Poster Session C

Advanced Neutron Sources (C1 – C15)
Neutron Instrumentation III (C16 – C54)
Soft Condensed Matter III (C55 – C90)
Magnetism III (C91 – C159)
Material Science III (C160 – C207)
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MS: Charge, Lattice and Isotope Effects in High-Tc Superconductors (C241 – C246)
MS: Instrumentation at Advanced Pulsed Neutron Sources (C247 – 253)
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C-1 Polarised Neutrons Used in SANS Investigations of Magnetic Nanomaterials

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We report on SANS investigations of magnetic microstructures in extremely fine-grained materials materials, where we face the problem that weak magnetic scattering signals have to be analysed beside strong nuclear contributions from other sources. We shall demonstrate that polarised neutrons give access to the sign and absolute values of the magnetic scattering length densities providing additional information about the nature of interfaces of nanocrystalline particles which are not available in conventional SANS. The investigations have been performed using the new powerful polarisation option ”SANSPOL” , recently developed on the SANS instrument V4 of the HMI, Berlin [1]. Results on nanocrystalline materials with single domain magnetism are presented, namely n-Co and n-Fe_3O_4 particles in magnetic liquids, n-particles of Fe_3Si and Fe in amorphous matrix of Fe-Si-B-Nb-Cu or Fe-Nb-B alloys. [1]T. Keller et al J. Nuclear Instruments A451(2000),474-479

C-2 Neutronic analysis of a liquid ^{4}He source for UCN production and storage

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UCN production and storage in a liquid ^{4}He source are evaluated by means of a multigroup neutron transport analysis. Using the cross section model developed by the authors, a set of group constants for liquid ^{4}He at many different temperatures down to 0.1 K is generated. Major results thus obtained are as follows. As temperature is decreased below about 0.5 K, UCN density shows saturation behavior because of no significant up-scattering and UCN loss by neutron β-decay only. Single down-scattering of a 1 meV neutron and also multiple scattering of a higher energy neutron contribute largely to UCN production. High UCN density of 1x10^5 cm^{-3} is possible with a high reflectivity of a storage vessel, say, over 0.9999.

C-3 Development of cross-section models for liquid H_2 and solid CH_4

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In order to clarify neutronic performance of a pulsed cold-neutron source, scattering properties of some typical hydrogenous moderators are studied. Cross section models for liquid ortho- and para-H_2 between 14 and 20.4 K and liquid and solid CH_4 at temperatures down to 20 K are developed. A set of group constants for liquid H_2 is also generated: 80 groups between 0.1 μeV and 10 eV in a P_3 approximation. Major results are as follows. (a)Cold neutron production due to para-to-ortho transition and upscattering of lower-energy neutrons by ortho H_2. (b)Neutron slowing-down by rotational excitation of a CH_4 molecule especially at 20 K. And (c) an optimum condition of a liquid H_2 source for cold neutron production.

C-4 New Approaches in Plasma Neutron Sources

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Possibilities to improve yield parameters of compact neutron sources ($\approx$1m) based on the ion acceleration in plasma systems including laser-produced plasma bundles are considered. Among such systems, generating d-d and d-t neutrons, are the same: a) high voltage discharge with inertial electrostatic confinement; b) shock waves colliding at some angle in plasma; c)nonstationary laser plasma, produced by interaction of intensive laser irradiation with solid targets. The laser-produced plasma is used as a neutron target or a medium of ions collective acceleration. Preliminary results have pointed that in pulse operation mode of (a) and (c) systems it is possible to reach neutron yield up to 100 millions - 10 billions n/pulse without using traditional combination of solid neutron target and ion acceleration by external electrical field. Neutron pulse duration is not more than 10 microsecond, and device power consumption is about a few kJ/pulse. Some schemes of presented neutron sources are discussed. The neutron emitting part of such source may be of a few cubic cm.

C-5 First Nuclear Research Centre in Morroco

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The rapid development of a number of special and economic sectors such as medicine, agriculture, environment .. requires the input of new technologies. Thus Morocco decided the construction of a nuclear research center which will be operationnal in 2002. The poster will describe the main activities which will be undertaken in this center with emphisis on experiments to be set up around a 2MW research reactor.

C-6 First neutron results from JESSICA, the ESS-like target mock-up and moderator test facility

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The JESSICA short pulse ESS-like spallation target mock-up facility is designed for prototyping experiments on the optimisation of a target/reflector/ moderator system of the European spallation source (ESS). A full-size 1:1 scaled liquid Hg target is placed in a short pulsed proton beam of the COSY proton accelerator to produce spallation neutrons at ESS-like proton energies. The neutronics and technical feasibility of advanced cold moderators will be investigated by neutron time-of-flight technique and the aim is to validate complex simulation methods of particle interaction and nuclear transport and to optimise the technical layout of an ESS-type target-reflector-moderator system. JESSICA experiments will result in: A) a set of nuclear transport and neutronic performance data of an ESS-type liquid mercury target/moderator/reflector system and its individual components, B) an optimised geometry of the target to moderator and target to reflector position and C) neutron spectra and neutron time distributions to validate MCNPX coded simulation models of target station concepts and scattering kernels for cold sources. Here, we report on recent results of reference data taken with an ambient water moderator, the start-up device of a number of advanced cryogenic moderators to be investigated in due course.

C-7 Facility and Instrument Upgrades at the Manuel Lujan Jr Neutron Scattering Center at LANSCE

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Exciting developments at the Lujan Scattering Center at LANSCE will be reviewed. After a long outage, the facility has returned to operations with renewed strength and power. Three new instruments are in commissioning stage and others are in design and prototype stage. Upgrades to several existing instruments take advantage of the enhanced flux resulting from upgrades to the accelerator, storage ring, and target-moderator systems. A revolutionary chopper synchronization protocol solves long-standing problems faced by pulsed spallation sources locked to power grid timing. The unique science enabled by the LANSCE source and Lujan instruments will be discussed.

C-8 Design of neutron guide systems at the Australian Replacement Research Reactor

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Australia's new research reactor will cater for neutron beam science and radioisotope production from the end of 2005, with unperturbed neutron flux of 4 x 10^{14} n/cm^2/s and at least eight working neutron beam instruments. The neutron beam facility will have cold and thermal neutron beams based around supermirror reflecting guides. The design of in-pile and out-of-pile segments has been optimized to deliver maximum usable neutron flux at neutron scattering instruments located at the reactor face and in the neutron guide hall. The conceptual design will be discussed including key performance issues and simulations of flux profiles and spectra at critical points in the system.

