflectometer at SINQ. Using this instrument, we compared angle dispersive reflectometry to a TOF mode setup, in respect to resolution and intensity, respectively.

B-24 Asymmetric diffraction geometry of the bent perfect crystal monochromator A way for a further improvement of properties of strain diffractometers

P. Mikula[1], R. Lin Peng[2], J. Saroun[1], M. Vrana[1],
[1] Nuclear Physics Institute, 250 68 Rez, Czech Republic
[2] Studsvik Neutron Research Laboratory, S-61182 Nykoeping, Sweden

An advantageous exploitation of asymmetric diffraction geometry of bent perfect crystal(BPC) monochromators has been studied with the aim of further increase of detector signal and/or resolution of strain diffractometers. It has been experimentally demonstrated that in the case of strain diffractometers the asymmetric diffraction geometry of the BPC monochromator with the output beam extension can be considerably superior over the symmetric geometry or asymmetric geometry with the output beam compression usually used in powder diffractometry. Monte Carlo simulations and experimental results obtained on the strain diffractometers in NFL Studsvik and NPI Řež will be presented.

B-25 On using of cylindrically bent perfect crystals (CBPC) for TOF spectrometery

P. Mikula[1], M. Furusaka[2],
[1] Nucl. Phys. Inst., 250 68 Rez, Czech Republic
[2] Neutron Sc. Lab., KEK, Oho 1-1, Tsukuba 305, Japan

CBPC neutron monochromators/analyzers have been proved as an excellent alternative of mosaic crystals providing a way how to increase luminosity and angular/energy resolution of diffractometers at reactors. However, in the case of scattering devices working in the TOF regime, the CBPC elements have not been used practically. We present the results of promising TOF tests carried out with the fully asymmetric diffraction geometry (FADG) of silicon CBPC slabs. The length and the curvature of the slab determine the range of Δk/k ($\sim 10^{-2}$) that could be investigated with the accuracy Δk/k $\sim 10^{-4}$. The obtained results indicate that the FADG analyzer in combination with 1d-PSD can be a good candidate for a high-resolution analyzer. The use of PSD increases the speed of data collection considerably.

B-26 MACS Low Background Doubly Focusing Neutron Monochromator

S.A. Smee[1,2], J.D. Orndorff[3], G.A. Scharfstein[3], Y. Qiu[3], P.C. Brand[2], C.L. Broholm[3,2], D.K. Anand[1],
[1] Department of Mechanical Engineering, University of Maryland, College Park, MD 20742, USA
[2] National Institute of Standards and Technology, Gaithersburg, MD 20899, USA
[3] Department of Physics and Astronomy, Johns Hopkins University, Baltimore, MD 21218, USA

A novel doubly focusing neutron monochromator has been developed as part of the Multi-Analyzer Crystal Spectrometer (MACS) at the NIST Center for Neutron Research. The instrument utilizes a unique vertical focusing element that enables active vertical and horizontal focusing with a large, 357-crystal ($\approx$1400 cm^2), array. The design significantly reduces the amount of structural material in the beam path as compared to similar instruments. Electromechanical and optical measurements verify the excellent focal performance of the device. Analytical and Monte Carlo simulations predict that, when mounted at the NIST cold neutron source, the device should produce a monochromatic beam (ΔE = 0.2 meV) with flux $\phi > 10^8$ n/cm^2/s.

B-27 Neutron imaging with multi-wafer monochromators

M. Popovici[1], A. D. Stoica[2],
[1] University of Missouri Research Reactor (MURR), Columbia, MO 65211, USA
[2] Spallation Neutron Source (SNS), Oak Ridge National Laboratory (ORNL), Oak Ridge, TN 37831, USA

Multi-wafer monochromators for neutron scattering have been developed at MURR. Units made of commercial thin silicon [100] wafers and of non-standard [511] and [110] wafers have been fabricated for stress mapping machines at MURR, ORNL and NIST. The phase space optics of multi-wafer assemblies was worked out (JAC, in press). It revealed that neutron imaging can be done with thick packets of wafers at the spatial

resolution of a single thin wafer. Imaging may be dispersive (like with prisms) with respect to the neutron energy, direction or a combination of these, but it may also be non-dispersive (like with mirrors). Experiments have confirmed these conclusions. Dispersive and non-dispersive images were obtained with multi-wafer units at spatial resolutions comparable with those of single wafers. For non-dispersive imaging the acceptance window did not depend indeed on the neutron wavelength.

B-28 Development of ^{3}He neutron spin filter cells at the HMI

A. Gorzel[1], J. Klenke[1], A. Rupp[1],
[1] Hahn-Meitner-Institut GmbH

The spin dependent cross section for thermal and epithermal neutrons gives ^{3}He a high importance in neutron scattering. Due to the expected experimental possibilities, the construction of a ^{3}He neutron spin filter is a main point of the instrument development at the HMI. Of substancial importance is in addition to a high transmission the reduction of relaxation losses owing to wall collisions and magnetic field gradients. Refillable cylindrical quartz cells were evacuated, heated and coated with Cs. They were filled with compressed polarized ^{3}He (p $\approx$ 1bar) at the university of Mainz (Prof. Heil). Scattering experiments with polarized and unpolarized neutrons (λ = 0.24nm) revealed time constants between 33h and 50h. NMR measurements at low pressure cells (p = 3.5mbar) varified these results. The transmission of the empty cells was around 80%.

B-29 The influence of background on neutron polariser optimisation

D. J. Goossens[1], L. D. Cussen[2],
[1] Research School of Chemistry, Australian National University, Canberra ACT 0200 Australia
[2] Neutron Scattering, Australian Nuclear Science and Technology Organisation, Menai, NSW 2234, Australia

The optimisation of neutron spin filter polarisers is of current interest. A commonly used criterion is the maximisation of τp^2 where τ and p are the transmission and polarisation of an unpolarised beam. Here, we present new optimisation criterion for measurement of the flipping ratio and related quantities. We find that this criterion gives pathological results when filter medium polarisation is very high or the sample is strongly polarising. We explore the sensitivity of this criterion to background, and find that in all but the most extreme cases a background of 0.5% of the peak count rate removes the pathological behaviour. Hence the criteria developed is robust and potentially of wide use.

B-30 Development of spin flippers with steady current for a TOF-NSE spectrometer at a pulsed spallation neutron source

T Takeda[1], H Seto[1], Y Kawabata[1],
[1] Faculty of Integrated Arts and Sciences, Hiroshima University, Higashi-Hiroshima 739-8521, Japan

We designed π and $\pi/2$ flippers for a TOF-NSE spectrometer at a pulsed spallation neutron source. The flippers operate with steady current for a white neutron beam. The pi flipper consists of a compact modified current sheet and Helmholtz coils. The current sheet produces magnetic fields parallel to the sheet surface without magnetic fields perpendicular to the sheet surface at the surface of the sheet for the neutron beam cross section. The $\pi/2$ flipper consists of a rectangular coil and Helmholtz coils. We present the results of performance tests of the new-type flippers.

B-31 Magnetic Design of Polarized Neutron Reflectometer

J. Füzi[1], L. Cser[1], Gy. Török[1],
[1] Budapest Neutron Centre, Research Institute for Solid State Physics and Optics, Budapest, Hungary

The polarization option for the Budapest Neutron Centre reflectometer has been designed and realized. The magnetic fields of polarizing mirrors, guide field magnets and flippers - both Mezei type and solid state flipper - has been calculated by numerical 3D magnetostatic computation. The obtained configuration of the magnetic flux density distribution was measured and the accuracy of the calculations verified. The first results of neutron experiments are presented.

B-32 Development of radio-frequency neutron spin flipper applicable to pulsed sources

R Maruyama[1], T Ebisawa[2], S Tasaki[2], D Yamazaki[1], S Kawakami[1], T Kawai[2],
[1] Department of Nuclear Engineering, Kyoto Univ.
[2] Research Reactor Institute, Kyoto Univ.

In Japan, a new pulsed neutron source with high intensity is now under construction. We have a plan to install modified neutron spin echo spectrometers using radio-frequency (r.f.) neutron spin flippers at the pulsed source, although we are developing these spectrometers at continuous monochromatic beams from reactors. We need an r.f. flipper system applicable to a pulsed source. The dependence of the r.f. flipper on neutron wavelength is related to the amplitude of the oscillating field. Therefore the amplitude of the oscillating current should be varied in inverse proportion to the neutron flight time. In this paper, we describe the r.f. spin flipper system applicable to pulsed neutron sources and discuss the experimental results of its performances.

B-33 Large angle neutron polarisation analyser

Th Krist[1], H Fritzsche[1], K Temst[2], F Mezei[1],
[1] Hahn-Meitner-Institut Berlin, Glienicker Str. 100, 14109 Berlin, Germany
[2] Lab. v. Vaste-Stoffysica en Magnetisme, K. U. Leuven, Celestijnenlaan 200 D, 3001 Leuven, Belgium

A new device for the polarisation analysis of neutrons over a large angular range was tested at the reflectometer V 6 at BENSC. It consists of a bent stack of Si wafers coated with a polarising supermirror and an absorbing layer and has a length of 75 mm. This stack was divided into sub-stacks which were tilted against each other by 0.2 deg to analyse a total angular interval of 2.4 deg. Rotating the detector arm holding the device in front of a 2D detector without a sample inserted shows that the expected angular range can be analysed with a flipping ratio above 70 and a transmission of 60% of the spin up component. In addition, neutrons which are reflected from a regular array of Co dots on Si in a specular and a non specular beam were spin analysed. Such a device can easily be expanded to cover any arbitrary angular range!

B-34 Loss-free Polarisation of Pulsed Neutron Beams

S. Müller[1], G. Badurek[1],
[1] Atominstitut der Österreichischen Universit"aten, Stadionallee 2, A-1020 Wien

The concept of so-called dynamical neutron polarization should allow to polarise a beam of slow neutrons without loosing, at least in principle, even a single particle. It is based upon the spin-dependent energy splitting of monochromatic neutrons transmitted through a NMR-like arrangement of crossed static and oscillating magnetic fields, which causes different interaction times of the two opposite spin states with a subsequent static precession field. If this Larmor precession is stopped at a position where the two states are oriented parallel to a given direction all neutrons are in the same spin state, however, on the cost of a tiny energy difference between them. For pulsed beams this new method should be applicable even to polychromatic neutrons if one exploits the spatial dispersion of the particles in combination with a suitably chosen time dependence of either the splitting or the precession field. However, until no efforts have been undertaken to work out its details. Therefore, in order to proof the feasibility of this method and to determine the achievable degree of polarisation under realistic conditions we have performed both analytical and numerical simulations, which go far beyond the simple iterative approach of the original proposal.

B-35 'CRYOPADUM', an improved, hybride, zero-field, neutron polarimeter design for Spherical Neutron Polarimetry

F. Tasset[1], L.-P. Regnault[2], E. Lelievre-Berna[1], M. Thomas[1], E. Bourgeat-Lami[1], S. Pujol[1],
[1] Institut Laue-Langevin, Grenoble, France
[2] CEA-G DRFMC/SPSMS/MDN, Grenoble, France

Cryopad-II, the unique ILL polarimeter, is routinely used on IN20 and D3 for antiferro-magnetic structure investigations. The elastic mode of operation has now been fully demonstrated, up to high momentum transfer, allowing for example the spectacular determination of the covalent magneto-electric magnetisation density in Cr_2O_3 by P. J. Brown et al. We discuss here the tentative inelastic magnetic measurements made on IN20 with Cryopad-II which allowed us to acquire the proper control of this technique, to demonstrate its feasibility and to understand its potential strength in detecting mixed nuclear-magnetic excitations. Within the frame of ENPI, a European Network for the development of Neutron Polarimetry, an intense simulation work has been recently accomplished for a hybride (Nb & Mu-Metal) magnetic design, holding the promise of a 2° precision even with a 2cm diameter sample size and a 2° beam divergence. Three such optimised Cryopadum devices are being presently built for ILL, CEA and JAERI, which should represent a dramatic improvement in the neutron scattering community access to Spherical Neutron Polarimetry.

B-36 Towards High Resolution Polarisation Analysis using Double Polarisation and Ellipsoidal Analysers

D. Martín y Marero[1],
[1] ISIS Facility, Rutherford Appleton Laboratory

Classic polarisation analysis methods lack the combination of high resolution and high-count rate necessary to cope with the demand of modern condensed matter experiments. In this work, we present a method to achieve high-resolution polarisation analysis based on a Double Polarisation system. Coupling this method with an Ellipsoidal Wavelength Analyser a high-count rate can be achieved whilst delivering a resolution of around 10 μeV. This method is ideally suited to pulsed sources, although it can be adapted to continuous sources as well.

B-37 NRSE phenomena with adiabatic passage of neutron spin through resonant coils

S.V. Grigoriev[1,2], W.H. Kraan[2], M.Th. Rekveldt[2], W.G. Bouwman[2]
[1] Petersburg Nuclear Physics Institute, Gatchina, St.Petersburg 188350, Russia
[2] Interfacultair Reactor Instituut, TU-Delft, 2629 JB Delft, The Netherlands

Neutron Resonance Spin Echo phenomena, produced by resonance coils with adiabatic passage of the neutron spin, are investigated experimentally and theoretically. The solution of the Schrödinger equation was obtained for the required configuration of the magnetic fields. The whole spectrum of the neutron wavelength is involved in the precession. The precession phase inside the coil consists of three contributions in the rotating frame approach. The first, biggest contribution is the phase of the rotating frame. The second is the precession phase of the neutron spin in the rotating frame since it follows adiabatically the effective field as seen in this frame. The third, smallest contribution is Berry's phase since the magnetic field rotates over an angle approaching π in this rotating frame. All three contributions have been experimentally studied.

B-38 Spin-Echo SANS based on adiabatic HF flippers in dipole magnets with skew poles.

W.H. Kraan[1], S.V. Grigoriev[2], M. Th. Rekveldt[1], W.G. Bouwman[1], O. Uca[1],
[1] Interfacultair Reactor Instituut TU-Delft, 2629 JB Delft, The Netherlands
[2] Petersburg Nuclear Physiscs Institute, 188350 Gatchina, Petersburg District, Russia

We built a Spin-Echo set-up having precession devices each made up of 2 adiabatic HF flippers. To realise the angle labelling of our coarsely collimated neutron beam, the poles of the dipole magnets for the HF flippers were shaped as parallellograms. Good polarisation can be obtained over large beam cross sections in dipole fields up to 750 gauss, i.e. HF equal to 2 MHz. SANS in a sample placed somewhere in the beam shows up as depolarisation, i.e. a decrease of the amplitude of the SE signal. Measuring the depolarisation at various positions of the sample inside one of the precession devices is equivalent to probing the sample's correlation function $g(r)$. We will show examples of spin-echo SANS measurements in which this function was determined up to r=60 nm.

B-39 Magnetised foils as π-Flippers in Spin-Echo Spectroscopy

M. T. Rekveldt, W. H. Kraan, W. G. Bouwman,
[1] IRI, NM, TU Delft, Mekelweg 15, 2629 JB Delft, The Netherlands

In Larmor precession devices, such as used in neutron spin-echo systems, field line integrals have to be homogeneous over the cross-section of the neutron beam. Inhomogeneities in these line integrals arise where the magnitude of the field changes along the neutron paths. Mostly correction coils are applied to correct for these inhomogeneities. In spin-echo systems using π-flippers in the region between these inhomogeneities, an automatic correction for the main contribution of the inhomogeneities is obtained that avoids complicated current correction coils. In this paper the application of such π-flippers in a spin-echo spectrometer for small-angle scattering will be considered and discussed. The principle can be used in conventional spin-echo spectrometers as well.

B-40 Applicability of spin-echo small-angle neutron scattering

Wim G. Bouwman, S. V. Grigoriev, O. Uca, W. H. Kraan, J. Plomp, M. T. Rekveldt,
[1] Interfacultair Reactor Instituut, Delft University of Technology, Mekelweg 15, 2629 JB, The Netherlands

Spin echo small angle scattering (SESANS)[1] is a novel polarised neutron spin echo technique to measure small angle neutron scattering with a divergent beam. Calculations indicate that the method works best with strong scattering samples. It appears that the counting statistics are independent on the wavelength used at the upper tail of the Maxwellian wavelength spectrum. Large particles give more scattering than small ones that make the technique most suitable for large particles where the resolution is problematic in conventional SANS. Calculations and SESANS measurements illustrate these principles. 1] W. G. Bouwman, M. van Oossanen, O. Uca, W. H. Kraan, and M. Th. Rekveldt., J. Appl. Cryst., 33, 767–770, 2000.

B-41 Line integral corrections in Larmor precession devices

O. Uca[1], W. H. Kraan[1], W. G. Bouwman[1], J. Plomp[1], M. T. Rekveldt[1],
[1] Interfaculty Reactor Institute, Delft University of Technology, the Netherlands

Larmor precession devices need homogeneous line integrals of the magnetic field along the neutron trajectories over the beam cross-section. Line integral inhomogeneities must be homogenized or corrected in order not to spoil the initial polarization. It has been shown that these inhomogeneities can be corrected with coils in the SESANS instrument with foils [1]. The coils generate a vertical field gradient opposite to the precession field. Actually these coils transform a gradient of the line integral in the field direction to a direction perpendicular to it. The same idea of correction is investigated for more general applications, theoretically and experimentally.[1] Line integral corections in SESANS, Accepted for publication in Physica B, 2001

B-42 Development of modified neutron spin echo spectrometers applicable to pulsed neutron sources

S Tasaki[1], T Ebisawa[1], R Maruyama[2], N Achiwa[3], T Kawai[1], Y Kawabata[1], M Hino[1], D Yamazaki[1], S Kawakami[2],
[1] Research Reactor Institute Kyoto Univ., Kumatori Osaka 590-0494, Japan
[2] Department of Nuclear Engineering, Kyoto Univ., Sakyo-ku, Kyoto 606-8501, Japan
[3] Graduate School of Sciences Kyushu University, Higashi-ku Hakozaki 812-8581 Fukuoka,Japan

Modified neutron spin echo is developing method based on neutron spin interferometry principle. There are three types of spectrometer are now being developed to apply to reactor neutron sources. Advantages of these spectrometers are 1. they do not require huge uniform magnetic field, 2. since the size of the spectrometer can be much smaller, then it will be possible to combine with other spectrometers, and 3. have possibility of increasing spin echo time. Application of these spectrometers, however, has not yet performed. We present results of preliminary experiments of the modified neutron spin echo spectrometers applicable to pulsed sources, and discuss on the feasibility of these spectrometers.

B-43 Larmor precession picture and quantum aspects of neutron spin behavior

N.K. Pleshanov[1],
[1] Petersburg Nuclear Physics Institute, 188350 Gatchina, Russia

The interest to quantum aspects of the neutron spin behavior in magnetic fields has recently been stirred up by developments in neutron techniques. In some of the papers the Larmor precession picture has been revoked as inconsistent with the exact quantum picture. However, one may show that in these cases the Larmor precession picture can be reconciled with the quantum approach to the neutron spin behavior in homogeneous fields. Particularly, the use of such notions as *zero field precession*, *optical spin rotation* and *quantum precession* introduced to oppose the *Larmor precession* can certainly be avoided. On the other hand, the conditions are obtained when the Larmor precession picture fails and quantum aspects of the neutron spin behavior do come into play. Examples of polarized neutron experiments are given to illustrate this.

B-44 Neutron spin-echo spectrometer at BARC Trombay

S.L. Chaplot[1], R. Mittal[1], P. Goel[1],
[1] Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai 400085, India

At one of the cold neutron guides at the Dhruva reactor at Trombay, we are testing a modestly designed neutron spin-echo spectrometer, which would be suitable for the study of dynamics at an intermediate length of about 1 nm and time up to 1 ns. We use a BeO- filtered quasi-monochromatic beam; and a multi-stage soller type design of the supermirror polarizer and analyser which allows focussing of the neutron beam by a suitable choice of the angles between the various columns of the supermirrors. The spin-echo signal has been observed for the direct beam, and further calibration experiments are in progress.

B-45 Instrumental Design and Performance of a New Pulsed Neutron Reflectometer (ARISA) for Free Surface at KENS

N. Torikai[1], M. Furusaka[1], H. Matsuoka[2], Y. Matsushita[3], M. Shibayama[4], A. Takahara[5], M. Takeda[6], S. Tasaki[7], H. Yamaoka[8],
[1] Neutron Science Lab (KENS), KEK, Tsukuba, Japan
[2] Dept. of Polymer Chemistry, Kyoto Univ., Kyoto, Japan
[3] Dept. of Applied Chemistry, Nagoya Univ., Nagoya, Japan
[4] Neutron Scattering Lab, ISSP, The Univ. of Tokyo, Tokai, Japan
[5] IFOC, Kyushu Univ., Fukuoka, Japan
[6] Physics Dept., Tohoku Univ., Sendai, Japan
[7] Research Reactor Institute, Kyoto Univ., Kumatori, Japan
[8] Dept. of Materials Science, Univ. of Shiga Prefecture, Hikone, Japan

A new pulsed-neutron reflectometer (ARISA) with a vertical scattering-plane geometry was installed at one of the thermal neutron ports of KENS. The neutron beam is guided downward onto sample surface. Specular reflection can be measured up to 4 nm^{-1} in neutron momentum transfer along the vertical direction for liquid sample using neutrons within wavelength range of 0.07 nm - 0.4 nm. A liquid trough and a high-temperature cell were prepared as sample environment equipment. The performance tests have been started using nickel films and a few polymer systems.

B-46 Wide angle NSE : the spectrometer SPAN at BENSC

C. Pappas[1], A. Triolo[1], R. Kischnik[1], F. Mezei[1],

[1] BENSC, HMI Berlin, Glienicker Str. 100, D-14109 Berlin, Germany

The peculiarity in the design of SPAN is in the NSE precession field, which is created by three pairs of coils with diameters 1, 3 and 4.8 m respectively. The set-up has a cylindrical symmetry around a vertical axis, which crosses the scattering plane at the sample position. The resulting magnetic field does not change with the scattering angle and thus enables simultaneous NSE measurements over a wide angular range. SPAN is also characterized by its broad incident wavelength band, which ranges from 9 Åto 2.5 Åi.e. from cold neutrons to the thermal spectrum. At the lowest wavelength of 2.5 $Å^{-1}$ Q_{max}=4.8$Å^{-1}$, which opens up new possibilities in probing coherent dynamics in the high Q range, where localized motions should occur. That high Q values have never been accessible by any other NSE spectrometer before and have up to now only been reached by the combined thermal TAS-NSE spectrometers TASSE-IN20 at ILL and PONTA at ISSP-JAERI

B-47 Calculations on spin-echo coils.

S. Prokudaylo[1], R. Gähler[1], T. Keller[1], M. Bleuel[1], M. Axtner[1], A. Selvachev[2],

[1] Physik Department E21, Technische Universität München, D-85747 Garching, Germany

[2] Institute of Computer Aided Design, Russian Academy of Science, Moscow, Russia

The perfomance of the coils used in Spin-Echo setup is simulated to obtain the optimum parameters. The possibility to use round wire instead of band for coil production is proved. The parameters of the static bootstrap coils were varied in 2D approach and a more advanced configuration as being used was found. The coil for normal spin escho with field perpendicular to the optical axis is considered in 3D simulations. First results are cited.

B-48 Viscosities and densities of melts measured with dynamic neutron imaging and the falling sphere technique

A. Kahle[1], B. Winkler[1], B. Hennion[2], P. Boutrouille[2], G. Bayon[3],
[1] Universität Kiel, Institut für Geowissenschaften, Mineralogie, Olshausenstr. 40, 24098 Kiel, Germany
[2] CEA, Centre d' Etudes de Saclay DSM/DRECAM/LLB, 91191 Gif-sur-Yvette Cedex, France
[3] CEA, Centre d' Etudes de Saclay DRN/DRE/SIREN, 91191 Gif-sur-Yvette Cedex, France

We demonstrate that viscosities and densities of silicate melts can be accurately determined using neutron imaging combined with the falling sphere technique. Investigations include the determination of the viscosity and density of a pure SiO_2 melt at temperatures up to 2000°C and experiments on the viscosities of partially crystallized melts.

B-49 Methyl Group Dynamics in a Crystal and its Glassy Counterpart by Neutron Scattering

A. J. Moreno[1], A. Alegr[1], J. Colmenero[1], B. Frick[2],
[1] Dpto. Fisica de Materiales y Centro Mixto CSIC-UPV/EHU. Apdo. 1072, 20080 San Sebastián, Spain
[2] Institut Laue Langevin, BP 156X, F-38042, Grenoble, France

Methyl group dynamics in a same sample of sodium acetate trihydrate in crystalline and glassy state has been investigated by neutron scattering. Measurements have been carried out in the whole temperature range, covering the crossover from the rotational tunneling to the classical hopping regime. The results in the crystalline sample have been analyzed according to the usual single-particle assumption while those in the glass in terms of a Gaussian distribution of single-particle potentials, this distribution resulting from the structural disorder present in the glass. It is found that the average potential barrier in the glass takes, within the experimental error, the same value as the single barrier in the crystal. The half-width of the distribution takes a value similar to those obtained in the quite different structural glasses (polymers) that had been investigated up to now.

B-50 Neutron scattering study of low energy excitations in triphenyl phosphite

J. Mayer[1], J. Krawczyk[1], J. Janik[1], M. Massalska-Arodz[1], I. Natkaniec[1,2], O. Steinsvoll[3],
[1] H.Niewodniczanski Institute of Nuclear Physics, 31-342 Krakow, Poland
[2] Frank Laboratory of Neutron Physics, JINR, 141980 Dubna, Russia
[3] Institute for Energy Technology, 2007 Kjeller, Norway

Triphenyl phosphite (TPP) was studied by a wide range of experimental methods [1]. In this paper we present the results concerning the low energy excitations measured by inelastic incoherent neutron scattering for all phases of TPP with two different instruments. The preliminary results obtained with a direct geometry spectrometer revealed a weak boson peak in glassy state, what is in agreement with large value of fragility of TPP. The more detailed results obtained with the inverted geometry spectrometer are also presented. The density of states presented, being a real property of the material, seems to be more correct way of describing the low energy processes than scattering law measured in direct geometry experiment [2]. [1] M. Mizukami, K. Kobashi, M. Hanaya, M. Oguni, J.Phys.Chem. B 103 (1999) 4078. [2] J.Mayer, J.Krawczyk, J.A.Janik, M.Massalska-Arodz, I.Natkaniec, O.Steinsvoll, submitted to Physica B.

B-51 Characterization of "Strong/Fragile" Behaviour of Glass-Forming Aqueous Solutions by Neutron Scattering

C. Branca[1], S. Magazù[1], G. Maisano[1], O. Migliardo[1],
[1] Dipartimento di Fisica and INFM, Università di Messina, P.O. Box 55, 98166 S. Agata, Messina, Italy

In this contribution we report the results of a study on glass-forming aqueous solutions. This study is principally addressed to the comparison of the vibrational properties of the two homologous disaccharides across the glass transition. The neutron scattering measurements have been performed on trehalose/H_2O and sucrose/H_2O mixtures by using the spectrometer MIBEMOL at the Laboratoire Leon Brillouin (LLB, Saclay) as a function of temperature and concentration. In order to characterize the different rigidity of both the disaccharide/H_2O mixtures, we have analysed the temperature behaviour of the Debye-Waller factor. For the trehalose/water mixtures, also the dependence of fragility on concentration has been also investigated.

B-52 Study on Destructuring Effect of Trehalose on Water by Neutron Diffraction

F. Migliardo[1], G. Maisano[1], P. Migliardo[1],
[1] Dipartimento di Fisica and INFM, Università di Messina, P.O. Box 55, 98166 S. Agata, Messina, Italy

α,α-trehalose, a glass-forming disaccharide, shows an excellent bioprotective capability in several living beings under environment stress conditions, maintaining activity and leavening capacity of several desiccation-resistant organisms. Raman scattering findings on aqueous solutions of trehalose and homologous disaccharides suggests the hypothesis that the cryoprotective action of trehalose on biological structures is to be connected with its capability to reduce the amount of freezable water and to destructure so the H-bond network of water. By neutron diffraction data, collected by using Sandals diffractometer at the ISIS facility (UK), we evidence the characteristic peaks changes of the partial structure factors and distribution functions in comparison with water spectra and as a consequence of an increase of temperature and concentration, and obtain the confirm that a decreasing of the tetrahedrality degree of water occurs.

B-53 Neutron Scattering Study on the Vibrational Behaviour of Disaccaride Aqueous Solutions

G. Romeo[1], F. Migliardo[1], P. Migliardo[1],
[1] Dipartimento di Fisica and INFM, Universit'a di Messina, P.O.Box 55, 98166 S. Agata, Messina, Italy

In recent years there has been a rapid growth in biochemical and biomedical studies involving disaccharides. Most disaccharides display similar H-bonding properties and possess a relatively large number of OH groups, that interface easily with the H-bond network of the closely associated waters. To understand the remarkable functional differences among homologue disaccharides, it is important to characterise and compare highly resolved data from proton-sensitive techniques. In this contribution we report a neutron scattering study of the vibrational properties of trehalose, maltose and sucrose aqueous solutions by using the TOSCA spectrometer at the ISIS facility (UK). We have analysed vibrational spectra of hydrated samples of three disaccharides, in order to investigate the extent to which certain unusual low-frequency differences between trehalose and the other homologues disaccharides are reflected in specific features at higher frequencies, and to characterize the effects of disaccharides on the dynamics of ice.

B-54 Neutron Scattering Study of Molecular Motions in Glassy BPA-Policarbonate.

S. Arrese-Igor[1], A. Alegríma[1], A. Arbe[1], J. Colmenero[1], B. Frick[2],

[1] Dpto Dpto de Física de Materiales, Universidad del País Vasco y Unidad de Física de Materiales (CSIC-UPV/EHU). Apdo 1072, 20080, San Sebastian, Spain.

[2] ILL, BP 156, 38042 Grenoble, France.

Most of the engineering thermoplastics, materials with a well-known technological significance, are glassy polymers. The mechanical properties of these polymers, being the basis of most of these applications, are directly related with the dynamical processes occurring at the molecular scale. For example, it is believed that the energy dissipation caused by the activation of dynamic processes related to secondary relaxation are responsible of the good impact resistance of engineering polymers. In order to shed new light into the comprehension of the relationship between molecular dynamics and mechanical properties of these polymers, we have studied the dynamics of glassy Polycarbonate (PC). Methyl group deuterated and fully deuterated samples were measured by means of Quasielastic Neutron Scattering (QNS) and Dielectric Spectroscopy (DS). It is shown that the occurrence of only phenyl ring p-flips is not enough to explain the NS data observed. Moreover, some additional center of mass movement is inferred from the fully deuterated sample spectra, where movements which do not involve structural changes, like phenyl ring p-flips, would not contribute to the quasielastic signal.

B-55 Characterization of Conformational Properties of Protein/Trehalose/Water System by Neutron Scattering

F. Migliardo[1], G. Maisano[1], P. Migliardo[1],

[1] Dipartimento di Fisica and INFM, Università di Messina, P.O.Box 55, 98166 S. Agata, Messina, Italy

The present work concerns with an experimental study of the conformational properties of an important protein dUTPase as a function of temperature and in presence and in absence of trehalose. Since trehalose plays an important role as stabilizer of cellular structures in particular stress conditions, by protecting biological membranes and enzymes under conditions of dehydration and elevated temperatures, this kind of study allows to test the stabilizing effect of trehalose on biological systems. The attention has been addressed to the temperature stabilization of dUTPase, an essential determinant of fidelity of DNA replication by effectively reducing the dTTP/dUTP ratio in cells undergoing active mitosis. To elucidate whether a direct protein-trehalose interaction takes place, SANS measurements have been performed by V4 spectrometer (BENSC, Germany). From this investigation we have obtained information on the changes of the protein structure as a function of temperature and in presence of trehalose.

B-56 Analysis of Vibrational Properties Changes of Water in Presence of Disaccharides

G. Romeo[1], P. Migliardo[1],

[1] Dipartimento di Fisica and INFM, Università di Messina, P.O.Box 55, 98166 S. Agata, Messina, Italy

The growing interest on trehalose and homologues disaccharides is based on the circumstance that they reveal great effective bio-protective effects. Among various functions, disaccharides increase tolerance to freeze-drying, inhibit virus growth in cell cultures and prolong the life of organs for transplantation. To understand the unique effectiveness of trehalose, neutron scattering is a powerful spectroscopic technique to be used in conjunction with simulation of the molecular mechanisms of the biological action. In this contribution we report the results obtained by using MARI spectrometer (ISIS, UK). The findings reveal that trehalose is most effective in destructuring the open (low density) conformation of ice, followed by maltose and sucrose, showing the effects of disaccharides on the structural arrangements and on the vibrational dynamics of water.

B-57 Characterization of Trehalose Aqueous Solutions by Neutron Spin Echo

C. Branca[1], A. Faraone[1], S. Magazù[1], G. Maisano[1], A. Mangione[1], C. Pappas[2], A. Triolo[2],

[1] Dipartimento di Fisica dell Università di Messina and INFM, 98166 Messina, Italy

[2] Hahn-Meitner-Institut, BENSC (NI), Glienicker Strasse, D-14109 Berlin, Germany

The work reports Neutron Spin Echo (NSE) results on aqueous solutions of trehalose, a naturally occurring disaccharide of glucose, showing an extraordinary .bioprotective effectiveness against dehydration and freezing. We collected data using the SPAN spectrometer (BENSC, Berlin) on trehalose aqueous solutions at different temperature values. The aim of the work is to furnish new results on the dynamics of the trehalose/water system on the nano and picoseconds scale.

B-58 The protons dynamics of ethylene glycol

A. G. Novikov[1], M. N. Rodnikova[2], O. V. Sobolev[1],

[1] Institute for Physics and Power Engineering, Bondarenko Sq.1., Obninsk, Kaluga Reg., Russia.

[2] Kurnakov Institute of General and Inorganic Chemistry, Russian Academy of Sciences, 117907, Moscow, Russia

The results of the inelastic neutron scattering experiment on ethylene glycol at T= 348K and T = 393 K by using ”direct geometry” double time-of-flight neutron scattering spectrometer DIN-2PI (Frank Laboratory of Neutron Physics, JINR, Dubna) are presented. The quasi-elastic and inelastic components of the incoherent scattering function S(Q,ω) have been considered. The diffusion characteristics and generalised frequency distributions (GFD) for protons of ethylene glycol molecules were obtained from the neutron scattering spectra.

B-59 Vibrational Dynamics of Hydration Water in Amylose

N. Angelini[1,3], F. Cavatorta[1,2], A. Deriu[1,2], G. Albanese[1,2],

[1] Istituto Nazionale di Fisica della Materia, Unitá di ricerca di Parma, Italy

[2] Dipartimento di Fisica dell’ Universitá di Parma, Italy

[3] CNR Istituto Biofisica - Pisa -Italy

We present a study on the dynamical properties of hydration water in amylose, based on low temperature vibrational spectra collected on the TOSCA at ISIS. The structural constraints of the polysaccharide chains favour the formation of a high density structure for water, that has been suggested by Imberty et al.[1] on the basis of conformational analysis. According to this model, hydration water can only enter the pores formed by six adjacent helices and completely fills the pore at 27%w/w, reaching a density originally quoted as 1.4 g/cm^3. Our measurements show that the dynamical behaviour of hydration water is similar to that observed in high density amorphous ice. Amylose shows therefore peculiar characters when compared to other porous materials where water forms structures having a liquid-like density. [1]Imberty A, Perez S, Biopolymers. 27,1205 (1988)

B-60 Inelastic Neutron Scattering in Amorphous Systems at Low Momentum Transfer

W. Schmidt[1,2], M. Ohl[1,2], U. Buchenau[1],
[1] Forschungszentrum Jülich, Institut für Festkörperforschung, 52425 Jülich, Germany
[2] Institut Laue Langevin, 38042 Grenoble, France

We studied inelastic scattering at low momentum transfer for polybutadiene [1], an amorphous polymer, and for water. The measurements were done on the cold-neutron three-axis spectrometer IN12 studying protonated and deuterated samples to distinguish between incoherent and coherent scattering. A large vacuum tank around the sample was used to eliminate the strong air scattering at low scattering angles, close to the incoming beam. Multiple-scattering calculations were performed and validated in the experiments. For the incoherent scattering, the expected Q^2-dependence could be confirmed. On the contrary, the coherent scattering shows a small, but clearly non-zero additional contribution down to the lowest accessible Q-vectors. The results are interpreted in terms of an elastic distortion around low frequency localised modes [2]. For IN12 a polarisation analysis with reduced air scattering is currently under construction. In addition to magnetic experiments also a separation of coherent and incoherent scattering at small momentum transfer will be available with high accuracy. This work has been funded by the BMBF under contract number 05-300-CJB-6. [1] W. Schmidt, M. Ohl, U. Buchenau, Phys. Rev. Lett., 85, (2000) 5669. [2] U. Buchenau, A. Wischnewski, M. Monkenbusch, W. Schmidt, Phil. Mag. B 79 (1999) 2021.

B-61 SANS study of the critical behaviour in a confined binary liquid mixture

M. Bonetti[1], Y. Alméras[1], F. Formisano[2], J. Teixeira[3],
[1] Service de Physique de l'Etat Condensé, CEA-Saclay, 91191 Gif-sur-Yvette Cedex, France
[2] INFM-OGG c/o ILL, 6 rue J. Horowitz, BP 156 38042 Grenoble Cedex 9, France
[3] Laboratoire Léon Brillouin, CEA/CNRS-Saclay, 91191 Gif-sur-Yvette Cedex, France

We report here some of the results obtained through a SANS experiment performed at the PAXE diffractometer of the LLB (Saclay, France) on the binary mixture n-octane+n-perfluorooctane soaked in a Vycor porous glass at the bulk critical composition. This experiment allowed the study of the critical behaviour in a temperature range extended with respect to a previous measurement [1] on a similar mixture to be performed. We have detected a low-Q intensity that increases more and more when lowering the temperature, even at temperatures much lower than the bulk critical one. The possibility that critical fluctuations could survive in an extremely broad temperature domain because of confinement is therefore discussed. [1] F. Formisano and J. Teixeira, Europ. Phys. J. E 1, 1 (2000).

B-62 Structural Changes and Diffusive Consequences in Sodium Disilicate Melts

A. Meyer[1], H. Schober[1,2], D. B. Dingwell[3],
[1] Physik Department E13, Technische Universität München, 85747 Garching, Germany
[2] Institut Laue-Langevin, 38042 Grenoble, France
[3] Institut für Mineralogie, Petrologie und Geochemie, Universität München, 80333 München, Germany

We investigate $Na_2Si_2O_5$ melts with inelastic neutron scattering at temperatures up to 1600 K. The elastic structure factor shows at $\simeq 0.9\,\text{Å}^{-1}$ an emerging prepeak which becomes more pronounced with increasing temperature. The partially destroyed Si-O tetrahedral network relaxes on a time scale of ns, whereas the Na ion relaxation dynamics occurs on a time scale of 10 ps. The temperature dependence of the latter is given by the sum of two nearly equally strong contributions: a faster diffusion and an increasing number of diffusing atoms. Our results on structure and dynamics can be rationalized using results of recent molecular dynamics simulations.