C-9 Renewal of KENS TMRA and Its Performance

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KENS (spallation neutron source of KEK) was renewed by replacing the whole target-moderator-reflector assembly (TMRA) with new one. The gadolinium poison giving sharper pulses was installed in the ambient moderator. Decoupling energy of the B4C decouplers were optimized to give higher neutron fluxes without loosing sharpness of neutron pulse. Tantalum clad tungsten target was developed to increase source intensity by about 20%. The neutron performance was measured at several spectrometers. Cold neutron intensity is fully recovered and epithermal neutron fluxes are increased as the neutronic design calculations indicated. The scattered neutron profile becomes more symmetrical by the reduced tail. At the total scattering spectrometer, the radial distribution function obtained by the Fourier transform of S(Q) shows better resolution in position and reduction in spurious hump. The stainless steel shields on the B_4C decoupler gives very low background at the new reflectometer. As a whole, it can be said that new KENS has a quite good ability to investigate the materials.

C-10 Concept design of a new liquid metal target station for high power neutron scattering facilities

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We have designed a liquid metal target station without a window wall for high power charged particle beams to pass through. The beams are irradiated directly from above into the free surface of the liquid metal in a target tube soaked vertically in a reservoir tank of the liquid metal. A large hollow chamber is equipped above the target tube. This chamber works as a getter pump to evacuate the system and a heat siphon to remove the heat fed by the beam, where the liquid metal works as the working liquid on both functions. Results of the feasibility study will be discussed at the meeting.

C-11 AUSTRON and its notable new features

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The 10Hz/0.5MW AUSTRON neutron spallation source is dedicated for high resolution structural and dynamical investigations of condensed matter and for new fundamental research with neutrons. New magnetic focussing and bunching systems are under development which create additional intensity gain factors of 10 - 20. Clean room conditions including vibration, temperature and humidity control will improve the standard of neutron optical and neutron reflectometry experiments considerably. Narrow band neutron perfect crystal resonators and storage systems are forseen for a novel beam tailoring. A dedicated new ultra-cold neutron station will open a new horizon for experiments in the sub-neV region. Recently the project got additional support of the Austrian governmental Board for Research and Technological Development which recommended the forced continuation of the project, the installation of a professional Project Group and the cooperation with the European spallation project and with the neighbouring countries.

C-12 The new cold neutron research facility at the Budapest Research Reactor

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Since February 2001 the new cold neutron research facility is routinely operated at BNC. This ensemble of equipment consists of the liquid hydrogen cold neutron source (CNS), the optimised supermirror neutron guide system and a number of experimental stations located in the neutron guide hall. The cold neutron channel has a take-off for three beams. The first guide serves for a triple axis spectrometer with a PG monochromator at the 21 m position from the CNS. The end of this guide is used for a prompt gamma activation analysis station, which - dividing the beam in height into two parts - enables the operation of two pair-mode gamma spectrometers symmetrically at both sides of the guide. A small angle scattering spectrometer is installed on the middle guide. The third guide serves for a reflectometer (with polarisation option) with a PG monochromator take-off. The end-position of this guide is used as a test beam, so far. These instruments are available for the international ! user community.

C-13 Correction for Thermal Diffuse Scattering in Single-Crystal Time-of-Flight Neutron Diffraction: First Applications

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The thermal diffuse scattering (TDS) correction developed by Popa & Willis [Acta Cryst. (1997) **A53**, 537 - 545] for single crystal pulsed neutron diffraction is examined via a series of experimental data sets collected at the spallation neutron source IPNS. The effect on the derived temperature parameter values is assessed and compared with reference structures obtained from gamma-ray diffraction. The importance of carrying out TDS corrections is emphasized. Suggestions are made how to evaluate the TDS in situations where the elastic constants are unknown.

C-14 ISIS Target Station II :: Preliminary Target and Moderator simulations

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When ISIS was first constructed the target and moderators where optimised to exploit the large epi-thermal fluxes of neutrons that are inherent to pulsed neutron sources. Since then experience has shown that pulsed sources can effectively compete with reactors for certain applications even in the thermal and cold neutron regions. The plan to build a second target station at ISIS, that is specifically designed to use these low energy neutrons, has prompted this design study. The second target station will use one pulse in five from an upgraded 300 micro-amp synchrotron giving a total power of 48 kW. This low power makes it possible to use target station designs that recoup a large fraction of the flux lost due to the small number of incident protons. In this preliminary report we present our current thoughts on the design of the second target station and the results of Monte-Carlo calculations of flux and pulse shape.

C-15 First results from the neutron Time Of Flight (n_TOF) facility at CERN

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Recently a neutron time of flight facility (n_TOF) has started its activity at CERN allowing to the neutrons a flight path of 185 m. The 20 GeV/c high intensity proton beam delivered by the CERN PS produces spallation neutrons with energies ranging from thermal to GeV energies. In fact, 4 pulses of 7×10^{12} protons, distant by 1.2 s and a width of 6 ns, are impinging every 14.4 s on a lead target followed by a 5 cm water moderator. The neuton spectral function is almost isolethargic and the total number of neutrons at the end of the flight path generated by a proton pulse is close to 1×10^5 neutrons/cm^2 for the current collimator configuration. The intense flux and the excellent resolution of this neutron beam allow one to study systematically neutron cross-sections with very modest mass samples. Results of the first commissioning measurements concerning the spectral function, resolution, target behaviour are presented.

C-16 TOSCA neutron spectrometer: the final configuration

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The forward and backward scattering parts (phase II) of the new neutron spectrometer, TOSCA, replacing the old TFXA and TOSCA (phase I), have been successfully installed at the ISIS pulsed neutron source. The results show a significant enhancement in the counting rate due to the larger detector area. The improved resolution (to $\sim$ 1.5% of the energy transfer) as compared with the previous instruments (TXFA 3%, TOSCA-I 2%) has been achieved by increasing the primary flight path from 12 m to 17 m. A chopper has been added in order to avoid neutron frame overlap and to reduce the fast neutron background. Additional diffraction capability will be installed in the near future.

C-17 Neutron Fourier diffractometer FSD for internal stress analysis: first results

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At the IBR-2 pulsed reactor in Dubna a new neutron Fourier diffractometer FSD is under construction. FSD continues the development of neutron Fourier diffractometry at long pulse neutron sources, which has been started several years ago with High Resolution Fourier Diffractometer (HRFD) at the IBR-2. Whereas HRFD is mainly used for precise structure refinement, FSD is optimised for internal stress measurements in bulk materials. The FSD design satisfies the requirements of high luminosity, high resolution, specific sample environment, wide range of d$_{hkl}$, and fixed scattering angles $\pm 90^\circ$. It consists of mirror neutron guide, fast Fourier chopper for the neutron beam intensity modulation, $\pm 90^\circ$ MultiCon ZnS(Ag) detector system with both geometrical and electronic focusing, 5-axis goniometer *Huber* and loading machines, VME-based RTOF-analysers for data acquisition. Examples of the first experimental results obtained with FSD are presented.