B-63 Chemical-isomeric effects on propanol glassy structure

G. J. Cuello[1], C. Talón[2], F. J. Bermejo[3], C. Cabrillo[3], M. A. Ramos[2], S. Vieira[2],
[1] Institut Laue Langevin, 6 rue Jules Horowitz, F-38042 Grenoble, France
[2] Laboratorio de Bajas Temperaturas, UAM, Cantoblanco E-28049, Madrid, Spain
[3] Instituto de Estructura de la Materia, CSIC, Serrano 123, E-28005 Madrid, Spain

We have studied the structure of both propanol isomers in their glassy and crystalline states by neutron diffraction. The glass-transition temperatures of 1- and 2- propanol are about 98 and 115 K, respectively, and even surprisingly larger differences are observed for the melting temperatures of the stable crystals, which are 148 and 185 K, respectively. Their supercooled liquid phases show rather different relaxation spectra, 1-propanol manifesting strong deviations from Debye behavior, whereas 2-propanol showing a far weaker effect. We discuss the spectra obtained for the static structure factor and the static correlation function g(r). There is a noticeable difference in the position of the FSDP, which clearly indicates a density change, well correlated with the period of the intermolecular oscillations shown by the g(r).

B-64 Observation of Crossover from 3D-Ising to isotropic Lifshitz critical Behavior and Double Critical Point in a ternary Polymer Blend

V. Pipich[1], D. Schwahn[1], L. Willner[1],
[1] Forschungszentrum Jülich GmbH, Institut für Festkörperforschung

A ternary polymer blend consisting of a critical polybutadiene/polystyrene mixture (PB/PS) and a symmetric diblockcopolymer PB-PS was studied by SANS. In principle, the diblockcopolymer acts as a surfactant thus enhancing the system compatibility. For diblock concentrations below and above the so-called Lifshitz line (LL) the, respectively, characteristic phase behavior of blends and diblockcopolymers is observed. The "blend" regime below LL shows an upper critical solution temperature which is decreasing with enhanced diblock content ϕ and is terminated at $\phi = 0.074$ when approaching LL. We could identify a crossover from 3d-Ising to isotropic Lifshitz critical behavior near $\phi = 0.05$ and found the existence of a double critical point (DCP) at $\phi_{DCP} = 0.074$. A properly consideration of the DCP has to be performed with the field variable $t_{UL} = \mid (T - T_L)(T - T_U) \mid /T^2$ its use leads consistently to the Lifshitz critical exponents $\gamma = 1.68$ and $u = 0.88$.

B-65 Self and collective dynamics of ordered star polymer solutions

J. Stellbrink[1], J. Allgaier[1], M. Monkenbusch[1], D. Richter[1], G. Ehlers[2], P. Schleger[2],
[1] Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany
[2] Institut Laue-Langevin, F-38042 Grenoble, France

We investigated self and collective dynamics of ordered star polymer solutions well above their overlap concentration c^*. Only at low Q self and collective dynamics become discernible. The collective short time diffusion coefficient D_{eff} is well described by the term $D_0 H(Q)/S(Q)$ as

known from colloid dynamics. For covering the slowed down dynamics at Q_m, the peak position in S(Q), the dynamic time range of NSE was extended for the first time up to 350ns using long wavelengths, (=19Å, at IN15(ILL, Grenoble). Here we found that S(Q,t)/S(Q,0) relaxes into a concentration dependent plateau. The plateau height gives the mean square displacement of star cores, which is related to the blob size of the surrounding star polymer solution obtained by dynamic light scattering.

B-66 Dynamic Neutron Scattering on Partially Deuterated Polybutadiene

S. Kahle[1], L. Willner[1], M. Monkenbusch[1], D. Richter[1], A. Arbe[2], J. Colmenero[2], B. Frick[3],
[1] Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany
[2] Departamento de Fisika de Materiales, Universidad del Pais Vasco, 20080 San Sebastian, Spain
[3] Institut Laue-Langevin, 38042 Grenoble Cedex, France

The molecular nature of the secondary relaxation (Johari Goldstein relaxation, β process) and its relationship with the a relaxation is in most cases still unknown. In order to access these processes on a molecular level, it is necessary to get spatial information of the relaxation. Through the momentum transfer dependence of the dynamic structure factor S(q,t) this information can be provided by quasielastic neutron scattering techniques. The large difference in scattering lengths between hydrogen and deuterium allows to accentuate certain correlations between atoms in a polymer melt. Here, we like to report on recent results on a polybutadiene melt, where the double bond was hydrogeneous, while the methylene groups carried deuterons (d4h2-PB). In this way the correlations between the double bonds are emphasised. We will show that the double bond / double bond correlation function, generated in this way, shows the same temperature dependence as the viscosity at higher temperatures at the structure factor peak maximum, but at lower temperatures the spectra decay faster than predicted from the viscosity time scale, th. However, the fully deuterated sample (d6-PB) has shown that the intermediate scattering function at the structure factor peak maximum shows the same temperature dependence over the complete temperature range[1]. This indicates the prevalence of a different process below a certain temperature TC, observed in the d4h2-PB sample. A similar temperature-dependence shows the β process observed with dielectric spectroscopy. [1] A. Arbe, D. Richter, J. Colmenero, B. Farago, Phys. Rev. E 54 (1996) 3853

B-67 Slow Dynamics of n-Butoxyethanol/water Mixture by Neutron Spin Echo Technique

K. Yoshida[1], T. Yamaguchi[1], M. Nagao[2], Y. Kawabata[3], H. Seto[3],
[1] Faculty of Science, Fukuoka University, Fukuoka 814-0180, Japan
[2] Institute for solid State Physics, University of Tokyo, Ibaraki 319-1106, Japan
[3] Faculty of Integrated Arts and Science, Hiroshima University, Higashi-Hiroshima 739-8521, Japan

n-butoxyethanol/water mixtures undergo phase separation at a lower critical solution temperature (LCST) of 49°C. Previously, large small-angle neutron scattering was observed in the mixtures at temperatures below LCST, suggesting that microheterogeneity occurs prior to macroscopic phase separation. In this study, neutron spin echo (NSE) measurements have been carried out at a cold neutron port C2-2 of JRR-3M, JAERI on an n-butoxyethanol/water mixture of alcohol mole fraction 0.09 at 25 and 37°C. The diffusion coefficients obtained from the time dependent echo signals based on a Brownian motion approximation were 6.6×10^{-11} and 7.8×10^{-11} $m^2 s^{-1}$ at 25 and 37°C, respectively. These values are about 10^2 times smaller than those of pure water and alcohol, probably reflecting the motion of molecular aggregates formed in the mixture. Dynamics of cluster formation in n-butoxyethanol/water mixtures will be discussed.

B-68 Dynamic and Static Properties of Star-burst and Star-like Dendrimers

S. Rathgeber[1], T. Pakula[2], V. Urban[3], M. Monkenbusch[4], S. Longeville[5],
[1] Forschungzentrum Jülich, IFF - Weiche Materie, 52425 Jülich, Germany
[2] Max-Planck-Institut für Polymerforschung, 55021 Mainz, Germany
[3] European Synchrotron Radiation Facility, 38043 Grenoble Cedex, France
[4] Forschungzentrum Jülich, IFF - Neutronenstreuung, 52425 Jülich, Germany
[5] Laboratoire Leon Brillouin, 91191 Gif-sur-Yvette Cedex, France

We studied the static and dynamic properties of star-burst and star-like dendrimers under good solvent conditions by means of small angle neutron- and X-ray scattering as well as neutron spin-echo (NSE) spectroscopy. From the form factor S(Q) we derived the radius of gyration, the sphere radius, the range of hydrodynamic interaction and the fractal dimension. Internal segment distributions have been characterized by the pair distance distribution function and the segment density profile, both obtained from S(Q) via an inverse Fourier transform algorithm. The experimental findings are in excellent agreement with MC computer simulation results using the cooperative motion algorithm. From a first cumulant evaluation of the NSE data we derived the relaxation rates on length scales smaller and larger than the overall dendrimer dimension. For the star-like dendrimers we were able to resolve length scales smaller than the extent of the linear units between the branching points.

B-69 Dynamics of flexible counter-ions in conducting polyaniline: A Quasielastic Neutron Scattering Study

M. Bee[1,2], D. Djurado[1], J. Combet[3], M. A. Gonzalez[2], P. Rannou[4], B. Dufour[4],
[1] Laboratoire de Spectrometrie Physique Universite J. Fourier Grenoble-I, B.P. 87 38402, Saint Martin d Heres Cedex, France
[2] Institut Laue-Langevin, 6 rue Jules Horowitz, B.P. 156, 38042, Grenoble Cedex, France
[3] Institut Charles Sadron, 6 rue Boussingault, 67083 Strasbourg Cedex, France
[4] CEA Grenoble, DRFMC, SI3M, LPMS, 17 avenue des Martyrs, 38054 Grenoble Cedex 9, France

Films of conducting polyaniline containing flexible counter-ions were investigated by quasielastic incoherent neutron scattering. In addition to promote high conductivity, these new ions also act to increase elasticity of samples. As in the case of more rigid counter-ions, polymer chains appear as very stiff objects whose dynamics is completely out of the investigated time-scale. Conversely the counter-ion dynamics was proved to be of major importance in relation with the charge transport since a dynamical transition is observed precisely in the temperature range where the electronic properties change from a metallic to a semiconducting regime.

B-70 Structure and Dynamics of Mixed Amphiphilic Membranes. A combined SANS-NSE study.

M. Mihailescu[1], M. Monkenbusch[1], J. Allgaier[1], D. Richter[1], J. Stellbrink[1],
[1] IFF, Forschungszentrum Jülich, Germany

Amphiphilic molecule such as the non-ionic $C_{10}E_4$ -tetraethyl- monodecyl-ether, consisting basically of a hydrophilic head and a hydrophobic tail, can built soft interfacial membranes of various topologies between immiscible fluids (e.g. water/oil). The average conformation and the

time relaxation of the fluctuating membranes, at mesoscopic length-scales, are investigated with Small Angle Neutron Scattering and Neutron Spin Echo techniques, respectively. Two example structures, i.e. in spherical and planar geometries, built by $C_{10}E_4$ surfactant in the presence of analogous polymeric macro-surfactants such as $PEP - PEO$ are presented. Informations on physical parameters like the bending elasticity moduli are extracted based on available theories, and the influence of block-copolymer on the membrane structure and interaction is discussed. [1] V.Lisy and B.Brutovsky,Phys.Rev.E,61(4),4045-4053,(2000) [2] A.G.Zilman and R.Granek, Phys.Rev.Lett.,77(23),4788-4791,(1996) [3] A.Caillé, C.R.Acad.Sci.274B,891-893,(1972)

B-71 Dynamic studies of Poly(di-n-alkyl itaconate)s

P. F. Holmes[1], V. Arrighi[1], S. Gagliardi[1], I. J. McEwen[1], J. M. G. Cowie[1], J. Combet[2], M. T. F. Telling[3],
[1] Heriot-Watt University, Edinburgh, UK
[2] Institut Laue-Langevin, 38042 Grenoble Cedex, France
[3] ISIS, Rutherford Appleton Laboratory, Didcot, UK

We report a dynamic study of poly(di-n-alkyl itaconate)s and present data from the backscattering spectrometers IRIS (ISIS) and IN10 (ILL). Elastic window scan measurements carried out on IN10 indicate that molecular motion is detected well below the glass transition temperature. It is possible to distinguish different dynamic processes where the temperature range over which these are observed is dependant on the length of the side chain n. The intermediate scattering function, I(Q,t) determined from the QENS data collected at IRIS was found to obey time-temperature superposition. We show that the I(Q,t) data at different temperatures can be overlapped using the same time-scale shift factors. This indicates that the relaxation process is common to all the polymers investigated.

B-72 Component dynamics in polymer blends. A combined QENS and dielectic spectroscopy investigation

S. Hoffmann[1], D. Richter[1], A. Arbe[2], J. Colmenero[2], B. Farago[3],
[1] Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany
[2] Departatmento de Física de Materiales, Universidad del Pa
is Vasco, Apartado 1072, E-20080 San Sebastián, Spain
[3] Institut Laue-Langevin, B. P. 156, F-38042 Grenoble Cedex 9, France

The individual dynamics of the two constituants of a binary polymer blend have been studied by means of QENS and dielectric spectroscopy (DS). In combining neutron spin-echo and backscattering techniques, the complete cross over from entropy driven, Rouse-like chain dynamics to the alpha-relaxation in the local segmental motion which is governed by local potentials and steric hindrances has been revealed. The observed blending effects on the respective relaxation times suggest a purely dynamic origin of the dynamic heterogeneity in polymer blends at temperatures well above the glass transition temperature without the assumption of any kind of local phase separation. The studies were continued towards lower temperatures by DS indicating systematic deviations from the mean-field behaviour observed by QENS which lead to an increased heterogeneity of the local dynamics of the system.

B-73 Fullerene-containing polymeric Stars in bulk and solution by Neutron Spin-Echo

V.T. Lebedev[1], Gy. Torok[2], L. Cser[2], D.N. Orlova[1], V.A. Berstein[3], V.N. Zgonnik[4], E.Yu Melenevskaya[4], L.V. Vinogradova[4],
[1] Petersburg Nucl. Phys. Inst., 188300 Gatchina, St.Petersburg dist., Russia
[2] Res. Inst. for Solid State Phys. and Optics, POB-49, H-1525, Budapest, Hungary
[3] Ioffe Physico-Techn. Inst.,194021 Polytechnicheskaya 26, St.Petersburg, Russia
[4] Inst. of Macromol. Compounds, 199004 Bolshoy pr.31, St.Petersburg, Russia

The benzene solutions of Stars with C_{60} fullerene core and poly(styrene) arms and the bulk polymer matrix have been investigated by Neutron Spin-Echo. The behaviours of Stars (~ 6 arms, mass $M \sim 5 \cdot 10^3$) at momentum transfer $q = 0.2 - 0.6nm^{-1}$ and in the time range $t = 0.01 - 20ns$ at $T = 20 - 90^\circ C$, were compared with dynamics of free PS-chains. Displaying depressed molecular mobility, the Stars did not obey usual dynamic Zimm or Rouse model. The influence of specific architecture and polymer-fullerene interaction on their dynamics is treated in terms of stretched auto- and pair correlation of chain units in Stars.

B-74 Molecular dynamics of poly(N-vinylcaprolactam) hydrate

V.T. Lebedev[1], Gy. Torok[2], L. Cser[2], Gy. Kali[3], A.I. Sibilev[1],
[1] Petersburg Nuclear Phys. Inst., 188300 Gatchina St.-Petersburg dist., Russia
[2] Research Inst. for Solid State Phys, POB 49, H-1525, Budapest, Hungary
[3] Hahn-Meitner Inst., Glienicker st.100, D-14109 Berlin, Germany

The poly(N-vinylcaprolactam) $(PVCL) - D_2O$ complex has been studied by NSE at temperatures from -60 to $+40^\circ C$, when the hydration transforms the originally amorphous rigid chain polymer to elastic one. The polymer $(M = 2 \cdot 10^6)$ shows a remarkable decrease of glass transition temperature from $T_G \sim 147^\circ C$ (dry polymer) to $T_G \sim -20^\circ C$ (7 water molecules per unit). We explain it with forming hydration shells (hydrogen bonds with $C = O$ -groups). This system undergoes a phase decomposition at $T \sim 50^\circ C$. So the polymer mobility has a maximum within window $T = -20^\circ C + 5^\circ C$, where the S(q,t) correlation function was measured. (time $t = 0.003 - 5ns$, momentum transfer $q = 0.55nm^{-1}$). It displays the specific chain dynamics being hybridization of slow reptation and fast transversal chain motion.Such kind of dynamics in polymer systems was not observed yet.

B-75 Dynamics of complexes of poly(N-vinylpyrrolidone)-C_{60} in aqueous solution

Gy. Torok[1], V.T. Lebedev[2], L. Cser[1], D.N. Orlova[2], A.I. Sibilev[2], V.N. Zgonnik[3], E.Yu. Melenevskaya[3], L.V. Vinogradova[3], M.A. Sibileva[4],
[1] Research Inst. for Solid State Phys., POB-49, H-1525, Budapest, Hungary
[2] Petersburg Nuclear Phys. Inst., 188300 Gatchina, St.-Petersburg dist., Russia
[3] Inst.of Macromol. Compounds, 199004, Bolshoy pr.31, St.-Petersburg, Russia
[4] Univ. of St.-Petersburg, 198904, University pr.2, Peterhof , St.-Petersburg, Russia

Hydration of complexes of poly(N-vinylpyrrolidone) (PVP) with fullerene C_{60} has been studied by SANS and NSE to elucidate the origin of strong polymer self-assembly induced by extremely low amounts of fullerene ($\sim 10^{-6} wt.\%$) in solution. As compared to free PVP-coils in D_2O, the complexes (C_{60}-molecule per PVP-chain), forming mass fractal structures, demonstrate intense segmental motion (time range t=0.2-20 ns) at temperatures $T = 20 - 80^{\circ}C$. This anomalous increrase of relaxation rate of chains in complexes at segmental scale should be related to the influence of fullerene on water shell around PVP. These results agree with viscometry data obtained for aqueous solutions of complexes at different fullerene content.

B-76 Conformation of a side-chain liquid crystal polymer in solution

D. Rousseau[1], J.-D. Marty[2], M. Mauzac[2], P. Martinoty[1], A. Brandt[3], J.-M. Guenet[4],
[1] Laboratoire de Dynamique des Fluides Complexes CNRS-ULP UMR 7506, 4 rue Blaise Pascal, F-67070 Strasbourg cedex, France
[2] Laboratoire des Interactions Moleculaires et de Reactivite Chimique et Photochimique, CNRS-UPS UMR 5623, 118 route de Narbonne, F-31062 Toulouse cedex, France
[3] BENSC - Hahn-Meitner Institut, Glienicker Strasse 100, D-14109 Berlin, Germany
[4] Institut Charles Sadron CNRS UPR 022, 6 rue Boussingault, F-67083 Strasbourg cedex, France

We have carried out a study of the conformation of liquid crystal polymer in diluted solutions. Our measurements have been taken in different solvents as a function of the grafted mesogens fraction. We have observed that, for mesogens fractions between 0% and 100%, the radius of gyration inscreases by a factor 2 independent of the solvent. As we will discuss during this communication, this observation corresponds to an increase by a factor 4 of the backbone's persistence length, and is in favor of Frederickson's theory [1]. [1] G.H. Frederickson, Macromolecules, 26, 2825, (1993)

B-77 Multiple-phase behavior and its memory effect for 4-acrylamidosalicylic acid gel

M. Annaka[1], R. Motokawa[1], M. Sugyama[2], K. Hara[3], T. Nakahira[1],
[1] Department of Materials Technology, Faculty of Engineering, Chiba University, 1-33 Yayoi-cho, Inage-ku, Chiba 263-8522, Japan
[2] Department of Physics, Graduate School of Science, Kyushu University, 6-10-1 Hakozaki, Higashi-ku, Fukuoka 812-8581 Japan
[3] Institute of Environmental Systems, Faculty of Engineering, Kyushu University, 6-10-1 Hakozaki, Higashi-ku, Fukuoka 812-8581 Japan

4-acrylamidosalicylic acid gel exhibits multiple phases as characterized by distinct degrees of swelling; the gel can take one of four different swelling values, but none of the intermediate values, which appears as a result of the combination of hydrogen bonding and hydrophobic interaction between polymer segments. The gel has remarkable memory: the phase behavior depends on whether the gel has experienced the most swollen phase or the most collapsed phase in the immediate past. The information is stored and reversibly erased in the form of a macroscopic phase transition behavior. The structure factors corresponding to these four phases were obtained by SANS, which indicated the presence of characteristic structures depending on pH and temperature, particularly in the shrunken state.

B-78 INS as a sensitive probe of inter-monomer angles in polymers

L. Eijck, van[1], F.C. Grozema[1], L.D.A. Siebbeles[1], G.J. Kearley[1],
[1] Interfaculty Reactor Institute, Delft University of Technology, Delft 2629 JB 15, Netherlands

We have explored the use of INS and numerical methods to obtain one of the most important structural parameters in conducting polymers: the angle between neighbouring aromatic rings. This is achieved by comparing the measured INS vibrational spectra of oligothiophenes in the crystalline state with those calculated using periodic DFT methods. The variation of the spectrum as a function of the angle between the thiophene rings, arises mainly from the soft out-of-plane coordinates. Potential functions for these coordinates are calculated and shown to be highly anharmonic. The angle sensitivity of the INS spectra from this work can be extended to non crystalline polythiophenes.

B-79 Dynamics of confined Polymer Electrolytes.

A. Triolo[1], L. Bronstein[2], J. W. Zwanziger[2], V. Arrighi[3], R.E. Lechner[1], R. Triolo[4],
[1] Hahn-Meitner Institut, BENSC, Berlin, Germany
[2] Dept. of Chemistry, Indiana University, Bloomington, USA
[3] Dept. of Chemistry, Heriot-Watt University, Edinburgh, UK
[4] Dept. of Physical Chemistry, University of Palermo, Palermo, Italy

The segmental dynamics of Poly Ethylene Oxide confined in Inorganic-Organic Composites is probed by means of the QENS technique. As a consequence of the confinement, PEO chains show a much slower relaxation behavior as compared to the bulk. The results are compared with evidences from other techniques. The effect of salt doping of PEO is also probed.

B-80 QENS Investigation of filled rubbers

A. Triolo[1], F. Negroni[2], V. Arrighi[3], R. E. Lechner[1], F. Lo Celso[4], R. Triolo[4],
[1] Hahn-Meitner Institut, BENSC, Berlin, Germany
[2] Pirelli Pneumatici S.p.A, Milan, Italy
[3] Dept. of Chemistry, Heriot-Watt University, Edinburgh, UK
[4] Dept. of Physical Chemistry, University of Palermo, Palermo, Italy

The QENS technique is applied to investigate the effect of inert filler addition to polymer dynamics. The segmental dynamics of styrene-butadiene rubber is found to be strongly affected by addition of SiO_2. Our preliminary data confirm the existence of a thin layer of bound polymer around the filler surface, whose dynamics is highly hindered as compared to bulk.

B-81 NSE and TOF investigation of coherent dynamics of atactic polypropylen

A. Triolo[1], C. Pappas[1], V. Arrighi[2],
[1] Hahn-Meitner Institut, BENSC, Berlin, Germany
[2] Dept. of Chemistry, Heriot-Watt University, Edinburgh, UK

The coherent dynamics of fully deuterated atactic polypropylene has been investigated by means of combined Neutron Spin Echo and Time of Flight Neutron Spectroscopy (covering more than four decades in time) between Tg+10 K and Tg+200 K. The segmental dynamics of aPP has been probed at different values of the momentum transfer ($0.5 \leq Q(Å^{-1}) \leq 1.8$). Time-temperature superposition was obtained, following the viscoelastic shift law. TOF-QENS indicates the existence of a faster relaxation, which is a precursor of the α-process. A thorough discussion on the two relaxation processes will be reported.

B-82 Segmental dynamics in Polymer Electrolytes

A. Triolo[1], F. Lo Celso[2], V. Arrighi[3], R. E. Lechner[1], R. Triolo[2],
[1] Hahn-Meitner Institut, BENSC, Berlin, Germany
[2] Dept. of Physical Chemistry, University of Palermo, Palermo, Italy
[3] Dept. of Chemistry, Heriot-Watt University, Edinburgh, UK

Polymer dynamics in PEO-salt mixtures is explored by means of the QENS technique. The reported results are the first QENS evidence that dynamic heterogeneities are induced in PEO-salt mixtures as a consequence of salt addition. In agreement with Molecular Dynamics simulation, this behavior can be rationalized assuming the existence of a bimodal relaxation: a fast process corresponding to the normal bulk one and a slower relaxation attributed to the formation of PEO-cation complexes, which considerably slows down chain dynamics.

B-83 Anomalies in the dynamics and structure of poly(vinyl chloride)

A. Arbe[1], A. Moral[1], A. Alegria[1], J. Colmenero[1], W. Pyckhout-Hintzen[2], D. Richter[2], B. Farago[3], B. Frick[3],
[1] Departamento de Fisica de Materiales, Universidad del Pais Vasco, and Unidad de Fisica de Materiales (CSIC-UPV/EHU), San Sebastian, Spain
[2] Institut für Festkörperforschung, Forschungszentrum Jülich, Jülich, Germany
[3] Institut Laue-Langevin, Grenoble, France

The structural and dynamical properties of poly(vinyl chloride)(PVC) have been studied by Small Angle Neutron Scattering (SANS) and combining dielectric spectroscopy, coherent and incoherent neutron scattering respectively. SANS reveals the existence of structural heterogeneities. The dynamics study shows deviations of the spectral shape and the Q-dependence of the alpha-relaxation from those exhibited by common glass-forming polymers. A model considering the coexistence of different regions leading to a distribution of characteristic times $g(\log\tau)$ gives account for the experimental observations. A unique functional form for the alpha-relaxation - determined from the coherent scattering data at the first peak of the static structure factor S(Q) - is assumed for all regions in the sample. The $g(\log\tau)$ found is compatible with the distribution of only one variable, the glass transition temperature. The origin of this anomalous dynamical behavior can be related to the structural heterogeneities identified in the SANS study.

B-84 Neutron diffraction Study of Zinc-Nickel Ferrites Powders Prepared by Combustion Synthesis

J. S. Lee[1], Y. Choi[2], Hae S. Shim[1], ,
[1] Korea Atomic Energy Research Institute, HANARO, Daejeon, 305-600, S-Korea
[2] Sunmoon University, Asan Chungnam, 336-840, S-Korea

The chemical composition and magnetic properties of $Zn_xNi_{1-x}Fe_2O_4$ powders prepared by self-propagating high temperature synthesis were determined by neutron diffraction analysis and with a vibrating sample magnetometer. The SHS reaction rate of the reactant mixture with tap density had an extreme value of 8.9 mm/sec at the oxygen pressure of 5 MPa. The ferrite spinel in the SHS products increased as the iron content in the reactants increased. The coercive force and residual magnetization were 7.99 Oe, 75.8 emu/g, whereas, the maximum magnetization, susceptibility and curie temperature were 0.791 emu/g and 0.001937 emu/gOe, respectively. The powder neutron diffraction patterns measured at room temperature using the 32-detector high resolution powder diffractometer (HRPD) at KAERI showed that monochromatic neutrons with a wavelength of 0.18339 nm were obtained from a Ge(331) monochromator with a 90 take-off angle. The Rietveld refinement of each patterns converged to good agreement(χ^2=1.88 2.24). In view of the improved magnetic properties and productivity, the non-stoichiometric number of the Ni-Zn ferrites formed by self-propagating high temperature synthesis method significantly depended on the initial powder size, oxygen pressure and the relative amount of iron to oxide.

B-85 Neutron diffraction investigation of the spontaneous and field induced spin-reorientation transition in Tm_2Fe_{17}

A. Pirogov[1], J. Park[2], J.-G. Park[2], C.H. Lee[3], K. Prokes[4], E. Valiev[1], N. Kudrevatykh[5], D. Sheptyakov[6],
[1] Ural State University, 620083 Ekaterinburg, Russia
[2] Department of Physics, Inha University, 402-751 Inchon, Korea
[3] Korean Atomic Energy Research Institute, 305-600 Taejeon, Korea
[4] Hahn-Meitner-Institute, SF-2, 14109 Berlin, Germany
[5] Institute of Metal Physics, 620219 Ekaterinburg, Russia
[6] Joint Institute for Nuclear Research, 141980 Dubna, Russia

Neutron diffraction measurements were carried out in order to study the spontaneous and induced spin-reorientation transitions of the "easy axis-easy plane" type in the poly- and single-crystalline samples of the Tm_2Fe_{17} compound. The temperature dependencies of the orientations and the values of the Tm- and Fe-ion magnetization were determined. The large magnetization anisotropy of Tm-ion magnetization was observed. Using for Tm_2Fe_{17} the two-sublattice model we have estimated the values of the magnetic crystallographic anisotropy constants of Tm- and Fe-sublattices.

B-86 Neutron diffraction investigation of the metamagnetic transition in $ErCo_2$

A. Podlesnyak[1,2], A. Mirmelstein[2], A. Pirogov[2], A. Teplykh[2], Th. Strässle[1], A. Furrer[1], A. Ermakov[3],
[1] Laboratory for Neutron Scattering, ETH Zürich & Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland
[2] Institute for Metal Physics RAS, 620219 Ekaterinburg GSP-170, Russia
[3] Ural State University, 620083 Ekaterinburg, Russia

In contrast to other Laves phase compounds, in which the d-electron subsystem is either non-magnetic ($LnNi_2$) or bears a stable magnetic moment ($LnFe_2$), $LnCo_2$ exhibits an intermediate behavior and undergoes a metamagnetic transition. Surprisingly, very few data on $LnCo_2$ by means of neutron scattering have been published so far, although in many cases the determination of the magnetization by neutron diffraction techniques is invaluable in the interpretation of the bulk phenomena. Neutron diffraction was employed to study the magnetic state of the $ErCo_2$ as a function of temperature and external magnetic field in the paramagnetic state. The metamagnetic transition has been confirmed directly with magnetization values 6.0(5) and 0.57(9) μ_B for the Er and Co sublattices, respectively.

B-87 Investigation of Atomic Ordering in Fe-Cr-Co Alloys

B. E. Vintaikin[1], E. Z. Vintaikin[2], K. Mikke[3], J. J. Milczarek[3], J. Jankowska-Kisieliñska[3],
[1] Bauman State Technical University, Moscow, Russia
[2] Institute of Physical Metallurgy, Moscow, Russia
[3] Institute of Atomic Energy, Swierk, Poland

Neutron diffraction study of atomic ordering in hard magnetic Fe-Cr-Co alloys was performed. High coercivity in these alloys is achieved by spinodal decomposition into ferromagnetic and paramagnetic phase. Elastic neutron scattering at (100) and (200) rlp allowed to determine the long range ordering in the ferromagnetic phase. The formation of the B2-type LRO at temperatures from 770 K to 920 K was investigated. It was shown that the B2-type LRO is formed at 770 K for Co concentrations higher than 16 at.% and that this feature was only weakly affected by increase of Cr concentration. At lower Co concentration only the SRO is observed at 770 K.

B-88 Effect of magnetic field on the itinerant Co-subsystem in $Ho_{0.423}Y_{0.577}Co_2$

A. A. Yermakov[1], R. Schneider[2], N. V. Baranov[1],
[1] Institute of physics & applied mathematics, Ural State University, 620083, Ekaterinburg, Russia
[2] Hahn-Meitner-Institute, BENSC, D-14109, Berlin, Germany

The rare earth intermetallic compounds $Ho_{1-x}Y_xCo_2$ belong to the Laves phases and have two interacting subsystems: the itinerant d-electrons of cobalt and the localized 4f-moments of rare earth metal. The Co-subsystem exhibits the properties of an itinerant metamagnet. The magnetic state of the d-electron subsystem is determined by the effective molecular field acting from rare earth atoms. As it is suggested the small external field produces an ordering effect on the R - subsystem of the compound with the Y-content just below x_c (0.58). It is found that the application of the small magnetic field enhances significantly the intensity of Bragg reflections and depresses the intensity of diffuse scattering in $Ho_{0.423}Y_{0.577}Co_2$. This behavior results from the metamagnetic transition in the itinerant d-band and magnetization growth of both R- and Co-subsystems.

B-89 Sublattice magnetisations in $ErCo_3$

E. Gratz[1], A. Markosyan[2], V. Paul-Boncour[3], A. Hoser[4], I. Gaidukova[2], V. Rodimin[2],
[1] Institute for Experimental Physics, T.U. Vienna, 1040 Wien, Wiedner Haupstrasse 8-10, Austria
[2] Faculty of Physics, M.V. Lomonosov MSU, Moscow, Russia
[3] LCMTR, CNRS, 94320 Thiais, France

[4] Forschungszentrum, Jülich, IFF, Germany
Measurements of the thermal expansion of ferrimagnetic $ErCo_3$ (T_C=401K) revealed an anomaly in the range of 60 to 80K. Interestingly no anomalous change was found in the temperature variation of the bulk magnetisation M. In order to understand the origin of the volume anomaly neutron diffraction studies were performed at the E6 diffractometer at HMI Berlin. The neutron data revealed that the Er-sublattice magnetisation M_{Er} decreases drastically above 80K, which causes also a decrease of the Co-sublattice magnetisation M_{Co}. This temperature induced reduction of the Co magnetisation is connected with the observed decrease of the unit cell volume ($\delta V/V = 0.3$ %). However due to the antiparallel alignment, M_{Er} and M_{Co} compensate and thus smooth the temperature variation of M. This work was supported by RFBR (project 00-02-17844) and TU Vienna, Austria.

B-90 Magnetic structures of $TmCu_2$

A. Kreyssig[1], H. Schneider[2], A. Schneidewind[1], C. Ritter[3], O. Isnard[3], G. Behr[4], M. Loewenhaupt[1],
[1] Technische Universität Dresden, Institut für Angewandte Physik (IAPD), D-01062 Dresden, Germany
[2] Technische Universität München, FRM-II, D-85747 Garching, Germany
[3] Institut Laue-Langevin, BP 156, F-38042 Grenoble, France
[4] Institut für Festkörper- und Werkstofforschung Dresden, Postbox 270116, D-01171 Dresden, Germany
$TmCu_2$ with the orthorhombic $CeCu_2$ structure shows three different magnetic structures: AF1 for $T \leq$3.1K, AF2 for 3.1K$<T\leq$4.4K and AF3 for 4.4 K $< T \leq T_N$ = 6.4 K. Neutron diffraction experiments on polycrystalline samples were carried out on D1B and D2B (ILL Grenoble) to determine the temperature dependence of the magnetic order and to characterize the three magnetic structures. In contrast to the commensurate propagation vector along *a*-axis for the phase AF1, the propagation vectors for AF2 and AF3 are incommensurate with additional small components along the *c*-axis and the *b*-axis, respectively.

B-91 Crystal field effects in $RAgSb_2$ intermetallic compounds (R=Tm, Ho, Er)

I. Sashin[1], A. Szytula[2], E. Goremychkin[3],
[1] Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research
[2] Institute of Physics Jagellonian University
[3] IPNS, Argonne National Laboratory
The influence of crystal field is an important source of magneto-crystalline anisotropy and in order to explain the differences in the magnetic structures of the tetragonal $RAgSb_2$(R=Ho,Er,Tm) compounds we have carried out investigation of the crystal field potential in these compounds by inelastic neutron scattering on the time-of-flight spectrometer KDSOG-M at the pulsed reactor IBR-2, Dubna, Russia. The crystal field parameters and corresponding level scheme have been determined from profile refinement of the neutron spactra. The anisotropic single crystal magnetic susceptibility and specific heat data can be described well with the crystal field potential determined from the neutron scattering spectra.

B-92 Magnetic order in RAuIn (R=Tb, Dy, Ho) compounds

M. Kolenda[1], B. Penc[1], N. Stüsser[2], A. Szytula[1], A. Zygmunt[3],
[1] Institute of Physics, Jagellonian University, 30-059 Krakow, Poland
[2] BENSC, Hahn-Meitner Institute, D-14109 Berlin-Wannsee, Germany
[3] Institute of Low Temperatures and Structural Research, PAS, 50-950 Wroclaw, Poland
Neutron diffraction data indicate that above the Neel temperatures equal to 51 K for R=Tb, 11 K for R=Dy and 5.1 for R=Ho these RAuIn comounds crystallizes in the hexagonal ZrNiAl-type of crystal structure. In the case of the TbAuIn compound below T_N an additional phase transition connected with the change of the magnetic structure is observed. In low temperatures magnetic orderings of TbAuIn and DyAuIn are similar to those observed in isostructural TbPdIn and DyPdIn [1]. For TbAuIn above T_t equal to 3.7 K a change of the magnetic structure to the sine-wave modulated is observed. For HoAuIn below T equal to 5.1 K the diffusion peaks of the magnetic origin are observed. [1] P. Javorsky at al., Mater. Sci. Forum 321-4 (1999) 705

B-93 Neutron diffraction study of CePtSn

B. Janousová[1], P. Svoboda[1], V. Sechovsky[1], K. Prokes[2,1], I. Cisarova[3],
[1] Charles Univ., Dept. of El. Structures, 121 16 Prague 2, Czech Rep.
[2] BENSC, HMI, D-14109 Berlin, Germany
[3] Charles Univ., Dept. of Inorg. Chem., 128 43 Prague 2, Czech Rep.

The orthorhombic CePtSn exhibits two antiferromagnetic (AF) transitions at $T_N = 7.8$ K and $T_M = 5.2$ K. The neutron and X-ray diffraction reveal the space group of its structure to be centrosymmetric $Pnma$, contrary to the previously reported non-centrosymmetric ε-TiNiSi-type structure. Our neutron diffraction data support the proposed "spin-slip" magnetic structure with basic propagation vector $\mathbf{q} = (0, 1/2, 0)$ and sample dependent spin-slips resulting in different observed propagation vectors. In contradiction to previous neutron diffraction study of CePtSn, we have found the coexistence of the two propagation vectors $q_1 = (0, 0.422, 0)$ and $q_2 = (0, 0.47, 0)$ below T_M while only q_2 exists between T_N and T_M.

B-94 Internal Magnetic Structure of Mn12-actetate

R. A. Robinson[1], P. J. Brown[2], D. N. Argyriou[1], D. N. Hendrickson[3], S. M. J. Aubin[3], G. Christou[4],
[1] Los Alamos National Laboratory, Los Alamos, NM 87545, USA
[2] Institut Laue Langevin, Grenoble, France
[3] University of California San Diego, La Jolla, CA 92093, USA
[4] University of Indiana, Bloomington, IN 47405, USA

The internal magnetic structure of $[Mn_{12}O_{12}(CD_3COO)_{16}(H_2O)_4].2CD_3COOH.4H_2O$ as determined by polarised-beam single-crystal neutron diffraction is reported. The standard picture, in which the inner tetrahedron of (S = 3/2) Mn^{4+} ions is polarised antiparallel to an outer ring of eight (S = 4) Mn^{3+} ions, is confirmed directly. While the total magnetisation for the molecule is in good agreement with bulk measurements, the individual moment components on each of the three symmetry-independent Mn sites are less than predicted by the standard picture. There is no evidence for net moments on the oxygen atoms, but overlap of positive and negative magnetisation on the oxygen sites cannot be ruled out. The results are compared with recent theoretical calculations.

B-95 Crystal Distortion and Magnetic Structure of γ-MnPt Alloys

T. Hori[1], Y. Tsuchiya[2], H. Shiraishi[1], Y. Ishii[3,4], K. Hojou[4],
[1] Shibaura Institute of Technology, Oomiya 330-8570, Japan
[2] Department of Fusion Engineering Research, Japan Atomic Energy Reseach Institute, Naka-machi 319-0193, Japan
[3] Advanced Science Research Center, Japan Atomic Energy Research Institute, Tokai, Ibaraki 319-1195, Japan
[4] Department of Materials Science, Japan Atomic Energy Reseach Institute, Tokai 319-1195, Japan

As is well known, most Mn-rich γ-Mn alloys undergo a distortion from the face centered cubic structure to a face centered tetragonal (f.c.t.) structure with $c/a < 1$ below the Néel temperature. We have found that there are the f.c.o. region and the f.c.t. region with $c/a > 1$ in γ-MnPt alloys. Neutron diffraction experiments have been made by a diffractometer installed at the JRR-3M reactor at JAERI. We determined that the γ-Mn alloy with 8 at% Pt shows the f.c.o. structure and the non-collinear antiferromagnetic structure below 420 K.

B-96 Magnetic structures of Er_6Ni_2Sn

O. Syshchenko[1], V. Sechovsky[1], K. Prokes[2], M. Hofmann[2],
[1] Department of Electronic Structures, Charles University, 121 16 Praha 2, The Czech Republic
[2] Hahn-Meitner-Institute, SF-2, D-141 09, Berlin, Germany

Er_6Ni_2Sn is one of the rare-earth (RE) RE_6Ni_2Sn intermetallics that crystallize in the orthorhombic Ho_6Ni_2Ga -type structure. Anomalies observed in Er_6Ni_2Sn bulk properties (temperature dependence of magnetization, AC susceptibility, specific heat and electrical resistivity) indicate magnetic phase transitions at 35 (T_N), 17 and 7 K, respectively. The magnetization curves measured at various temperatures below 35 K are suggestive of antiferromagnetic ordering at low temperatures. We performed a neutron diffraction study of this compound at various representative temperatures between 1.7 and 50 K in order to elucidate different magnetic phases on microscopic scale. The results suggest a propagation vector q = (0,0,0) for all magnetic structures of this compound below T_N. While the magnetic structure between T_N and 17 K is body centered, that one below 17 K is primitive. No transition at 7 K has been detected in the neutron diffraction experiment.

B-97 TOF Neutron Diffraction and Rietveld Refinement of Crystal and Magnetic Structures of $Tb_{1-x}R_xCu_2$

A. Schneidewind[1], W. Kockelmann[2], G. Behr[3], A. Kreyssig[1], M. Loewenhaupt[1]
[1] TU Dresden, Institut für Angewandte Physik (IAPD), D-01062 Dresden, Germany
[2] Universität Bonn, Mineralogisch-Petrologisches Institut, Poppelsdorfer Schloss, D-53115 Bonn, Germany
[3] IFW Dresden, POB 270116, D-01171 Dresden, Germany

RCu_2 compounds (R = rare earths excluding La) crystallize in the $CeCu_2$ structure which can also be described as distorted AlB_2 structure. To study the relations between crystal and magnetic structures in detail we have performed TOF neutron powder diffraction on $Tb_{1-x}R_xCu_2$ containing magnetic (Dy) and non-magnetic (Pr, Y) atoms on the rare earth sites. The mixed compounds crystallize in the same structure as the pure RCu_2. The R atoms are randomly distributed on the 4e sites. The most sensitive lattice parameter on the variation of x is found to be b. The same type of magnetic ordering as in $TbCu_2$ is observed. A broadening of the reflections according to the third harmonic of the wave vector is observed.

B-98 Magnetic ordering of Er and Co sublattices in $Er_{1-x}Y_xCo_2$ studied by neutron diffraction

A. Kolomiets[1], H. Nakotte[2], V. Sechovsky[1], L. DeLong[3],
[1] Charles University, Prague, Czech Rep.
[2] New Mexico State University, Las Cruzes, USA
[3] University of Kentucky, Lexington, USA

$ErCo_2$ is a C15 cubic Laves-phase intermetallic with itinerant electron magnetism (IEM) in the Co sublattice. When $ErCo_2$ is diluted with 40% of Y, the 1st order ferromagnetic phase transition is split into two. This was assigned to the separate ordering in Er and Co sublattices [1]: first order the Er moments, and then the IEM transition in Co sublattice takes place. Here we present an alternative point of view based on the neutron diffraction performed on $ErCo_2$ and $Er_{0.6}Y_{0.4}Co_2$. We tend to ascribe each transition temperature to magnetic ordering of clusters with a characteristic mean Er-Y composition. [1] R. Hauser, et al., Phys. Rev B, 62 (2000) 1198.

B-99 Magnetic domain structure in polycrystalline Fe

V. Wagner[1], D. Bellmann[2],
[1] Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany
[2] GKSS Research Centre GmbH, 21502 Geesthacht, Germany

The magnetic domain structure in a polycrystalline Fe foil was observed by 3-dimensional Depolarization Analysis (NDA) of transmitted neutrons (λ = 0.15 nm). The sample consisted of rolled foil of high impurity Fe (25 microns thick), which displayed a small coercive field. By NDA the mean domain size and the magnetic texture as well as the bulk magnetization were followed along a complete magnetization loop. In the virgin state the sample was magneticlly isotropic with domain size of about 1 micron. The domain size distribution in the virgin state was determined in an alternative way using Ultra Small-Angle Neutron Scattering (λ = 0.44 nm) at the DCD of the Geesthacht Neutron Facility.

B-100 Magnetic correlations in $(Nb_{1-y}Fe_{2+y})$

P. M. Bentley[1], R. Cywinski[1], J. R. Stewart[2],
[1] Department of Physics and Astronomy, University of Leeds, Leeds LS2 9JT, England
[2] Institut Laue Langevin, B.P.156, 38042 Grenoble, Cedex 9, France

The C14 Laves phase compound $(Nb_{1-y}Fe_{2+y})$ has extremely weak itinerant Fe moments with competing ferro- and antiferromagnetic correlations co-existing on a potentially frustrated 2d Kagome net-like structure. Stoichiometric ($NbFe_2$) is antiferromagnetic below (T_N)=18K, although ferromagnetism can be induced by weak external fields of $\sim$0.4T or by excursions to either side of stoichiometry for y$> +0.005$ or y< -0.005 [1]. We report a SANS study of the evolution of ferromagnetic correlations with temperature and concentration in $(Nb_{1-y}Fe_{2+y})$. The SANS data follows a Lorentzian plus squared Lorentzian function. There is little evidence of well-defined critical scattering at the reported Curie points of the alloys, and a modest increase in the correlation range close to (T_c) is observed only for y<0. The correlation range never exceeds 8nm implying an essentially inhomogeneous or clustered ferromagnetic state. [1] M R Crook and R Cywinski, J. Mag. Magn. Mater, 140-144 (1994) 71

B-101 On the magnetic structures of holmium-erbium alloys

H. M. Ronnow[1], J. Jensen[2], D. F. McMorrow[3],
[1] DRFMC, CEA Grenoble, France
[2] Orsted Laboratory, University of Copenhagen, Denmark
[3] Materials Research Department, Risø National Laboratory, Denmark

The two rare earth metals holmium and erbium have similar exchange interactions but opposite sign of the crystal-field parameters, which upon alloying the two elements leads to a remarkably complex phase diagram with a pentacritical point. The competing crystal fields are also responsible for a very unusual disordered isotropic phase completely surrounded by ordered phases. We have performed a neutron scattering investigation of the magnetic structures in two single-crystal Ho/Er alloys with respectively 10% and 50% holmium content. The results are compared to mean-field calculations in the virtual-crystal approximation with parameters given by the detailed models that exist for pure holmium and erbium respectively. The possibly most notable observation is that the 10% sample at low temperatures exhibits a broadening of the magnetic Bragg reflections. We demonstrate that the system has a single well-defined modulation vector 7/36, but with local disorder where blocks of 3/36 and 4/36 follow each other in a random sequence.

B-102 Intra- and inter-multiplet neutron transitions in an Fe_4 magnetic cluster

G. Amoretti[1], R. Caciuffo[2], S. Carretta[1], A. Cornia[3], D. Gatteschi[4], E. Liviotti[1],
[1] INFM, Universita di Parma, 43100 Parma, Italy
[2] INFM, Universita di Ancona, 60131 Ancona, Italy
[3] Universita di Modena, 41100 Modena, Italy
[4] Universita di Firenze, 50144 Firenze, Italy

We report the results of neutron spectroscopy for a tetranuclear Iron cluster, $Fe_4(OCH_3)_6(dpm)_6$, having an $S = 5$ spin ground-state [1]. The experiments were carried out on a deuterated powder sample at the ILL, in Grenoble. The transitions within the ground multiplet, below $0.3meV$, were measured with a high-resolution TOF spectrometer. Taking into account the presence of three different isomers, the parameters of the ZFS Hamiltonian have been determined. The results are discussed with reference to high-field EPR data [2]. A non-dispersive peak at $7.8meV$, detected at $T = 1.4K$ using a 3-axis spectrometer with polarisation analysis, is interpreted as the transition between the $S = 5$ ground state and the two degenerate $S = 4$ excited multiplets. The Q dependence of the cross-section is discussed in comparison with theoretical models. [1] A.L. Barra et al., J. Am. Chem. Soc. **121**, 5302 (1999). [2] A. Bouwen et al., J. Phys. Chem. B **105**,2658 (2001).

B-103 On the magnetic structure of $RbNiF_3$

K. Krezhov[1],
[1] Institute for Nuclear Research and Nuclear Energy, Bulgarian Academy of Sciences,72 Tzarigradsko chaussee, BU-1784 Sofia, Bulgaria

In contrast to the large majority of other ABX_3 compounds being orthorhombic the transparent magnetodielectric $RbNiF_3$ (T_c = 133 K, S.G. $P6_3/mmc$) is a representative of a much smaller group of halcogenides with hexagonal crystal symmetry. In this study results from the full profile analysis (FullProf code) of powder neutron diffraction patterns taken at different temperatures both above and below T_c are presented. The sets of positional, thermal and lattice parameters at RT and 150 K are compared. The magnetic structure determination is based on the 4.2 K pattern. The

discussion takes into account models with two, three and four magnetic sublattices tested for description of the magnetic structure. The temperature dependence of the nearly pure magnetic reflection (002) has been measured and used for comparison with the corresponding curve reconstructed from the sublattices magnetization calculated in the frames of mean field theoretical models

B-104 Evidence for boron-carbon disorder in $YNi_2{}^{10}B_2C$.

A.D. Hillier[1], R.I. Smith[1], W.I.F. David[1], R. Cywinski[2],
[1] ISIS Facility, Rutherford Appleton Laboratory, Chilton, Oxon, OX11 0QX, U.K.
[2] Physics and Astronomy Department, University of Leeds, Leeds, LS2 9JT, U.K.

There has been a tremendous interest in the RNi_2B_2C (R=rare earth or Y) family of superconductors since their discovery. This results partly from their relatively high superconducting transition temperature and partly from the opportunities they offer for the study of the coexistence of superconductivity and long range magnetic order. The compounds crystallise with a modified $ThCr_2Si_2$ structure (I4/mmm) with C occupying the interstitial (0,0,1/2) site. Several authors have reported a marked sensitivity of the electronic properties of the RNi_2B_2C compounds to thermal treatment and it has been suggested that boron-carbon site disorder may be responsible for the observed behaviour. Whilst natural B and C have similar neutron and X-ray scattering lengths, and the low absorption ^{11}B isotope has precisely the same neutron scattering length as C. However, that of the highly absorbing ^{10}B is significantly different from that of C. We have therefore used pulsed neutron time of flight diffraction to study a sample of isotopically enriched $YNi_2{}^{10}B_2C$. Rietveld refinement of the resulting diffraction pattern indeed confirms that the B-C disorder may be as high as 10% in these compounds. The results of the structure refinement will be presented.

B-105 Antiferromagnetic phase transitions of spinels, $Zn_{1-x}Cu_xCr_2Se_4$; x=0.50 and 0.60

M. Hidaka[1], N. Tokiwa[1], T. Wai[1], H. Fujii[2], M. Mito[3], K. Takeda[3],
[1] Department of Physics, Faculty of Sciences, Kyushu University, Fukuoka 812-8581, Japan
[2] Department of Physics, Faculty of Education, Oita University, Oita 870-1192, Japan
[3] Department of Applied Quantum Physics,Faculty of Engineering,Kyushu University,Fukuoka 812-8581, Japan

Magnetic and crystallographic properties have been studied by neutron powder diffraction and of magnetizations for spinels $Zn_{1-x}Cu_xCr_2Se_4$ with x=0.50 and 0.60. It is found that the spinels of x=0.50 and 0.60 show the antiferromagnetic phase transition at about 24 K and 28K (T_N), respectively, in addition to a ferromagnetic phase transition at about 420 K. These spinels show the satellite-like magnetic reflections having an indexes of (h q, k,l);q=0.47 below T_N and the short range order of spins (spin glass-like) above T_N.

B-106 Neutron diffraction studies of $R_5Rh_4Ge_{10}$ (R=Tb,Ho,Er)

M. Kolenda[1], M. Hofmann[2], J. Leciejewicz[3], B. Penc[1], A. Szytula[1],
[1] Institute of Physics, Jagiellonian University, 30-059 Krakw, Poland
[2] BENSC Hahn-Meitner Institute D-14109 Berlin-Wannsee, Germany
[3] Institute of Nuclear Chemistry and Technology 03-169 Warszawa, Poland

Neutron diffraction patterns recorded in the paramagnetic state confirmed that $R_5Rh_4Ge_{10}$ (R=Tb,Ho,Er) compounds exhibit the tetragonal $Sc_5Co_4Si_{10}$ (P4/mbm space group)-type crystal structure. In this structure rare earth atoms R occupy three nonequivalent atomic positions. The low temperature neutron diffraction data confirm the change of the magnetic structure at T_t=3.8, and at the Néel temperature T_N=11.5 K for R=Tb, at T_N=7 K for R=Ho, and at T_t=4.2 K and T_N=5.5 K for R=Er. Low temperatures data indicate that in all these compounds the rare earth atoms form complex antiferromagnetic structures: collinear in the case of Tb- and Ho- compounds, sine modulated for $Er_5Rh_4Ge_{10}$ with the vave vector k=(1/4,1/4,0) for 1.5 K<T<4.2 K and (1/3,1/3,0) for 4.2 K up to T_N. The magnetic moment values are different in different sublattices.

B-107 Evolution of magnetic structures in UNi_2Si_2 – UPd_2Si_2 system

J. Vejpravova[1], P. Svoboda[1], V. Sechovsky[1], C. Ritter[2],
[1] Charles Univ., Dept. of Electronic Struct., 121 16 Prague 2, The Czech Republic
[2] ILL, 38042 Grenoble, France

The influence of Pd–Ni substitution on the formation of magnetic phases in the tetragonal $U(Ni_{1-x},Pd_x)_2Si_2$ system and concentration magnetic phase diagram are presented. The series of different substitutions was prepared and detailed studies by powder neutron diffraction were performed for x=0.25, 0.5 and 0.75. All compounds order antiferromagnetically, form ferromagnetic basal planes stacked along *c*-axis (q = (0 0 q_z) propagation). The ground-state phase (AF3) of UNi_2Si_2 is an uncompensated AF structure (+ + − stacking, (q_z=2/3)). In $UPd_2Si_2$the ground-state phase corresponds to the simple AF structure – AF2 (+ − + − ($q_z = 1$)). In Pd–Ni compounds, no traces of the AF3 phase were found already for x=0.25. The ground-state powder patterns correspond to AF2 for x≥ 0.25.

B-108 Magnetic Properties of $(Mn_{1-x}Ru_x)_3Ga$ Alloys

T. Hori[1], M. Akimitsu[1], H. Miki[2], K. Ohyama[2], Y. Yamaguchi[2],
[1] Shibaura Institute of Technology, Oomiya 330-8570, Japan
[2] Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan

We have found that the alloys $(Mn_{1-X}Ru_X)_3Ga$ with $0.33 \leq x \leq 0.67$ have an ordered b.c.c. structure. The alloy with $x = 0.33$ i.e. Mn_2RuGa shows a ferromagnetism; the saturation magnetization extrapolated to 0 K is 24 emu/g, and the Curie temperature is 460 K. The Curie temperature of $(Mn_{1-X}Ru_X)_3Ga$ decreases almost linearly with increasing *x*, and vanishes around $x = 0.67$ ($MnRu_2Ga$). We have made neutron diffraction experiments using a powder sample of Mn_2RuGa, and found that the alloy has an ordered atructure of $CuHg_2Ti$ type. The magnetic Mn atoms occupy the 4a (0,0,0) and 4d (3/4,3/4,3/4) sites. It may be considered that the magnetic moments of Mn atoms on the 4a and 4d sites are antiparallel to each other.

B-109 Incommensurate-commensurate phase transition in the frustrated antiferromagnet $CsCuCl_3$

A. Hoser[1,2], N. Stüßer[1], U. Schotte[1], M. Meschke[1], M. Meißner[1],
[1] Hahn-Meitner Institut, Glienicker Str.100, 14109 Berlin, Germany
[2] Institut für Kristallographie, RWTH-Aachen, 52056 Aachen, Germany

In zero field the spin 1/2 moments of the Cu^{+2}-ion in the hexagonal perovskite $CsCuCl_3$ form a helical spin structure along the c-axis and a 120°

structure on the triangular lattice in the a-b plane. It was shown in the past that quantum and thermal fluctuations have large effects on the magnetic structure in magnetic fields, lifting the degeneracy caused by frustration. Here we present new results of our successful neutron diffraction work performed in order to study the IC-C phase transition occurring at 2 Kelvin at about 16 Tesla with the field applied in the a-b plane. For these experiments the 14.5 Tesla superconducting magnet VM1 of BENSC and a Dy-booster was used to get fields up to 17 Tesla.

B-110 Magnetic Field Induced Phase Transition in $Ce_2Fe_{17-x}Mn_x$ Compounds

A. Teplykh[1], A. Pirogov[1], A. Kuchin[1], O. Prokhnenko[2,3], C. Ritter[3], Z. Arnold[2], O. Isnard[4],
[1] Institute for Metal Physics, S.Kovalevskaya 18, Ekaterinburg, 620219 Russia.
[2] Institute of Physics AS CR, Cukrovarnicka 10, 16253 Prague 6, Czech Republic
[3] Institute Laue Langevin, BP 156, 38042 Grenoble Cedex 9, France
[4] Laboratoire de Cristallographie, CNRS, BP 166, 38042 Grenoble cedex 9, France.

Neutron diffraction technique was used to investigate the atomic and magnetic structure of the $Ce_2Fe_{17-x}Mn_x$ compounds with x=0.5 and 1.0 under magnetic field up to 1.2 T over the temperature range 2-300 K. The magnetic reflexes observed at temperatures 2-208 K and H=0 T for x - 0.5 correspond to an incommensurate helical antiferromagnetic structure [1] with wave vector is 0.034 $Å^{-1}$ at 2 K. This structure is suppressed in an external magnetic field and a ferromagnetic phase in fields higher than 0.6 T is induced in agreement with the earlier made assumption [2]. In the contribution the complex transformation of the magnetic structures under magnetic field and temperature is analysed and discussed. The work was partially supported by SSTP (No 107-19 (00) -P-DO1) and RFBR (grant No 99-02-16395). [1] D.Givord, R.Lemaire, IEEE Trans. Magn. Mag-10. 109 (1974) [2] A.G.Kuchin et al., J.All.Com. , 313 , (2000), p. 7-12

B-111 An Influence of Magnetic State on Phonons and Martensitic Transformation in the γ-$Fe_{72}Ni_6Mn_{22}$ Alloy.

Y. Mikhailov[1] , S. Dubinin[1],
[1] Institute of Metal Physics, S. Kovalevskoi Str.18, Ekaterinburg, 620219 Russia.

Dispersion curves of phonons were measured at T=340K in single crystal of the antiferromagnetic γ-$Fe_{72}Ni_6Mn_{22}$ alloy (T_n=358K), which was undergoing martensitic transformation γ to ϵ (M_s=320K). The obtained results were compared with the earlier known dispersion curves of phonons in ferromagnetic γ-Fe_xNi_{1-x} (x=0.65; 0.70) and antiferromagnetic γ-$Fe_{70}Mn_{30}$ alloys near γ to α and γ to ϵ transformations, respectively. The considerable differences in longitudinal and transverse dispersion curves of phonons are observed before martensitic transformations of various types, they take place in the alloys with magnetic orders which differ one from another. We suppose that such behaviour of dispersion curves of phonons happens because of different magnetic orders and a certain extent of inhomogeneity of magnetic structures, which are the consequence of competing exchange interaction in these magnetics.

B-112 Magnetic diffuse scattering Tb

R. P. Schneider[1,2], T. Chatterji[2], J.-U. Hoffmann[1,2], D. Hohlwein[1,2],
[1] Institut für Kristallographie, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany
[2] Dept. SF2, Hahn-Meitner Institut Berlin, Glienicker Str. 100, 14109 Berlin, Germany
[3] Institut Laue-Langevin, Grenoble, France

Rare earth metal terbium exhibits very large magnetic moments localised on a hexagonal lattice with high crystal field anisotropy. Below the N'eel-point $T_N = 228$K an incommensurate helical magnetic structure stabilises which transforms into a ferromagnetic one below $T_C = 218$ K. Using the Flat-Cone diffractometer E2 at BENSC it is possible to obtain scattering distributions within complete planes of reciprocal space. Diffuse scattering intensity in the (hol) plane was observed at several temperatures within the ferromagnetic, helical and paramagnetic phase. An extended molecular field theory was fitted to the experimental diffuse scattering data yielding information about the magnetic exchange interactions. In all three phases we found a long-ranged interaction of RKKY-type mediated by the conduction electrons.

B-113 Critical Scattering Studies of $CsCo_{0.83}Mg_{0.17}Br_3$: An Intrinsic Random Field State

J. van Duijn[1], D.B. Gaulin[1], W.J.L Buyers[2], M.A. Lumsden[1],
[1] Department of Physics and Atronomy, McMaster University, Hamilton, ON, L8S 4M1, Canada
[2] NPMR, NRC, Chalk River, ON, K0J 1J0, Canada

We have performed critical neutron scattering studies on $CsCo_{0.83}Mg_{0.17}Br_3$, a dilute, stacked-triangular lattice, Ising-like antiferromagnet. Its parent compound, $CsCoBr_3$, displays two magnetic phase transitions, at 28 and 14 K. The high temperature transition is to a partially-paramagnetic, three-sublattice Neel state, ordered in an up-down-paramagnetic spin arrangement. Our studies on single crystal $CsCo_{0.83}Mg_{0.17}Br_3$ show the onset at 28 K of a two component lineshape. The two components are attributed to an intrinsic random field state, generated by the presence of quenched non-magnetic Mg impurities imbedded in the partially-paramagnetic Neel state. At temperatures below 15 K, the sharp component dominates the broad, and the scattering at the ordering wavevectors continues to evolve to temperatures as low as 4 K

B-114 Magnetic interactions and Onsager reaction field from paramagnetic-diffuse neutron scattering

D. Hohlwein[1,2],
[1] Institute of Crystallography, University Tübingen, 72076 Tübingen, Germany
[2] Hahn-Meitner-Institut, BENSC, 14109 Berlin

Magnetic interactions in solids are mostly determined from magnon dispersion curves within the ordered phase. If there is no long-range ordering or if the interaction parameters change with temperature, the magnetic interactions have to be deduced from the diffuse scattering. The magnetic-diffuse scattering is proportional to the q-dependent susceptibility. At high temperature the susceptibility can be described with a mean-field theory using interaction parameters. At lower temperatures the theory has to be modified. We used an additional parameter f , for the Onsager reaction field, to describe the diffuse intensity distribution. The possibility to determine the interaction parameters as well as f is shown for the model system MnF_2. Diffuse intensity distributions in the (h0l) layer have been measured as a function of temperature with the Flat-cone diffractometer E2 at the Berlin reactor. The Onsager parameter f can also be calculated by a Fourier transformation of the diffuse intensity distribution. We show that this parameter correctly describes the deviation from the mean-field theory in the temperature range from $T_N + 3$ K up to 2.4 T_N.

B-115 Anomalous critical scattering from a three-dimensional percolating antiferromagnet, $RbMn_{0.31}Mg_{0.69}F_3$

S. Itoh[1], K. Iwasa[2], H. Ikeda[1], M. Bull[3],
[1] Neutron Science Laboratory, High Energy Accelerator Research Organization, Tsukuba, 305-0801, Japan
[2] Department of Physics, Tokyo Metropolitan University, Hachioji, Tokyo, 192-0397, Japan
[3] ISIS Facility, Rutherford Appleton Laboratory, Didcot, Oxon, OX11 0QX, UK

We performed a neutron diffraction experiment to measure critical scattering from the three-dimensional percolating antiferromagnet, $RbMn_{0.31}Mg_{0.69}F_3$, whose magnetic concentration is just at the percolation concentration for a cubic lattice, $c_p = 0.312$. The magnetic scattering was observed at around the superlattice point, (1/2,1/2,1/2). We found that the scattering function exhibits a non-Lorentzian lineshape, $S(q) = (q^2 + \kappa^2)^{-x}$, with the exponent of $x = 0.6 \pm 0.1$ at the low temperature of 1.6 K, and that the exponent is attributed to the fractal structure of the percolating network.

B-116 Lattice anomalies in unstable valence compound CeNi

V.N. Lazukov[1], E.V. Nefeodova[1], V.V. Sikolenko[2], U. Staub[3], P.A. Alekseev[1], M. Braden[4], K.S. Nemkovski[1], C. Pradrvand[3], I.P. Sadikov[1], L. Soderholm[5], N.N. Tiden[1],
[1] RRC, "Kurchatov Institute", 123182 Moscow, Russia
[2] JINR, Dubna, Moscow region, Russia
[3] SLS, PSI, Switzerland
[4] LLB, CEA/Saclay, France, INFP Karlsruhe, Germany
[5] Chemistry Division, Argonne National Laboratory, USA

Measurements of CeNi structural parameters by neutron diffraction as well as Ce valence by X-ray absorption spectroscopy at temperatures 10 K - 295 K have been performed. No evidence of a phase transition was observed, but some nearest neighbor distances between ions have clear peculiarities in the temperature range 100 K - 150 K. The valence of Ce is changed smoothly with temperature and could not result in this effect as well as the nonmonotonic phonon frequency temperature dependence. An influence of spin correlation in Ce sublattice and gap-like magnetic excitation spectrum developed at low temperatures on lattice parameters is discussed.

B-117 Yb-ion correlations and crystal field in Kondo-insulator YbB_{12}

P.A. Alekseev[1], J.-M. Mignot[2], K.S. Nemkovski[1], N.Yu. Shitsevalova[3], R.I. Bewley[4], R.S. Eccleston[4], E.S. Clementyev[1], V.N. Lazukov[1], E.V. Nefeodova[1], I.P. Sadikov[1], N.N. Tiden[1],
[1] RRC "Kurchatov Institute", 123182 Moscow, Russian Federation
[2] LLB, CEA/Saclay, F-91191 Gif sur Yvette, France
[3] IPM NASU, 252142 Kiev, Ukraine
[4] ISIS, RAL, Didcot, Oxon, OX110QX, UK

The influence of the coherence breakdown in the Yb sublattice on the excitation spectra of the YbB_{12} -based systems and characteristics of the crystal field potential have been studied by the inelastic neutron scattering on $Yb_{1-x}Lu_xB_{12}$ and $Yb_{0.9}Er_{0.1}B_{12}$ samples. The spectral shape was considerably changed in the near-gap region due to Lu substitution with respect to the pure YbB_{12}. The crystal field potential has been determined by use of the Er^{3+} ions as a sensor. The possible splitting of Yb^{3+} multiplet due to crystal field appears to be comparable with the gap energy, as well as with the Kondo temperature and energy of the only inelastic peak in YbB_{12} spectra at $T>T_{Kondo}$

B-118 Crystal field-phonon coupling in the Kondo lattice $CeCu_2$

U. Witte[1,2], S. Kramp[1], M. Braden[3], P. Svoboda[4], M, Loewenhaupt[1],
[1] TU Dresden, IAPD, D-01062 Dresden
[2] HMI Berlin, Glienicker Str. 100, D-14109 Berlin
[3] LLB Saclay, F-91191 Gif-Sur-Yvette Cedex
[4] Charles University, CZ-12116 Praha

The Kondo lattice $CeCu_2$ shows antiferromagnetic order below 3.5 K. Measurements on a polycrystalline sample showing an anomaly in the inelastic neutron spectra at about 14 meV footnoteM. Loewenhaupt et al., JMMM 76&77 (1988) 415 and Physica B163 (1990) 427 and at temperatures of 100-150 K lead to the assumption of a coupling between a crystal field transition and phonons. Inelastic neutron measurements on a single crystal confirm this assumption. We find an unusual energy shift (up to 15%) of certain phonons with increasing temperature, depending on their symmetry. At the same time the magnetic response is strongly broadened due to the coupling to the phonons.

B-119 Vortex Magnetism in High-temperature Superconductors

B. Lake[1], G. Aeppli[2,3], K. Lefmann[3], H. M. Ronnow[4,5], N. B. Christensen[3], D. F. McMorrow[3], K. N. Clausen[3], P. Vorderwisch[6], P. Smeibidl[6], M. Mangkorntong[7], N. E. Hussey[7,8,9], T. Sasagawa[7], M Nohara[7], H. Takagi[7], T. E. Mason[1], A. Schröder[10],
[1] Oak Ridge National Laboratory, P.O. Box 2008, MS 6430, Oak Ridge TN 37831-6430, U.S.A.
[2] N.E.C. Research Institute, 4 Independence Way, Princeton, NJ 08540-6634, U.S.A.
[3] Materials Research Department, Risø National Laboratory, 4000 Roskilde, Denmark.
[4] CEA-Grenoble (MDN/SPSMS/DRFMC), 17 Av. des Martyrs, 38054 Grenoble cedex 9, France.
[5] Institut Laue-Langevin, 6 rue Jules Horowitz, BP 156, 38042 Grenoble Cedex 9, France.
[6] BENSC, Hahn-Meitner Institute, Glienicker Strasse 100, 14109 Berlin, Germany.
[7] Department of Advanced Materials Science, Graduate School of Frontier Sciences, University of Tokyo, Hongo 7-3-1, Bunkyo-ku, Tokyo 113-8656, Japan.
[8] Department of Physics, University of Loughborough, Loughborough, LE11 3TU, U.K.
[9] H. H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol BS8 1TL, U.K.
[10] Department of Physics, University of Karlsruhe, D-76128 Karlsruhe, Germany.

There is strong evidence that magnetic interactions play a crucial role in the mechanism driving high-temperature superconductivity in cuprate superconductors. To investigate further this we have done a series of neutron scattering measurements on $La_{2-x}Sr_xCuO_4$ (LSCO) in an applied magnetic field. Below T_c the field penetrates the superconductor via an array of normal state metallic inclusions or vortices. Phase coherent superconductivity characterized by zero resistance sets in at the lower field-dependent irreversibility temperature (T_{irr}). We have measured optimally doped LSCO (x=0.16, T_c=38.5K) and underdoped LSCO (x=0.10, T_c=29K); both have an enhanced antiferromagnetic response in a field. Measurements of the optimally doped system at $H = 7.5T$ show that subgap spin fluctuations first disappear with the loss of finite resistivity at T_{irr}, but then reappear at a lower temperature with increased lifetime and correlation length compared to the normal state. In the underdoped system elastic antiferromagnetism develops below T_c in zero field, and is significantly enhanced by application of a magnetic field. Phase coherent superconductivity is then established within the antiferromagnetic phase at T_{irr}; thus, the situation in underdoped LSCO is the reverse of that for the optimally doped LSCO where the zero-resistance state develops first before the onset of antiferromagnetism.

B-120 Uniaxial pressure dependence of the weak antiferromagnetic order in UPt_3

N.H. van Dijk[1], P. Rodière[2], A. Huxley[2], J. Flouquet[2], M.T. Fernandez-Diaz[3], F. Yakhou[4], B. Fåk[2,5],
[1] IRI, NM, TU Delft, Mekelweg 15, 2629 JB Delft, The Netherlands
[2] CEA, DRFMC/SPSMS, 38054 Grenoble Cedex, France
[3] ILL, BP 156, 38042 Grenoble Cedex, France
[4] ESRF, BP 220, 38043 Grenoble Cedex, France
[5] ISIS Facility, RAL, Chilton, Oxon OX11 0QX, UK

The weak antiferromagnetic order of the heavy-fermion superconductor UPt_3 has been investigated by elastic neutron scattering under applied uniaxial pressure up to 6 kbar along the a and c axes of the hexagonal crystal structure. For $p||a$ the small moment of 0.02 μ_B/U-atom shows a non-linear decrease for increasing pressures. For $p||a$ a significant increase in the magnetic Bragg peak intensity is observed, which suggests a domain repopulation and confirms the presence of a single-k structure instead of the recently proposed triple-k structure. The results are discussed in relation to the understanding of the unconventional superconducting phase diagram.

B-121 Soft mode driven magnetic ordering in the singlet ground state system PrNi.

E.S. Clementyev[1,2], P.A. Alekseev[2], P. Allenspach[1], V.N. Lazukov[2],
[1] Laboratory for Neutron Scattering, ETHZ & Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland
[2] RRC, "Kurchatov Institute", RU-123182 Moscow, Russia

The measurements of the dispersion of the low-energy magnetic modes have been performed by inelastic neutron scattering technique for the

singlet ground state system PrNi above the Curie temperature (Tc=20.5 K) in the energy transfer range up to 7 meV. A progressive softening of one of the magnetic modes in the paramagnetic phase at temperatures approaching Tc has been observed at the magnetic Bragg point in PrNi. The temperature dependence and the character of the dispersion of the magnetic excitations in PrNi are indicative of an induced magnetic ordering mechanism in this compound with dominating ferromagnetic exchange interactions between the Pr ions.

B-122 Resonating Spin wave excitation in localized 5f uranium intermetallics $U_3Pd_20Si_6$

N. Metoki[1], Y. Koike[1], N. Aso[2], M. Kohgi[3], K.A. McEwen[4], N. Tateiwa[5], Y. Haga[1], N. Kimura[6], T. Komatsubara[6], H. Aoki[6], Y. Morii[1],
[1] ASRC, Japan Atomic Energy Research Institute, Tokai, Naka, Ibaraki 319-1195, Japan
[2] NSL-ISSP, University of Tokyo, Tokai, Naka, Ibaraki 319-1106, Japan
[3] Graduate School od Sci., Tokyo Metropolitan University, Hachioji, Tokyo 192-0397, Japan
[4] University College London, London WC1E 6BT, United Kingdom
[5] Research Center for Materials Science at Extreme Condition, Osaka University, Toyonaka, Osaka 560-8531, Japan
[6] Center for Low Temp. Sci., Tohoku University, Sendai 980-8545, Japan

We present unusual magnetic excitation in an uranium intermetallics $U_3Pd_20Si_6$. $U_3Pd_20Si_6$ is a localized 5f system, which shows clear crystalline electric field excitations about 20 - 30 meV. In the AFM state of 8c uranium site below T_N = 19 K strong AFM spin wave excitation was observed whole in reciprocal space up to 3 meV at zone boundary. The dispersion relation can be described by the nearest-neighbor interaction with an anisotropy gap of about 1 meV. Surprisingly, however, the gap was collapsed by a continuum spin excitation existing near AFM zone center. This continuum is connected to a low energy dispersive ferromagnetic fluctuation, most likely, due to uranium 4a site. The dispersive ferromagnetic fluctuation exists even in paramagnetic state of 4a site. The unusual low energy response represents a new type of spin dynamics due to the dynamical inter-site coupling of uranium spins.

B-123 Effect of pressure and Mn substitution on magnetic ordering of $Ce_2Fe_{17-x}Mn_x$

O. Prokhnenko[1,2], C. Ritter[1], Z. Arnold[2], O. Isnard[3], A. Teplykh[4], J. Kamarad[2], A. Pirogov[4], A. Kuchin[4],
[1] Institute Laue Langevin, BP 156, 38042 Grenoble Cedex 9, France
[2] Institute of Physics AS CR, Cukrovarnicka 10, 16253 Prague 6, Czech Republic
[3] Laboratoire de Cristallographie, CNRS, BP 166, 38042 Grenoble cedex 9, France
[4] Institute for Metal Physics, S.Kovalevskaya 18, Ekaterinburg, 620219 Russia

To clarify the interplay of volume and Mn in $Ce_2Fe_{17-x}Mn_x$ neutron diffraction experiments under high pressure were performed on Ce_2Fe_{17} and $Ce_2Fe_{16}Mn$ compounds. The existence of collinear ferromagnetic (below 95 K) and incommensurate helical antiferromagnetic structures in Ce_2Fe_{17} was confirmed at ambient pressure. A helical structure, similar to Ce_2Fe_{17}, exists down to low temperatures in $Ce_2Fe_{16}Mn$. The corresponding propagation vector $\tau = (0, 0, \tau_z)$ changes from 0.333 r.l.u. at 100 K to 0.407 r.l.u. at 200 K in the case of Ce_2Fe_{17} and stays $\tau \approx 0.378$ r.l.u. below 210 K for $Ce_2Fe_{16}Mn$. The ferromagnetic phase in Ce_2Fe_{17} is suppressed by a pressure of 3 kbar and is substituted by the new incommensurate antiferromagnetic phase. The complex pressure effect and the appearance of a new non-collinear phase in $Ce_2Fe_{16}Mn$ is in agreement with the magnetic measurements. The possible models of the pressure induced phases are discussed. The work was partially supported by RFBR 99-02-16395.

B-124 Small-angle polarized neutron scattering in $YBa_2(Cu_{0.9}Fe_{0.1})_3O_{7-y}$ ceramics at T=290 - 550 K

G.P. Kopitsa[1], V.V. Runov[1], A.I. Okorokov[1], I.S. Lyubutin[2], K.V. Frolov[2],
[1] Petersburg Nuclear Physics Institute, Russian Academy of Sciences, Gatchina, Leningrad district, 188300, Russia
[2] Institute of Crystallography, Russian Academy of Sciences, Moscow, 117333, Russia

Small-angle polarized neutron scattering (SAPNS) measurements were performed on deoxygenated $YBa_2(Cu_{0.9}Fe_{0.1})_3O_{7-y}$ ceramics in vacuum at temperature range 290<T<550 K and magnetic fields 0<H<50 Oe. Anomalies in the temperature curves of the scattering intensity I(T,q) (where q is momentum transfer) and polarization P(T) of transmitted beam were observed at 300<T<500 K. From analysis of SAPNS and depolarization data it was found that the magnetic correlations of ferromagnetic type with a scale of few hundred angstrom exist in the system. These results are agreed to data of Mößbauer spectroscopy. The nature of these effects is discussed.