C-18 Upgrade of the TOF-Diffractometer EPSILON

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Due to a flight path of 102 m a resolution of $\Delta d/d < 5 \cdot 10^{-3}$ was achieved at the diffractometer Epsilon (IBR-2, Dubna). To overcome poor intensity a renewing was made for the whole data acquisition system, including nine radial collimators, consisting of 48 GdO$_2$ coated foils (angle distance 20' of arc) and covering a range of 20° in 2Θ. A range of 20° is covered in the other direction. Three of the pyramidical shaped collimators are grouped to a unit of 66°. The rear end of the collimators is planar $(24 \cdot 24cm^2)$ and the distance between the foils is 4 mm, but 1 mm at the front end, - their transparency is expected to be 95%. Single ^3He-counter tubes are used, which are 10 mm in diameter and 20 mm long. Each collimator/detector-block is mounted on a ring with its surface plane perpendicular to the incident neutron beam. The scattering angle 2Θ for all detectors is unique and equals 90°. All blocks have the possibility of adjustment in three directions. The intensity gain is $>$10.The work was supported by the German BMBF under the project 03-DUBPOT-9 and the GeoForschungsZentrum Potsdam.

C-19 Conceptual analysis for a 1.4 μeV backscattering spectrometer at the European Spallation Source ESS

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The instrument presented is a backscattering, crystal-analyzer spectrometer designed to provide highest energy resolution together with an extended range of momentum transfer. Therefore the secondary spectrometer if used with Si(111) crystal analyzers will provide a high energy resolution of approximately 1.4 μeV at the elastic peak and a Q-range of 0.1 to 2.0 Å^{-1}. A second analyzer system using Si(311) crystals will provide a more modest energy resolution of approximately 6 mueV with an extended Q-range of 0.2 to 3.8 Å^{-1}. A Mica analyzer system will likely allow an improvement of energy resolution to 0.5 μeV. The combination of high count rate, extended dynamic range in energy transfer along with the energy resolution characteristics of classical reactor spectrometers result in a spectrometer that will provide unprecedented opportunities for new science to the neutron scattering community. We compare the new setup with other spallation source backscattering spectrometers, i.e. the IRIS/ SNS type, and show the advantages of the new design which offers a standard energy resolution which is competitive to reactor type instruments.

C-20 Building a high resolution total scattering powder diffractometer - Upgrade of NPD at LANSCE

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The Neutron Powder Diffractometer NPD at the Lujan Neutron Scattering Center at Los Alamos National Laboratory is the highest resolution neutron powder diffractometer in the US. We are currently upgrading NPD by adding a large number of position sensitive detectors in the backscattering position. This will optimize the instrument for total scattering measurements. The upgraded instruments will make it possible to collect data from a powder sample over a wide range in Q as well as with very good Q resolution. The total scattering includes Bragg- as well as diffuse scattering and holds the key to determining the crystallographic average structure as well as the local structure, often responsible for the properties of complex materials.

C-21 The new MAPS spectrometer at ISIS

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The scientific programme on the new inelastic scattering spectrometer MAPS has recently started at the pulsed neutron source ISIS. MAPS is a direct geometry spectrometer that has been optimised to measure collective excitations in single crystals. Its principal innovation is the use of position sensitive detectors that provide close to continuous coverage over a large detector area in the forward scattering direction. This allows the freedom to take cuts from the data on any plane or along any direction in reciprocal space, with the resolution tuneable in software. The design and technical specification of MAPS will be presented, and the performance of the detector system described. The use of the spectrometer to measure excitations in single crystals will be illustrated by a variety of experimental data taken from the scientific commissioning programme.

C-22 Improvement of the performance of the chopper spectrometer, INC

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The INC spectrometer is the chopper spectrometer at KENS (Neutron Science Laboratory, High Energy Accelerator Research Organization). A guide tube comprising supermirrors, of which the critical wavenumber is three times as large as that of natural nickel, was installed in the primary flight path of INC. Also, the characteristics of the ambient-temperature water moderator, which INC is facing, was changed by renewal construction of the neutron source at KENS. Through these constructions, the performance of INC was drastically improved. A huge intensity gain at low energies due to installing the supermirror guide tube and a gain of factor 2 at high energies due to changing the characteristics of the neutron source were observed without any increase in the background noise. The observed gain of the guide tube was in very good agreement with a calculation. We, for the first time, have demonstrated the effectiveness of a supermirror guide tube for higher energy neutrons than cold neutrons for which a guide tube has been known to be effective. Moreover, the poisoning of the ambient-temperature water moderator provided INC more symmetric energy resolution function as well as an increase in the peak intensity in the time-of-flight spectra. The present constructions resulted in a great improvement concerning all aspects of the performance.

C-23 A new single-crystal diffractometer for neutron protein crystallography (BIX-4)

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A neutron diffractometer (BIX-3) at JRR-3M of JAERI has been applied to the structure determination of wild-type/mutant rubredoxin and myoglobin in 1.5 Å resolution. Those results increase activity of the neutron protein crystallography and the requirements of a much higher performance. A new diffractometer (BIX-4) uses an elastically-bent perfect-Si crystal monochromator and neutron imaging plates as BIX-3. In addition, several optimizations of the monochromator house and modifications from BIX-3 are carried out as follows, (1) 1.4 Å is used as a wavelength for an incident neutron which gives a maximum intensity at a sample position. (2) 3Q super mirror is installed inside of a flight tube. The intensity at a sample position is estimated to be about 5 times larger than current BIX-3.

C-24 Design of a low energy multi-chopper spectrometer for a spallation source

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A multi-chopper (MC) direct geometry spectrometer has the advantage of giving the user complete flexibility over the incident energy, the resolution (within the limits of the choppers) and the resolution lineshape. In addition, one can match the two main resolution contributions, thus obtaining the maximum possible flux for a certain resolution. Although several MC spectrometers already exist on steady state reactor sources, at present there is not a single example of one on a pulsed spallation source. This is surprising, as our simulations presented in this paper show that a MC spectrometer is ideally suited to a spallation source. We also show that if such an instrument were built at ISIS it would outperform any MC spectrometer existing in the world at present.