B-125 Zn-doping effect seen in neutron-scattering-study on $La_{2-x}Sr_xCuO_4$ superconductor

H. Kimura[1], M. Kofu[2], K. Hirota[2], M. Aoyama[3], Y. Koike[3], K. Yamada[4], Y. Endoh[5],
[1] Research Institute for Scientific Measurements, Tohoku University
[2] Department of Physics, Tohoku University
[3] Department of Applied Physics, Tohoku University
[4] Institute for Chemical Research, Kyoto University
[5] Institute for Material Research, Tohoku University

Spatially modulated static antiferromagnetic (AF) correlations coexists and competes with superconductivity have been systematically studied through neutron-scattering measurements with focusing on Zn-doped $La_{2-x}Sr_xCuO_4$ (LSCO). The static AF correlations for Zn-doped LSCO with $x = 0.12 \sim 0.21$ have almost the same appearing temperature T_m ($\sim$ 20 K) and the correlation length xi_m ($\sim$ 80 Å), which is lower and shorter than those for Nd or Ba-codoped LSCO, Stage-4 La_2CuO_{4+y}, and LSCO with $x \sim 1/8$. In the former (Zn-doped) system, the T_m has an energy resolution dependence suggesting the glassy nature of static spin correlations, while in the latter one, T_m is almost resolution dependent indicating the phase transition into a long-ranged AF order. These results can be explained by *incoherent* and *coherent* pinning mechanism of AF spin fluctuation. In the former mechanism, pinning centers *i.e.* Zn atoms are introduced randomly on CuO_2 plane and uncorrelated with each other. On the other hand, the latter one is originated from the periodically induced potential due to structural changes. The proposed *incoherent* pinning model might clarify the role of Zn doping in the antiferromagnetism of La-214 cuprates.

B-126 Critical magnetic scattering in invar $Fe_{65}Ni_{35}$ alloy

A.I. Okorokov[1], S.V. Grigoriev[1], S.V. Maleyev[1], H. Eckerlebe[2], G. Kozik[2],
[1] Petersburg Nuclear Physics Institute, 188350 Gatchina, St.Petersburg, Russia
[2] GKSS Forchungszentrum, 21502 Geesthacht, Germany

The critical SAPNS experiment on invar alloy $Fe_{65}Ni_{35}$ was performed in the magnetic field $\vec{H}$ using special "inclined" geometry ($\vec{H}$ is inclined to the wavevector $\vec{k_0}$). Three contributions to the critical scattering were studied at different magnetic fields (10-1000 G) in the temperature range: $T_C \pm 0.1T_C$. First, the pair spin correlations with their amplitude and the correlation length $R_C(T, H)$ were measured. Second, the three-point dynamical spin correlations were investigated by extracting an asymmetric part of the polarization dependent scattering. The data are interpreted in terms of the static and dynamic scaling theory. Third, the nuclear-magnetic interference term, showing the spin-lattice coupling, was obtained from the symmetric polarization - dependent scattering.

B-127 Crystal field in RNiAl compounds studied by inelastic neutron scattering

P. Javorský[1], H. Nakotte[2], H. Mutka[3], V. Sechovský[1],
[1] Department of Electronic Structures, Charles University, Ke Karlovu 5, 121 16 Prague 2, The Czech Republic
[2] Physics Department MSC 3D, New Mexico State University, Las Cruces, NM 88003-8001, USA
[3] Institut Max von Laue Paul Langevin, rue Jules Horowitz, 38042 Grenoble Cedex 9, France

RNiAl compounds crystallize in the ZrNiAl-type hexagonal structure, the point symmetry at the rare-earth sites is orthorhombic. Crystal field plays an important role in the magnetic behaviour of these materials. We present an inelastic neutron scattering study of the crystal field in PrNiAl, NdNiAl, ErNiAl and ErCuAl. The selected rare-earth ions are near both ends of the lanthanide series where one usually expects a stronger influence of the crystal field. The results are compared with the specific-heat data, and the lower part of the crystal-field energy level scheme is determined.

B-128 Neutron Diffraction and Mössbauer Spectroscopy Study of $La_{0.6}Sr_{0.4}Fe_{1-x}Co_xO_{3-y}$ (x = 0,0.5) Perovskites

S. Neov[1], L. Dabrowski[2], M. Hofmann[3], H. Bouwmeester[4],
[1] Institute for Nuclear Research & Nuclear Energy, 1784 Sofia, Bulgaria
[2] Institute of Atomic Energy, 05-400 Swierk, Poland
[3] Hahn-Meitner-Institut, D 14109 Berlin, Germany
[4] University of Twente, 7500 AE Enschede, The Netherlands

Crystal and magnetic structure of substituted perovskites $La_{0.6}Sr_{0.4}Fe_{1-x}Co_xO_{3-y}$ (x = 0, 0.5) were studied by neutron diffraction and Mössbauer spectroscopy. Below the room temperature the oxides have $R\bar{3}c$ structure. The occupancy of crystallographic (18e) positions by oxygen atoms varies from 2.82(2) to 2.92(2). Below T = 154 K, Mössbauer spectra of x = 0.5 sample show Zeeman sextet, characteristic for a regular arrangement of Fe- spins. Neutron diffraction did not register a significant change of the G-type AF structure at this temperature. The mean magnetic moment at T = 40 K is 1.61 μ_B per B-site, for x=0.5, and 2.63 μ_B for the x = 0 composition. An increase of T_N and oxygen deficiency was observed as a result of the heating to 850 K. The structure of $La_{0.6}Sr_{0.4}Fe_{0.5}Co_{0.5}O_{2.84}$ at 850 K is cubic, space group Pm3m.

B-129 Geometrical frustration and incommensurate magnetic ordering in CePdAl

L. Keller[1], A. Dönni[2], H. Kitazawa[3],
[1] Laboratory for Neutron Scattering, ETH Zürich & PSI, CH-5232 Villigen PSI, Switzerland
[2] Department of Physics, Niigata University, Niigata 950-2181, Japan
[3] National Research Institute for Metals (NRIM), Tsukuba 305-0047, Japan

The ordering of the Ce magnetic moments in the heavy-fermion compound CePdAl was investigated by means of neutron powder diffraction measurements of high-quality polycrystalline samples at temperatures down to 180 mK. CePdAl crystallizes in the hexagonal ZrNiAl-type structure. The triangular coordination symmetry of the magnetic ions gives rise to geometrical frustration and leads to an incommensurate antiferromagnetic structure at $T_N = 2.8$ K, exhibiting a coexistence of ordered and frustrated disordered Ce moments. The magnetic propagation vector shows a pronounced temperature dependence below T_N and locks in to $\mathbf{k} = (1/2, 0, \tau)$, $\tau = 0.35$, below 1.9 K. The previously suggested second magnetic phase transition at lower temperatures could not be confirmed.

B-130 Neutron Polarisation Analysis of the Spin Glass Phase of $Y(Al_{1-x}Fe_x)_2$

J.M. Preston[1], J.R. Stewart[1], R. Cywinski[2], W. Steiner[3], M. Reissner[4],
[1] Institut Laue Langevin, 6 rue Jules Horowitz, B.P. 156, 38042 Grenoble, France
[2] Department of Physics, E.C. Stoner Building, University of Leeds, Leeds, LS2 9JT, West Yorkshire, UK
[3] Wiedner Haupstr. 8-10, A-1040, Wien, Austria

[4] Technische Universität, Wien, Austria
The cubic C15 Laves phase system $Y(Al_{1-x}Fe_x)_2$ has a low temperature spin glass state for x=0.1-0.75, but is essentially ferromagnetic for x>0.75. Extensive susceptibility, Mössbauer and μSR measurements [1-3] indicate inhomogeneous magnetisation processes in the spin glass regime, dominated by strong dynamic ferromagnetic correlations above T_g. The magnetic and atomic short-range order have been studied using neutron polarisation analysis on the diffuse scattering spectrometer, D7 at the ILL, enabling extraction of the Warren-Cowley short-range order parameters and the magnetic spin correlations. [1] M Reissner *et al* J Phys F Metal Phys **14** (1984) 1249 [2] J Bogner *et al* J Phys Conds Matter **10** (1998) 9849 [3] MTF Telling *et al* Physica B **289** (2000) 213

B-131 CEF-effects and disorder versus Kondo lattice behavior in $CeMSi_3$ (M=Rh, Ir)

A. Krimmel[1], M. Reehuis[1], A. Loidl[1],
[1] Institut für Physik, Universität Augsburg, Universitätsstr. 1, 86159 Augsburg, Germany
On the basis of specific heat, magnetic susceptibility and electrical resistivity measurements, $CeMSi_3$ (M=Rh, Ir) have recently been characterized as magnetically ordering Kondo lattice compounds. However, no magnetic Bragg peaks could be observed by powder neutron diffraction, resulting in an upper limit of the ordered magnetic moments of 0.25 μ_B. An additional quasielastic neutron scattering study on $CeRhSi_3$ did not reveal any appreciable magnetic signal at low temperatures 1.5 K $\leq T \leq$ 40 K and only very weak scattering contributions at elevated temperatures 40 K $\leq T \leq$ 300 K. For a proper characterization of $CeMSi_3$ (M=Rh, Ir) we propose to include crystal field effects and nonmagnetic atomic disorder. This may also hold true for other compounds of the $CeTX_3$ (T=transition metal, X=Si, Ge) intermetallics showing similar magnetic behavior.

B-132 Valence and Magnetic transitions in $YbMn_2Si_{2-x}Ge_x$

M. Hofmann[1], S. J. Campbell[2], A. V. J. Edge[2],
[1] Rutherford Appleton Laboratory, ISIS, Chilton, OX11 0QX, UK
[2] School of Physics, University College, The University of New South Wales, ADFA, Canberra, ACT 2600, Australia
Rare-earth intermetallic compounds containing ytterbium exhibit a wide range of interesting and unusual physical and magnetic properties. This occurs mainly as a result of their mixed valence states (II/III) or changes from one valence state to the other. Nowik [1] has recently investigated the magnetic phase transitions in the $YbMn_2Si_{2-x}Ge_x$ series by magnetisation and Mössbauer effect studies on ^{57}Fe doped samples. A number of transitions were observed in the limiting $YbMn_2Ge_2$ and $YbMn_2Si_2$ compounds. We have carried out a neutron diffraction investigation of $YbMn_2Si_{2-x}Ge_x$ to delineate details of the valence and related magnetic transitions that take place. As well as determining the magnetic structures, our neutron diffraction experiments provide evidence for a change in the Yb valence state from trivalent in $YbMn_2Si_2$ to divalent in $YbMn_2Ge_2$ around a critical Ge concentration x$\sim$1.6. [1] I Nowik, I Felner and E R Bauminger, JMMM, 185 (1998) 91

B-133 Inelastic Neutron Scattering Study on two Mixed Valence Dodecanuclear Polyoxovanadate Clusters

R. Basler[1], G. Chaboussant[1], P. Koegerler[2], A. Müller[2], H. U. Güdel[1],
[1] Department of Chemistry, University of Berne, Freiestrasse 3, 3000 Berne 9, Switzerland
[2] Faculty of Chemistry, University of Bielefeld, Postfach 100131, 33501 Bielefeld, Germany
Energy splittings resulting from magnetic exchange interactions in the mixed valence dodecanuclear clusters $A_4[V_8^{IV}V_4^{V}As_8O_{40}(H_2O)]\cdot xH_2O$ (A = Na^+ or $(NHEt_3)^+$) were investigated by an inelastic neutron scattering (INS) study using both cold and thermal neutrons. The low temperature magnetic properties can be described by considering an antiferromagnetically coupled tetramer, of four vanadium(IV) ions. Up to four magnetic transitions were observed within the ground state multiplet. The transition energies and the relative INS intensities were modeled with an appropriate exchange Hamiltonian. The whole study was performed on undeuterated samples and we were able to resolve magnetic transitions in the 0..4 meV energy range. The ability of using undeuterated samples for INS on spin clusters becomes important as deuteration is often prohibitive.

B-134 Field-induced Magnetic Structures in UNiGe

K. Prokes[1], H. Nakotte[2], E. Brück[3], P. F. de Châtel[3], V. Sechovský[4],
[1] Hahn-Meitner-Institute, SF 2, D-14109 Berlin, Germany
[2] MSC3D, New Mexico State University, Las Cruces NM 88003, USA
[3] University of Amsterdam, NL-1018 XE Amsterdam, The Netherlands
[4] Charles University, DES, CZ-121 16 Prague 2, The Czech Republic

At temperatures lower than T_N = 50K, the orthorhombic UNiGe exhibits an incommensurate (INC) antiferromagnetic structure, which becomes commensurate below 42.5 K. At 4.2 K, there are two field-induced transitions at 17 and 25 T for the b-axis and at 3 and 10 T for fields applied along c. We have reinvestigated all the magnetic structures of UNiGe including the field-forced ferromagnetic structure, which is established above the upper critical field. While the intermediate field-induced phases have a propagation vector (0, 1/3, 1/3), the INC phase is characterized by a propagation vector (0, d1, d2). The ferromagnetic phase is non-collinear even in 14.5 T with a significant a-axis component similar to low-field phases. This suggests that the magnetic ordering in UNiGe is governed by anisotropic exchange interactions.

B-135 Preparation, Crystal and Magnetic Structure of the Double Perovskite Ba_2FeWO_6

A. K. Azad[1,2], A. Mellergård[1], S. G. Eriksson[1,2], S. Ivanov[3], J. Eriksen[1], H. Rundlöf[1],
[1] Studsvik Neutron Research Laboratory, Uppsala University, SE-61182, Nyköping, Sweden
[2] Dept. of Inorganic Chemistry, University of Gothenburg, SE-412 96, Göteborg, Sweden
[3] Karpov Institute of Physical Chemistry, 103064, Moscow, Russia

Single-phase polycrystalline material of the double perovskite Ba_2FeWO_6 has for the first time been prepared and characterized by x-ray and neutron powder diffraction (NPD). The crystal structure was tetragonal with lattice parameters a = b = 5.7479(4) and c = 8.1444(9)Åat room temperature (295K). NPD data at 10K shows the evidence of an antiferromagnetic ordering of the Fe atoms. Reverse Monte Carlo modelling was used to find the magnetic structure, which show that it is based on a unit cell related to that of nuclear structure by the propagation vector (0 $\frac{1}{2}$ $\frac{1}{2}$). An ordering of non-collinear spins was found with alternate layears in the c-direction or a-b plane. The model was checked by Rietveld refinement and the magnetic moment of iron was found to be 3.39(2) μ_B.

B-136 Inelastic neutron scattering spectra in f-electron compounds: First principles calculations

M. Divis[1], J. Rusz[1], V. Nekvasil[2],
[1] Charles University, Department of Electronic Structures, Ke Karlovu 5, 121 16 Prague 2, Czech Republic
[2] Institute of Physics, Czech Academy of Sciences, Cukrovarnicka 10, 162 53 Prague, Czech Republic

Theoretical investigation of the rare earth (RE^{3+}) localized 4f electron states and band energy spectrum of $REGa_2$, $REAl_2$, $REAl_3$ intermetallics and $REBa_2Cu_3O_6$, $REBa_2Cu_3O_7$, RE_2CuO_4 cuprates was performed. A parameter free first principles method based on the density functional theory was used to calculate the crystal field interaction. This approach is shown to provide a a reasonable theoretical description of the experimental data (e.g. inelastic neutron scattering INS, magnetization, susceptibility) in various RE intermetallic compounds. In cuprates the same approach, combined with a semi-phenomenological superposition model, allows to account for special features in the INS, RAMAN AND IR spectra associated with non-regular RE sites.

B-137 Long-range magnetic order in intermediate-valence Ce-Lu alloys

P.P. Deen[1], J.P. Goff[1], A.M. Toader[1], J. Klenke[2], F. Yakhou[3], R.C.C Ward[4], M.R. Wells[4],
[1] Department of Physics, University of Liverpool, U.K.
[2] Hahn Meitner Institut, Germany
[3] European Synchrotron Radiation Facility, France
[4] Clarentdon Laboratory, University of Oxford, U.K.

Intermediate-valence Ce alloys are found to exhibit particularly rich magnetic phase diagrams with both long and short-range magnetic order. Single crystal Ce-Lu alloys with a DHCP structure were grown using molecular beam epitaxy and are ideal for testing this unusual behaviour. Neutron diffraction studies using the triple-axis spectrometer, E1, at HMI show that long-range magnetic ordering, of the β-Ce type, occurs for all compositions of Ce-Lu alloys. X-ray magnetic resonant scattering studies using ID20 at the ESRF show that the Ce in Ce-Lu alloys adopt an intermediate valence behaviour. The results show that the intermediate valence behaviour in Ce alloys is due to chemical pressure, and that this phenomenon is decoupled from the diffuse magnetic response.

B-138 Magnetic Ordering in $U_{0.7}Th_{0.3}S$

O. Zaharko[1], P. Fischer[1], K. Mattenberger[2], O. Vogt[2],
[1] Labor fÑeutronenstreuung, ETHZ & PSI, CH-5232 Villigen
[2] Labor für Festkörperphysik, ETH, CH-8093 Zürich

Dilution of U by nonmagnetic Th in the pseudobinary system $U_{1-x}Th_xS$ ($0 \leq x \leq 1$) changes the degree of localization of 5f electrons and the strength of ferromagnetic exchange. This leads to a decrease of the Curie temperature and of the effective magnetic moment [1]. Neutron diffraction studies of a $U_{0.7}Th_{0.3}S$ single crystal have been performed at the SINQ TRICS and TASP instruments. The U-moments order ferromagnetically at T_C = 99.0(1) K. The ordered moment value is 1.7(5) μ_B/U at 10 K. The crystal symmetry remains cubic below T_C. An anisotropic broadening of all reflections with the evolution of magnetic order is observed. Strong magneto-strictive effects introduce local strains and/or formation of microdomains. The The estimated coherence lengths are 65 Åand 45 Åat 10 K in the longutudinal and transversal directions, respectively. Other single crystals of $U_{1-x}Th_xS$ system are under investigation. [1] O. Vogt, K. Mattenberger, J. Löhle, JMMM submitted.

B-139 The Loss of Antiferromagnetism in Fe-substituted (YMn_2)

R. Cywinski[1], S. H. Kilcoyne[1], C. Ritter[2],
[1] Department of Physics and Astronomy, University of Leeds, Leeds LS2 9JT, UK
[2] ILL, B.P.156, 38042 Grenoble, Cedex 9, France

Neutron powder diffraction has been used to map the evolution of the magnetic structure of YMn_2 with Fe substitution. The transition from a spin fluctuating Pauli paramagnetic state to long range helical antiferromagnetism, and the accompanying discontinuous volume expansion, observed for pure (YMn_2) on cooling below 100K [1] maintains its discontinuous character on addition of Fe. Although the magnitude of the ordered

moment, of 2.8 Bohr magnetons, and the 5%volume expansion at the Neel point do not change appreciably with Fe substitution, the temperature of the transition decreases rapidly to zero at the composition ($YMn_{1.95}Fe_{0.05}$). The period of the antiferromagnetic helix in the ordered state is found to be strongly dependent on concentration and temperature. [1] R Cywinski, S H Kilcoyne and C A Scott, J Phys :Condensed Matter 3 (1991) 6473

B-140 Crystal Structure, Superconductivity and Magnetism in the New Class of Heavy-Fermion Materials:$Ce_mT_nIn_{3m+2n}$ (T = Co, Rh, Ir)

E. G. Moshopoulou[1], J. D. Thompson[2], P. G. Pagliuso[2], J. L. Sarrao[2], Z. Fisk[2,3],
[1] National Center for Scientific Research "Demokritos", Institute of Materials Science, 15310 Agia Paraskevi, Greece
[2] Los Alamos National Laboratory, Los Alamos, NM 87545 USA
[3] National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL 32306 USA

A recent advance in the physics and chemistry of heavy-fermion materials has been the discovery of the first homologous series of heavy-fermion materials $Ce_mT_nIn_{3m+2n}$ (T = Co, Rh, Ir). The crystal structure and the structural aspects associated with phase transitions of various members of the series, have been determined by high-resolution powder and single crystal neutron diffraction. The ordered, intergrowth crystal structure of the series implies an evolution of spatial dimensionality among its various members. The detailed crystal structure, the fascinating properties and the unusual phase transitions of these new materials as well as the structure-property relationship will be discussed at the conference.

B-141 Magnetic excitations in strongly-interacting rare earth compounds

A.T. Boothroyd,
[1] Department of Physics, Oxford University, Oxford, OX1 3PU, U.K.

I will describe neutron inelastic scattering investigations of several rare-earth-containing compounds whose properties depend on interactions acting on the $4f$ states. The presentation will include recent results on (i) the spin excitations in the anomalous non-superconducting cuprate $PrBa_2Cu_3O_{6+x}$, showing the importance of Pr–Pr and Pr–Cu coupling in determining its properties, (ii) the nature of the ground state involving hybridization of $4f$ electrons and conduction band states in heavy fermion $YbNi_2B_2C$, a material which apparently exhibits a temperature-dependent Kondo temperature, and (iii) the strong magnetoelastic coupling in PrO_2 that causes a dynamic Jahn-Teller effect in the ground state and a continuum of vibronic excited states in the energy spectrum. I will show how quantitative modelling of the magnetic excitation spectra has brought us an understanding of the microscopic properties of these materials.

B-142 Experimental study of vortex lattice transitions in YNi_2B_2C

S. Levett[1,2], C. Dewhurst[1], D. McK Paul[2],
[1] Institut Laue Langevin
[2] University of Warwick

We have performed extensive high-resolution small angle neutron scattering (SANS) measurements of the vortex lattice in single crystals of YNi_2B_2C for B$\|$c. The data suggests that there is a macroscopic transition width consisting of a coexistence of the low and high-field distorted hexagonal vortex lattice phases. We find no evidence for a continuous distortion of the vortex lattice between the two states. Rather, the smooth variation in scattered intensity corresponds to a redistribution of populations between the two types of domains. We will compare our results to those predicted theoretically by Knigavko et al. [1], who suggest that the reorientation occurs as two successive second order phase transitions. Also, experimental data related to the temperature dependence of the lattice transitions will be discussed. [1] A. Knigavko et al., Phys. Rev. B, 62, 111 (2000)

B-143 Magnetic excitations in quadrupolar ordered UCu_2Sn

J. P. Allen[1], K. A. McEwen[1], R. I. Bewley[2],
[1] Department of Physics and Astronomy, University College London,Gower Street, London WC1E 6BT, UK
[2] ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, OxonOX11 0QX, UK

Quadrupolar ordering in uranium intermetallic compounds is rather rare. The best known example is UPd_3, but recent elastic constant measurements have strongly indicated that UCu_2Sn exhibits quadrupolar ordering below 16K [1]. We have examined the spin dynamics of UCu_2Sn using the HET chopper spectrometer at ISIS. Our results show clear evidence of temperature dependent magnetic scattering in the energy range 5 - 15 meV. Intermultiplet excitations at 350 meV indicate that the U ions have the $5f^2$ configuration. We will compare our data with the predictions of the crystal field model given in [1]. [1] T. Suzuki et al, Phys. Rev. B 62 (2000) 49

B-144 Magnetic excitations in f electron compounds RCu_6 (R = Ce, Pr)

Y. Koike[1,2], N. Metoki[1], Y. Morii[1], Y. Onuki[1,3],
[1] Advanced Science Research Center, Japan Atomic Energy Research Institute, Tokai, Ibaraki 319-1195, Japan
[2] Japan Science and Technology Corporation, Kawaguchi, Saitama 332-0012, Japan
[3] Graduate School of Science, Osaka University, Toyonaka 560-0043, Japan

We have carried out the inelastic neutron scattering experiments on RCu_6 (R = Ce, Pr) in order to investigate the magnetic inelastic response of these systems. These compounds have the same monoclinic crystal structure, space group $P2_1/c$ at low temperatures but different magnetic properties. In $CeCu_6$, a new magnetic excitation mode was found at around (1 0 0.5) with the excitation energy of about 0.3 meV. We found that this new antiferromagnetic correlation showed very similar field and temperature dependence to the other antiferromagnetic mode around (100) and (001) reported before. In $PrCu_6$, we measured the crystalline electric field excitation at various wave vectors using a single crystal. We observed the energy excitation of about 1.5 meV and 2.6 meV. These excitations would be corresponding to J_x and J_y-mode respectively. These excitations had a weak wavevector dependence due to the RKKY interaction between the $4f$ electrons. The 1.5 meV excitation mode split into two branches at around (020).

B-145 Magnetic correlations in the bilayered ruthenate $Sr_3Ru_2O_7$

L. Capogna[1], E. M. Forgan[1], S. M. Hayden[2], J. A. Duffy[2], R. S. Perry[1], A. P. Mackenzie[1], S. Ikeda[3], A. Wildes[4], N. Burton[1], G. McIntyre[4], P. G. Kealey[1], Y. Maeno[3],
[1] School of Physics and Astronomy, University of Birmingham, Edgbaston, Birmingham B15 2TT, UK

[2] H.H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol BS8 1TL, UK
[3] Department of Physics, Kyoto University, Kyoto 606-8502, Japan
[4] Institut Laue-Langevin, 6 rue Jules Horowitz, BP 156-38042, Grenoble Cedex 9, France

$Sr_3Ru_2O_7$ is the bilayered member of the ruthenate compounds $Sr_{n+1}Ru_nO_{3n+1}$. This family displays a wide variety of phases, including unconventional superconductivity in the single layered Sr_2RuO_4 compound. $Sr_3Ru_2O_7$ is very close to a ferromagnetic instability and the balance can be tipped by impurities, magnetic field and pressure. We report on the magnetic properties of high purity single crystals of $Sr_3Ru_2O_7$ as observed by inelastic and elastic neutron scattering measurements. In particular, we present the first observation of spin fluctuations and show that they indicate a crossover in the nature of the magnetic correlations in $Sr_3Ru_2O_7$.

B-146 On the Interaction of Hydrogen and Deuterium with Dislocations Studied by Small Angle Neutron Scattering

R. Kirchheim[1], M. Maxelon[1], A. Pundt[1], W. Pyckhout-Hintzen[2], J. Barker[3],
[1] Institut für Materialphysik, Universität Göttingen, Hospitalstr. 3-7, D-37073 Göttingen
[2] Institut für Festkörperforschung, FZ Jülich, Germany
[3] Center for Neutron Research, NIST, Gaithersburg, USA

Small angle neutron scattering (SANS) measurements on Pd samples containing dislocations with a density of a few 10^{11} cm^{-2} reveal an additional intensity for a scattering vector of 0.02 to 0.2 $Å^{-1}$ after loading with hydrogen or deuterium. The corresponding net cross section is proportional to the reciprocal scattering vector as expected for line type scattering objects with a superimposed exponential decrease stemming from scattering within the Guinier-regime. This experimental finding is in accordance with a model where extended segregation of H or D within the dilated regions of edge dislocations occurs. In a first order approximation this corresponds to a precipitation of cylindrically shaped hydrides along the dislocation line and can be treated quantitatively yielding radii in agreement with SANS data. Whereas gas volumetric measurements at the same total concentration reveal no difference for the amount of H- and D-segregation, there is a pronounced effective difference in SANS intensities which cannot be explained by the different scattering lengths alone. However, the different sign of the latter quantity in combinations with an expected volume expansion within the hydride/deuteride region provides a reasonable explanation of the intensity difference observed. Knowing the amount of segregated H or D from gas volumetry and the dislocation density from electron microscopy the SANS results can be explained in a self consistent way.

B-147 Local structure of deuterated Ti-Zr amorphous alloy

T. Fukunaga[1], K. Itoh[1], K. Hashi[2], K. Aoki[2],
[1] Research Reactor Institute, Kyoto University, Kumatori-cho, Sennan-gun, Osaka 590-0494, Japan
[2] Department of Materials Science, Kitami Institute of Technology, 165 Koencho Kitami. Hokkaido 090-8507, Japan

Ti-Zr alloy system is isomorphous over the total concentration range. A neutron zero-scattering alloy can be obtained at the composition Ti-32.4at%Zr because of negative and positive coherent neutron scattering amplitudes of Ti and Zr respectively. Moreover, $(Ti_{0.676}Zr_{0.324})D_{0.31}$ amorphous alloy was synthesized by mechanical alloying under D_2 gas atmosphere in order to get information of the location of D atom. The concentration-concentration correlation of the Ti-32.4at%Zr neutron zero scattering alloy indicates no fluctuation except for the small negative peak at about 0.3 nm due to Ti-Ni pair correlation. In contrast, small negative and positive peaks became definitely visible in the atomic correlation function G(r) of the $(Ti_{0.676}Zr_{0.324})D_{0.31}$ amorphous alloy. The modulation was originated from D-Ti and D-Zr correlations. The stronger correlation of the D-Zr pair than that of the D-Ti pair was observed in the G(r) of the $(Ti_{0.676}Zr_{0.324})D_{0.31}$ amorphous alloy.

B-148 Geometric Isotopic Effect in Hydrogen-containing Crystals in three dimensional Model for H-Bond Approximation

A. Barabash[1], E. Shadchin[1],
[1] Institute of Physics of National Academy of Sciences of Ukraine

The geometric isotopic effect, that is connected with the isotopic changes of the fre-quencies of the stretching and bending vibrations of the H-bonds in hydrogen-containing crystals of the KDP-type. is investigated. The mechanism that is responsible for changing of hydrogen bond length due to the isotopic proton substitution of the H-bonds is proposed. According to the three-dimensional Morse potential for a proton in the H-bond the dependencies of the frequencies for the stretching and bending vibrations as a function of the hydrogen bond length is obtained. It was shown that in the frame of the three-dimensional model for H-bond based on Einstein approximation for enharmonic oscillators the best agreement between experimental and theoretical data related to the observed lengthening of the H-bonds at isotopic substitution can be achieved if the inter-actions between the nearest hydrogen-bonded chains in crystal is regarded.

B-149 Hydrogen Vibrations in Austenitic Steel

S. Danilkin[1], H. Fuess[2], V. Gavriljuk[3], M. Hoelzel[2], A. Ivanov[4], T. Wieder[2], H. Wipf[2],
[1] Hahn-Meitner Institut, Berlin, Germany
[2] Darmstadt University of Technoligy, Darmstadt, Germany
[3] Institute for Metal Physics, Kiev, Ukraine
[4] Institute Laue-Langevin, Grenoble, France

Hydrogen in austenitic stainless steel causes embrittlement, but all the factors determining these hydrogen effects are not yet fully understood. We report on a diffraction and INS study of H-doped Fe-18Cr-16Ni-10Mn austenitic steel with two different hydrogen contents (0.33 and 0.27 at.%). The INS measurements were performed at 80, 145, 197, 246 and 300K with the IN1 spectrometer (ILL). For both H contents, the observed peak from the hydrogen vibrations had a two-component structure at T$<$250K. The relative intensity of the components (1) and (2) at $\sim$125 meV and $\sim$135 meV, correspondingly, depends on sample temperature. At the temperatures 145 and 197 K, the intensity ratio I(1)/I(2) was smaller in the sample with lower H content. This indicates a possible structural change due to the formation of a H-induced phase with bigger Me-H distance, probably metastable gamma(H)-phase and/or epsilon(H)-martensite.

B-150 Density and Hydrogen Concentration of Amorphous Carbon Nitride Thin Films by X-ray and Neutron Reflectivity

S. Santucci[1], L. Lozzi[1], L. Valentini[2], J. M. Kenny[2], A. Mennelle[3],
[1] Dipartimento di Fisica - Unità INFM, Università dell'Aquila - Italy
[2] Materials Engineering Center, Università di Perugia - Italy
[3] Laboratoire Leon Brillouin, CEA/Saclay - France

Due to difficulties in measuring hydrogen concentration, there still exist several unanswered questions regarding the effects of the presence of hydrogen on the structure and bonding of hydrogenated amorphous carbon nitride films. Specular reflectivity of neutrons and x-rays can be used to determine the scattering length density profile of a material perpendicular to its surface. We have applied these techniques to study hydrogenated amorphous carbon nitride thin films. By the combination of these two techniques we obtain not only the mass density, but also the concentration of hydrogen, which varies in our case between 10% and 30%. This method is a new and nondestructive way to determine the concentration of hydrogen within an error of less than 2 at.% in samples with sharp interface. It is especially suited for amorphous carbon films.

B-151 In-situ neutron diffraction study of reversible deuteration in nanocrystalline $LaNi_{5+x}$ (x∼1)-Ni alloy.

F. Cuevas[1], J.-M. Joubert[1], M. Latroche[1], A. Percheron-Guegan[1], O. Isnard[2],
[1] LCMTR-ISCSA-CNRS. 2-8 rue Henri Dunant, 94320 Cedex. France.
[2] CRG-D1B. ILL-Grenoble. France

$LaNi_5$-substituted alloys are used as negative electrodes in nickel metal-hydride batteries. In real devices, substitutions include costly cobalt to obtain a long cycle-life, though this could be attained for over-stoichiometric $La(Ni,M)_{5+x}$ compounds such as $LaNi_5Cu$. Although over-stoichiometry in non-substituted $LaNi_{5+x}$ is limited to x=0.4 at equilibrium, we were able to prepare $LaNi_6$ powders (x=1) by mechanical alloying. Such powders are nanocrystalline and are decorated by Ni precipitates. We here report on the crystallographic changes, as studied by in-situ neutron diffraction, in both $LaNi_{5+x}$ and Ni phases during reversible deuteration. Measurements were conducted at 298 K for deuterium pressures between $10^2$and 10^7Pa.

B-152 Short-lived proton entanglement in yttrium hydrides

E. B. Karlsson[1], C. A. Chatzidimitriou-Dreismann[2], T. Abdul-Redah[2], T. J. Udovic[3], B. Hjörvarsson[4],
[1] Dept.of Physics, Uppsala University, Sweden
[2] I.N.Stranski-Institute for Physical and Theoretical Chemistry, Technical University, Berlin, Germany
[3] Materials Science and Engineering Laboratory, NIST, Gaithersburg, USA
[4] Dept.of Materials Physics, Royal Institute of Technology, Stockholm, Sweden

Earlier experiments on $NbH_{0.8}$ and $PdH_{0.6}$ [1] have shown large anomalies in the cross sections for protons, when studied by neutron Compton scattering. Here, these investigations are extended to the metallic hydrides YH_2, YH_3, YD_2 and YD_3 and $Y(H_xD_{1-x})_2$. Strongly reduced cross sections for hydrogen are observed both in YH_2 and YH_3, but only minor ones for YD_2 and YD_3. The scattering time depends on the neutron scattering angle [1], which allows a time-differential analysis where the time window lies around one femtosecond. The anomalies persist longer in YH_2 and YH_3 than in $NbH_{0.8}$ and $PdH_{0.6}$. The reduced cross sections are interpreted as a result of quantum entanglement between protons, surviving for a few fs in the solids. [1] E. B.Karlsson, C. A. Chatzidimitriou-Dreismann, T. Abdul Redah, R. M. F.Streffer, B. Hjorvarsson, J. Ohrmalm, and J. Mayers, Europhys.Lett.,46 (1999) 617.

B-153 Irradiation Stimulated Phase in Titan Hydride $TiH_{1.95}$

I. Khidirov[1], N. Mukhtarova[1], K. Baktibaev[1], U. Gafurov[1],
[1] Institute of Nuclear Physics, Tashkent 702132, Uzbekistan

Gamma -irradiation stimulated phase transition FCC→VCT in titan dihydride TiH_2 (irradiation temperature T∼100°C) by X-ray- and neutron - diffraction methods has been shown. Ti and H atoms coordinates were determined using the Rietveld method analysis of neutron diffraction data. The founded phase was metastable and transites into stable FCC phase that corresponds to equilibrium phase diagram of Ti-H system at temperatures T $\geq$37°C. The similar VCT structure has been found at T$\leq$ 37°C by other authors: it was a result of temperature effect. Gamma-irradiation increase the phase transition temperature; the radiation-stimulated phase differs from termo-stimulated phase.

B-154 Crystal Structure and Phase Transformations of solid Solutions Ti-N-H and Ti-N-D

I. Khidirov[1], U. Gafurov[1],
[1] Institute of Nuclear Physics, Tashkent Ulugbek 702132, Uzbekistan

Phase correlation and structure peculiarities of phase in the solid solution for Ti-N-H and -Ti-N-D systems by neutron and X-ray diffraction methods has been investigation. All the systems had order-disorder phase transition so distribution of nonmetal atoms depends on temperature. The new ordered monoclinic phase $Ti\text{-}2N_{1-x}H(D)_{2-x}$ was found and crystal structure was determined. It was shown the different solid solutions TiN0,26Ho,15 and TiN 0,26D 0,15 were isostructural at the high temperature (1270 K) and nonmetal atoms arrangement in interstitials was identical.

B-155 Effect of ordering of the oxygen in Ti-O-H on localization of hydrogen

S. Morozov[1], N. Primakov[1], V. Semenov[1],
[1] Institute for Physics and Power Engineering, Obninsk, Russia

The results of dynamics investigation of the hydrogen and oxygen atoms in Ti-O-H alloys are presented for different temperatures and concentrations of impurities. It is shown that the hydrogen dissolve in a hexagonal matrix of metal only , when alloy has formed ordered on oxygen superstructure. Part of hydrogen is precipitates in hydride phase $TiH_{1.5}$ at the concentration of oxygen less then 10 at.% because the alloy is not ordered totally. The other part is remaining in α-phase. The low-temperature measurements show that the α-phase Ti-O-H is stable up to 10K. The present research is supported by Russian Foundation of Basic Research, grant No. 01-02-96001

B-156 Combination of SANS and 3D Stochastic Reconstruction Techniques for the Study of Equilibrium and Dynamic Properties of Nanostructured Materials

E. S. Kikkinides[1], K. Stefanopoulos[2], T. Steriotis[2], N. Kanellopoulos[2], W. Treimer[3],
[1] CPERI/CERTH, 6th km. Charilaou-Thermi Rd, 57001 Thermi-Thessaloniki, Greece
[2] NCSR "Demokritos", 153 10 Agia Paraskevi Attikis, Greece
[3] HMI, Glienicker Strasse 100, 14 109 Wannsee, Berlin

Ceramic nanostructured materials have recently received scientific and industrial interest due to their unique properties. A series of such nanoporous structures were characterised by SANS techniques carried out at HMI, Berlin. The resulting scattering curves were analysed to obtain basic structural information regarding pore size distribution and autocorrelation function of each material. Furthermore, stochastic reconstruction models were employed to generate 3D images with the same basic structural characteristics obtained from SANS. Finally, simulation results of diffusion on the reconstructed images provide very good agreement with experimental data obtained on the actual materials.

B-157 Grain Size Dependent Atomic Dynamics of Nanocrystalline $Ni_{80}P_{20}$

S. Mentese[1], J.-B. Suck[1], V. Reat[2],
[1] TU Chemnitz, Institute of Physics, Materials Research and Liquids, D - 09107 Chemnitz
[2] Institut Laue-Langevin, B.P. 156, 38042 Grenoble Cedex 9 - France

We investigated the influence of the grain size (grain boundary fraction) on the atomic dynamics of nanocrystalline materials. The nano-scaled materials were obtained by crystallizing amorphous starting material of the same chemical composition. The inelastic neutron scattering experiments were performed at the time-of-flight spectrometer IN 5 (ILL, Grenoble). From the time-of-flight spectra we determined the generalised vibrational density of states and the dynamic structure factor. In reference to the polycrystalline sample the nanocrystalline material show an enhancement in the low energy region (below 15 meV) of the density of states. The difference is larger the smaller the grain size.

B-158 Vibrational and magnetic properties of supersaturated $Cu_{100-x}Fe_x$

F. Jurányi[1], J.-B. Suck[1], S. Janssen[2],
[1] TU-Chemnitz, Institute of Physics, Materials Research and Liquids,D 09107 Chemnitz, Germany
[2] Paul Scherrer Institute, Laboratory for Neutron Scattering,CH 5232 Villigen, Switzerland

We investigated the atomic dynamics and the magnetic properties of the $Cu_{100-x}Fe_x$ system. Samples with nominal Fe concentration of 5, 17.5, 30 and 45 at% were prepared in the same manner by mechanical alloying in a planetary ball mill. All samples are nanocrystalline supersaturated solid solutions, without crystalline Fe phase and amorphous matrix. The inelastic neutron scattering measurements were performed at room temperature at FOCUS (PSI, SINQ). In the dynamic structure factor with increasing Fe concentration we observe enhanced intensities at low energies. Furthermore one can see a shift towards higher energies and a broadening of transverse and longitudinal modes.

B-159 Study of the Nanocrystalline Ball Milled $Cu_{80}(Fe_{0.3}Co_{0.7})_{20}$ Compound

S. Galdeano[1], M.H. Mathon[1], L. Chaffron[2], C.H. de Novion[1],
[1] Laboratoire Léon Brillouin, Bat. 563, CEA Saclay, F-91191 Gif-sur-Yvette
[2] Section de Recherches de Métallurgie Physique, Bat. 520, CEA Saclay, F-91191 Gif-sur-Yvette

The aim of this work is to study the influence of the ball milling temperature and intensity on the nanostructure of the $Cu_{80}(Fe_{0.3}Co_{0.7})_{20}$ compound. The ball milling of powders of Cu-Fe and Cu-Co supersaturated solid solutions allows the formation of a very fine $Fe_{30}Co_{70}$ precipitation in the Cu matrix, interesting for its magnetoresistive properties. Powder neutron diffraction and SANS, coupled to magnetic measurements and EXAFS experiments, allowed to correlate the ball milling conditions to the nanostructure and the magnetic properties of the ternary compound.

B-160 Nanostructures and magnetic correlation in Ferrofluids studied by SANS

A. Hoell[1], M. Kammel[1], A. Wiedenmann[1],
[1] Hahn Meitner Institute Berlin, Glienickerstrasse 100 D-14109 Berlin Germany

New magnetic colloids ("ferrofluids") susceptible for medical applications have been prepared based on nanoparticles of Co or Fe_3O_4 and stabilised electrostatically or by coating with various types of surfactants. Small Angle Neutron Scattering measurements have been performed at the instrument V4 at the BERII reactor of the Hahn-Meitner-Institute, Berlin using polarised neutrons (SANSPOL)[1]. The combination of SANSPOL with conventional contrast variation using different H/D mixtures of the carrier liquid allowed the unknown structure and size distributions of core and shell and magnetic structures to be determined. Inter-particle correlation have been evaluated as a function of concentration and external magnetic field and by freezing the carrier liquid. Work supported by the DFG program WI1151/2-1) [1] A. Wiedenmann, J. Appl. Cryst. 33 (2000)428-432

B-161 Neutron diffraction study of (Co-Ti) substituted Ba-hexaferrite fine particles

Z. Somogyv[1], Gy. Mészáros[1], E. Somogyvári[1], K. Krezhov[2], F. Bour[3], I. Nedkov[4],
[1] Research Institute for Solid State Physics and Optics, H-1525 Budapest, POB 49, Hungary
[2] Institute for Nuclear Research and Nuclear Energy, BU-1784 Sofia, Bulgaria
[3] LLB CEA-CNRS CEN Saclay, 91191 Gif-sur-Yvette, France

[4] Institute of Electronics BU-1784 Sofia, Bulgaria

In recent years use of nanoparticle systems is of enhanced interest in the efforts to achieve higher recording density. In this paper we report the effect of nanometric grain sizes on the structural parameters of $BaFe_{12-2x}Co_xTi_xO_{19}$, ($x$ = 0.45 - 0.85) based on neutron diffraction measurements. The structure of pure $BaFe_{12}O_{19}$ hexaferrite ($P6_3mmc$ space group, block type ferrimagnetic spin arrangement) was adopted in the Rietveld full profile analysis. Beside the sublattice substitution rates the atomic position parameters and the magnetic moment values were determined. The detailed crystallographic and magnetic structural parameters are presented and discussed by comparing nano- and microcrystalline samples.

B-162 Structure and Subatomic Properties of Nanocrystalline $LaMnO_3$

S. G. Bogdanov[1], E. Z. Valiev[1], A. N. Pirogov[1], A. E. Teplykh[1], A. A. Ostroushko[2], A. E. Udilov[2],
[1] Institut of Metal Physics, 18, Kovalevskaya St., 620219 Ekaterinburg, Russia
[2] Institut of Physics and Applied Mathematics, USU, 620083 Ekaterinburg, Russia

Samples of nanocrystalline $LaMnO_{3+\delta}$ were synthesized by pyrolysis of polymer-salt compounds. Those were annealed at various temperatures up to T_{an}=1100°C in air for 4 h. For the samples annealed at $T_{an} < 600$°C, nonstoichiometry parameter $\delta \leq 0.1$ and $\delta \cong 0.16$ for the others. They were investigated by neutron and X-ray diffraction and by small angle neutron scattering (SANS). It was found that the annealed at $T_{an} \geq 600$°C samples are crystallized in rhombohedral syngony (space group $R\bar{3}c$) and the others have double-phase structure (orthorhombic Pnma + rhombohedral). Diffraction peaks are broadened by reason of small value of coherent block size. As follows from SANS and broadening peak magnitude, the particle size is about 20 nm at the low T_{an}. It increases with annealing and becomes $\geq$ 100 nm at $T_{an} = 1100$°C. The investigated samples have surface fractal properties with fractal dimension D_S=2.6-2.2. The work was partially supported by SSTP (No. 107-19(00)-P-DO1) and RFBR 00-02-16211.

B-163 The recrystallisation of amorphous Er_7Fe_3

P. Manuel[1], S. Kilcoyne[1],
[1] Dept of Physics and Astronomy, University of Leeds, Leeds LS2 9JT, UK

In our studies of binary rare earth - transition metal phase diagrams using kinetic neutron techniques, we have adopted a novel preparation technique involving annealing amorphous precursors in the neutron beam and monitoring the subsequent phase formation and transformations via neutron thermograms. Here we present an in-beam neutron diffraction study of the initial crystallisation, phase formation and subsequent transformation of an amorphous Er_7Fe_3 alloy. The final product of the crystallisation process is the well known C15 Laves phase compound $ErFe_2$, however there are indications of the formation of a hitherto unreported intermetallic compound at intermediate temperatures. The neutron data are complemented by Mössbauer spectroscopy measurements of the precursor material and final $ErFe_2$ phase.

B-164 A kinetic neutron diffraction study of the recrystallisation of amorphous Y_7Co_3

S. Kilcoyne[1], P. Manuel[1],
[1] Department of Physics and Astronomy, University of Leeds, Leeds LS2 9JT, UK

The reported Y-Co equilibrium phase diagram is rich in intermetallic phases. However, the details of this phase diagram are generally established in far from equilibrium conditions. Here we adopt a novel kinetic neutron diffraction technique of studying the development of intermetallic Y-Co phases in-beam via observation of the crystallisation and subsequent phase formation and transformation of an amorphous Y_7Co_3 precursor.

B-165 SANS and TEM Investigation of Photoluminiscent Si Nanoparticles Obtained by Laser-induced Synthesis

S. Botti[1], R. Coppola[2], F. Gourbilleau[3], R. May[4], R. Rizk[3], M. Valli[5],
[1] ENEA-Frascati, FIS, CP 2400, 00100 Roma - Italy
[2] ENEA- Casaccia, FIS, CP 2400, 00100 Roma - Italy
[3] LERMAT, ISMRA, 14050 Caen - France
[4] ILL, 156X 38042 Grenoble -France
[5] ENEA-Bologna, FIS, V. Don Fiammelli 1, 40138 Bologna -Italy

Nanometer-sized Si particles synthesized by laser-induced de composition of gas precursors are very promising for Si-based optoelectronic devices. The Si nanoparticles were characterized by small-angle neutron scattering (SANS) and conventional and high resolution transmission electron microscopy (TEM & HREM) to determine how their size distribution, in relation with the preparation conditions. The particle average size and width distribution, obtained by the SANS measurements performed by the D22 instrument at Institut Laue Langevin (Grenoble, France) were compared to the size histograms deduced from TEM and HREM observations. Both kinds of data were subsequently correlated to the photoluminescence spectra. The role of interference effects arising form interparticle spatial correlations is also discussed.

B-167 The Premartensite Phenomena in Quenched $Ti_{49}Ni_{51}$

S. Teploukhov[1], S. Dubinin[1], V. Parkhomenko[1], V. Grishkov[2], A. Lotkov[2],
[1] Institute for Metal Physics, Kovalevskaja Str. 18, Ekaterinburg, 620219, Russia
[2] Institute of Strengh Physics and Material Science, Academicheskii Av.2/1, Tomsk, 634021, Russia.

The atomic structure of single crystal $Ti_{49}Ni_{51}$ was investigated by neutron diffraction method. The martensitic transformation from cubic (B2) to monoclinic (B19) phase take place at 175K after qwenching from 1120K to water. It is shown for the first time that the short order of atomic distortions in initial cubic phase is observed up to 420K. The largest diffraction effects take place at (111) reciprocal lattice plane. The wave vector of atomic distortions in quenched alloy corresponded 1/5211 at 300K. The role of premartencitic phenomena in mechanism reconstructive transformation is discussed. The work was partially supported by STTP (No 107-19(00)-I-D01.

B-168 Pressure-induced Structural Phase Transition in $NdAl_xGa_{2-x}$

Th. Straessle[1], D. P. Kozlenko[2], V. P. Glaskov[3], B. N. Savenko[2], K. Conder[1], A. Furrer[1],
[1] Laboratory for Neutron Scattering, ETHZ & PSI, CH-5232 Villigen, Switzerland
[2] Frank Laboratory of Neutron Physics, JINR, Dubna, Russia
[3] Russian Scientific Center Kurchatov Institute, Moscow, Russia

High-pressure neutron diffraction experiments on the Laves phase $NdAl_xGa_{2-x}$ revealed a pressure-induced isostructural phase transition for

$x = 1.00$ and 1.08 above about 1.5 GPa at room temperature. Within its hexagonal AlB_2 structure the compound changes its lattice ratio c/a discontinuously from 0.96 to 0.84 in analogy to chemical pressure for $x > 1.12$. Pressures up to 5.2 GPa did not result in a pure high-pressure phase but rather in a mixture of both phases. The intermetallic MN_2 phases of the AlB_2 structure are known to appear in two distinct groups with different c/a ratios. The observed isostructural transition is discussed within the framework of near-neighbor diagrams.

B-169 Neutron depolarization study on the austenite/pearlite transformation in steel

S. E. Offerman[1,2], L. J. G. W. van Wilderen[1,2], N. H. van Dijk[1], M. Th. Rekveldt[1], J. Sietsma[2], S. van der Zwaag[2],
[1] IRI, NM, TU Delft, Mekelweg 15, 2629 JB Delft, The Netherlands
[2] TNW, TU Delft, Rotterdamseweg 137, 2628 AL Delft, The Netherlands

Three-dimensional neutron depolarization experiments have been performed in order to study the isothermal phase transformation from austenite into pearlite in eutectoidic steels. The polarization rotation during transmission through the sample is a measure of the ferromagnetic ferrite fraction, while the degree of depolarization determines the characteristic length scale of the lamellar pearlite microstructure. The rate of transformation is strongly dependent on the amount of undercooling. The relation between the evolving microstucture and the corresponding magnetic structure of the ferrite phase will be discussed.

B-170 Low temperature phase transition in the $Cs_5H_3(SO_4)_4 \times 0.5H_2O$ crystal

S. Lushnikov[1], P. Fischer[2], S. Gvasaliya[1], A. Balagurov[3], V. Pomjakushin[3],
[1] A.F.Ioffe Physical Technical Institute, RAS, St.Petersburg, Russia
[2] PSI, Villigen, Switzerland
[3] FLNP, JINR, Dubna, Russia

The crystals of $Cs_5H_3(SO_4)_4 \times 0.5H_2O$ (PCHS) have $P6_3/mmc$ symmetry at room temperature. At the lowering of the temperature the quasi-two-dimensional glass-like state in PCHS is realized. Using the HRPT (PSI, Villigen) diffractometer the structure of PCHS compound has been studied in the temperature range of 20 - 300 K. The appearance of additional reflexes which do not correspond to the $P6_3/mmc$ symmetry was observed. At present report the results of PCHS structure refinement will be presented. The possibility of the structure phase transition for the materials with glassy behavior will be discussed.

B-171 Structure and Transformations of Metastable Phases in (Zr,Ti)-(Nb,V) alloys

G. J. Cuello[1], G. Aurelio[2], A. Fernández Guillermet[2], J. Campo[3],
[1] Institut Laue-Langevin, F-38042 Grenoble, France
[2] CONICET, Centro Atómico Bariloche, 8400 Bariloche, Argentina
[3] Instituto de Ciencia de Materiales de Aragón, CSIC-Univ. de Zaragoza, 50009 Zaragoza, Spain

An experimental study is presented of the effect of an isothermal heat-treatment upon the structural properties of three metastable phases in (Zr,Ti)-(Nb,V) alloys, viz. α (hcp), β (bcc) and Ω, formed by quenching them from 1273K. By neutron diffraction, the constitution of the aged alloys and the structural parameters of the resulting aged phases were determined. The approach combines the lattice parameters measurements with previously established correlations in Zr-Nb and Ti-V alloys. In such way, new information on the composition of the aged phases was obtained. For long aging times the α and β phases seem to be approaching metastable equilibrium conditions. These results open up the possibility of using quenching-and-aging experiments to gain insight into the metastable phase diagram of these systems.

B-172 In-situ Neutron Diffraction Studies of Martensitic Transformations in NiTi Polycrystals upon Thermomechanical Loading

P. Lukás[1], P. Sittner[2], D. Neov[1], D. Lugovyy[1], M. Ceretti[3],
[1] Nuclear Physics Institute, 250 68 Rez, Czech Republic
[2] Institute of Physics, Na Slovance 2, Prague 8, 182 21, Czech Republic
[3] Laboratoire Leon Brillouin (CEA/CNRS), CE Saclay, 91191 Gif sur Yvette, France

Functional thermomechanical behaviors of martensitically transforming shape memory alloys are exploited for sensing, actuating or vibration control purposes in engineering applications. We have performed in-situ neutron diffraction experiments on NiTi polycrystalline alloy at dedicated stress/strain diffractometers equipped with thermomechanical testing device. The macroscopic data (stress, strain, temperatures) together with the diffraction data (lattice strains, phase compositions) collected during thermal, mechanical and thermomechanical recovery stress cycles characterize progress of the phase transformations processes between cubic B2 ordered austenite phase, rhomboedral R-phase and monoclinic B19' martensite phase in NiTi.

B-173 Neutron Diffraction Study of Stress Induced Martensitic Transformation in TRIP Steel

E. C. Oliver[1], P. J. Withers[1], M. R. Daymond[2], S. Ueta[3], T. Mori[1],
[1] Manchester Materials Science Centre, University of Manchester and UMIST, UK
[2] ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, UK
[3] Daido Steel Company Ltd, Nagoya, Japan

Neutron diffraction has been used to follow *in situ* the stress induced martensitic transformation during uniaxial tensile testing of Fe-25%Ni-0.4%C polycrystals. This method provides data on the extent of transformation, the development of crystallographic texture, and the evolution of lattice strain. Two types of specimen were examined: unswaged, and swaged at 200°C. The swaged material was further aged with greater yield strength, enhancing the transformation. Moreover, it exhibited stronger texture than the unswaged material. The extent of transformation is shown to be dependent on grain orientation. For example, in the swaged material, grains with $\langle 100 \rangle$ parallel to the tensile axis transform preferentially. Correspondingly, the majority of martensite grains formed have $\langle 110 \rangle$ along the loading direction. Analysis of the unswaged material behaviour is complicated by the extensive plastic deformation which precedes deformation, and the associated residual stresses and grain rotations.

B-174 Structural study of the high-temperature phases of the hexagonal perovskite $KCoCl_3$.

D. Visser[1,2,3], R. G. Delaplane[4], S. Levitt[1],
[1] Department of Physics, The University of Warwick, Gibbet Hill Road, Coventry CV4 7AL, UK
[2] IRI, Technical University Delft, Mekelweg 15, 2629JB Delft, The Netherlands
[3] CLRC, ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot OX11 0QX, UK

[4] Studsvik, Neutron Research Laboratory,Uppsala University, S- 61182 Nykoping, Sweden
Between room-temperature and its melting point at 625K, DSC measurement show that $KCoCl_3$ undergoes structural phase transitions at 398K and 593K. Neutron powder diffraction shows that the phase transition at 398K involves a unitcell volume change by a factor 3: aV3 × aV3 × c to a × a × c. The unit cell dimensions donot change at 593K. A comparison between the structural disorder of K-cation in the hexagonal perovskite $KNiCl_3$ (Physica B 276-278 (2000) 300-1) and K-cation disorder $KCoCl_3$ is presented.

B-175 The Equilibria in the AlN-Al_2O_3-Y_2O_3 Ternary System - Thermodynamic and Neutron Diffraction

M. Medraj[1], R. Hammond[3], J. Root[3], W. T. Thompson[2], R. A. L. Drew[1],
[1] McGill University, Montreal, Quebec, Canada
[2] Royal Military College, Kingston, Ontario, Canada
[3] Neutron Program for Materials Research, National Research Centre, Chalk River, Ontario, Canada
Aluminum nitride (AlN) is currently used in electronic packaging and engineering ceramics. It offers both higher thermal conductivity and superior electrical insulating properties compared with Al_2O_3. Yttria (Y_2O_3) is the best additive for AlN sintering, and it has been shown that AlN densifies by a liquid phase mechanism, where the surface oxide, Al_2O_3, reacts with the oxide additive, Y_2O_3, to form a Y-Al-O-N liquid that promotes particle rearrangement and densification. Construction of the phase relations in this multicomponent system is becoming essential for further development of the AlN. Binary diagrams of Al_2O_3-Y_2O_3, AlN-Al_2O_3, and AlN-Y_2O_3 were thermodynamically modeled. The obtained Gibbs free energies of components, stoichiometric phases and solution parameters were used for the calculation of isothermal sections and liquidus surface of AlN-Al2O3-Y2O3 system. The predicted ternary phase diagram was verified experimentally using in situ high temperature neutron diffractometry. The ternary phase diagram AlN-Al_2O_3-Y_2O_3 has been constructed for the first time in this work.

B-176 Neutron Diffraction Study of $K(H_{1-x}D_x)_2PO_4$

S. A. Kim[1], Y. N. Choi[1], C. H. Lee[1],
[1] HANARO Center, Korea Atomic Energy Research Institute, Taejeon 305-600, Korea
As the four circle diffractometer (FCD) has been set up in HANARO at the Korea Atomic Energy Research Institute, it has become possible to study single crystal structure by means of the neutron diffraction in KOREA. $K(H_{1-x}D_x)_2PO_4$ (DKDP) single crystals were grown from D_2O with reagent KH_2PO_4 and the crystal structure was determined as the practical sample. The crystals are tetragonal at room temperature with lattice parameters of a=7.4633(7), c=6.9785(5)Åand Z=4. Intensity data were collected on the FCD with Ge(331) monochromated neutron beam (λ=0.997Å). The structure was refined to final R and wR values of 0.041 and 0.096, respectively. In this crystal 66% of H-positions were substituted by D and the rest 34% occupied by H. The phase transition temperature of DKDP obtained with deuteration levels is 193K. This value agrees fairly well with the result of Differential Scanning Calorimetry measurement. The nuclear density distribution provides an observation of the disordered state of D/H in DKDP. Powder diffraction patterns were obtained from room temperature to 10K by the high resolution powder diffractometer in HANARO. The low temperature phase transition from the tetragonal to the orthorhombic was observed between 190 and 195K. This result agrees well also with the results of DSC and single crystal measurements. On cooling, the nuclear density distribution provides an observation of the disordered to the ordered state of D/H.

B-177 Phonon softening preceding the forward and reverse martensitic transformation in Ni_2MnGa

U. Stuhr[1], P. Vorderwisch[2], V.V. Kokorin[3],
[1] Paul Scherrer Institut, 5232 Villigen, Switzerland
[2] Hahn-Meitner-Institut, 14109 Berlin, Germany
[3] Institute of Magnetism, 252680 Kiev, Ukraine
Ni_2MnGa is the only Heusler alloy known to undergo a martensitic transformation in the ferromagnetic state. The transformation is associated with the shape-memory and a huge magnetostrain effect, which makes this alloy a promising actuator material. The transformation temperature T_M and other transformation characteristics are, in contrast to the Curie temperature, strongly influenced by deviations from the stoichiometric composition. We have investigated precursor phenomena of the forward transformation (phonon softening, "central peak") for a single crystal with T_M near room temperature. We furthermore succeeded to produce a nearly single-variant martensite which allowed, for the first time, the detailed investigation of phonon softening phenomena preceding the reverse transformation.

B-178 The First Observation of Boson Peak from Water Vapour Deposited Amorphous Ice

J. Li[1], A. Kolesnikov[1,2],
[1] Department of Physics, UMIST, P.O. Box 88, Manchester M60 1QD, UK
[2] IPNS, Argonne National Laboratory, 9700 S. Cass Av., Argonne, IL 60439, USA
Boson peak in the vibrational spectra of amorphous materials (e.g. silica) is a subject attracted considerable scientific attention in recent years. The excess of low-energy vibrational modes (the so-called Boson peak) coexisting with the sound waves from crystalline spectrum is still unresolved mystery. Understanding the physical mechanism of the source of the low-energy excitations is fundamentally important for us to understand the structure and dynamics of the amorphous materials. In this paper, we report the first observation of the Boson peak in the inelastic incoherent neutron scattering (IINS) spectrum from a low-density amorphous (LDA) form of ice obtained by vapour deposition on a cooled substrate (at 20 K) with low flow-rate (∼14 mg/h). The IINS spectrum of vapour deposited amorphous (VDA) ice clearly shows the low-energy excess excitations centred at 4 meV, while there was no excess scattering from other LDA ices studied before, which were obtained either by annealing the high-density amorphous ice or by hyper-quenching of water droplets of -size. In addition, the integrated intensity of the acoustical peak in the IINS spectrum for VDA ice (1-15 meV) is also noticeably larger compared to that for ice-Ih (by about 5%). The observation indicates that the Boson peak in VDA ice spectrum is more likely due to the broken hydrogen bonds in the glass material.

B-179 Partial dynamic structure factors in $Ni_{62}Nb_{38}$ metallic glass.

G. Syrykh[1], M. Zemlyanov[1], A. Ivanov[1,2],
[1] RRC "Kurchatov Institute", 1, Kurchatov sq., Moscow, RUSSIA
[2] ILL 6, rue Jules Horowitz, BP 156 X, F-38042, Grenoble Cedex 9, FRANCE
The total dynamic structure factors S(Q, E) in three $Ni_{62}Nb_{38}$ samples with different isotope content were investigated by inelastic neutron scattering, over a range of momentum and energy transfer: Q = 0.5-5 $Å^{-1}$ and E = 1-40 meV at IN6 spectrometer (ILL, Grenoble, France).

According to the Ashcroft-Langreth formalism [I], the partial structure factors S_{NiNi}(Q, E) S_{NbNb}(Q, E) and S_{NiNb}(Q, E) were reconstructed. It is the first experimental observation showing the existence of collective vibrational excitations in $Ni_{62}Nb_{38}$ metallic glass at partial level. [1] N.W. Ashcroft, D.C. Langreth - Phys. Rev. 159 (1967) 500

B-180 The effect of small angle scattering of thermal neutrons of titanium nickelide amorphized by fast neutrons

V. Parkhomenko[1], S. Bogdanov[1], S. Dubinin[1], S. Teploukhov[1],
[1] Institute for Metal Physics, S.Kovalevskaia Str.18, 620219, Ekaterinburg, Russia

Recently we suggested a model for titanium nickelide amorphized by fast neutrons. In the case of fast neutron effect, the amorphous structure of the alloy are results from the chaotic displacements of atoms from original crystal lattice sites. Atomic displacement centres in a crystal are combinations of the substitution defects and vacancies. This work was aimed to verify experimentally some statements of the model and, especially, to find micro-areas of a higher vacancy concentration in titanium nickelide amorphized by fast neutrons. The single crystal of Ti49Ni51 amorphized by fast neutrons, and the amorphous ribbon of the titanium nickelide-based alloy Ti50Ni25Cu25 quenched from a melt, were investigated. The effect of small angle scattering of thermal neutrons was detected only in the titanium nickelide irradiated by fast neutrons. Small angle scattering sections were calculated by the model of fractal clusters. Using the values of the correlation length, 2R=150A, the volume fraction of clusters, V=1%, and the vacancy concentration in a cluster, Cvac=10%, gave a good fit to the experimental data. The work was partially supported by STTP(No 107-19-(00)--D01) and RFFI(No 01-02-16877).

B-181 Structural studies on Na_2O-TeO_2-GeO_2 glasses

P. Balaya[1], P. S. R. Krishna[2], B. A. Dasannacharya[1],
[1] IUC-DAEF,Mumbai Centre, BARC, Mumbai 400085, India
[2] SSPD, BARC, Mumbai 400085, India

Structure of glasses $(Na_2O)_{0.2}$-$(TeO_2)_{0.8}$ (NT), $(Na_2O)_{0.2}$-$(GeO_2)_{0.8}$ (NG) and $(Na_2O)_{0.2}$-$(TeO_2)_{0.4}$-$(GeO_2)_{0.4}$ (NTG) has been studied using neutron diffraction up to 14.5 $Å^{-1}$. Analysis of our neutron data using Monte Carlo g(r) (MCGR) method revealed that NT mainly consists of TeO_4 and TeO_3 units with longer and shorter Te-O bonds. NG network is made up of GeO_4, GeO_5 and GeO_6 units. The mixed glass NTG consists of $Te_2O_5{}^{2-}$, GeO_4, GeO_5 and GeO_6 groups. $Te_2O_5{}^{2-}$ is made up of only TeO_3 and the long distance Te-O correlation has disappeared in NTG. It seems that local structure of NT melt, consisting of TeO_3 and Te_2O_5 units gets frozen in NTG due to the presence of GeO_2. Correlation with our Raman scattering measurements and with other physical properties will be attempted.

B-182 The effect, studied by SANS, of rapid quenching from ambient to subambient temperatures on the microstructure of some metallic glass ribbons

M. Calvo-Dahlborg[1], U. Dahlborg[1], F. Haeussler[2],
[1] Laboratoire de Science et Génie des Matériaux et de Métallurgie, Ecole des Mines de Nancy, F-54042 Nancy Cedex, France
[2] Institut für Massivbau und Baustofftechnologie, Universität Leipzig, D-04109 Leipzig, Germany

Small Angle Neutron Scattering (SANS) experiments have been performed on NiP and FeCoB metallic glass ribbons produced after different heat treatments of the melt. It was observed that a rapid quenching from ambient to liquid nitrogen temperature has a strong effect on the microstructure in a size range of 1 to 60 nm. Furthermore, after a subsequent heating to ambient temperature the microstructure has been found to be different from what it was before the quench. However, similar experiments performed on a ribbon containing of the order of 2% crystalline inclusions of an average size of about 15 nm revealed no effect. A detailed comparison of the microstructures using various correction and simulation programmes is presented.

B-183 Dynamic Correlations around the Glass Transition in Systems with different Degrees of Fragility.

O. Russina[1], M. Russina[2], F. Mezei[1,2], C. Dreyfus[3],
[1] Hahn-Meitner Institute Berlin, Glienicker Str.100, 14109 Berlin, Germany
[2] Los Alamos National Laboratory, MS H805, Los Alamos, NM 87545, USA
[3] Université Pierre et Marie Curie 4, Place Jussieu 75252 Paris cedex 05, France

We have investigated two ionic salt systems with different degrees of fragility, $Ca_{0.8}K_{1.4}NO_3$ (CKN) and $ZnCl_2$ by cold neutron spectroscopy. Using a new approach for multiple scattering correction we were able to analyse the microscopic dynamics in an extended range of Q, in particularly in the range of wave numbers corresponding to the length scale of several atomic distances and inaccessible up to now. The spectra were studied in detail around the glass transition temperatures. Vibrations dominate the dynamics in both systems below Tg. In CKN Boson peak has been observed for the first time by neutron scattering. With increasing temperature a strong anharmonic intensity in the picosecond range was observed in CKN, but it was absent in $ZnCl_2$. We have concentrated on the dynamics in the Q range of the intermediate range order, longest distance of structural correlations in disordered systems. The results reveal the first direct experimental evidence for the existence of heterogeneous correlated atomic motion in the supercooled liquid state and prove the relaxational nature of so-called picosecond processes around the glass transitions, being the subject of a decade old controversy. We will also discuss possible explanations of the marked difference in the dynamic behaviour of CKN and $ZnCl_2$.

B-184 Structural studies on PbO-TeO_2 glasses

P. S. R. Krishna[1], S. L. Narasimhan[2], V. Sudarsan[3],
[1] Solid State Physics Division, BARC, Mumbai-400085, India
[2] High Pressure Physics Division, BARC, Mumbai-400085, India
[3] Novel Materials and Structural Chemistry Division, Mumbai-400085, India

We present the structural studies on (x)PbO – (1-x)TeO_2 glasses for x=0.1,0.2 and 0.3 using Neutron Diffraction up to a $Q_{max} = 14Å^{-1}$ and correlate the results with the ^{125}Te NMR studies on these glasses. Analysis of the neutron data using Monte Carlo g(r) (MCGR) method reveals that the short range order in our glasses is consistent with the network having building blocks of TeO_4 polyhedra at lower x=0.1 and TeO_3 polyhedra at x=0.3. At x=0.2 TeO_{3+1} units with one long bond are prevalent. A small shoulder at $Q \approx 1.4Å^{-1}$ is building up as x increases which shows that Intermediate range order is going up.

B-185 Pressure Induced Change of Atomic Dynamics in Densified GeO_2 Glasses

K. Shibata[1], K. Suzuya[2], N. Umesaki[3], N. Kitamura[4], S. Kohara[3],
[1] Institute for Materials Research, Tohoku University, Katahira,Aoba, Sendai 980-8577, Japan
[2] Japan Atomic Energy Research Institute, Tokai, Naka, Ibaraki319-1195, Japan
[3] Japan Synchrotron Radiation Research Institute, Mikazuki, Sayo,Hyogo 679-5198, Japan
[4] Osaka National Research Institute , Midorigaoka, Ikeda, Osaka563-8577, Japan

Neutron inelastic measurements have been performed on normal and pressure-compacted GeO_2 glasses using LAM-D spectrometer at KENS spallation pulsed neutron source. Four cylindrical GeO_2 samples, which had been subjected to pressures 0 (ambient pressure), 2 , 4, and 6 GPa, respectively, were studied. The boson peak of the dynamical structure factor, S(Q,E), shifts higher energy transfer magnitude with increasing density (preparation pressure), indicating a modification of the intermediate range order resulting from a compaction of the germania rings. The vibrational density of states, G(E), does not change drastically on densification, except for an energy shift of spectrum.

B-186 DMPC membrane and mixed DMPC/C12E8 micelles orientation in strong magnetic fields

M.A. Kiselev[1], M. Janich[2], P. Lesieur[3], A. Hoell[4], J. Oberdisse[5], J. Pepy[5], T. Gutberlet[4],
[1] FLNP, JINR, Dubna, Russia
[2] Martin Luther University, Halle, Germany
[3] LURE, Orsay, France
[4] HMI, Berlin, Germany
[5] LLB, Saclay, France

The orientation of lipid membranes in magnetic fields can be helpful to understand the structure orientation behavior of mixed lipid/surfactant aggregates and pure lipid membranes, which is of specific interest in medical and fundamental applications. The orientation of DMPC multilamellar vesicles above and below the main phase transition and of mixed DMPC/C12E8 micelles at different detergent concentrations in strong magnetic fields was studied via SANS for magnetic field range of 0-4T. The results for the mixed lipid/surfactant system show with increase of the magnetic field a change of the structure of a Gaussian coil of rod-like micelles. The isotropic coil structure is strained under the magnetic field to a more anisotropic one. In the case of spherical-like micelles no orientation effect was detected.

B-187 A Neutron Diffraction Study of Hydration Effect on Stratum Corneum

G. Charalambopoulou[1], T. Steriotis[1], T. Hauss[2], K. Stefanopoulos[1], A. Stubos[1],
[1] NCSR "Demokritos", 153 10 Agia Paraskevi Attikis, Greece
[2] HMI, Glienicker Strasse 100, 14 109 Wannsee, Berlin

The primary barrier to transdermal diffusion resides in Stratum Corneum (SC), the outer layer of skin which consists of an array of keratin cells embedded in a multilamellar lipid domain. SC hydration is important in determining the rate of percutaneous permeability. Despite its great importance, the actual mechanism of water-SC interaction is yet unresolved. Recently, membrane neutron diffraction was employed aiming to reveal important structural details of SC and ultimately enable the localization of water molecules in the two phases of the tissue. The resulting scattering pattern of hydrated SC depicts a strong diffraction peak at Q=1 nm^{-1}, corresponding to a periodicity of 6.28 nm. A slight shift of the peak towards lower Q was observed upon prolonged deuteration. This behavior implies that excess hydration might disturb to some extend the organisation of the lamellar structure.

B-188 Structural characterization of phosphatidylcholine-diacylglycerol system by neutron scattering and X-ray diffraction

H. Takahashi[1], K. Nagura[2], M. Imai[3], Y. Matsushita[4], I. Hatta[2],
[1] Department of Physics, Gunma University, Maebashi 371-8510, Japan
[2] Department of Applied Physics, Nagoya University, Nagoya 464-8603, Japan
[3] Department of Physics, Ochanomizu University, Tokyo 112-8610, Japan
[4] Department of Applied Chemistry, Nagoya University, Nagoya 464-8603, Japan

Diacylglycerol (DAG) is recognized one of most important lipids for biological functions in biomembranes. To understand the functions of DAG, it is indispensable to study the effect of DAG on phosphatidylcholine (PC) which is one of main lipid components in biomembranes. Previously, we have suggested that addition of DAG increases the thickness of the PC membranes. To study the detailed mechanism we performed neutron scattering and X-ray diffraction experiments for vesicle and oriented bilayer systems. These data imply that addition of DAG induces the change of the tilt angle of lipid molecules in the membrane, as a result the membrane thickness increases.

B-189 Hybrid biomembrane substructure determination by contrast variation analysis

T. Gutberlet[1], R. Steitz[1], J. Howse[2], I. Estrela-Lopis[3], B. Kloesgen[4],
[1] Hahn-Meitner-Institut Berlin, Glienicker Str. 100, 14109 Berlin, Germany
[2] Iwan-N.-Stranski Institut f. Physikal. u. Theor. Chemie, TU Berlin, Str. d. 17. Juni 112, 10623 Berlin, Germany
[3] Max-Planck-Institut für Polymer- und Kolloidforschung, Am Mühlenberg 1, 14476 Golm, Germany
[4] Fachbereich Physik, FU Berlin, Arnimallee 14, 14195 Berlin, Germany

Controlled design of supported lipid bilayer probes as model biomembranes is a central challenge in the development of biosensors or as tools for basic biophysical features. Ideally, such a probe bases on a solid plate with a polymer coverage and an adsorbed lipid monolayer. This surface is a soft cushion for the condensation of free floating fluid membranes from an aqueous lipid vesicle suspension. In situ neutron reflectometry serves to monitor the build-up of the sandwich (PS-coated Si-single crystal, adsorbed lipid monolayer and DMPC bilayer). Taking the data step by step, and applying a layer model for the refractive index yields reasonable values for the hybrid structure. Experimental resolution is distinctly enhanced by contrast variation via D_2O/H_2O exchange and by use of deuterated components (e.g. d54DMPC, dPS). The method is highly sensitive: even minor contaminations of protonated compounds, and their effect on the desired structure, show up clearly at the appropriate contrast variation. Thus the interaction of membranes with interfaces or structural changes as effected by membrane active molecules (proteins, DNA, detergents) can be studied.

B-190 Interaction of Alzheimer's β-amyloid with anionic and zwitterionic lipid membranes.

T. Hauß[1,2], S. Dante[1,3], N. A. Dencher[3],
[1] Hahn-Meitner-Institut Berlin, Berliner Centrum für Neutronenstreuung
[2] Heinrich-Heine-Universität Düsseldorf, Institut für PhysikalischeBiologie
[3] Technische Universität Darmstadt, Institut für Biochemie

One hallmark of Alzheimer's disease (AD) are senile plaques found in brains of patients with AD, and the main protein component of the plaques are β-amyloid (Aβ) peptides. There is an ongoing discussion, if the plaques are the main cause of the dementia, or if the Aβ peptide itself plays an important role in the pathogenesis of AD. We have investigated the interaction of the Aβ (25-35) fragment with lipid membranes by neutron diffraction. Selectively deuterated β-amyloid was synthesized to localize the C-terminal end of the peptide. The neutron diffraction spectra of the lipid membranes containing labeled and unlabeled peptide allow the reconstruction of the scattering length density profile and the localizing of the deutereted part of the peptide in the membranes.

B-191 Association of DNA with poly(N-vinylpyrrolidone)-C_{60} complex in D_2O

Gy. Török[1], V.T. Lebedev[2], L. Cser[1], D.N. Orlova[2], O.K. Kaboev[2], A.I. Sibilev[2], M.A. Sibileva[3], V.N. Zgonnik[4], E.Yu Melenevskaya[4], L.V. Vinogradova[4],
[1] Res. Inst. for Solid State Phys. and Optics, POB-49, H-1525 Budapest, Hungary
[2] Petersburg Nucl.Phys.Inst., 188300 Gatchina, St.Petersburg dist., Russia
[3] Univ. of St.Petersburg, 198904 University pr.2, Peterhof, St.Petersburg, Russia
[4] Inst. of Macromolec. Compounds, 199004 Bolshoy pr.31, St.Petersburg, Russia

Interaction of DNA with poly(N-vinylpyrrolidone)-C_{60} $(PVP-C_{60})$ complex in D_2O by SANS has been studied at physiological temperatures $T = 20-40^{\circ}C$ to elucidate the mechanism of antiviral activity of fullerenes. Varying the concentration of complex (C_C=0.1-1.0 %wt.) at a constant DNA content ($C_\star$=0.1 % wt.) we observed a strong association with DNA as compared to free poly(N-vinylpyrrolidone) (PVP). It was revealed in an increased interference between DNA and polymer chains. The $PVP-C_{60}$ complex forms large clusters with DNA (size $\sim 30nm$)whereas the free PVP creates smaller associates ($\sim 8nm$) only.