C-25 The OSIRIS diffractometer and polarisation analysis spectrometer at ISIS: New developments and ^{3}He spin-filter polarisation analysis

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OSIRIS combines a long-wavelength powder diffractometer with a polarisation analysis backscattering spectrometer. The diffractometer can access wavelengths up to 70 with a resolution of better than 1% Δd/d. The very high counting-rate at shorter wavelengths is ideal for in-situ, real-time and parametric experiments. The spectroscopy section incorporates a large array of graphite crystals arranged in near-backscattering to give a high counting rate with $25 \mu eV$ energy resolution. The incident beam is polarised using a supermirror bender and the scattered beam is polarisation-analysed by a ^{3}He spin-filter in the process of being constructed. The spin-filter system consists of a fibre laser, a peristaltic pump and a wide-angle banana-shaped quartz cell in a continuous-flow setup. The scattered beam passes twice through the spin-filter cell, thus doubling the optical path length in the cell. The aim is to achieve 70% nuclear polarisation with no variation in time.

C-27 EXCED - Epithermal Neutron Diffractometer at KENS

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A new epithermal neutron diffractometer (EXCED) was installed at the KENS spallation pulsed-neutron source. EXCED is designed to be a small scattering angle diffractometer using an incident neutron energy ranging from ∼0.5 eV to ∼5 eV for determining the crystal and magnetic structures of the high absorption materials. By this diffractometer, we have been able to measure the nuclear and magnetic Bragg peaks of Gd compounds which have been known as the best absorber of thermal neutrons. The instrumental details of EXCED and the preliminary results of the neutron diffraction from a single crystal of the Gd alloy are reported.

C-28 The Neutron Bonse-Hart Diffractometer for USANS at NIST

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In April 2000 the Perfect Crystal Diffractometer at NIST's Center for Neutron Research started operation. The performance of the instrument will be presented. Design measures taken to optimize its performance will also be discussed. The instrument is located on a dedicated thermal neutron beam port and utilizes a vertically focussing pyrolytic graphite pre-monochromator to provide higher neutron intensity (n/sec) on the perfect-crystal monochromator. The channel-cut monochromator and analyzer crystals for the instrument are large Si(220), triple-bounce, crystals (19 cm long x 6 cm high with a 4.4 cm wide channel) to provide a beam, of fixed wavelength 2.4±0.1 Å, with a cross section at the sample position of up to 5 cm x 5 cm. The Q-range of instrument is $3x10^{-5}$Å^{-1}¡Q¡0.01Å^{-1}. The maximum beam current is 30,000 n/sec. Recent experimental results will be presented to characterize instrument performance. The instrument is part of the NIST/NSF Center for High Resolution Neutron Scattering (CHRNS) with up to 2/3rd of the available beam time to be allocated to outside-user experiments.

C-29 The Backscattering Spectrometer at the NIST Center for Neutron Research

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The neutron backscattering technique extends the dynamic range of neutron time-of-flight and conventional triple axis spectrometers down to μeV energies and is ideal for the study of mechanisms such as slow motions in complex liquids, jump diffusion and quantum rotational tunneling. We report on the performance of the new high flux backscattering spectrometer (HFBS) at the NIST Center for Neutron Research. Compared with other backscattering spectrometers, the HFBS achieves a higher neutron intensity through the use of a device called the phase space transformation chopper and the incorporation of a larger analyzer array. A custom designed Doppler drive for the monochromator provides a triangular velocity profile which extends the dynamic range of the spectrometer by more than a factor of two over similar instruments.

C-30 A New Thermal Neutron Spectrometer/Diffractometer for Polarization Analysis (SV30) at the research reactor FRJ-2

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A new spectrometer for polarization analysis is under construction at the Research Center Jülich. The spectrometer is constructed as a multiple purpose instrument, which can be used both as a triple-axis spectrometer and a diffractometer for applications of polarized neutron scattering in triple-axis spectroscopy, crystallographic investigations and measurements of magnetic diffuse scattering. Therefore, the spectrometer is equipped with two exchangeable detector modules that carry an analyzer unit with a single detector and an image plate neutron detector. Two double focusing monochromators (Cu(200) and PG(220)) allow for a high flux of neutrons with an energy up to 125 meV at the sample position. The use of ^{3}He filters as a polarizer and an analyzer together with the image plate neutron detector makes possible a polarization analysis for high energy neutrons over a large solid angle of 60° x 60°.

C-31 The new reflectometer with polarization analysis in Jülich

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In the neutron guide hall ELLA at the research reactor FRJ-2 (DIDO) in Jülich we built a new neutron reflectometer with polarization analysis. The instrument is equipped with a 2D position sensitive detector and a polarization analyser covering the complete detector area. The neutron optical setup is designed, not to reduce the resolution of the instrument compared to the use of unpolarized neutrons and leaves the opportunity, to perform experiments with the complete flux of unpolarized neutrons. This instrument allows to measure efficiently diffuse scattering under grazing incidence from magnetic layered systems with polarization analysis, allowing to draw conclusions about lateral structures in the magnetization of the sample. The instrument has been equipped with electronics complying with the *Munich standard*, i.e. Linux computers for data treatment and experiment control and standardized industrial components with Profibus communication for driving the motors and position control. The communication between the workstation and the mechanical and detector components uses the TACO protocol, the first user software is written in psh, a scripting language developed at FZ Jülich.

C-32 Project of High Resolution Direct Geometry Spectrometer on New Neutron Source (TROITSK, Russia)

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Unique time-of-flight spectrometer of inelastic neutron scattering in direct geometry with relative energy resolution of 1-3% is proposed. The main idea of device is inelastic and small angle neutron scattering combination. As the new generation time-of-flight machine the proposed instrument is able to successful operate in the wide field of condensed matter physics. It will be very convenient to research the coherent excitations both the magnet and phonon, as in amorphous materials so in monocrystals with large elementary cell by this device. Apart from that it is possible to use it for small angle neutron diffraction measurements. In this paper the spectrometer optimization results and its basic parameters are presented.

C-33 The salient features of a newly developed medium resolution double crystal based small-angle neutron scattering instrument at Trombay

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A double crystal based moderate resolution small-angle neutron scattering instrument has been built and commissioned at the guide laboratory of Dhruva reactor, Bhabha Atomic Research Centre, Trombay, India. The instrument consists of a non-dispersive (1,-1) setting of 111 reflections of silicon single crystals with the sample between the two crystals. The neutron wavelength used is 0.312 nm. The accessible range of wave vector transfer q has been found to be 0.003-0.173 nm^{-1} for a typical experiment with sintered alumina.