B-192 Neutron Scattering from Magnetically Aligned Biomimetic Substrates

T. Gutberlet[1], A. Hoell[1], M. Kammel[1], J. Katsaras[2],
[1] Hahn-Meitner-Institut Berlin, Glienicker Str. 100, 14109 Berlin, Germany
[2] NRC Chalk River Laboratories, Chalk River,Ontario K0J 1J0, Canada

Binary mixtures of long-chain and short-chain phospholipids or bile salt analogues can form disk-shaped bilayered micelles (diameter 10-100 nm, thickness 4-6 nm) which have been shown to orient themselves in a magnetic field, serving as a self-orienting biomimetic substrate [R. Sanders, J. Prestegard, Biophys. J. 58, 1990, 447; R. Prosser et al., JACS 188, 1996, 269]. As demonstrated by neutron diffraction the bicellar system is highly alignable (¡ 1.0° mosaic) within the magnetic field [J. Katsaras et al., PRL 78, 1997, 899], exhibiting a rare temperature and concentration dependent nematic-smectic phase transition [G. Raffard et al., Langmuir 16, 2000, 7655]. The structural changes during this phase transition and the effect of water content and shearing on the bicelle system have been investigated by SANS and neutron diffraction at various magnetic field. Results on the structure of the disk-like micelles and the superstructural aggregation in the smectic phase will be presented.

B-193 Inelastic Incoherent Neutron Scattering Studies of the Hydration Water in DNA and Proteins

J. LI[1], I. Michalarias[1], R. Ford[1], V. Ruffle[1],
[1] UMIST, Department of Physics, Manchester, UK

Neutron vibrational spectroscopy is a powerful way to study the structure and dynamism of water inside and around biological molecules, because the translational frequencies will change with local structure of water around DNA and proteins and can be observed in the measured inelastic neutron scattering spectrum with very high accuracy even at very low concentrations of water present due to very large cross-section of hydrogen atom. On the other hand the scattering from the biomolecules are very weak and in different energy transfer range, we can observe the vibrations largely due to water-water interaction perturbed by the biomolecules. In the paper, we will present a series of neutron spectroscopic measurements for a range of proteins (e.g. photo system II and anti-freeze proteins), biopolymers and DNA materials using newly developed instruments such as TOSCA and HET at ISIS in the energy transfer range from 2 to 500 meV (15 cm^{-1} to 4000 cm^{-1}). The spectra show interesting features, indicating that the local structure of water are highly disordered around DNA molecules for instance, this could be due to strong interactions of water with DNA molecule, preventing "good" ice-like structure to form and resulting in spread of O-O-O bond angles and O-H-O lengths.

B-194 SANS study of micelle formation in the fractal structure of protein-detergent complexes

E. Seth[1], V.K. Aswal[2],
[1] Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai 400 085, India
[2] Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland

Small-angle neutron scattering (SANS) measurements have been carried out from the micellar solutions of the detergent sodium dodecyl sulfate (SDS) and its complexes with the protein bovine serum albumin (BSA). These studies show the fractal nature of the micellar packing in the protein-detergent complexes. It is found that when the detergent interacts with the protein it results in unfolding of protein molecules, and the micelle-like clusters of detergents are formed along the polypeptide chain. The structure of these micelle-like clusters bound to the protein in protein-detergent complexes is different from those of normal micelles in the pure detergent solutions. In protein-detergent complexes, the micelles tend to be spherical with much less number of aggregation of detergent molecules than those in normal micelles, and it is independent of the shape and aggregation number of the micelles in the corresponding pure detergent solutions.

B-195 Small Angle Polarized Neutron Scattering Studies of Selectively Polarized Proton Domains in Macromolecules

B. van den Brandt[1], S. F. J. Cox[2], H. Glättli[3], P. Hautle[1], H. Jouve[4], J. Kohlbrecher[1], J. A. Konter[1], E. Leymarie[3], S. Mango[1], R. May[5], H. Stuhrmann[4], O. Zimmer[6],
[1] Paul Scherrer Insitute, CH - 5232 Villigen PSI, Switzerland
[2] ISIS Facility, Rutherford Appleton Lab, Chilton, Oxon, OX11 0QX, UK
[3] CEA Saclay, SPEC, F - 91191 Gif-sur-Yvette, France

[4] Institut de Biologie Structurale Jean-Pierre Ebel, F - 38027 Grenoble Cedex 1, France
[5] Institut Laue Langevin, BP 156, F - 38042 Grenoble Cedex 9, France
[6] Technische Universität München, James-Franck-Strasse, D - 85748 Garching, Germany

We aim at taking advantage of the possibility to create clusters of polarized protons in organic materials in order to investigate with higher resolution at will different parts of complex macromolecules by polarized neutron scattering. Small angle polarized neutron scattering in organic substances doped with a low concentration of free radicals has shown that strong proton polarization gradients can be created at the free radical sites by dynamic nuclear polarization (DNP) methods, HF saturation and or adiabatic fast passage polarization reversal. In a magnetic field of 3.5 T and at a temperature of 1 K decay times of the non-uniform proton spin polarization between 1 s and 10 s were observed by time resolved measurements at D22 of the ILL. Work is in progress for a better understanding of the proton spin dynamics involved and for refining different aspects of an interesting, eventually powerful application of DNP in neutron scattering.

B-196 Chasing experiments on the E. coli Chaperonin system

J. Holzinger[1,2], E. Manakova[2], R.P. May[1], M. Roessle[2], K. Vanatalu[3], S. van der Vies[2], H. Heumann[2],
[1] Institut Laue-Langevin, 38042 Grenoble, France
[2] Max Planck Institut für Biochemie, 82152 Martinsried, Germany
[3] Institute for Biophysics, Tallin, Estonia
[4] Vrije Universiteit, 1081 HV Amsterdam, Netherlands

E. coli chaperonin GroEL binds and releases denatured substrate protein in an ATP dependent process, accompanied by its co-chaperonin GroES. Bacteriophage T4 encodes a specialised protein, GP31 that interacts with GroEL at the place of GroES. We prepared partially deuterated GroEL and GroES that can be made invisible in 99% D_2O. Assembly and disassembly of GroEL-co-chaperonin complexes in equilibrium was studied by a chasing of protonated co-chaperonin with partially deuterated GroES. This allowed us to estimate binding constants and to compare the two co-chaperonins.

B-197 Intramolecular and surface-coupled protein motions

W. Doster[1], M. Diehl[1], H. Schober[2], W. Petry[1],
[1] Technische Universität Mn̈chen, Physik Department E 13, 85747 Garching, Germany

To unravel the complex molecular dynamics of proteins requires the support of computer simulations but also of experiments which allow to discriminate between different types of motions. A practical approach is to change the properties of the protein environment, which selects surface-coupled from intramolecular modes. We discuss neutron scattering experiments with proteins in very different environments: dehydrated (vacuum), fully hydrated and solidified in a glucose glass. The analysis shows that a particular class of dihedral transitions (main chain and side chain) and those of methyl groups do not communicate with the protein surface. Dihedral transitions of surface side chains and concerted motions of secondary structure depend strongly on the viscosity of the solvent. Low frequency vibrations in the Terahertz regime are also strongly affected by the solvent. We show that the vibrational relaxation of the heme in group in myoglobin interacts with delocalized protein modes.

B-198 Effect of pressure and pressure-denaturation on fast molecular motions of solvated myoglobin

W. Doster[1], R. Gebhardt[1], H. Schober[1], J. Wiedersich[1],
[1] Physik Department E13, Technische Universität München, 85747 Garching, Germany

The increase in packing density with pressure should enhance both, polar and non-polar interactions and thus protein stability. The onset of pressure denaturation of globular proteins is presumably triggered by a breakdown of intra-molecular voids which are penentrated by water The influence of pressure in the range up to 8 kbar on the pico-second dynamics of myoglobin and its hydration shell has been studied by neutron time-of-flight spectroscopy. The quasi-elastic scattering decreases with pressure due to a reduction in the rate and amplitude of hydrogen bond fluctuations. Irreversible denaturation occurs around 4 kbar. The hysteresis observed on completing the pressure cycle suggests a structural contribution to the dynamic effects of less than 10 %: Water interacts more strongly with the unfolded state. We determine activation volumes associated with folding-unfolding fluctiations.

B-199 A neutron crystallographic analysis of a rubredoxin mutant

T. Chatake[1], K. Kurihara[1], I. Tanaka[1], M. W. W. Adams[2], F. E. Jenney, Jr[2], N. Moiseeva[3], R. Bau[3], N. Niimura[1],
[1] Japan Atomic Energy Research Institute, Ibaraki 319-1195, Japan
[2] Dept. of Biochemistry, University of Georgia, Athens, GA 30602, USA
[3] Dept. of Chemistry, University of Southern California, Los Angeles, CA 90089, USA

In order to reveal the thermostabilization mechanism of rubredoxin, the structure of a rubredoxin triple mutant was solved at 1.5 Angstrom resolution by neutron crystallographic analysis using BIX-3 of JRR-3M, JAERI. The positions of non-hydrogen atoms are almost the same as the native rubredoxin, but the positions of hydrogen atoms and hydration are changed in some region, suggesting that such difference may contribute to thermostabiliy of the rubredoxin. Various types of solvent peaks were observed in the solvent region.

B-200 Molecular Motions of Benzene Adsorbed in ZSM-5 Zeolite: QENS Study

S. Mitra[1], R. Mukhopadhyay[1], A. K. Tripathy[2], N. M. Gupta[2],
[1] Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai, 400085 India
[2] Applied Chemistry Division, Bhabha Atomic Research Centre, Mumbai, 400085, India

We report dynamics of benzene molecules contained in the pores of HZSM-5 and CaZSM-5 zeolites as studied by QENS spectrometer at Trombay, India at room temperature. Benzene molecules are found to undergo 6-fold jump rotation in the channel intersections. Residence times obtained for benzene in the pores of HZSM-5 and CaZSM-5 zeolites are found to be close to that of solid benzene. It is also seen that the rotational dynamics of benzene in CaZSM-5 zeolites is slower than that in HZSM-5 zeolites indicating strong cation exchange effect. Fourier Transformed Infrared (FTIR)study indicated a strong intermolecular interaction, which seems to give rise to a solid like state of benzene in the pores of these zeolites.

B-201 Dynamics of Confined Water in Porous Alumina: Neutron Scattering Study

R. Mukhopadhyay[1], S. Mitra[1], I. Tsukushi[2], S. Ikeda[3],
[1] Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai 400085, India.
[2] Department of Physics, Chiba Institute of Technology, Chiba, Japan.
[3] KENS, KEK, 1-1 Oho, Tsukuba, Japan.

Dynamics of water molecules contained in the pores of alumina gel has been studied by high resolution LAM80-ET spectrometer at KEK, Japan and medium resolution QENS spectrometer at Trombay, India, in the temperature range of 300-250 K. In the picture of single particle dynamics a clear evidence of two types of water are found to be present in the pores of alumina gel. Water molecules attached to the surfaces are localized and others undergo hindered diffusion in the middle of the pores. Localisation radius and diffusion constant (D_{local}) characterizing the local dynamics and also the diffusion constant (D_t) and residence time of the water molecules diffusing inside the pores are obtained.

B-202 Dynamics of Propane in Na-Y Zeolite

S. Mitra[1], R. Mukhopadhyay[1], A. Sayeed[2], S. Yashonath[2], S.L. Chaplot[1],
[1] Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai 400 085, India.
[2] Solid State and Structural Chemistry Unit, IISc., Bangalore, 560 012, India.

Dynamics of propane adsorbed in Na-Y zeolite has been studied at 300, 325, 350 K, using QENS spectrometer at Trombay, India. The data have been found to be consistent with the model in which the propane molecules undergo translational diffusion characterised by a gaussian distribution of jump lengths inside the Na-Y zeolite cage. Rotational motion of the propane does not seem to contribute in the measured data (ΔE=200 μeV). Diffusion constant and root mean square jump length are determined at each temperature. The present results are consistent with PFG-NMR results of diffusion of propane in zeolite Na-X, a similar system. We have also carried out molecular dynamics simulation and the results are in very much agreement with the experimental data.

B-203 Neutron diffraction and $^{1}3$C MAS NMR studies of chemisorbed zeolites with methylium ions

S. Vratislav[1], M. Dlouhá[1], V. Bosáèek[2],
[1] Faculty of Nuclear Sciences and Physical Engineering CTU Prague, Bøehová 7, 115 19 Prague 1, Czech Republic
[2] J. Heyrovský Institute of Physical Chemistry, Dolejskova 3, 182 23 Prague 8, Czech Republic

Some organic cations like methylium or ethylium, create chemisorbed, with more or less polarized, but covalently bonded alkoxy species in zeolitic structures. Careful ^{13}C MAS NMR measurements make possible to distinguish between signals of bridging and terminal methoxy groups. Neutron powder diffraction patterns were collected from evacuated ampoules with samples at room and 7 K on the KSN-2 diffractometer which is placed at the LVR-15 research reactor in e? near Prague. The complete structural parameters (including chemisorbed methylium ions at O1 and O4 in NaX and at O1 in NaY) were determined by Rietveld analysis using GSAS package. Redistribution of Na^{+} cations in the lattice of both structures after chemisorption was detected.

B-204 Structural Studies of Supercritical CO_2 in Confined Space

T. Steriotis[1], K. Stefanopoulos[1], A. Mitropoulos[2], N. Kanellopoulos[1], M. Hofemann[3],
[1] NCSR "Demokritos", 153 10 Agia Paraskevi Attikis, Greece
[2] Department of Petroleum Technology, Cavala Institute of Technology, 65404 Ag. Lucas, Cavala, Greece
[3] HMI, Glienicker Strasse 100, 14 109 Wannsee, Berlin

The behavior of CO_2 adsorbed on a microporous carbon substrate, at an isothermal temperature above the critical one, is studied by in situ neutron powder diffraction. The diffraction patterns provide evidence that the adsorbed phase gains liquid-like properties at a pressure about half way the critical one. Such a transition affects the flow of CO_2 in confined spaces and a maximum appears on the permeability curve.

B-205 Orientational Disorder in Solid Monolayers of Tetramethylsilane Adsorbed on Graphite and MgO (100) Surfaces

N. Sakisato[1], A. Inaba[1], T. Matsuo[1],
[1] Department of Chemistry, Graduate School of Science, Osaka University, Toyonaka, Osaka 560-0043, Japan

Tetramethylsilane (TMS) molecules form a 2-D solid on the surface of graphite. According to our calorimetric study, the solid monolayer formed at submonolayer coverages exhibits a phase transition at 107 K and melts at 146 K. The large transition entropy suggests an orientational disorder of the molecules in the high-temperature phase. To investigate the dynamical aspect, we performed an incoherent neutron scattering experiment. A large decrease in the elastic scattering intensity around 100 K demonstrates that the molecules are in static order in the low-temperature phase and in dynamic disorder in the high-temperature phase. The similar results were obtained also for the monolayers of TMS on the (100) surface of MgO.

B-206 Micellization in the mixed system of cationc and non-ionic surfactants in heavy water by SANS method.

A. Rajewska[1,3], R. F. Bakeeva[2], A. I. Kuklin[1], A. H. Islamov[1],
[1] Joint Insitute for Nuclear Research, Laboratory of Neutron Physics, 141980 Dubna, Russia
[2] Kazan State Technological University, Kazan, Russia
[3] Institute of Atomic Energy, 05-400 Swierk-Otwock, Poland

The mixed system Triton X-100 / CTAB / D_2O was investigated by small-angle neutron scattering. Measurements were carried out on the time-of-flight small-angle neutron scattering (TOF SANS) spectrometer of the IBR-2 pulsed source [1], at FLNP, JINR, Dubna, Russia. Formation of mixed micelles was detected for dilute and high concentration solutions. The influence of varying temperature and composition on the differential cross section was observed. Triton X-100 was nonionic detergent but the CTAB (cethyltrimethylammonium bromide) the cationic one. From our measurements we were able to deduce that ionic surface-active materials interact with non-ionic surface -active compounds to form weakly charged mixed micelles [2,3]. For the fitting procedure we used a FISH program. [1] Yu. M. Ostanievich, Makromol.Chem., Marcomol. Symp.,15 (1988) 91 [2] Chevalier Y., Zemb Th., Rep. Prog. Phys., 53 (1990) 279 [3] Rathman J. F., Scamehorn J. F., Langmuir, 3 (1987) 372

B-207 Dynamics of the Proton in $HCrO_2$ and $HCoO_2$

R.G. Delaplane[1], T. Gustafsson[2], M. Ichikawa[3], T. Tsuchida[4], S.F. Parker[5],
[1] The Studsvik Neutron Research Laboratory, Uppsala University, Nyköping, Sweden
[2] Department of Materials Chemistry, Ångström Laboratory, Uppsala University, Uppsala, Sweden
[3] Division of Physics, Hokkaido University, Sapporo, Japan
[4] Division of Materials Science and Engineering, Hokkaido University, Sapporo, Japan
[5] ISIS facility, Rutherford Appleton Laboratory, Chilton, Didcot, UK

Inelastic neutron scattering has been used to study the dynamics of the proton in $HCrO_2$ and $HCoO_2$. Spectra were measured for samples of $HCrO_2$, $HCoO_2$ and $DCrO_2$(5%H) on the instrument TOSCA at the ISIS neutron spallation source. The crystal structure (hexagonal cell) of $HCrO_2$/$HCoO_2$ consists of a layer of Cr/Co atoms perpendicular to the **c** axis lying between two sheets of O atoms. The O-Cr-O layers are joined together by strong hydrogen bonds parallel to the **c** axis. The $HCrO_2$ spectrum is dominated by an intense H bond bending mode at about 1240 cm^{-1} which is similar for $HCoO_2$ since the O-H...O distance is about 2.47Å. The bending mode of H in $HCrO_2$ is split due to coupling but appears a a single peak when diluted in $DCrO_2$. Implications of these results for the form of the potential for the vibration of H/D will be discussed.

B-208 Temperature-Dependent Effects in Low-Barrier Hydrogen Bonds.

J. A. Cowan[1,2], G. J. McIntyre[1], P. Smith[2], J. A. K. Howard[2], S. Mason[1], S. M-.F. Lo[3], I. D. Williams[3],
[1] Institut Laue Langevin, Grenoble, France.
[2] University of Durham, Durham, United Kingdom.
[3] Hong Kong University of Science and Technology, Hong Kong, China.

While there is a wealth of neutron-diffraction data on short low-barrier O-H O hydrogen bonds, the equally biologically important N-H O / N H-O cases have been neglected. We report the results of high-quality neutron-diffraction experiments on samples containing a wide variety of these bonds. We also report the revealing behaviour of one of these bonds on changing the temperature and upon deuteration. Monochromatic and multi-wavelength Laue experiments have been performed at the ILL, and we will compare the advantages and disadvantages of both techniques.

B-209 Mesoscopic order in liquid mixtures studied by small-angle scattering

L. Almásy[1], L. Cser[1], G. Jancsó[2],
[1] Research Institute for Solid State Physics and Optics, Budapest, Hungary
[2] Atomic Energy Research Institute, Budapest, Hungary

Small-angle neutron scattering was used to determine the mesoscopic order in binary aqueous solutions exhibiting strongly non-ideal mixing behavior. The Kirkwood-Buff theory was used for modeling the structural characteristics - the fluctuations in particle density and concentration, and the preferential clustering of the solute and the solvent molecules. The capability of this method is demonstrated on the n-propanol - heavy water mixture, the results are compared with those of earlier SAXS[1], light scattering[2] and thermodynamic[3] studies. [1] H. Hayashi, K. Nishikawa, T. Iijima, J. Phys. Chem. 94, 833 (1990) [2] G. H. Grossman, K. H. Ebert, Ber. Bunsenges. Phys. Chem. 85,1026 (1981) [3] I. Shulgin, E. Ruckenstein, J. Phys. Chem. B, 103 2496 (1999)

B-210 Decoherence of Entangled Protons and Attosecond Dynamics of C-H Bond Breaking

T. Abdul-Redah[1], C. A. Chatzidimitriou-Dreismann[1],
[1] Technical University of Berlin, Institute of Chemistry, Sekr. ER 1, Strasse des 17. Juni 112, D-10623 Berlin, Germany

In previous work we investigated the attosecond dynamics and dissociation of C-H bonds of solid H-polystyrene (PS) at $T \approx 295$K using neutron Compton scattering (NCS). A striking decrease of the neutron scattering cross section density of H of ca. 20% with respect to that of the carbon nucleus was found. A theoretical explanation grounding on protonic quantum entanglement (QE) and decoherence has been given [1]. Here we present recent NCS results of solid H-/D-PS mixtures and of liquid H-/D-benzene mixtures. Extending our previous work on liquid H_2O/D_2O mixtures [2], the results of the hydrocarbon systems indicate that the considered QE effect is mainly of intramolecular origin. [1] C. A. Chatzidimitriou-Dreismann, T. Abdul-Redah, J. Sperling, J. Chem. Phys., **113** (2000) 2784. [2] C. A. Chatzidimitriou-Dreismann, T. Abdul-Redah, R. M. F. Streffer, J. Mayers, Phys. Rev. Lett., **79** (1997) 2839.

B-211 Temperature evolution of the thermal expansion tensors of ammonium Tutton salts

W. Kockelmann[1,2], A. Meents[1], A. Kirfel[1],
[1] Mineralogisch-Petrologisches Institut, Universität Bonn, 53115 Bonn, Germany
[2] Rutherford Appleton Laboratory, ISIS, Chilton, OX11 0QX, United Kingdom

The temperature dependencies of the lattice parameters and thermal expansion tensors of isotypic ammonium Tutton salts $(ND_4)_2MII_2(SeO_4)_2$ $6D_2O$ (MII=Co, Zn), which crystallize in space group P21/a, were studied between 5 to 380 K by time-of-flight neutron powder diffraction. In contrast to the temperature behaviour of the Jahn-Teller compound $(ND_4)_2Cu_2(SO_4)_2$ $6D_2O$ [1] and a $K_2Co_2(SO_4)_2$ $6D_2O$ reference sample, the Co and Zn ammonium Tutton salts exhibit very similar negative thermal expansions of the monoclinic cell along the c-direction. The temperature evolutions of the thermal expansion tensors are attributed to the additional hydrogen bonds of $(ND_4)^+$ and their dynamic behaviour. [1] B.J. Hathaway, A.W. Heat, J. Sol. State Chem. 51 (1984) 364.

B-212 Guest-Host Coupling in Xenon Hydrate

J. Baumert[1], C. Gutt[1], W. Press[1], J. Tse[2],

[1] Institut für Experimentelle und Angewandte Physik, Universität Kiel, Germany
[2] National Research Council, Ottawa, Canada
Gas hydrates are inclusion compounds formed by an ice like network with small guest molecules included. One of their outstanding physical properties is their thermal conductivity that is unusually low and displays a temperature dependence similar to that of glasses. This is thought to arise from a strong coupling between guest molecule and host lattice vibrations. We recently confirmed this coupling in a high-resolution inelastic neutron experiment (INS) on Xenon hydrate by finding three distinct low energy excitations at 2.05meV, 2.87meV and 3.94meV. Xe-hydrate has the cubic structure I consisting of 6 large and 2 small cages in the unit cell. The Xe-atoms in the small spherical cage vibrate with the highest frequency and in the larger ellipsoidal cage with two lower frequencies. This leads to resonant (low energy) modes [1] in the frequency range of the localized Xe-modes, mediated by scattering from the ice framework. [1]J.S.Tse, V.P.Shpakov, V.V.Murashov, V.R.Belosludov, J.Chem.Phys., 107, 9271(1997)

B-213 Bound Water around the Core of Ionic Micelles?

S. Vass[1], H. Grimm[2], K. Haimer[3], M. Klapper[3], T. Gilányi[4],
[1] KFKI Atomic Energy Research Institute, Budapest, Hungary
[2] Institut für Festkörperforschung, FZ Jülich, Jülich, Germany
[3] Max-Planck-Institut für Polymerforschung, Mainz, Germany
[4] Eötvös Loränd University, Budapest, Hungary
From the analysis of the interaction potential acting between pure hydrophobic surfaces immersed in water one concluded that such surfaces are able to reorganize the local structure of water by forming ”rigid” solvent layers in their vicinity. Although the rigid solvent layer structure have been assumed to be destroyed if ions are present, the analysis of the hard-sphere radius of the DLVO potential acting between various sodium alkyl sulphate micelles versus alkyl chain length contradicts this assumption. Neutron backscattering experiments made in micellar solutions of ionic ABA- and BAB type triblock coplymers indicate the existence of slowly moving solvent molecules. The work was supported by BMfBF, BASF AG, Germany, and by OTKA, Hungary, contract No. T029958.

B-214 Ammonium ion behaviour in the $LiRb_{1-x}(NH_4)_xSO_4$ mixed crystals

M. Martinez Sarrion[1], L. Mestres[1], L. Smirnov[2],
[1] Inorganic Chemistry Department, University of Barcelona, 08028 Barcelona, Spain
[2] SUC SSC RF Institute of Theoretical and Experimental Physics, 117259 Moscow, Russia
$LiNH_4SO_4$ undergoes phase transition: I-459.5K-II-283K-III-27K-IV phase, where sp. gr. of phases are respectively Pnam, Pna21, P21/c, and Cc. The $LiRb_{1-x}(NH_4)_xSO_4$ (RBAS) mixed crystals are crystallised at room temperature in phase II with ammonium concentration up to x=0.8 [1]. There are presented the results of the investigation of RBAS carried out by neutron scattering at temperatures from 300 to 20 K for x=1.0, 0.91 and 0.77. Spectra of inelastic incoherent neutron scattering (IINS) in phases II and III at high temperature for x=1.0 contain the contributions of quasielastic incoherent neutron scattering which fully disappear with cooling to 20 K. The generalised phonon density of states, calculated from the IINS spectra, shows noticeable broadening of translational and librational bands at 20 K with increasing ammonium concentration. 1. M.L.Martinez Sarrion, L.Mestres, A.A.Bakkali, E.H.Bocanegra, Material Research Bulletin, 33 (1998) 269.

B-215 Critical Exponents for the Ferromagnetism in Colossal Magnetoresistance Manganites

N Furukawa[1], Y Motome[2],
[1] Department of Physics, Aoyama Gakuin University, Tokyo, Japan
[2] Institute of Matrials Science, University of Tsukuba,Japan

Critical phenomena of the colossal magnetoresistance manganites are theoretically studied. Regarding the critical exponents for the ferromagnetic transition in the colossal magnetoresistance manganites, there exists a contradiction: Neutron scattering estimates show Heisenberg-like universality class, while some d.c. and r.f. magnetization measurements give mean-field like exponents. In order to clarify the intrinsic nature of the phase transition, comparison with theoretical prediction is necessary. Here we show the Monte Carlo results for the critical phenomena of the double exchange model. Our estimate for the critical exponents are consistent with those by neutron scattering measurements.

B-216 Magnetic order parameter in the perovskite system $CaMn_7O_{12}$

R Przenioslo[1], I Sosnowska[1], E Suard[2], T Hansen[2], ,
[1] Institute of Experimental Physics, Warsaw University, Hoza 69, PL 00681 Warsaw, Poland
[2] Institut Laue-Langevin, Grenoble, F 38042, France
[3]

The magnetic ordering in the distorted perovskite system $CaMn_7O_{12}$ has been studied by powder neutron diffraction with the high flux diffractometer D20. The magnetic ordering in $CaMn_7O_{12}$ consists of two phases: one ferrimagnetic and one modulated [1]. The magnetic peaks due to both phases disappear at the same temperature. The temperature dependence of the intensity $I(T)$ of magnetic peaks due to both these phases can be described for 55 K $< T <$ 90 K with a power-law characteristic for critical scattering $I(T) \propto (T_N - T)^{2\eta}$ where T_N = 89.6(6) and η = 0.31(5). This value of η agrees with the prediction for a 3-dimensional Ising model. Models of possible magnetic orderings in $CaMn_7O_{12}$ are discussed. [1] R. Przeniosl o, I. Sosnowska, D. Hohlwein, T. Hauss, I.O. Troyanchuk Solid State Comm. 111 (1999) 687.

B-217 Crystal and magnetic structures of new layered oxides A_2GaMnO_{5+y} (A = Ca, Sr)

D.V. Cheptiakov[1], E.V. Antipov[2], A.M. Abakumov[2], A.M. Balagurov[3], P. Fischer[1], L. Keller[1], M.V. Lobanov[2], V.Yu. Pomjakushin[3],
[1] Labor für Neutronenstreuung, ETHZ & PSI, CH-5232 Villigen PSI, Switzerland
[2] Department of Chemistry, Moscow State University, Moscow 119899, Russia
[3] Frank Laboratory of Neutron Physics, JINR, 141980 Dubna, Russia

Crystal and magnetic structures of new complex manganese oxides A_2MnGaO_{5+y} (A = Ca, Sr) were studied by neutron diffraction. Being a perovskite type derivatives, their crystal structures belong to a brownmillerite type and consists of alternating (MnO_2), (CaO) and (GaO) layers. At $T_N \approx 160K$, these compounds undergo a transition into an antiferromagnetic state. The magnetic ordering is purely three-dimensional with Mn magnetic moments aligned at opposite directions within the MnO_2 layer and between neighboring MnO_2 layers as well. Such a type of antiferromagnetic ordering seems to be quite unexpected, since the three-dimensional antiferromagnetism is realized in a strongly two-dimensional layered chemical structure matrix.

B-218 Oxygen Isotope Effect on Crystal and Magnetic Structure of $(La_{1-y}Pr_y)_{0.7}Ca_{0.3}MnO_3$

A.M. Balagurov[1], V.Yu. Pomjakushin[1], D.V. Sheptyakov[1], N.A. Babushkina[2],
[1] Frank Laboratory of Neutron Physics, JINR, 141980 Dubna, Russia
[2] RSC, "Kurchatov Institute", 123182 Moscow, Russia

The oxygen $^{16}O/^{18}O$ isotope effect on the crystal and magnetic structure of $(La_{1-y}Pr_y)_{0.7}Ca_{0.3}MnO_3$ has been studied by neutron powder diffraction in the temperature range from 15 to 293 K. The isotope enriched samples have been found identical in crystal and magnetic structure down to the temperature of transition of the sample with ^{16}O into the metallic ferromagnetic phase, while at low temperature, both crystal and magnetic structures of the samples with ^{16}O and ^{18}O are different. In particular, for composition with y=0.75, the precise structural analysis shows a clear difference in Mn-O1 distances and Mn-O1-Mn valence angles along b-axis (Pnma sp. gr.) whereas in-plane distances and angles are the same. For large y values, the magnetic structure of saturated ^{18}O samples is pure AFM of pseudo-CE type. The study of the samples with partial isotope substitution shows that both FM-phase fraction and T_{FM} strongly depend on ^{18}O oxygen content disappearing at about 60% of ^{18}O. On the contrary, the temperature of AFM transition does not depend on isotope content. Accordingly, it could be suggested that heavier oxygen isotope influences mainly the FM-metallic phase favoring the charge localized state.

B-219 Influence of a magnetic field on the magnetic soliton lattice of copper metaborate

J. Schefer[1], B. Roessli[1], M. Boehm[1,2], U. Staub[3], G.A. Petrakovskii[4], B. Ouladdiaf[2], A. Vorotinov[3], L. Bezmaternikh[3],
[1] Laboratory for Neutron Scattering, ETH Zurich and Paul Scherrer Institute, CH-5232 Villigen, PSI
[2] Institut Laue-Langevin, Av. des Martyrs, 38042 Grenoble, France
[3] Swiss Light Source, Paul Scherrer Insitute, CH-5232 Villigen, PSI
[4] Institut of Physics, SB RAS, 660036 Krasnoyarsk, Russia

Copper metaborate, CuB_2O_4, forms a magnetic soliton lattice below T=10K in absence of an external magnetic field [1] due to the Dzyaloshinskii-Moriya interaction and anisotropy of order n=4 in the tetragonal plane. In the temperature range 10K $\leq$ T $\leq$ 21K, the magnetic structure is commensurate compared with the chemical lattice and characterised by a non-collinear spin arrangement. We show that temperature and magnetic field influcence the ordering of the magnetic lattice in the same way, as expected for a spiral structure caused by relativistic interactions [2]. [1]B. Roessli, J. Schefer, G.A. Petrakovskii et al., Phys. Rev. Lett. **86**, 1885 (2001). [2]Yu.A. Izyumov and V.M. Laptev, Sov. Phys. JETP **62**, 755 (1986).

B-220 Theoretical Prediction of the Spin-Wave Spectra in Charge Ordered 3D and Layered Manganites: Interrelation of Crystal, Charge, Orbital, and Magnetic Structures

L.E. Gontchar[1], A.E. Nikiforov[1],
[1] Urals State University, Department of Physics

The manganites with general formulas $R_{0.5}A_{0.5}MnO_3$ (3D-manganite), $R_{0.5}A_{1.5}MnO_3$ (layered manganite), and $RA_2Mn_2O_7$ (double-layered manganite), where R^{3+} is rare-earth ion, A^{2+} is alkaline-earth ion, are known as charge ordered compounds at low temperatures with some R and A. In present work it is shown how the charge ordering and crystal structure form the orbital and magnetic ones. The model of orbitally-dependent

superexchange and single-ion anisotropy is used. The model presented in this work allows to explain the CE- and A- magnetic structures in terms of charge and orbital structures. The magnetic structures and spin-wave dispersion curves of some certain compositions are calculated. This research is supported by Awards CRDF REC-005 and Russian Ministry of Education #E00-3.4-277

B-221 The Lattice Dynamics of $LaMnO_3$: the Role of the Orbital Degrees of Freedom

A.E. Nikiforov[1], S.E. Popov[1],
[1] Urals State University, 620083, Russia, Ekaterinburg Lenin av. 51, The Department of Physics

For $LaMnO_3$ strong coupling of the spin, charge, and orbital degrees of freedom is characteristic. The strong coupling is usually attributed to the strong electron-vibrational coupling due to the Jahn-Teller(JT) effect. That is why lattice dynamics of the pure $LaMnO_3$ depends on the orbital structure. We have calculated both the fundamental phonon frequencies of the undoped $LaMnO_3$ and the phonon frequencies across Brillouin zone. The calculation has been performed in the framework of the interionic pair potentials and shell model. In the pair potential model we explicitly include JT term. As the result of comparison the calculations result with different experiments the most intense Raman lines of A_g and B_{2g} symmetry are active in the JT effect. We have calculated the dependence of the Raman active phonons frequencies on JT constant value. We believe that our calculations could be transferred on other low doped orthorhombic manganites. The research was made possible in part by Award N REC 005 of the CRDF and Ministry of Eduction of RU N E00-3.4-277

B-222 Magnetic properties and crystal-field excitations in the $Ln_{1-y}Sr_yCoO_{3-\delta}$ (Ln=La, Pr, Ho)

A Podlesnyak[1,2], A Mirmelstein[2], N Golosova[2], E Mitberg[3], I Leonidov[3], V Kozhevnikov[3], I Sashin[4], F Altorfer[1], A Furrer[1],
[1] Laboratory for Neutron Scattering, ETH Zürich & Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland
[2] Institute for Metal Physics RAS, 620219 Ekaterinburg GSP-170, Russia
[3] Institute of Solid State Chemistry RAS, 620219 Ekaterinburg GSP-145, Russia
[4] Joint Institute for Nuclear Research, 141980 Dubna, Moscow region, Russia

The members of the $Ln_{1-y}Sr_yCoO_{3-delta}$ solid solution have received much attention in recent years due to their unique magnetic and transport properties and possible applications as oxidation catalysts, electrode materials and oxygen permeable membranes. Magnetic and structural studies in the series $Ln_{1-y}Sr_yCoO_{3-\delta}$ (Ln=La, Pr, Ho) have been carried out by powder neutron diffraction. The inelastic neutron scattering has been employed to study the crystalline-electric-field (CEF) interaction in the title compounds. We have succeeded to reproduce the CEF splitting using the extended point charge model with screening length as the only adjustable parameter. The results obtained allow to relate the CEF response with the peculiarities of the oxygen defect structure in the nonstoichiometric cobalt perovskites.

B-223 Sr substitution effect on $Bi_{0.125}Ca_{0.875}MnO_3$

T. Ishigaki[1], T. Kudo[1],
[1] Department of Materials Science and Engineering,Muroran Institute for Technology, Muroran 050-8585, Japan

Polycrystalline samples of $Bi_{0.125}Ca_{0.875-y}Sr_yMnO_3$ ($y = 0.15$ and 0.25) were studied with neutron powder diffraction and magnetic measurements. The crystal structure of samples were monoclinic in contrast with orthorhombic for $Bi_{0.125}Ca_{0.875}MnO_3$. Magnetic measurement for $y = 0.15$ sample showed the anti-ferromagnetic state ($T_N \approx$ 250K) and a ferromagnetic like behaviour below 100K. The temperature dependence for the Mn-O-Mn bond angle is in good agreement with its for magnetisation below 100K.

B-224 Spin waves, charge/orbital ordering and antiferromagnetism of $LaSr_2Mn_2O_7$

T. Chatterji[1,2], G.J. McIntyre[1], R. Suryanarayanan[3], G. Dhalenne[3], A. Revcolevschi[3],
[1] Institut Laue-Langevin, BP 156, F-38042 Grenoble Cedex, France
[2] Max-Planck-Institut für Physik Komplexer Systeme, Noethnizerstrasse 38, D-01187 Dresden, Germany
[3] Laboratoire de Phisico-Chimie, Université Paris-Sud, 91405 Orsay Cedex, France

Neutron scattering investigations of the charge/orbital and magnetic ordering, spin correlations and spin waves of the bilayer manganite $La_{2-2x}Sr_{1+2x}Mn_2O_7$ have been performed for x = 0.4 and 0.5. $La_{2-2x}Sr_{1+2x}Mn_2O_7$ shows the maximum colossal magnetoresistance effect for x = 0.4 close to the ferromagnetic phase transition $T_C approx 128$ K. Inelastic neutron scattering measurements have been used to investigate the magnetic excitations of $La_{1.2}Sr_{1.8}Mn_2O_7$. The dispersion of both the acoustic and the optic modes along [100] and [001] have been measured and by using a effective localised spin model the complete set of exchange interactions has been determined. The strong anisotropy in the exchange interactions suggests that $La_{1.2}Sr_{1.8}Mn_2O_7$ can be considered as a quasi two-dimensional ferromagnet consisting of weakly coupled ferromagnetic bilayers. The charge/orbital ordering of the 50% hole-doped bilayer manganite $LaSr_2Mn_2O_7$ has been determined by means of X-ray and neutron diffraction on a single crystal. The temperature variation of the superlattice reflections corresponding to the propagation vector $\vec{k} = (-\frac{1}{4}, \frac{1}{4}, 0)$ indicates the development of a coupled charge/orbital ordering below $T_{CO} \approx 225$ K which starts melting at about the same temperature at which antiferromagnetic ordering ($T_N \approx 170$ K), detected by neutron diffraction, sets in.