C-34 The small angle neutron spectrometer at the HANARO reactor, Korea

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The small angle neutron spectrometer(SANS) had been constructed without cold neutron source at the HANARO Research Reactor, KAERI, Korea and the performance test was carried out. The SANS is to be used for the study of microstructual inhomogeneities in materials in the 1 nm to 100nm rage in size. The spectrometer is 9m long due to limitation of reactor hall space and utilizes a neutron velocity selector with 10% wavelength resolution and a pinhole collimation to provide a continuous incident beam whose wavelength is variable from 0.4nm to 1nm. The neutron detector is a two dimensional position sensitive detector of 128 x 128 pixels with 5mm x 5mm spatial resolution. The sample to detector distance can be varied from 1.5m to 4.5m and the detector can be rotated about the sample position to extend the angular range of spectrometer. The low Q limit of the spectrometer is 0.06nm^{-1}. In this paper, the design and characteristics of the spectrometer were introduced in detail and several SANS results of standard samples were presented which illustrate its performance.

C-35 Polarized neutron reflectometer at the Budapest Research Reactor

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The reflectometer is installed on the curved neutron guide at the cold neutron source of the Budapest Research Reactor (BRR). The neutron beam is monochromatized (lambda = 4.3 Å) by the use of pyrolitic graphite single crystal together with a Be-filter. The scattering plane is horizontal. Prior the installation the polarization option was carefully designed. The parameters and abilities of the device are demonstrated by test measurements.

C-36 The new Thermal Time of Flight Spectrometer at NFL, Sweden

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At NFL, Studsvik, the Swedish center for neutron scattering, a new Thermal Time Of Flight (TTOF) spectrometer has recently been completed, and the instrument is now open for proposals. The construction is similar to the IN4 spectrometer at the Institute Laue Langevin (ILL) in France.The TTOF consists of a monochromator of graphite. The monochromator is both vertically and horizontally focusing the beam towards the sample position to achieve as high a flux as is possible. A Fermi chopper chops up the beam in pulses. After being scattered the neutrons are detected by an array of ^{3}He detectors, and the signal is fed into the instrument computer. The sample position is designed to accommodate exactly the same equipment as on the SLAD (Studsvik Liquid and Amorphous Diffractometer). This is to make it easy to perform diffraction and spectroscopy on the same sample under exactly the same conditions.

C-37 Status of POLDI - the new time-of-flight diffractometer at PSI

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The new high resolution time-of-flight (tof) diffractometer POLDI for the investigation of residual strains shall go into operation this year. In order to enhance the intensity of a tof-diffractometer at a continuous neutron source, the instrument concept allows that neutrons of several pulses arrive the detector at the same time. The dependency of the arrival time on the scattering angle is used to reconstruct the diffraction pattern. This special concept and the short flight path of 12 m required the development of special instrument components (focusing neutron mirror, time-focusing ^{3}He-detector) and data analysis methods. We will present the concept and present status of the instrument, some simulation results, the neutron beam properties and hopefully first results of the overall instrument performance.

C-38 The Single Crystal Diffractometer at the Replacement Research Reactor at ANSTO

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The Australian Replacement Research Reactor is scheduled to have a single-crystal diffractometer when it starts operating in 2005. A preliminary comparison for possible designs will be presented.

C-39 Current Status of TRR-II Neutron Spectrometer Designs

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The objective of the Taiwan Research Reactor Project is to modify the old Taiwan Research Reactor (TRR) into a multi-purpose medium flux research reactor (TRR-II). The project started in 1998, and the new reactor is scheduled to be first critical at the end of 2006. The estimated maximum unperturbed thermal neutron flux ($E<0.625$ eV) is approximately 2.7×10^{14}n/cm^{2}sec, which will be the most advanced neutron source in Taiwan. The new TRR-II reactor will have five thermal neutron beam tubes (BT2-6), and a cold neutron source (CNS) with two extended cold neutron beam tubes (BT1 and BT8). Four neutron guides inside BT8 will be installed to guide cold neutrons to the guide hall, and four spectrometers are planned in this project. The four planned spectrometers are: a 40 m small-angle neutron scattering instrument (SANS), a high-resolution powder diffractometer (HRPD), a vertical focusing reflectometer (RF), and a triple-axis spectrometer (TAS). Both SANS and RF will be installed at the guide hall using cold neutrons, and HRPD and TAS will be installed at the reactor building using thermal neutrons. The four spectrometers are still on conceptual design phase and may subject to continueous modifications based upon inputs from demestic users. However, the conceptual design will be completed by the end of 2001.

C-40 QENS TOF-Spectrometers at Continuous and Pulsed Sources

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Intensity-resolution optimization of direct geometry (MTOF) spectrometers for high-resolution QENS experiments is discussed in view of further developing this technique to allow continuous, more extensive variation of time scales, on one and the same instrument. We show, that the total intensity of a modern MTOF spectrometer - as compared to the best existing - can be increased by two orders of magnitude at a continuous source and by at least three orders of magnitude at future pulsed sources. Consequently an appreciable extension of the range of time scales towards longer times will be possible. Pulse-width ratio (PWR) intensity-resolution focussing employing static phase-space transformers, neutron wavelength band-pass filters, and position-sensitive detectors for intensity-resolution optimization will be discussed in detail.

C-41 Current and future neutron scattering development in CIAE

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Currently, the 15 MW Heavy Water Research Reactor (HWRR) at CIAE in Beijing is the unique neutron source available for neutron scattering experiments in China. A 60 MW tank-inCpool inverse neutron trap-type research reactor, China Advanced Research Reactor (CARR), now is being built at China Institute of Atomic Energy in Beijing to meet the increasing demand of neutron scattering research in China. According to design, the maximum unperturbed thermal neutron flux would be expected to be $8 \cdot 10^{14} n/cm^{2}$s in the reflector. Seven out of nine tangent horizontal beam tubes will be used for neutron scattering experiments. A cold source, a hot source and a 30x60 m^{2} guide tube hall will be constructed. In this paper, a brief introduction of HWRR, the existing neutron scattering facilities and research activities at HWRR, CARR, and the facilities to be built at CARR are presented.

C-42 Neutron Beam Facilities at the Australian Replacement Research Reactor

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Contracts have placed for a new 20-MW research reactor to be constructed at Lucas Heights, just outside Sydney, Australia, to replace the existing DIDO-class HIFAR reactor. The new multipurpose facility will feature an excellent large liquid-D2 cold source, supermirror guides and a large modern guide hall. We plan to have 8 neutron-beam instruments available when the facility comes on line in 2005: 2 powder diffractometers, small-angle neutron scattering, reflectometer, 3-axis spectrometer, polarised-neutron spectrometer, single-crystal diffractometer and residual-stress diffractometer. The facility and conceptual details of the instruments will be described.

C-43 Cold Neutron Scattering Instrumentation Upgrades at the Oak Ridge High Flux Isotope Reactor

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During the period 2001-2003, a number of projects will be undertaken at High Flux Isotope Reactor, including a high-performance cold source, new beam lines and neutron scattering instrumentation. The cold source will consist of a supercritical hydrogen moderator (500 ml at 20K), which will support four cold neutron guides that will extend into a guide hall. The cold instruments will include a medium-resolution 35m SANS facility, designed for SANS studies of biological molecules, a high resolution 40m SANS instrument, a reflectometer and a cold neutron test station, which will be used to test components for the Spallation Neutron Source. The 40m and 35m SANS instruments (SANS1 and SANS2) will have variable wavelength with neutron fluxes comparable to the best current SANS facilities worldwide, along with large area (1m x 1m) high count rate detectors. The installation will commence in late-2001 and the HB4 beam line and instrumentation will be installed in 2002 and should be operational in 2003.

C-44 Instrumentation for the Long Wavelength Target Station at SNS

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[1] Intense Pulsed Neutron Source

The Spallation Neutron Source (SNS), under construction at Oak Ridge National Laboratory by the U.S. Department of Energy, will operate with 2 MW proton beam power and 60 Hz pulsing rate. From the outset, the design of SNS has provided for two differently optimized target stations. The first, High Power Target Station (HPTS), will offer both ambient-temperature and cryogenic moderators, designed to deliver the highest-intensity beams for applications that can exploit the 60-Hz pulsing frequency. The proposed second, Long Wavelength Target Station (LWTS), will operate at a significantly lower frequency, and permit the use of colder, more effi-cient moderators for producing long-wavelength neutrons. With the use of couple solid methane moderators, the LWTS is designed to deliver, on average, a factor of three more neutrons per pulse than the HPTS. The LWTS will optimize long-wavelength applications by closely tailoring moderator spectra and pulse shape resolution to instruments that operate best with the coldest spectra and long intervals between pulses, and will give advantages for some high-resolution ap-plications of medium-wavelength neutrons. The technical concept for the LWTS provides for up to 21 independent neutron spectrometers; 9 viewing a coupled slab moderator, 10 viewing a decoupled slab moderator, and 3 viewing a front wing-like moderator. Instruments proposed for the LWTS are selected on the basis that they serve the needs of the scientific community and that they exploit the large bandwidth and high cold-neutron brightness provided by the LWTS. This suite of instruments will augment the range and performance of existing instruments by probing structure and interactions on long length scales and large ranges of length scale, 10-10,000Å, and slow processes occurring on large ranges of timescale, 10^{-7}s to 10^{-13}s.11 instruments well suited to the unique capabilities of the LWTS were described in the pro-posal for construction of the LWTS. Three instruments-Broad-Range Intense Multipurpose SANS (BRIMS), 200-neV backscattering spectrometer, and magnetism and diffuse scattering spectrometer (MiDaS)-were worked out in considerable detail to confirm the performance projections. The remaining 8 instrument concepts are less detailed, but are sufficient for per-formance comparisons with existing instrumentation or proof-of-principle tests. While these in-strument concepts are based on existing technology, and could be built immediately, an ongoing R&D effort will extend the designs for greater optimization. The Intense Pulsed Neutron Source at Argonne National Laboratory is funded by the U.S. Department of Energy under Contract W-31-109-ENG-38. This work was partially supported by funding from the U.S. National Science Foundation.

C-45 Neutron Scattering at High Magnetic Fields and Low Temperatures

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During the last years the Berlin Neutron Scattering Center (BENSC) has concentrated on the development of special sample environment for neutron scattering experiments at extreme conditions. BENSC offers structural research at the highest vertical magnetic fields available for neutron scattering (up to 17 T) and simultaneously temperature variation between 80 K and 1.5 K. For vertical fields up to 14.5 T and horizontal fields up to 6 T measurements can be performed at temperatures between 300 K and 0.03 K. Future developments will be a 9 T vertical magnet with a room temperature bore for research with organic materials at temperatures between 600 K and 250 K, as well as a dilution unit equipped with a magnetic cooling stage, which may extend the accessible temperature region down to 0.001 K.

C-46 High Pressure Clamp Cells For Neutron Scattering At Low Temperatures

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Two high pressure clamp cells made from TiZr zero alloy are presented in this report.The first cell has a steel support around the TiZr inner part and a window in the support for neutron scattering- 90o . The height of a sample is 6 mm and the diameter is 10 mm. The outer diameter of the cell is 62 mm; this allows putting the cell into a standard ILL orange cryostat. The cell was tested under pressure up 15kbars at temp. 4K. The support, nuts, and pistons are made from hard steel alloy, and some pistons are from WC6.The other clamp cell was made from TiZr without the support and permitted achieving the pressure up to 10kbars. The diameter of the inner hole for a sample is 7 mm and the height is 25 mm. For inelastic scattering, we have made a clamp cell from Al alloy, allowing the pressure up to 9 kbar (the sample diameter is 7.2 mm and the height is 40 mm). All these cells were tested in PSI and were used for the investiagations of the magnetic spiral in ZnCr2Se4 and TN in the colliner antiferromagnetic Cu0.5In0.5Cr2S4 under pressure with NaCl (a pressure calibrant) and Fluorinert (a pressure medium).

C-47 Liquid He-free 10 T superconducting magnet for neutron scattering

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A new-type superconducting magnet which is directly cooled down by two 4 K-GM cryocoolers (i.e., without the use of liquid-He) has been developed for neutron scattering experiments. The magnet consists of a split-pair of a $(Nb,Ti)_3Sn$ inner coil and a NbTi outer coil; and the gap for the neutron-beam path is 29 mm. These upper and lower coils are supported by three rings of Al alloy (4.5, 7.5, and 8 mm in thickness) and a block of Al alloy (42.5 degree in angle). The total thickness of Al alloys in the neutron-path is 52 mm, and the transmission of the beam is about 60% for neutrons with 20 meV. The bore is 51 mm in diameter at room temperature. In this bore one of sample cooling-systems (He-free 4 K or dilution refrigerators) is inserted. The maximum field of 10 T is fairly stably obtained. Several results on the magnetism of strongly correlated electron systems obtained by using of this cryomagnet are presented.

C-48 Operation of the Cold Neutron Source at the Budapest Research Reactor

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A liquid hydrogen cold neutron source (CNS) with cryogenic system of a direct cooling moderator assembly for enhanced performance and improved safety characteristics has been installed at the 10 MW power Budapest Research Reactor. After commissioning the operating licence was obtained and the equipment is in routine operation since February 2001. Neutronic and cryogenic properties as well as the optimisation of the operating conditions have been studied. The installation of the CNS has been followed by the replacement of the old neutron guide system by a new supermirror guide assembly both for the in-pile and out-of pile part. Four experimental stations are using the cold neutron beams. The ensemble of the CNS and new guides provides an intensity gain as high as the factor of 30-60.