B-225 Neutron diffraction magnetic scattering in ordered and disordered Sr_2FeMoO_6

D. Sánchez-Soria[1], J.A. Alonso[1], M. García-Hernández[1], M.J. Martínez-Lope[1], J.L. Martínez[1], A. Mellergard[2],
[1] Instituto de Ciencia de Materiales de Madrid, CSIC, Cantoblanco, E-28049 Madrid, Spain
[2] NFL-Studsvik, Uppsala University, S-611 82 Nykoping, Sweden

The interesting magnetotransport properties of the double perovskite Sr_2FeMoO_6 have been shown to be strongly influenced by cationic anti-site disorder, although the real effect in the electronic properties of the system is subject to controversy. We have performed temperature dependent neutron powder diffraction in two Sr_2FeMoO_6 samples with a very different degree of cationic order, 70% for the called *ordered* sample and 18% for the *disordered*. Although X-Ray diffraction and magnetic measurements show clear differences between both samples, that is, absence of low angle superstructure peak, lower Ms and smoother decay of the magnetization around the FM transition temperature in the disordered sample, the neutron signals are surprisingly similar. We propose that this unexpected strong magnetic scattering in the disordered sample arises from antiferromagnetically ordered Fe-rich patches in which strong AFM Fe^{3+}-O-Fe^{3+} superexchange interactions are promoted, being the long range coherence of this AFM structure maintained by Fe-O-Mo AFM interactions.

B-226 Long scale phase separation versus homogeneous magnetic state in $(La_{1-y}Pr_y)_{0.7}Ca_{0.3}MnO_3$

V Pomjakushin[1], A Balagurov[1], V Aksenov[1], P Fischer[2], L Keller[2], D Sheptyakov[2], O Gorbenko[3], A Kaul[3], N Babushkina[4],

[1] Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, 141980, Dubna, Moscow region, Russia

[2] Laboratory for Neutron Scattering, ETH Zurich and Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland

[3] Chemistry Department, Moscow State University, Moscow, Russia

[4] RSC Kurchatov Institute , Kurchatov sq.1, 123182, Moscow, Russia

The magnetic structure of the series $(La_{1-y}Pr_y)_{0.7}Ca_{0.3}MnO_3$ for y from 0.5 to 1.0 (including $^{16}O/^{18}O$ isotope substitution) has been studied by neutron powder diffraction in the temperature range from 10 to 293 K and in external magnetic fields perpendicular to the scattering plane up to 4 Tesla at DMC/SINQ (Villigen). We show that the phase diagram has a border region of concentrations between y=0.6 and y=0.8 separating the homogeneous FM metallic and canted AFM (pseudo CE-type) insulating states. In this region the low temperature magnetic state is macroscopically ($\geq$ 1000Å) incoherently spatially separated into AFM an FM phases. The FM phase has a small non-collinearity of C-type, presumably due to interfaces to the AF-phase. The macroscopical clusters can be induced by disorder on the carriers hopping amplitude caused by natural dispersion of the A-cation radius near the metal-insulator transition around y=0.7.

B-227 Charge and spin configurations in $Pr_{1-x}Ca_xMnO_3$ and $Pr_{1-x}Sr_xMnO_3$ ($x = 0.5 - 0.75$)

Z. Jirak[1], C. Martin[2], M. Hervieu[2], J. Hejtmanek[1],

[1] Institute of Physics ASCR, Na Slovance 2, 18221 Prague 8, Czech Republic

[2] Laboratoire CRISMAT, ISMRA, Bd du Marechal Juin, 14050 Caen, France

The mixed valence perovskite manganites exhibit very rich structural and magnetic phase diagrams. Apart of a dependence on the actual Mn^{3+}/Mn^{4+} ratio there are other factors which influence the character of manganese e_g electrons and resulting crystal states, such as average size of large cations and their size variance. The present report summarizes the high resolution neutron diffraction results, completed with electron microscopy and physical measurements, for two analogous praseodymium manganites substituted with smaller calcium and larger strontium cations, respectively. The crystal and magnetic structures determined are discussed in relation to the e_g electron localization (including various kinds of the long range charge ordering), the electron itinerancy in clusters and the metallic e_g states with different degree of orbital polarization.

B-228 Structural evidence against charge ordering in $Pr_{1-x}Ca_xMnO_3$ ($x \approx 0.5$) perovskites

M. A. Daoud-Aladine[1], J. Rodriguez-Carvajal[1], L. Pinsard-Gaudart[2], M.T. Fernandez-Diaz[3], A. Revcolevschi[2],

[1] Laboratoire Leon Brillouin, CEA-CNRS Saclay,91191 Gif sur Yvette

[2] Institut Laue Langevin, 38042 Grenoble

[3] Laboratoire de Physico-Chimie de l Etat Solide, Universite Paris Sud, Bat. 414, 91405 Orsay

The structural model obtained from unconstrained structure refinement of the neutron diffraction data collected in the paramagnetic phase of a $Pr_{0.6}Ca_{0.4}MnO_3$ single crystal below the structural phase transition at T_{CO} contradicts the expected one from the charge and orbital ordering picture. The modulated lattice distortion reflects rather the trapping and the spatial ordering of magnetic bi-polarons (MBP) spreading over two Mn sites, suggesting the MBP are the new paramagnetic units with a doubled effective paramagnetic moment. The CE-type magnetic ground state is alternatively viewed as the antiferromagnetic ordering of these MBP. Since the Mn valence state, investigated by the XANES local probe, have been confirmed to be mixed at all temperatures in another powder sample of $Pr_{1/2}Ca_{1/2}MnO_3$, our results give clear evidence against charge ordering in half doped manganites. At last, composition fluctuations are likely to occur in our floating-zone grown single crystals since synchrotron X-ray powder diffraction reveals that the single phased crushed crystal at RT splits into three macroscopic phases below T_{CO}.

B-229 Orbital, Charge and Spin Ordering in $Bi_{1-x}Ca_xMnO_3$ (x>0.5): Implications for Phase Segregation

A.Llobet Megias[1,2], J.L. García-Muñoz[1], C. Frontera[1], C. Ritter[3], M. Respaud[4], J.M. Broto[4], M.J. Martínez-Lope[5], M.A.G. Aranda[6],
[1] Institut de Ciència de Materiales de Barcelona, C.S.I.C. Spain
[2] Los Alamos National Lab, Los Alamos, New Mexico 87545, USA
[3] Institute Laue Langevin,Grenoble, France
[4] SNCMP and LPMC, INSA, Complexe scientifique de Rangueil, Toulouse, 31077 France
[5] Instituto de Ciència de Materiales de Madrid, C.S.I.C., Spain
[6] Departamento de Química Inorgánica, Cristalografía y Mineralogía, U. de Málaga, Spain

The tendency toward the formation of charge inhomogeneities in manganites and other transition metal oxides is stimulating considerable experimental and theoretical research. The presence of lattice polarons, disordered or forming ordered stripes is intimately related to the transport properties of these materials. The strong relationship between CMR and phase separation makes nanoscopic and macroscopic phase segregation a current hot topic that deserves much attention. We have investigated (i) charge/orbital -ordering and (ii) phase segregation phenomena in $Bi_{1-x}Ca_xMnO_3$ (0.5<x<1) using high-resolution neutron (NPD), ultra-high resolution synchrotron (SXRD) powder diffraction and magneto-transport techniques. We focus on the low temperature phase segregation phenomena observed in this portion of the phase diagram, the percolative nature of the metal-insulator transitions and CMR effects. The very precise results show that the presence of tiny compositional fluctuations is at the origin of the macroscopic phase segregation for x>0.75. Our study proposes a revision of the single-phase concept referred to these oxides.

B-230 Neutron scattering studies for the field-induced ordered state of TbB_2C_2

K. Kaneko[1], S. Katano[2], M. Matsuda[2], K. Ohoyama[1], H. Onodera[1], Y. Yamaguchi[1],
[1] Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan
[2] Advanced Science Research Center, JAERI, Tokai 319-1195, Japan

TbB_2C_2 which is isostructural with the antiferroquadrupolar (AFQ) ordering materials DyB_2C_2 and HoB_2C_2 exhibits no AFQ order under $H = 0$. However, from detailed magnetization measurements, it is presumed that an AFQ order is realized in TbB_2C_2 under $H > 0$. To confirm the field-induced AFQ order, neutron diffraction experiments on $Tb^{11}B_2C_2$ were carried out under fields up to 10 T. The results indicate that the magnetic structure of TbB_2C_2 under $H = 0.5$ T is basically the same as those of the ground state of DyB_2C_2 and HoB_2C_2 where the AFQ and AFM order coexist. Therefore, we suppose that a field-induced AFQ order is realized in TbB_2C_2.

B-231 Spin Fluctuations in Half-Doped 2D Mn and Co Oxides

K. Nakajima[1], T. Sawada[1], T. Iihama[2], H. Yoshizawa[1], K. Kakurai[3], Y. Endoh[4],
[1] Neutron Scattering Laboratory, Institute for Solid State Physics, University of Tokyo
[2] Department of Physics, Tohoku University
[3] Advanced Science Research Center, Japan Atomic Energy Research Institute
[4] Institute for Materials Research, Tohoku University

We have studied the magnetic excitations in hole-doped $La_{0.6}Sr_{1.4}MnO_4$ and $La_2CoO_{4.24}$ by means of the inelastic neutron scattering experiments. In half-doped manganites and cobaltates, distinct charge ordered phases are observed, in which Mn^{3+} and Mn^{4+}, or Co^{2+} and Co^{3+} are ordered in the checkerboard arrangement in the 2D plane. In $La_{0.6}Sr_{1.4}MnO_4$, well-defined antiferromagnetic spin-wave excitations are observed at a low-energy region. The spin-waves have a 2D nature, which is same as those in non-doped La 2-1-4 systems. The intensity of the excitations rapidly decreases at a high-energy region, $\Delta E > 6$ meV, as observed in charge ordered phases of La_2NiO_4. We also measured the spin-wave excitations in oxygen doped $La_2CoO_{4.24}$. The obtained results will be compared with those from non-doped systems, hole-doped cuprates and nickelates.

B-232 Study of the magnetic structures in $La_{0.1}Pr_{0.6}Ca_{0.3}MnO_3$ by means of neutron diffraction.

V. Naish[1], T. Novoselova[1], A. Pirogov[1],
[1] Institute for Metal Physics, S.Kovalevskaya Str.18, Ekaterinburg GSP-170, Russia

The weak-doped antiferromagnetic manganites are known to show such very unusual phenomena as a charge and an orbital ordering in addition to a magnetic ordering. In this paper we organize the correct task setting in the neutron diffraction patterns decoding in order to get the reliable information about the magnetic structures of the manganites. The complete set of the antiferromagnetic structures obtained over either one or another irreducible representations of the symmetry group are given. It has been applied to the decoding of the neutron powder diffraction data taken on $(La_{0.1}Pr_{0.6})Ca_{0.3}MnO_3$ at different temperatures by the Rietveld method (GSAS program [1]). We have to admit that our results appeared to be quite different from the literature data [2,3]. [1] Larson A.C., GSAS, (1994) Copyright, The Regents of the University of California. [2] Martin C. , Phys.Rev.B (2000) Vol.62, No.10: 6442 [3] Balagurov A.M., Phys.Rev.B (1999) Vol.60, 383

B-233 Probing the Local Structure of Doped Manganites using the Atomic Pair Distribution Function.

Th. Proffen[1], S.J.L. Billinge[2],
[1] Los Alamos National Laboratory, LANSCE-12, MS H805, Los Alamos, NM 87545, USA
[2] Department of Physics and Astronomy, Michigan State University, East Lansing, MI 48824-1116, USA

The electronic and magnetic properties of the manganite $La_{1-x}Ca_xMnO_3$ are the subject of extensive study. In the doping range between $x = 0.17$ and $x = 0.5$ these materials show a metal-to-insulator (MI) transition transforming from a ferromagnetic metal (FM) at low temperature to a paramagnetic insulator (PI). For these high-T_c materials no macroscopic inhomogeneities are observed as e.g. for the low-T_c manganite $Pr_{1-x}Ca_xMnO_3$. We have used atomic pair distribution function (PDF) analysis based on neutron powder diffraction data to investigate local structure for doping $x = 0.25$ as a function of temperature. We can probe the charge distribution of the sample using the PDF by searching for evidence of Jahn-Teller (JT) distorted octahedra implying the presence on Mn^{3+} ions. A two phase model based on the local structures of the FM and PI phases was used to refine the experimental PDFs quantitatively. We observe the co-existance of both phases over a wide temperature range: A small fraction of the localized JT phase (PI) is present at the lowest temperature ($T = 10\ K$), whereas at room temperature only nearly half of the sample has remained in the delocalized (FM) phase.

B-234 Evidence for a Dynamic Jahn-Teller Effect in PrO_2

C.H. Gardiner[1], A.T. Boothroyd[1], S.J.S. Lister[1], P. Santini[1], B.D. Rainford[2], L.D. Noailles[3], D.B. Currie[4], R.S. Eccleston[5], R.I. Bewley[5],

[1] Department of Physics, University of Oxford, Oxford, OX1 3PU, United Kingdom
[2] Department of Physics, University of Southampton, Southampton, SO17 1BJ, United Kingdom
[3] Inorganic Chemistry Laboratory, University of Oxford, Oxford, OX1 3QR, United Kingdom
[4] Department of Chemistry, University of Southampton, Southampton, SO17 1BJ, United Kingdom
[5] ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, OX11 0QX, United Kingdom

Recent neutron scattering research into the properties of PrO_2 has produced unusual results which are suggestive of a strong magneto-elastic coupling between phonon modes and crystal field states [1,2]. This leads to a dynamic Jahn-Teller effect in the ground state and a bound state between a phonon and a crystal field excitation. Measurements of the magnetic excitation spectrum of PrO_2 over the energy range 0–1200 meV show broad features as well as crystal field excitations characteristic of a Pr^{4+} ion. The ordered magnetic moment of the Pr^{4+} ion has been measured in a single crystal, and found to be anomalously small, in agreement with measurements made on polycrystalline samples [2]. The reduction of the ordered moment from that expected in a cubic crystal field and the broad features in the excitation spectrum can be reproduced qualitatively by a model based on magneto-elastic coupling. [1] A.T. Boothroyd et al Phys. Rev. Lett. **86**, 2082 (2001) [2] S. Kern et al, Solid State Communications **49**, 295 (1984)

B-235 Phase Separation from Competing Orbital and Magnetic Degrees of Freedom

D. N. Argyriou[1], U. Ruett[1], C. Adams[2], J. Gardner[3], J. Mitchell[1], P.G. Radaelli,
[1] Argonne National Laboratry, Argonne, IL, 60439, USA
[2] Reactor Radiation Division, National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA
[3] NPMR, Chalk River Laboratories, Chalk River, ON, KOJ 1JO, Canada.
[4] Rutherford Appleton Laboratory, Chilton, Didcot, Oxon Ox11 0QX, UK

We observe experimentally that competing orbital and magnetic degrees of freedom lead to long range phase separation in the manganite perovskites. Examples of this competition and phase separation are found both in layered perovskites such as $LaSr_2Mn_2O_7$ and three-dimensional materials such as $Pr_{0.7}Ca_{0.3}MnO_3$. Neutron and X-ray diffuse scattering measurements show that in both cases short range CE-type charge and orbital ordering correlations are observed at 300K and with decreasing temperature long range order develops. The stability of the CE-type phase is challenged by magnetic degrees of freedom, with the effect of either melting the CE-type phase in the case of $LaSr_2Mn_2O_7$, or producing a mixed phase ground state in $Pr_{0.7}Ca_{0.3}MnO_3$. Indeed diffuse scattering measurements suggest that the onset or melting of the CE-type phase is akin to an orbital order-disorder transition. Our observations are consistent with recent two-orbital Monte Carlo simulations of manganites where phase separation is predicted close to ferromagnetic-metallic ground states. Indeed this proximity is seen clearly in $Pr_{0.7}Ca_{0.3}MnO_3$ where application of a magnetic field at low temperatures leads to a ferromagnetic metallic state.

B-236 $La_{1.5}Sr_{0.5}NiO_4$ Charge-Ordered Phase: Structure and GPDOS.

A. E. Nikiforov[1], V. A. Smorkalov[1], A. Yu. Zaharov[1],
[1] Urals State University, Lenin av.51, 620083 Ekaterinburg, Russia

The computer simulation of charge-ordering (CO) phenomenon in $La_{1.5}Sr_{0.5}NiO_4$ has been carried out. The microscopic mechanism responsible for the CO phase stabilization were revealed and GPDOS was predicted. The CO state was associated with holes arrangement over Ni sites in chess-board manner within NiO_2 layers. The calculations were performed within the framework of pair potential approach and shell model. Harmonic approximation was used for the dynamics investigation. Total crystal energy minimization yielded that CO phase is stable and has lower energy than HTT one, and that during HTT to CO transition structure relaxation gives more energy gain than hole redistribution. It turned out that main interreaction decreasing crystal energy is Coulomb one Ni^{3+}-O^{2-}_{basal} which causes breathing phonon creation. Calculated GPDOS shows a good quality agreement with experimental one. So, in both cases the doublet splitting of one line in CO phase is observed. We conclude that it is owing to E_g or E_u oxigen vibration mode degeneracy vanishes.

B-237 Crystal-lattice modulation and phonon anomaly associated with strong p-f mixing effect of CeSb

K. Iwasa[1], A. Hannan[1], M. Kohgi[1], M. Braden[2,3], J.-M. Mignot[3], H. Kitazawa[4], T. Suzuki[5]
[1] Department of Physics, Faculty of Science, Tokyo Metropolitan University, Hachioji, Tokyo 192-0397, Japan
[2] Forschungszentrum Karlsruhe, Institut für Nuklear Festkörperphysik, Postfach 3640, D-76021 Karlsruhe, Germany
[3] Laboratoire L'eon Brillouin, 91191 Gif sur Yvette cedex (France)
[4] National Research Institute for Metals, Tsukuba, Ibaraki 305-0047, Japan
[5] Tsukuba Institute of Science and Technology, Tsukuba, Ibaraki 300-0819, Japan

CeSb shows various magnetic structures with sequences of two kinds of Ce^{3+}-ion layers. The respective layers are composed of paramagnetic Ce ions with crystal-field ground state of Γ_7 and ferromagnetically aligned Ce ions with almost fully polarized magnetic-moment values of $2\mu_{mB}$. The origin of the formation of the ferromagnetic layers has been attributed to the strong p-f mixing effect. The present paper reports the unusual crystal-lattice properties associated with the p-f mixing effect in CeSb. We observed X-ray satellite reflections below $T_{mN} = 17mK$. Since the 4f-electron orbital of the polarized Ce ion is rather anisotropic compared to the Γ_7 one, the result is interpreted by modulations of inter-layer spacing and 4f-electron orbital state. By inelastic neutron scattering, we found an anomalous phonon mode appearing only in the ordered phases. It exhibits a local-mode character with the atomic displacement within the p-f mixing plane. This phenomena may be explained by phonon-induced electronic transition between the polarized Ce-ion state and the excited states.

B-238 Structure and Magnetic Ordering in $La_{0.5}Sr_{1.5}MnO_4$

P. Reutler[1,2,3], O. Friedt[4], B. Büchner[3], A. Revcolevshi[2], M. Braden[4,5],
[1] II. Physik. Insititut, Universität zu Köln, D-50937 K"oln
[2] Laboratoire de Physico-Chimie de l'Etat Solide, Université de Paris-Sud, F-91405 Orsay Cedex
[3] II. Physik. Insititut, RWTH Aachen, D-52056 Aachen
[4] Laboratoire Léon Brillouin, CEA/CNRS, F-91191 Gif-sur-Yvette Cedex
[5] Forschungszentrum Karlsruhe, IFP, Postfach 3640, D-76021 Karlsruhe

The layered manganite $La_{0.5}Sr_{1.5}MnO_4$ exhibits a charge order below T_{CO}=217K and AFM ordering below T_N=110K being reflected in a respectively doubled and quadrupled unit cell. We have made a detailed neutron structure analyses on single-crystalline samples at temperatures of 25K (CO and Magnetic order), 130K (only CO), and ambient temperature including a determination of Debye-Waller factors. Only very weak intensities of superlattice reflections (e.g. I(1.5,1.5,2)/I(006)=10^{-4}) were observed, so that the complete static ordering of valence states of Mn^{3+} and Mn^{4+} along the [110] direction is a picture not applicable as it is in strong disagreement to a bond length analysis. Furthermore we have observed additionally to the 3 dimensional low temperature AFM ordering a strong diffuse scattering contribution of the magnetism.

B-239 Relation Between the Magnetic Resonance and the Low-Temperature Spectral Function in the High-Temperature Superconductors

J. Mesot[1], M. Boehm[1,2], N. Metoki[3], A. Hiess[2], J. C. Campuzano[4], K. Kadowaki[5],
[1] Laboratory for Neutron Scattering, Paul Scherrer Institute, CH-5232 Villigen, Switzerland.
[2] Institut Laue Langevin, BP 156, F-38042 Grenoble, Cedex, France.
[3] Advanced Science Res. Center, Japan Atomic Energy Res. Inst., Tokai, Ibaraki 319-1195, Japan.
[4] Department of Physics, University of Illinois at Chicago, Chicago, IL 60607, USA.
[5] Institute of Materials Science, University of Tsukuba, Ibaraki 305, Japan.

We show that, in the high-temperature superconductors YBCO and Bi2212, the magnetic resonance measured by inelastic neutron scattering is connected to the peak-dip-hump structure of the single particle spectral function obtained from angle resolved photoemission (ARPES) experiments. In particular, we find that the energy of the collective mode inferred from ARPES matches that of the resonance. We also show that this relation together with the wavevector of the resonance implies the absence of bilayer splitting in the electronic dispersion.

B-240 Polaron life-time in $La_{0.75}Ca_{0.25}MnO_3$

N Wakabayashi[1], P Dai[2], J Fernandez-Baca[2], Y Tomioka[3], Y Tokura[3,4],
[1] Department of Physics, Keio University
[2] Solid State Division, Oak Ridge National Laboratory
[3] Joint Research Center for Atom Technology(JRCAT)
[4] Department of Applied Physics, University of Tokyo

As part of continued effort to accurately characterize the nature of the polaron in perovskite manganese oxides, quasielastic neutron scattering measurements were performed on a single crystal sample of $La_{0.75}Ca_{0.25}MnO_3$. Energy scans at the wavevector for the short-range correlation peak in the paramagnetic insulator phase show that the line widths are resolution limited at all temperatures. In contrast, the line width of the diffuse part of the scattering due to uncorrelated polarons was found to be much larger and to increase rapidly as the temperature was increased. The width is as large as 4meV (FWHM) and of the same order of magnitude as that of magnetic scattering. This result is interpreted to show that the decrease in the resitivity is closely related to the decrease in the life-time of uncorrelated polarons as the temperature is increased in the insulator phase.

B-241 Magnetic diffuse scattering in a bilayer manganite $La_{2-2x}Sr_{1+2x}Mn_2O_7$

M Kubota[1], Y Oohara[1], H Yoshizawa[1], H Fujioka[2], K Hirota[2], Y Moritomo[3], Y Endoh[4],
[1] Neutron Scattering Laboratory, I. S. S. P., University of Tokyo, Tokai, Ibaraki, 319-1106
[2] CREST, Department of Physics, Tohoku University, Aoba-ku, Sendai, 980-8578
[3] PRESTO and CIRSE, Nagoya University, Nagoya, 464-8601
[4] CREST, Institute for Materials Research, Tohoku University, Aoba-ku, Sendai 980-8577

In $La_{2-2x}Sr_{1+2x}Mn_2O_7$ sample with $x = 0.45$, an antiferromagnetic (AFM) correlation generates the diffuse signal along c with the period of $1/z_o$ for $T_C < T < T_N$ (z_o; the distance of Mn ions within a bilayer along c). Below T_C, however, the period of a diffuse signal changes due to the appearance of a canted AFM structure with a canting angle θ_{cant} of 63.7 °. On the other hand, the diffuse signal with the canted AFM structure is almost invisible for x=0.40, which is reasonable considering a small θ_{cant} of 6.3°. These results indicate a phase separation does not occur between a FM and an AFM spin correlations along c.

B-242 Spin Order and Orbital Degrees of Freedom in YVO_3 and $LaVO_3$

C. Ulrich[1], G. Khaliullin[1], H. He[1], M. Ohl[2,3], A. Ivanov[2], Y Taguchi[4], Y. Tokura[4], B. Keimer[1],
[1] Max-Planck-Institut FKF, 70569 Stuttgart, Germany
[2] Institut Laue-Langevin, 38042 Grenoble, France
[3] Forschungszentrum Jülich, 52425 Jülich, Germany
[4] Department of Applied Physics, University of Tokyo, Japan

Transition metal oxides with the perovskite structure display a large variety of unusual properties such as high temperature superconductivity or colossal magnetoresistance. YVO_3 is of particular interest because it undergoes reversible sign changes in the magnetisation with temperature. In order to determine the spin dynamics an the orbital degrees of freedom in the Mott-Hubbard insulators YVO_3 and $LaVO_3$, we have studied their spin wave dispersion relations by single crystal inelastic neutron scattering (INS). YVO_3 has two magnetic phase, a C-type phase between 114 K and 78 K and a G-type phase at low temperatures. Or INS results indicate that the high temperature magnetic phase has an unusual ground state, analogous to the situation in $LaTiO_3$, where no orbital ordering is observed. This underlines that the quantum mechanical processes related to the spin and orbital degrees of freedom are much more complicated. In the low temperature phase of YVO_3 and in $LaVO_3$ (C-type) on the other side the VO_6 octahedra are distorted and the orbitals are locked to the lattice.

B-243 Phonon Density of States in $LaMnO_3$ doped with Ca nd Sr.

A. Ivanov[1], Ya. Mukovskii[2], D. Shuliatév[2], A. Arsenov[2],
[1] Institut Laue-Langevin, 38042 Grenoble, France
[2] Moscow State Steel and Alloys Institute, 117936 Moscow, Russia

Phonon densities of state in $La_{1-x}A_xMnO_3$ (A = Sr,Ca, x=0, 0.3) CMR compounds have been measured using neutron inelastic scattering technique. High-frequency dynamics is characterised by the pronounced bands of oxygen vibrations in the undoped and Sr-doped compounds. It was found that the shape of the phonon spectrum of the Ca-doped samples differs remarkably from the spectrum of Sr-doped samples. The shape of the spectral functions in both systems does not change appreciably going through the phase transitions. Certain changes are registered in the spectrum of the Ca-doped system when magnetic field is applied to the powder sample. It is suggested that the observed differences could be related to the different oxygen isotope effect in these CMR compounds.

B-244 Anomalously high orbital ordering temperature in $Bi_{0.5}Sr_{0.5}MnO_3$: $6s^2$ lone pair effect.

C. Frontera[1], A. Llobet[1,2], C. Ritter[3], M. Respaud[4], J. Vanacken[5], M. A. G. Aranda[6], J. L. García-Muñoz[1],
[1] ICMAB-CSIC, Bellaterra, Spain
[2] Los Alamos National Laboratory, Los Alamos, New Mexico, USA
[3] Institut Laue-Langevin, Grenoble, France
[4] L.N.C.M.P. and L.P.M.C., INSA, Toulouse, France
[5] LVSM, KU Leuven, Leuven, Belgium
[6] Dep. Quím. Inorg., U de Málaga, Málaga, Spain

We present a study of the structural and magnetic properties of $(Bi, Sr)MnO_3$ in the temperature interval $4.2 - 700K$. Based on neutron and synchrotron X-ray measurements we have found that $Bi_{0.5}Sr_{0.5}MnO_3$ presents OO/CO yet at room temperature [1]. The superlattice peaks associated with this OO/CO persist up to the surprisingly high temperature $T_{CO} \approx 500K$ [2]; more than $350K$ above the temperature predicted by the bandwidth tuning mechanism for its Mn-O-Mn bond bending. A detailed structural and magnetic study is presented both confirming the presence of charge-ordering and remarkable differences with respect to rare earth-based half-doped manganites [3].A new mechanism favoring orbital/charge ordering is proposed based on the lone-pair of $6s^2$ electrons of Bi^{3+}. [1]C. Frontera *et al.* J. of Phys.: Cond. Matt. **13**, 1071 (2001). [2]J.L. Garcia-Muñoz *et al.* Phys. Rev. B **63**, 064415 (2001). [3]C. Frontera *et al.* Phys. Rev. B (in press).

B-245 Manganites doped with Sr (x=0.1 and x=0.125): two steps before the metallic and ferromagnetic transition.

F. Moussa[1], M Hennion[1], P. Reutler[2,3,4], J. Rodriguez-Carvajal[1], F. Wang[1], L. Pinsard[2], B. Büchner[4],
[1] Laboratoire Léon Brillouin, CE Saclay, F-91191 Gif-sur-Yvette Cedex, France
[2] Laboratoire de Physico-Chimie de l' Etat Solide, Univ. Paris-Sud F-91405 Orsay Cedex, France
[3] II. Physik Institut, Universität zu Köln, D-50937, Germany
[4] II. Physik Institut, RWTH Aachen, D-52056 Aachen, Germany

Phonon and spin wave dispersion curves have been measured in $La_{0.9}Sr_{0.1}MnO_3$ and in $La_{0.875}Sr_{0.125}MnO_3$. $La_{0.9}Sr_{0.1}MnO_3$ is an example of an AF canted state with interactive F inhomogeneities. From the two measured anisotropic spin wave branches, a F and an AF exchange integrals have been determined together with an anisotropic coupling related to the F inhomogeneities revealed by the diffuse scattering. The phonons are nearly isotropic. They lie in the same range of energy as the magnons which propagate in the F basal plane. $La_{0.875}Sr_{0.125}MnO_3$ exhibits a JT transition at 290 K, a ferromagnetic transition at 175 K with an upturn of the resistivity and a reentrant structural transition at 159 K with again an insulating behaviour. This transition is shown to be driven by the softening of the TA mode at the point where Bragg peaks grow. This transition reveals also a strong magnon - phonon coupling specially at the zone boundaries. The neutron scattering results can bring some light on the nature of this still debated insulating F state.

B-246 Neutron and X-ray Critical Scattering from NaV_2O_5

Y. Fujii[1], N. Aso[1], K. Ohwada[1], K. Katsuki[1], N. Takesue[1], M. Nishi[1], K. Kakurai[1], H. Nakao[2], T. Yosihama[3], M. Isobe[4], Y. Ueda[4],
[1] Neutron Scattering Lab., ISSP, Univ. of Tokyo, 106-1 Shirakata, Tokai,Ibaraki 319-1106, Japan
[2] Photon Factory, KEK, 1-1 Oho, Tsukuba, Ibaraki 305-0801, Japan
[3] Adv. Sci. Res. Center, JAERI, Tokai, Ibaraki 319-1195, Japan
[4] Mater. Design & Character. Lab., ISSP, Univ. of Tokyo, 5-1-5Kashiwanoha, Kashiwa, Chiba 277-8581, Japan

A quarter-filled spin ladder compound NaV_2O_5 undergoes a novel phase transition at T_c=35K at ambient pressure associated with lattice dimerization[1] and charge-ordering between V^{4+}(S=1/2) and V^{5+}(S=0) both modulated with q=(1/2,1/2,1/4)[2] as well as spin-gap formation at q=(1,1/2,0)[3]. We observed a strong x-ray critical scattering resulting from fluctuation of the lattice dimerization near T_c [4]. In order to study dynamical behavior of the lattice system in this compound, we have carried inelastic neutron scattering experiments with a triple-axis spectrometer, that is, measurement of energy spectrum of critical scattering. It has been revealed that such a critical scattering doesn't result from any soft phonon but has a relaxation type response in energy, presumably expressed by a Lorentian although strong incoherent scattering from V atoms blocks information near the energy zero region. Based on the observed time-space correlation, we discuss a phase transition mechanism of this spin-charge-lattice coupled system of NaV_2O_5. [1] Y. Fujii et al., JPSJ 66 (1997) 326. [2] H. Nakao et al., PRL 85 (2000) 4349. [3] T. Yosihama et al., JPCS 60 (1999) 1099. [4] H. Nakao et al., Physica B241-243 (1998) 534.

B-247 Neutron beam line with triple axis spectrometer, powder diffractometer and a surface machine using a toroidally bent asymmetric crystal monochromator

V Siruguri[1], P. D. Babu[1], A. V. Pimpale[2], P. S. Goyal[1], B. A. Dasannacharya[2],
[1] IUC-DAEF, Mumbai Centre, R-5 Shed, BARC, Mumbai 400 085, India
[2] IUC-DAEF, Indore Centre, University Campus, Khandwa Road, Indore 452 017, India

A new beam line with three stations in tandem - a triple axis spectrometer (TAS), a powder diffractometer (PD) and a surface machine (SM) - is under development at the Dhruva reactor, BARC, Mumbai. Monte Carlo (MC) simulation programs are developed for studying the propagation of neutrons starting from reactor end and progressing through various optical elements - collimators, slits, monochromator crystal, sample and finally reaching the detector. The programs for the PD are validated by applying to an existing beam line using a plane crystal monochromator and then used to design the new high intensity beam line using a toroidally bent asymmetric crystal monochromator [1]. Simulation results show that a perfect bent crystal monochromator based PD provides an almost constant resolution of 0.5 deg (FWHM) over a wide scattering angle range 10 - 120 deg for detector angular resolution of 0.2 deg and a sample size of 6 mm dia. The status of the beam line along with ongoing MC simulation for the TAS and the SM will be presented. [1] M. Popovici and W. B. Yelon, J. Neutron Research 3(1995)1.

B-248 The new "BerSANS-PC" software package for reduction and treatment of small angle neutron scattering data

U. Keiderling[1,2],
[1] Technical University Darmstadt, Petersenstrasse 23, D-64287 Darmstadt, Germany
[2] Hahn-Meitner-Institut, Glienicker Strasse 100, D-14109 Berlin, Germany

Measurements on SANS instruments are typically characterized by a large number of samples, short measurement times for the individual samples, and a frequent change of visiting scientist groups. Besides this, recent advantages in instrumentation have lead to more frequent measurements of kinetic sequences and a growing interest in analyzing two-dimensional scattering data, all requiring special software tools which enable the users to extract physically relevant information from the scattering data with a minimum of effort. The new "BerSANS-PC" data processing software package has been developed for the SANS instrument "V4" at the Hahn-Meitner-Institut in Berlin, Germany, to meet these requirements and to support an efficiently working guest user service. Comprising some basic functions of the "BerSANS" program available at the HMI in the past, the software package is a completely new development for network-independent use on local PCs with a full-feature graphical interface.

B-249 Mosaic crystal algorithm for Monte Carlo

P A Seeger[1,2], L L Daemen[2],
[1] 239 Loma del Escolar, Los Alamos, NM 87544, USA
[2] Manuel Lujan Jr. Neutron Scattering Center, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

An algorithm is presented for calculating reflectivity, absorption, and scattering of mosaic crystals in Monte Carlo simulations of neutron instruments. The algorithm uses multi-step transport through the crystal with an exact solution of the Darwin equations at each step. It relies on the kinematical model for Bragg reflection (with parameters adjusted to reproduce experimental data). For computation of thermal effects (the Debye-Waller factor and coherent inelastic scattering), an expansion of the Debye integral as a rapidly converging series of exponential terms is also presented. Any crystal geometry and plane orientation may be treated. The algorithm has been incorporated in the Neutron Instrument Simulation Package (NISP).

B-251 The use of Multichannel Collimation in Small Angle Neutron Scattering: a Computer Simulation Study

A. N. Falcão, F. M. A. Margaça, F. G. Carvalho,
[1] Physics Dept., Nuclear and Technological Institute, E. N. 10, 2686-953 Sacavém, Portugal

In a computer simulation study, the use of converging multichannel collimation in a small angle neutron scattering arrangement is shown to lead to improved performance of typical instruments. The influence of the use of neutron guides (both straight and curved) to feed the instrument as well as that of guide interruptions, like those necessary to include velocity selection, on the overall performance of the instrument are discussed. The implementation of variable geometry is considered, and guidelines for the construction of variable geometry XY collimators are presented.

B-252 Monte-Carlo simulations of the neutron Brillouin spectrometer BRISP

J.-B. Suck[1], S. Jahn[1,2],
[1] Institute of Physics, Materials Research and Liquids, TU Chemnitz, D-09107 Chemnitz, Germany
[2] Institut Laue-Langevin, BP 156, F-38042 Grenoble Cedex 9, France

The thermal neutron Brillouin spectrometer BRISP will be a new type of instrument at the ILL using the time-of-flight technique and is aimed mainly for investigations of disordered matter and magnetic materials at small momentum transfers and relatively large energy transfers. Within this dynamic region transitions from macroscopic to microscopic properties of matter can be studied. Monte-Carlo simulations have been made to determine the possible performance of the instrument with respect to resolution and intensity. The neutron flux at the monochromator has been determined using the MCNP code and another program was used for the ray-tracing through the instrument. To find the optimal setup, i.e. a good resolution in energy and momentum transfer at acceptable intensity, different monochromator and collimator options have been tested. The chopper speed becomes important especially at small detector distances and high neutron energies.

B-253 Monte Carlo Simulation of the cold triple axis spectrometer (PANDA) at the FRM-II

R. Schedler[1], M. Rotter[1], M. Loewenhaupt[1], N.M. Pyka[2],
[1] Intitute for Applied Physics (IAPD), TU Dresden, 01062 Dresden,Germany
[2] FRM-II, Technische Universität München, 85747 Garching, Germany

The cold triple axis spectrometer PANDA will be among the first instruments to start operating at the new neutron source. Monte Carlo Simulations of the spectrometer have been performed in order to optimize the design of the neutron optics and provide information about the features of this new spectrometer (see http://www.physik.tu-dresden.de/iapd/index.php3). As a first step simulations were performed for the primary neutron path from the cold source to the sample. The vertical and optional horizontal neutron guides, the variable horizontal diaphragm, optional collimators and the double focusing monochromator have been included and different configurations of the spectrometer have been simulated. In a second step also the other parts of the spectrometer have been modelled. The energy spectrum of the cold source, the transmission of the collimators and the

reflectivity of the supermirrors have been taken into account. The simulations have been performed for several incident energies. Results include the resolution ellipsoid, the flux at the sample position and energy, divergence and spatial distribution of the neutron intensity at several locations such as monochromator, sample, analyser and detector.

B-254 Designing new guides and instruments at the ILL using the McStas Monte-Carlo neutron simulation package

E. Farhi[1],
[1] Institut Laue-Langevin, BP 156, 38042 Grenoble Cedex 9, France

With the increasing complexity of modern neutron scattering instruments, the need for powerful tools to optimize their geometry and physical performances (flux, resolution, divergence, etc.) has become essential. As the usual analytical methods reach their limit of validity in the description of fine effects, the use of Monte Carlo simulations, that can handle these latter, has become widely spread. The McStas program was developed at Risoe National Laboratory in order to provide neutron scattering instrument scientists with an efficient and flexible tool for building Monte Carlo simulations of guides, neutron optics and instruments. To date, the McStas package has extensively been used at the Institut Laue-Langevin, Grenoble, France, for various studies including cold and thermal guides with balistic geometry, diffractometers, triple-axis, backscattering, and time-of-flight spectrometers.