C-49 Intense Positron Source at the Munich Research Reactor FRM-II

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Principle and design of the in-pile positron source at the new Munich research reactor FRM-II are presented. Absorption of high energy prompt γ-rays from thermal neutron capture in ^{113}Cd generates positrons by pair production. For this purpose, a cadmium cap is placed inside the tip of the inclined beam tube SR-11 in the neutron field of the reactor, where an undisturbed thermal neutron flux up to 2×10^{14} n/cm^{2}s is expected. At this position the flux ratio of thermal to fast neutron will be better than 10^4. Monte Carlo calculation showed that a mean capture rate in cadmium between 4.5 and 6.0×10^{13} n/cm^{2}s can be expected. Inside the cadmium cap a structure of platinum foils is placed for converting the γ-radiation into positron-electron pairs. The heated foils also act as positron moderators to generate monoenergetic positrons. After acceleration to 5 keV the positron beam is formed by electric lenses and guided by magnetic fields. In the primary positron beam an intensity of about 10^{10} slow positrons per second can be expected.

C-50 Resolution of 3 axis spectrometers by Phase Space methods

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Phase space arguments are used to discuss the resolution of three axis spectrometers. The assumption of rectangular rather than Gaussian profile beam elements leads to significant insights into the optimum use of the instruments. In particular, the optimum choice of collimators and monochromators is discussed and the concept of the *focussing scattering angle* is developed. The knowledge gained can be transferred to the Gaussian profile approximation.

C-51 Monte Carlo Program to Compute the Instrumental Diffraction Line Profile for a Focussing High-resolution Configuration

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Recently [1] were proposed the principle and the construction of a high-resolution powder diffractometer with pneumatically bent monochromator crystal and flat thin sample. The instrumental profile is calculated for such a configuration by Monte Carlo procedure taking account of the real shape of the pneumatically bent monochromator and the misalignment parameters of the instrument. The algorithm and the input and output data files descriptions are given. Some test computations are presented too. These calculations will be important in a further effort to find instrumental corrections mainly for the reliable crystallite size and the strain of first and second kind determinations. [1].I.Ionita, A.D.Stoica, M.Popovici, N.C. Popa Nuclear Instr. and Meth. A431, 509 (1999)

C-52 Optimization Conditions in Pulsed Source TOF Neutron Spectroscopy

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In neutron diffractometry the optimal use of the neutrons supplied by the available neutron sources is of the greatest importance. The usual way to do it is to maximize the neutron flux at sample by using neutron guides, supermirrors or spatial focusing effects [1]. A different approach [2] is to obtain a very good resolution not by getting focused beams at sample or anywhere else, but only by decreasing as much as possible the scan variable variances. In the proposed paper the pulsed source TOF neutron spectrometry is considered. Both the direct and the inverse geometry corresponding to the monochromator placed before respectively after the sample, are taken into consideration. For the direct geometry both the situations when the monochromator is a crystal or a narrow curved slits chopper are treated. For the above mentioned experimental configurations focusing conditions are deduced by canceling the major contributions to the scan variable variances. The focusing conditions, deduced for the idealized case of thin moderator, sample, monochromator and detector, are related to the optimal positioning of the detector, sample and moderator or to an optimal choice of the crystal radius of curvature, for a crystal monochromator. The focusing conditions deduced for an idealized configuration can serve as ”0”-th order approximation in a numerical optimization process. [1] P. Böni, J. Neutron Research,5, 59-63 (1996). [2] I. Ionita, A.D. Stoica, M. Popovici, N.C. Popa, Nuclear Instr. & Meth., A 431, 509-520 (1999).

C-53 Asymmetry and peak width at the axially focusing E9 powder diffractometer - theoretical and experimental description

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The neutron powder diffractometer E9 at the research reactor BER II uses an axially focusing monochromator in combination with a wide detector opening in order to gain intensity. Common descriptions of the asymmetry at this type of instrument consider the effects from the heights of sample and detector only. However, with an axial convergence angle of about 7° from the monochromator this approximation is not sufficient. The high inclination of parts of the incoming beam in relation to the diffraction plane results in an increased asymmetry compared to a parallel beam. Moreover, this configuration results in broadening of the reflections even at diffraction angles of 90°. A thorough theoretical discussion of these effects on the peak shape of E9 will be presented together with additional minor effects influencing this instruments peak shape.

C-54 MC simulation of single crystal spectroscopy and diffraction at spallation sources

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The simulation package VITESS offers an advanced Monte Carlo technique for the numerical calculation of flux, count rates and resolution functions for single crystal neutron spectrometers and diffractometers. The comparison of various moderator (decoupled-poisoned, decoupled and coupled) and target (short and long pulse) options for backscattering spectrometers and single crystal diffractometers at the future European Spallation Source (ESS)is one of the main applications of VITESS. Single crystal instrument components highly determine both the wavelength selection and intensities measured in the detectors. Both intensity and beam divergence are highly influenced by the focussing geometry of the monochromators or analysers. Crystal sample modules are implemented to analyse the options mentioned above for single crystal diffraction at ESS.

C-55 Neutron spin echo and time echo studies on magnetite ferrofluids

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Dynamics of magnetite particles in heavy water based ferrofluids have been studied by a neutron spin echo (NSE) spectrometer PONTA in JRR-3M at the Bragg positions as well as by a newly constructed time echo neutron spectrometer of MIEZE type in JRR-3M. Since the structure factors of (111) and (311) Bragg reflections are mainly magnetic and non-magnetic, respectively, quasielastic scattering due to particle motions and magnetization fluctuatuions will give different contributions for these Bragg reflections. Whereas the time echo neutron spectrometer makes no difference for magnetic or non-magnetic, spin non-flip or spin flip scattering processes but just reflects the change of neutron velocities by the quasielastic scattering.

C-56 Neutron diffraction study of the quantum behavior of the pair correlation function of low-density ^{4}He

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An extensive neutron diffraction investigation on low-density (n¡4.3nm^{-3}) states of helium gas along the 6 K isotherm has been performed by means of both wide and small angle experiments, allowing for the extraction of the zero- and first-order density coefficients of the Fourier transform of the direct correlation function c(r) in a very wide wavevector region extending from k=1nm^{-1} to k=160nm^{-1}. The two independent measurements provide quantitatively consistent results and the experimental quantities show a good agreement both with corresponding quantum-mechanical calculations and with the k=0 thermodynamic data.