B-255 Simulation of the Backscattering Spectrometer IN16: How much can be gained by using the Phase Space Transformation technique?

M. A. Gonzalez[1], B. Frick[1],
[1] Institut Laue - Langevin, BP 156, 38042 Grenoble Cedex 9, France

IN16 is a backscattering spectrometer combining high flux and an excellent resolution. We have studied a possibility to improve both the flux and the dynamic range of this instrument by using the Phase Space Transformation technique to monochromate a white neutron beam. By using a crystal mounted on a chopper that moves perpendicularly to the average scattering vector of the incident neutrons it is possible to increase significantly the number of neutrons in a given wavelength band at the expense of worsening the Q-resolution. In order to obtain reliable information about the improvement that could be achieved by applying this principle to the existing instrument, we have performed simulations with the McStas package to compare the flux of IN16 in its present configuration with that of an hypothetical IN16B located at the end position of a straight focusing neutron guide. The simulations reproduce well several test experiments performed on IN16 and allow us to predict that a gain in flux up to a factor of 8 can be expected.

B-256 A new method of Debye-Scherrer pattern integration on 2D detectors demonstrated for the new Structure Powder Diffractometer (SPODI)

F. Elf[1], R. Gilles[2], G.R.J. Artus[3], S. Roth[4],
[1] Mineralogisches Institut der Universität Bonn, Poppelsdorfer Schloss, 53115 Bonn, Germany
[2] Fachbereich Material- und Geowissenschaften, TU Darmstadt, Petersenstr. 23, 64287 Darmstadt, Germany
[3] Neue Forschungs-Neutronenquelle, TU München, Lichtenbergstr.1, 85747 Garching, Germany
[4] Physik Department E13, TU München, James Franck Str. 1, 85747 Garching, Germany

Sample height and nonparallelism of the primary beam are responsible for vertically smeared Debye-Scherrer rings as measured by a 2D detector (Beseneffekt or umbrella effect). It will be shown that this effect can be reversed by mathematical algorithm of deconvolution. Intensity integration along the elliptic arcs reduces data to conventional 1D diffraction patterns without intensity loss and no significant peak broadening or asymmetry, suitable for Rietveld refinement programs. The diffraction data were obtained by Monte Carlo simulations (McStas).

B-257 Performance gains for next-generation neutron-scattering instruments resulting from improved supermirror coatings

Ch Rehm[1], M Agamalian[1],
[1] Spallation Neutron Source Project / Oak Ridge National Laboratory

Next-generation pulsed neutron-scattering facilities will offer instruments with unprecedented capabilities by simultaneous enhancement of source power and usage of advanced optical components. The Spallation Neutron Source (SNS), already under construction at Oak Ridge National Laboratory, will provide greater than an order of magnitude more usable neutron flux than current state-of-the-art facilities. Similar gain factors are also achievable by implementing new optical devices and instrument concepts. We analyzed how the performance of next generation neutron scattering instruments depends on the quality of supermirror coatings. A simulation program which allows different approaches for supermirror design has been developed. It was found that state-of-the-art supermirrors have not yet reached their theoretical limitations, particularly for high-critical angle supermirrors. We propose how to improve the reflectivity for the critical transfer momentum, and the resulting gains will be demonstrated on the basis of a conceptual design for the SNS magnetism reflectometer.

B-258 Optimization of the SNS Magnetism Reflectometer Design Using Monte Carlo Simulations

W.-T. Lee[1], F. Klose[1],
[1] Spallation Neutron Source, Oak Ridge National Laboratory

The Magnetism Reflectometer at the Spallation Neutron Source (SNS) will employ advanced neutron optics to achieve high data rate, improve the resolution, and extend the dynamic range. Utilized optical components include a polygonal and sectioned curved neutron guide and a TOF spin resonance energy filter. The results of a neutron beam interacting with these devices are rather complex. Further complications arise due to the spectral/time emission profile of the moderator and non-perfect neutron optical coatings. While analytic formulae for the individual components provide some design guidelines, a realistic performance assessment of the whole instrument can only be achieved by advanced simulation methods. In this contribution, we present an optimization of the Magnetism Reflectometer using Monte Carlo simulations. We will compare different instrument configurations and calculate the resulting data rates and resolutions.

B-259 Optimization of a focusing monochromator for neutron strain-scanning diffractometer

J. Šaroun[1,2], T. Pirling[2], R.W. Rogge[3],
[1] Nuclear Physics Institute, 25068 Řež near Prague, Czech Republic
[2] Institute Laue Langevin, 6 rue Jules Horowitz, BP 156, 38042 Grenoble Cedex 9, France
[3] National Research Council, Chalk River Laboratories, Chalk River, ON, Canada, K0J 1J0

Well-designed monochromator is obviously a key part of a neutron diffractometer for strain measurements. High incident flux is important priority for such an instrument, but it must not be achieved at the cost of worse resolution and/or diffraction peak shape. It is therefore necessary to assess the performance of the monochromator in the context of the whole instrument setup. We present a study based on Monte Carlo simulations, comparing several mosaic and elastically deformed crystals as possible candidates for optimum monochromators. A set of diffraction profiles measured at a conventional strain-scanning diffractometer is compared with simulations for validation. The results show that elastically deformed crystals can be optimized better than the mosaic ones for a limited range of wavelengths. This can be particularly useful for microstrain investigations, which need high angular resolution, but require lower number of reflections and more relaxed spatial resolution. On the other hand, a choice from both types of crystals is suggested when the instrument has to operate efficiently in a wide wavelength range.

B-260 Simulation of a complete inelastic neutron scattering experiment

H. Edwards[1], K. Lefmann[1], B. Lake[2], K. Nielsen[1], P. Skaarup[1],
[1] Department of Condensed Matter Physics and Chemistry, Risø National Laboratory, 4000 Roskilde, Denmark.
[2] Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

A quantitative simulation of an inelastic neutron scattering experiment on the high-temperature superconductor $La_{2-x}Sr_xCuO_4$ is presented. The complete experiment, including sample, is simulated using an interface between the experiment control program (TASCOM) and the simulation software package (McStas). Simulating the entire experiment is an attractive alternative to the usual method of comparing data to the folding of the theoretical cross section with the resolution function if the resolution function is nontrivial. Quantitative comparisons between experiment and simulation are made.

B-261 Design and simulation of the CG1 guide beamline at the HFIR cold source

S. E. Nagler[1], W. T. Lee[1], R. M. Moon[1],
[1] Solid State Division, Oak Ridge National Laboratory

In the near future a super-critical hydrogen cold source will be installed in the HB4 beam tube of the High Flux Isotope Reactor (HFIR), Oak Ridge National Laboratory. The cold source will illuminate four neutron guides. Here we discuss the design and simulation of the guide CG1, dedicated to a new triple axis spectrometer. The conceptual design for the HFIR guides, including CG1, was aided by numerical calculations of neutron trajectories and acceptance diagrams. The CG1 guide consists of a partially trumpeting two-channel bender and a straight guide section. The design was subsequently modeled in detail from source to specimen, utilizing the McStas program. The lessons learned from the McStas simulations resulted in some minor but important changes in the design, and these were also verified using the original method of calculation. The resulting combination of guide and vertically focusing monochromator should deliver a beam with excellent spatial and angular distributions in and out of the scattering plane. The available intensity will enable the construction of a powerful spectrometer for incident energies as large as 20-25 meV.

B-262 Simulation of the polarized neutron diffuse scattering spectrometer, D7

J.M. Preston[1], J.R. Stewart[1], E. Farhi[1],
[1] Institut Laue Langevin, 6 rue Jules Horowitz, B.P. 156, 38042 Grenoble, France

The 3-directional neutron polarization analysis technique provides a method of unambiguous separation of nuclear and magnetic scattering [1]. This method is used to examine magnetic configurational disorder and the interplay between such disorder and local atomic defect structures on the diffuse scattering spectrometer D7 [2] at the Institut Laue Langevin. As part of the ILL Millennium Programme, D7 is being upgraded and optimised. The installation of new focusing supermirror Schärpf bender polarizers and analysers will, it is estimated, increase the effective counting rate of the instrument by a factor of 60. As part of the design process, the McStas package [3] has been used to simulate the proposed polarization devices for the new D7. Results from the McStas simulation are presented here alongside preliminary test results of the new D7 polarizer. [1] O. Schärpf and H. Capellmann, Phys. Stat. Sol. **A135** (1993) 359 [2] J.R. Stewart *et al* J. Appl. Phys. **87** (2000) 5425 [3] K. Lefmann and K. Nielsen, Neutron News, **10/3** (1999) 20

B-263 Monte Carlo Simulations of Critical Scattering Experiments

M Hagen[1],
[1] Physics Department, Keele University, Keele, Staffordshire ST5 5BG, United Kingdom

The use of Monte Carlo ray tracing (simulation) techniques to study the performance of neutron scattering instrumentation is now becoming well established. As well as *what if* studies for instrument design, simulations can also be used to study, at least in general terms, how different instrument configurations and data-analysis procedures will perform in different experiments. In the study of critical phenomena the quantity one usually wishes to obtain is the correlation function. If this is to be done accurately via a diffraction experiment then the so-called Quasi-Static Approximation must be satisfied. Monte Carlo simulation has been used to examine how well this approximation is satisfied, for the cases of a two-axis diffractometer and an energy dispersive (time of flight) multi-detector diffractometer, for different experiments. Another approach to obtaining the quasi-static correlation function, for one and two dimensional magnetic materials, is the integration of spectra from inelastic scattering experiments. Again simulation has been used to assess how such a procedure will be affected by variations in the resolution across the inelastic spectrum. The results of these studies will be presented.

B-264 IDEAS - A Monte Carlo Simulation Package for Neutron Scattering Instrumentation

W.-T. Lee[1], X.-L. Wang[1], J. L. Robertson[2], F. Klose[1], Ch. Rehm[1],
[1] Spallation Neutron Source, Oak Ridge National Laboratory
[2] Solid State Division, Oak Ridge National Laboratory

The need to optimize the design of neutron scattering instruments at current and planned neutron sources has demanded detailed and realistic performance assessments. Such assessments often involve complex convolution calculations and require numerical simulations. We present here IDEAS (Instrument Design and Experiment Assessment Suite), a general-purpose software package for simulating the optics of neutron scattering instruments. Individual self-contained modules representing different neutron optical components are arranged in a sequence to form an instrument. To perform a simulation, the modules sequentially modify the physical parameters of a neutron (position, velocity, spin, and probability) subject to the physics of the interaction. A user interface incorporated in the software reduces the set up, modification, and simulation to virtually the click of a button, thus allowing a user to focus on the instrument design and carry out fast prototyping. The software was also optimized to maximize the

simulation speed. In addition, the only convention for incorporating new optical component module is the function header of the simulation code and the neutron parameters. Simulations for SNS instruments and the Neutron Optical Test Station at the future HFIR cold neutron guide hall will be presented as examples.

B-265 Upgrade of the backscattering spectrometer IN13 at ILL.

C. Mondelli[1,2], L. Alianelli[1,2], F. Natali[2], A. Paciaroni[2], C. Pfister[3], M. Bée[3],
[1] Institut Laue-Langevin, B.P. 156, F-38042 Grenoble Cedex 9, France
[2] Istituto Nazionale per la Fisica della Materia, Operative Group Grenoble, B.P. 220, F-38043 Grenoble Cedex 9, France
[3] Université Joseph Fourier, B.P.53, F-38041 Grenoble Cedex 9, France

The availability of high momentum transfers (0.3 ¡ Q(Å) ¡ 5.5) with an energy resolution of few μeV, makes of the spectrometer IN13 a very useful instrument for the study of the local dynamics of soft matter, such as polymers and biological systems. In the present configuration the performance of the instrument is overall limited by the low incident flux. A progressive upgrade of the instrument is planned in order to improve this feature and also to increase the instrument versatility. In this way different possibilities of changing the standard configuration will be available in order to allow for the best compromise between flux, energy resolution and Q-range for each experiment. The first step of this project consists on fully simulating the instrument and the modifications envisaged. This has been done using the McStas package and here we present the results of those simulations.

B-266 Bragg diffracting neutron energy filters

S. N. Klausen[1], H. M. Ronnow[2], R. Stancliff[3], B. Fortescue[3], K. Lefmann[1], A. R. Wildes[4],
[1] Materials Research Department, Risø National Laboratory, Denmark
[2] DRFMC, CEA Grenoble, France
[3] Department of Physics, University of Oxford
[4] Institut Laue-Langevin, France

We review the use of neutron energy filters based on the principle of Bragg diffracting unwanted neutrons out of the beam. Such filters are used in a wide range of neutron instruments, but we focus on the application to inelastic neutron scattering experiments. In almost any experiment, can the quality of the signal be improved by using a filter to remove higher order lambda/n contamination and to lower the background in general. But we also discuss more specialised applications such as removing a specific energy (e.g. the incident energy from the outgoing beam), using a cut-off filter as broad-band analyser, or to shape the resolution function defined by the rest of the instrument. On three axis spectrometers, the desired neutron energy is selected by Bragg reflection. But this principle can be inverted, so that Bragg diffraction is used to scatter unwanted neutron energies out of the beam. This can be done either with single crystals (e.g. silicon or germanium wafers), powder (berylium, berylium oxide or graphite) or intermediate pyrolytic graphite.Powder filters ideally scatter all neutrons with wave-vector larger than a cut-off wich is fixed for the given material. The two other types employ one particular reflection to expell a specific unwanted neutron energy, but all other reflections will give rise to parasitic dips in the transmssion function at other energies. Using Monte Carlo simulations for realistic experimental situations, the performance and design considerations for each of the three types of filters are evaluated.

B-267 MC- Simulation of double-bent monochromator and analyser crystals

P Link[1], G Eckold[1], J Neuhaus[2],
[1] Institut für Physikalische Chemie, Universität Göttingen, Tammannstr. 6, 37077 Göttingen, Germany
[2] Zentrale Betriebseinheit FRM-II, Technische Universität München, 85747 Garching, Germany

Modern neutron scattering instruments improve considerably their performance by focussing in real and reciprocal space. Here we present MC simulations of the thermal three-axis spectrometer PUMA. This instrument is equipped with double-bent monochromator and analyser crystals, which have been simulated as McStas [1] components. The monochromator component images the real crystal holder mechanics with its 117 individual crystals. The neutron flux distribution at the sample position for PG002 and Cu220 monochromator crystals has been calculated for different focussing modi and incident energies. Also the influence of the horizontal slit on the flux distribution and the resolution function has been studied. [1] K. Lefmann and K. Nielsen, Neutron News, 10/3 (1999) 20

B-268 Simulation and design of a primary spectrometer for RITA-1 at PSI

K. Lefmann[1], B. Roessli[2], D.F. McMorrow[1],
[1] Dept. Mat. Res., Risø National Laboratory,4000 Roskilde, Denmark
[2] Laboratory for Neutron Scattering, Paul-ScherrerInstitut,5232 Villigen, Switzerland

A number of neutron instruments are being moved from Risoe to PSI. Among them is the advanced triple axis spectrometer RITA-1. As the SINQ source at PSI is a (continuous) spallation source, the boundary conditions for the primary beam differs from those of the former DR3 at Risoe. Thus, the design of the primary spectrometer has to be reconsidered. We present a suite of possible designs and the corresponding simulated values of neutron flux and instrument resolution. The implications for the fast-neutron background is discussed.

B-269 Simulating IRIS@ISIS

S. N. Klausen[1], K. Lefmann[1],
[1] Materials Research Department, Risø NationalLaboratory

The inverted geometry time-of-flight spectrometer IRIS at ISIS is computer simulated using the neutron ray-tracing package McStas (http://neutron.risoe.dk/mcs
The dependence of the resolution on the neutron energy transfer is investigated and compared to real experimental results and other simulation results. The dependence of the resolution on the neutron momentum transfer is investigated too. The simulation results are used for analysis of magnetic dynamics from a powder sample of hematite nanoparticles.

B-270 Monte Carlo simulations of RITA2@PSI

S. N. Klausen[1], K. Lefmann[1], F. Altorfer[2],
[1] Materials Research Department, Risø National Laboratory,Denmark
[2] Laboratory for Neutron Scattering, Paul Scherrer Institute,Switzerland

The cold-neutron triple axis spectrometer RITA2 (see e.g. K. Lefmann et al. Physica B 283, 343 (2000)) designed and build at RisøNational

Laboratory will be installed at the neutron source SINQ at Paul Scherrer Institute. The spectrometer is planned to be operational from May 2001. In connection with the installation of RITA2 computer simulations using the neutron ray-tracing package McStas (http://neutron.risoe.dk/mcstas/) is performed. The simulation results are compared to real experimental results obtained at a powder sample. Especially the intensity and the resolution of the spectrometer is investigated.

B-271 Attempt of determination of a kind of residual stresses within a welding interface of bi-metal austenitic and ferritic steel tube from time-of-flight neutron diffraction spectra

Yu.V. Taran[1], H. Kockelmann[2], J. Schreiber[3], J.S. Wright[4],
[1] Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, 141980 Dubna, Moscow region, Russia
[2] MPA, Stuttgart University, D-70569 Stuttgart, Germany
[3] EADQ, Fraunhofer Institute for Nondestructive Testing, D-01326 Dresden, Germany
[4] ISIS, Rutherford Appleton Laboratory, Didcot, Oxon, OX11 0QX, UK

Shape welding of a ferritic steel layer on an austenitic steel tube is used to build compressive stresses on its outer surface and as a result, suppress stress corrosion. Investigations of residual stresses (RS) in such bi-metal tubes are important for developing optimal welding techniques applying in chemical and nuclear industry. Triaxial map of lattice parameter of both phases through tube cross-section was derived on the ENGIN stress-diffractometer at the ISIS pulsed neutron facility. Analysis of a kind of RS calculated from lattice parameters under different assumptions about a stress free phase lattice parameters was performed to make a correct comparison RS with results obtained by the destructive mechanical turning out technique and by the finite element method. The indication on domination of RS of the 1st kind within a welding interface is received.

B-272 Correlating Microstructure and Filtration Efficiency in Nafion Membranes using SANS

E. Gilbert[1], Y. Halpern[2], M. Henry[2], J. Hestekin[2], R. Datta[2],
[1] Intense Pulsed Neutron Source, Argonne National Laboratory, Argonne, IL 60439, USA
[2] Chemical & Biological Technology, Energy Systems Division, Argonne National Laboratory, Argonne, IL 60439, USA

Nafion membranes are hydrophilic, show extremely high oxidation stability but are non-porous. A chemical treatment has been developed that converts Nafion into a porous membrane that can potentially be used in highly oxidative conditions, for example, to recover hydrogen peroxide from hydrophobic solvents. To determine the impact of this treatment on the membrane microstructure, SANS experiments have been conducted on the control and chemically-treated material as a function of hydration. The scattering has been successfully fitted to a modified Local Order Model. Our results show that while the pore structure of both the treated and the control collapse on drying, by using an appropriate rehydration protocol, microstructural changes formed during the chemical treatment are maintained.

B-273 Neutron strain scanning in straightened eutectoid steel rods

M L Martinez[1], C R Borlado[2], F J Mompean[1], R L Peng[3], M R Daymond[2], J Ruiz[4], M. Garcia-Hernandez[1]
[1] ICMM, CSIC, ES-28049 Madrid, Spain
[2] ISIS Facility, CLRC, Chilton, Didcot, Oxon. OX11 0QX, UK
[3] NFL-Studsvik, Uppsala University, S-611 82 Nyköping, Sweden
[4] ETSICCP, UPM, ES-28040 Madrid, Spain

Neutron strain scanning has been performed on an eutectoid steel rod at a reactor based source (REST diffractometer, at NFL) and at a pulsed source (ENGIN diffractometer, at ISIS). The sample used is a primary rod obtained from a drawing process and has subsequently been subject to a bending and a straightening procedure, which induce residual stress. The material exhibits a pearlitic microstructure, with alternating ferrite (90% vol) and cementite (10% vol) layers. Strain profiles for the ferritic phase were measured on REST. Both phases were measured on ENGIN and analyzed by single-peak (ferrite) and Rietveld refinement (ferrite and cementite) methods. The agreement between REST and ENGIN data is excellent for the three measured directions in the ferritic phase. Total stress profiles have been evaluated by combining phase stresses using the rule of mixtures. The experimental results compare well with analytical models for a two-phase material subject to bending and straightening operations under pure bending and unbending moments with perfect elastic behavior up to the yield point and plastic Voce behaviour above this point.

B-274 Residual stress study by neutron diffraction in perforator s striker

A.V. Tamonov[1], G.D. Bokuchava[1], A.M. Balagurov[1], D.M. Levin[2], N.R. Shamsutdinov[1],
[1] Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Dubna, Russia
[2] Tula State University, Physics Department, Tula, Russia

Within the framework of co-operation with the industrial enterprises of Russia (TULAMASHZAVOD) test experiments on residual stress study in perforator s striker were carried out. The knowledge of residual stress level in such components is very important for equipment production in mineral resource industry. Two samples were measured. They had a cylindrical shape (outer diameter 24mm, inner - 8mm). Sample 1 was made of steel 65C2BA and in initial state the material was isothermally hardened with drawing afterwards. Sample 2 was made of steel 20-2-4- and in initial state it was carburized. The experiment was performed at High Resolution Fourier Diffractometer at the IBR-2 reactor in Dubna, Russia [1]. For the stress measurements we used the 90*-detector with gauge volume 2x2x5mm3. The back scattering detector was utilised for the investigation of diffraction peak broadening and the phase analysis. Looking at the diffraction pattern one finds the presence of austenitic phase in Sample 1. Presence of austenite phase was found in Sample 2 too. After analysis of peak intensities the estimation for the volume content of austenite had been found: c_α = (11.7+0.2) % (for Sample 1) and c_α = (6.7+0.2) % (for Sample 2). It is a pretty large amount comparatively to the homogeneity reported by samples producers. Also the strong peak broadening can be clearly seen in the both samples. This estimation of the microstrains gives quite a high value: e=0.012*0.004 (for Sample 1) and e=0.0107 +0.0040 (for Sample 2). The strain of this amplitude corresponds to the stresses above the yield strength of the material. But one must keep in mind the non-homogeneity of the samples, so the deformation has the limited nature, allowing stresses to exceed the yield strength. Radial and tangential components of the stress tensor are negative, i.e. compression is going on. In the sample s bulk they achieve high values. Axial component has a different behaviour. Firstly, in the places close to the edges, axial stress is positive, i.e. the material is under tension. In the core of the sample, the sign of stresses changes. Then, the sample has pretty high stress gradients. In addition to the combination of tension/compression near the edges this fact forms the complex stress state of the material. These circumstances badly damage the resistance of the sample. The measured stresses in Sample 2 changed in comparison with Sample 1. The carburizing altered the residual stress distribution: all components of the strain tensor are positive in the central parts of Sample 2. But the positive value of the residual stresses is decreasing in accordance with their interval to the outside surface and the inner surface. The tendency of changing their sign was observed. This is expected result, because the negative stresses had to be formed in near surface region about 1 mm thickness. So the carbonization layer is situated just near the surface. After analysing of the macro- as well as micro-stress state of Sample 1 we came to the conclusion, that material had no the optimal heat treatment. The fatigue resistance of this sample can be improved by 2-3 times by appropriate treatment. The residual stress distribution in Sample 2 is friendly more for increasing of the fatigue load resistance. Although this thick and hard carbonization

layer leaded to an appearance of the high value stresses in the centre of the perforator s striker, the found tendency allows us to consider that we can improve the process of the thermochemical treatment, which yields forming the optimum near the surface. [1] V.L.Aksenov, A.M.Balagurov, V.G.Simkin et al., JINR Communication, 13-96-164, Dubna, 1996.

B-275 Pressure-induced Magnetic Cooling - the Barocaloric Effect Investigated by Neutron Scattering

T. Straessle[1], A. Furrer[1],
[1] ETH Zuerich & Paul Scherrer Institut

The barocaloric effect found in many rare-earth compounds opens the way to novel magnetic refrigeration techniques which are rather based on the application of external pressure than on the application of large external magnetic fields as needed for cooling by the magnetocaloric effect. The effect occurs in rare-earth compounds which show a large pressure dependence of their crystal field via a pressure-induced structural and/or magnetic phase transition. In this context neutron scattering has proven to be the experimental method of choice in studying the crystal field and the detailed magnetic structure. Examples of compounds showing the barocaloric effect are presented. Direct measurements of the effect are compared with calculations based on microscopic properties determined by neutron scattering and macroscopic measurements.

B-276 A New Dynamical Diffraction-Based Technique of the Residual Stress Measurements in Thin Films

M Agamalian[1], E Iolin[1], Ch Rehm[1],
[1] Oak Rigde National Laboratory, Spallation Neutron Source Division

It has been shown that the back-face diffraction from a thick Si single crystal (so-called N̈eutron Camel)̈ is sensitive to the ultra-small deformation strain [1]. We have later used this effect to measure the bending radius, R, of the 8 mm thick Si substrate coated by a 2000 angstroms Ni film and convert R to the residual stress in the Ni film by the Stoney formula [2]. This experiments have clearly shown that the Neutron Camel can be applied for the residual stress measurements. The technique is extremely sensitive and can be used, in contrary to the conventional X-ray diffraction, on any (but not only crystalline) thin films deposited on the thick Si crystals. 1. M. Agamalian et al. Phys. Rev. Lett. 81, 602 (1998). 2. M. Agamalian et al. submitted to Phys. Rev. Lett. (2001).

B-277 Neutron Diffraction Measurement of Residual Stresses in Al-Cu Cold Cut Welding

M. Marcantoni[1,2], F. Fiori[2,3], , ,
[1] Dipartimento di Meccanica, University of Ancona, Italy
[2] Istituto Nazionale per la Fisica della Materia, Research Unit of Ancona, Italy
[3] Istituto di Scienze Fisiche, University of Ancona, Italy

Usually, when it is necessary to join different materials with a big difference in the melting point, welding should be avoided. To overcome this problem we have designed and built a device to obtain cold-cut-welding, which is able to strongly decrease oxidation problems of the surfaces to be welded. Thanks to this device it was possible to achieve good joining between different pairs of materials (Al-Ti, Cu-Al, Cu-Al alloys) without reaching the material melting. The mechanical and microstructural characterisation of the joining and the validation of its quality have been obtained using several experimental methods. In particular, in this work neutron diffraction experiments for the evaluation of residual stresses in Cu-Al junctions are described, carried out at the G5.2 diffractometer of LLB, Saclay (F). The measured stress behaviour is in good agreement with expectations. Neutron diffraction results are discussed and related to other experimental tests such as microstructural characterisation of the welded interface (through optical and scanning electron microscopy) and mechanical characterisation (tensile strength tests).

B-278 Neutron diffraction measurements for residual stress analysis in automotive steel gears

G. Annibali[1,2], G. Bruno[2,3], A. Giuliani[2,4,5], A. Manescu[2,4,6], M. Marcantoni[1,2,7], F. Rustichelli[2,4], F. Turquier[2,4],
[1] Università degli Studi di Ancona, Dipartimento di Meccanica, Via Brecce Bianche, I-60129 Ancona, Italy
[2] INFM-Istituto Nazionale per la Fisica della Materia, Research Unit of Ancona, Ancona, Italy
[3] HMI-BENSC, Glienicker Strasse 100, D-14109 Berlin, Germany
[4] Università degli Studi di Ancona, Istituto di Scienze Fisiche, Via Ranieri 65, I-60131 Ancona, Italy
[5] Università degli Studi di Ancona, Dipartimento di Fisica e Ingegneria dei Materiali e del Territorio, Via Brecce Bianche, I-60129 Ancona, Italy
[6] National R&D Institute for Welding and Material Testing, ISIM, Timisoara, Romania
[7] CEA, CEN Saclay, Laboratoire Léon Brillouin, 91191 Gif sur Yvette cedex, France

Standard production and machining of automotive components is still attractive, although it is not cost effective, if the life of the component has got the highest priority. An important parameter to increase the fatigue life of these components is the introduction of beneficial residual stress, especially in the most loaded superficial layers. The aim of the present study is to investigate the residual stress in two steel gears cut and machined from extruded bars and then submitted to tempering and nitriding. The results were compared with those obtained on sintered, nitro-carburised steel gears manufactured using the net-shape forming technique. They show a higher tensile stress level in the bulk of the component with lower Carbon and Chromium content, i.e. a strong influence of nitriding elements. Consequently, in the nitrided layers, the calculated compressive stresses reach relatively high values in the Al and C rich sample. These stresses are sensibly bigger than those found in the sintered and nitro-carburised wheels both in the surface and in the bulk.

B-279 Neutron Diffraction Measurements of Residual Stresses in Aerospace MMC Materials

G Bruno[1,2], M Ceretti[2,3], E Girardin[2,4,5], A Giuliani[2,4,5], A Manescu[2,4,6], F Rustichelli[2,4],
[1] HMI-BENSC, Glienicker Strasse 100, D-14109 Berlin, Germany
[2] INFM-Istituto Nazionale per la Fisica della Materia, Research Unit of Ancona, Ancona, Italy
[3] CEA, CEN Saclay, Laboratoire Léon Brillouin, 91191 Gif sur Yvette cedex, France
[4] Università degli Studi di Ancona, Istituto di Scienze Fisiche, Via Ranieri 65, I-60131 Ancona, Italy
[5] Università degli Studi di Ancona, Dipartimento di Fisica e Ingegneria dei Materiali e del Territorio, Via Brecce Bianche, I-60129 Ancona, Italy
[6] National R&D Institute for Welding and Material Testing, ISIM, Timisoara, Romania

We studied the effect of the forming process on the residual stress state of a component for aerospace application made of 2009+25% SiCp and extruded, proceeding in 3 steps, first studying the material as received (cast billets), then specimens after static loading and fatigue, and then studying the real components mentioned above. The micromechanical model developed in parallel can predict the stress and strain level in the microstructure. The results obtained by the measurements in the billet have been used as input for the model. Then the results of the measurements in the tensile specimens have been compared to the simulation of the fatigue and tensile behaviour of the material. The extrusion process has been simulated and according to the results of the modelisation, optimised extruded MMC components have been produced, a shaft has been extruded as simple shape aeronautical component. Residual stress level has been evaluated in the simple shape aeronautical component; experimental and calculated data are in good agreement.

B-280 Neutron diffraction a tool to optimize processing of niobium tubes

H Brokmeier[1,2], W Singer[3], H Kaiser[3],
[1] Institut für Werkstoffkunde und -technik, TU Clausthal, 38678 Clausthal-Zfd, Germany
[2] GKSS-Forschungszentrum Geesthacht, 21502 Geesthacht, Germany
[3] Deutsches Elektronen-Synchrotron, 22607 Hamburg, Germany

Among other techniques an accelerator unit can be processed by hydroforming of high purity niobium tubes. This pre-product undergoes a number of processing steps starting with casting till the final hydroforming which leads to the cavities. Very important for a high quality hydroforming is the texture homogeneity along the perimeter. Due to the fact that the texture was influenced by casting, by different deformation, by different annealing and by tube production the whole processing line was controlled by texture measurements. Neutron diffraction was carried out to handle the coarse grained material as well as to analyze the average texture of the tube wall non-destructively.

B-281 Characterisation of Industrial Materials at ILL: Small Angle Neutron Scattering

P Lindner[1], AW Wright[1],
[1] Institute Laue-Langevin, 6 rue Jules Horowitz, F-38042 Grenoble cedex 9

Neutrons are a unique tool for investigating the internal structure of matter; they are non-destructive and can penetrate deeply into most materials as they interact with the atomic nuclei. Over the last few years, several sectors of industry have used the facilities of the Institut Laue-Langevin, Grenoble, for their product research, control and development. In particular, small angle neutron scattering (SANS) is sensitive to dimensions in the range of nanometers to 0.2 micrometers and reveals detailed structural information that cannot be obtained by more conventional methods. The poster will show some examples from soft- and hard materials research.

B-282 SMARTS - a new neutron spectrometer for residual stress measurement

Mark Bourke[1], David Dunand[2], Ersan Ustundag[3],
[1] Los Alamos National Laboratory, USA
[2] Northwestern University, USA
[3] California Institute of Technology, USA

A spectrometer called SMARTS (spectrometer for materials research at temperature and stress) has been constructed at the Los Alamos neutron scattering center. Its design maximizes capability and throughput for two classes of measurement a) residual macrostrain in engineering components and b) in situ loading. SMARTS is scheduled to enter commissioning in July 2001. Initial results will be presented in the context of scientific and industrial opportunities. The instrument comprises; a source to sample flight path of 30.75 m, a water moderator, a Ni58 / 2theta super mirror guide and a t-zero chopper at 10 m. Two detectors comprising sets of 180 ^{3}He tubes are mounted at $\pm$90 to the incident beam with a secondary flight path of 1.5 m. Manipulation of engineering components is achieved using a translator with a capacity of 1500 Kg and positioning accuracy of 0.1mm. Definition of a sampling volume is achieved using incident collimation and a suite of 5 interchangeable radial collimators. Sample alignment, aperture and collimator alignment is achieved using a theodolite interfaced to a workstation. One significant SMARTS capability is a load frame/furnace suite capable of applying up to 200KN in uniaxial compression or tension and performing load tests up to 1500°C.

B-283 European Standardization Activities on Residual Stress Analysis by Neutron Diffraction

A. G. Youtsos[1], C. Ohms,
[1] Institute for Advanced Materials of the Joint Research Centre of the EuropeanCommission

A main objective of a recently completed European research project, RESTAND, was to develop industrial confidence in the application of the neutron diffraction technique for residual stress measurement, and its principal deliverable was a relevant draft code of practice. As no such standard is yet available, and on the basis of this draft standard document, the Technical Committee on NDT of the European Committee For Standardization (CEN/TC 138) has established a new Ad hoc Work Group (AHG7). The objective of this group is the development of a European Pre-standard on ”test method for measurement of residual stress by neutron diffraction”. The document contains the proposed protocol for making the measurements. It includes the scope of the method, an outline of the technique, the calibration and measurement procedures recommended, and details of how the strain data should be analysed to calculate stresses and establish the reliability of the results obtained.

B-284 Use of the Rietveld refinement with the generalized spherical-harmonic model for describing crystallographic texture in neutron powder diffraction data of NiTi shape memory alloys

H. Sitepu[1], W. W. Schmahl[1], J. K. Stalick[2],
[1] Institut für Geologie, Mineralogie und Geophysik, Ruhr-Universität Bochum,Universitätsstrasse 150, 44780 Bochum, Germany
[2] NIST Center for Neutron Research, Gaithersburg, MD 20899, USA

Quantitative analysis of crystallographic preferred orientation (texture) in polycrystalline shape memory alloys NiTi is of interest not only because preferred orientation give errors in quantitative phase analysis, but also in structure determination for every phase using diffraction data. In the present study, texture and phase fraction of polycrystalline shape memory alloys in Ti-50.14%Ni have been carried out with a BT-1 high-resolution, fixed wavelength, multi detectors powder diffractometer at the NIST Center for Neutron Research based on the DSC heating curve. The paper will describe the experimental procedure and illustrate with texture of cubic (B2) austenitic and monoclinic (B19) martensitic phases.

B-285 Residual Stresses and Hardening Near Crack Tip Regions of Austenitic Steel

M. Ceretti[1], K. Hirschi[1], B. Marini[2], J.-M. Sprauel[3], J.-P. Lauriat[4], E. Elkaim[4],
[1] Laboratoire Léon Brillouin (CEA-CNRS), CEA-Saclay, F-91191 Gif sur Yvette, France
[2] CEREM/SRMA, CEA-Saclay, F-91191 Gif sur Yvette Cedex, France
[3] Laboratoire MécaSurf, ENSAM, F-13717 Aix-en-Provence cedex 1, France
[4] LURE, Bât 209D Centre Universitaire, B.P. 34, F-91898 Orsay Cedex, France

Austenitic steel is used extensively in the field of nuclear industry, in the primary circuit of fast breeder reactors. As the normal operation temperature is about 650°C, it is very important to determine the role of residual stresses in the deformation and the fracture process in order to estimate the component’s lifetimes. The plastic deformation is also an important parameter related to the residual stress relaxation and its redistribution after fatigue loading. The aim of this work was to determine the residual stress field in cracked fatigue specimens by neutron diffraction techniques in order to use this data for quantifying the influence of the different loading parameters on the fatigue crack growth. On the other hand, some microstructural parameters, such as the average size of coherently diffracting blocks and the mean-square microstrain, were estimated by combining neutron and X-ray (synchrotron radiation) diffraction techniques.

B-286 Applied Neutron Network - ANNet

A. Wright[1], P. Lindner[1],
[1] Institut Laue-Langevin, 38042 Grenoble, France

The Applied Neutron Network, ANNet, is a newly created network of scientists, engineers and industrialists working together on applied and industrial R&D using neutrons. Its function is to build links between private companies, neutron scientists, applied research laboratories and the neutron facilities at the Institut Laue-Langevin (ILL), Grenoble, with the aim of finding solutions to applied and industrial research problems ANNet is operated by the ILL’s Industrial Liaison and Consultancy Group with the help of an international working party. It establishes communications between expert scientists, industrial companies and neutron experts and organises events on applied and industrial neutron research. Membership is open to all scientists and engineers from both private and public organisations who wish to contribute to the development of applied and industrial R&D using neutrons.

B-287 Polymer Surface Adsorption Measured by SANS

J. L. Hutter[1], H. E. King, Jr.[1], M. Y. Lin[2],
[1] ExxonMobil Research and Engineering Company, Annandale, NJ, 08801, USA
[2] National Institute of Standards and Technology, Gaithersburg, MD, 20899, USA

We use small angle neutron scattering to characterize a polymerichydrate inhibitor, poly(N-vinyl-2-pyrrolidone), adsorbed onto hydrate crystal surfaces. Gas hydrates are crystals in which water molecules encage small molecules such as propane or methane. Their stability at temperatures

above the freezing point of water presents a significant chanlange to oil and gas transport. Hydrate formation can be kinetically suppressed by certain polymeric inhibitors, but little is known about the mechanism of this effect. We measure a polymer coverage of 5 mg/m^2, but on only a small (2%) fraction of the available surface. Unlike the expected self-similar structure sean in other systems, this layer has the unusual property of a thickness several times the polymer coil dimension. Therefore, most of the polymer is not bound directly to the surface, suggesting the formation of surface aggregates. We speculate on the role of these aggregates in the growth inhibition of hydrate crystals.

Publishing with the Physical Review and Physical Review Letters

J. Kim-Zajonz
Physical Review B

General information and publications statistics for the journals of the American Physical Society will be presented. The international scope of these publications increases annually, as seen in the distributions of both authors and referees. Information about PROLA and other APS online features will also be available. The aim of the poster is to provide enough information to stimulate questions and discussion on a wide range of topics concerning publishing and peer review. Feedback on the journals, the review process and how the journals are perceived in the community will be appreciated.