C-57 Investigation of sheared liquids by neutron backscattering and reflectivity

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Recently we have shown that the macroscopic flow dynamics of lubricants can be explored by inelastic neutron scattering. To investigate this more carefully and optain in addition information on the diffusion processes parallel and perpendicular to the shear gradient we have built a shear cell specially for quasielastic and inelastic neutron scattering and another shear cell for neutron reflectivity. As a first sample we have investigated water solutions of the triblock copolymere P85, of which the structural properties are well known from SANS. In a reflectivity measurement (EVA at ILL) with a hydrophilic and a hydrophobic coated polishead silicon waver used in the shear device and a 33% (in weight) solution of P85 in deuterated water we find the polymere concentration right at the surface varying between 12% and 52% for different coatings, temperatures between 18° and 73°C and shear rates up to 5000 1/s, including also further structural changes. On the backscattering instrument IN10 we observe that the sample seems to ”stick” to the plates implying an unusual macroscopic velocity distribution differing from that found for lubrication oils. Moreover we report on the changes in the quasielastic line width for different temperatures and shear rates in the direction of the shear gradient.

C-58 An analytic form for the total neutron cross section of liquid para-hydrogen

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The total neutron cross section of liquid para-hydrogen, close to the triple point, has been measured in a wide range of wavelengths using the PEARL beamline at ISIS. The experimental results compare only qualitatively with the results of the Young and Koppel (YK) theory. However, this should be expected, due to the presence of the intermolecular interactions in the real system. In order to interpret the experimental data, we define, first, an effective temperature which takes into account the mean field effect due to the interactions. This improves the agreement in the intermediate energy range. In the long wavelengths regime, the results of the theoretical model are low and an effective molecular mass of the order of 24 a.m.u. should be taken into account for a good fit of the experimental data. In the high energy limit, instead, the extrapolation of the YK model gives a good analytic description of the measured cross section beyond 1 eV. Finally, we give an analytic expression for the total neutron cross section of liquid para-hydrogen, covering the wavelength range between 0 and 5Å.

C-59 Transition between hydrodynamic and fast sound in a binary mixture: a neutron Brillouin scattering experiment

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Several molecular-dynamics simulations, theoretical studies, and neutron and light scattering experiments have been devoted in the past fifteen years to the investigation of the phenomenon of fast sound propagation in the microscopic dynamics of two-component fluids. In the rare-gas mixture He-Ne a fast sound mode was studied by a neutron scattering determination of the dynamic structure factor. In order to study the transition between the fast and the normal acoustic mode in the hydrodynamic regime, Q values lower by about one order of magnitude than in usual experiments have to be probed. We describe here the results of the first neutron Brillouin scattering experiment performed with this purpose on the same system already investigated at larger Q.

C-60 The microscopic dynamics of condensed parahydrogen

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We have measured the almost-pure incoherent scattering function of liquid and solid parahydrogen, using inelastic neutron scattering. The experiments were carried out on TOSCA, a time-of-flight, inverse-geometry, crystal-analyzer spectrometer, operating at the ISIS pulsed neutron source (UK). The experiments have been planned taking advantage of the intrinsic incoherence introduced in the scattering process by the rotational transitions. The measured double differential cross-section gives a direct experimental access to the microscopic dynamics of condensed hydrogen. From the high energy region of the spectrum, where the impulse approximation for the center of mass motion applies, we have been able to extract the translational mean kinetic energy, which, as expected, turns out rather different from the classical value, and density dependent. The density behaviors of the liquid and solid mean kinetic energy are slightly different. In the low energy region we used the Gaussian approximation to compare, in the liquid phase, various models and a novel quantum simulation (namely Centroid Molecular Dynamics) with the experimental data. Results are encouraging, but suggest further work, possibly beyond the Gaussian approximation.

C-61 On-line Rheometry and SANS from Complex Fluids

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The powerful instrumentation for small angle neutron scattering (SANS) at the Institut Laue-Langevin (ILL), Grenoble, France, in combination with a state-of-the-art rheometer provides a unique possibility to directly correlate rheological properties of complex fluids with the underlying microstructure. For this purpose we installed at D11 a commercial Bohlin CVO 120 HR rheometer, which allows many different rheological tests like simple shear flow either at constant shear stress or constant shear rate, creep and creep recovery as well as low and large amplitude oscillatory shear deformation. A thermostated Searle-type shear cell has been developed in collaboration with FZ Jülich. Two different beam configurations can be achieved: one where the incident beam is aligned radially, i.e. along the direction of the velocity gradient and another one where the beam is parallel to the flow direction (”tangential” beam). As an example, we demonstrate the influence of added, water-soluble polymer on the structure and flow behaviour of a lyotropic lamellar phase.

C-62 Neutron Scattering Study on Vitamin C (L-Ascorbic Acid)/Water Aqueous Solutions

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From the physical chemistry point of view, Vitamin C (L-ascorbic acid), due to both its relatively small dimension and to the existence of H-bond interaction sites, can be considered as a model-system for the study of solute-solvent interaction mechanisms. It is well known that the antioxidant action of Vitamin C is on the basis of its positive effects on human health. Our purpose is to get information on molecular mechanisms regulating its biological functions, in which the hydrogen bonding plays a key role. In this contribution we show neutron scattering findings on L-ascorbic acid aqueous solutions. To estimate the strength of the L-ascorbic acid/water interaction and its influence on the diffusive dynamics of both L-ascorbic acid and water, we have determined the translational, rotational and vibrational contributions of the motion and quantitatively evaluated important quantities, such as the hydration radius, the hydration number and the mean-square displacement.

C-63 QENS and NMR studies of 3-picoline – water solutions

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We have studied mobility of the solute and the solvent in aqueous solutions of 3-methyl pyridine (3-picoline). This system has a closed-loop immiscibility region between 38.5 and 114^{circ}C at normal pressure, if heavy water is used as solvent, while it is fully miscible with light water at any concentration and temperature. In the present study the origin of the partial miscibility behavior is sought through microscopic dynamical features of the solute-solvent interaction. H-D substitution on both the solute and the water was used to separate the dynamics of the two species. At high picoline content the diffusion coefficient of water decreases strongly and becomes similar to that of the solute, indicating strong coupling between the motions of the solute and the solvent. Activation energies characteristic of the dynamic behavior of the methyl group were determined from ^{1}H spin-lattice relaxation rate measurements in the solutions above 40^{circ}C.

C-64 Scaling behavior of shear-induced sponge to lamellar transitions

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We report shear-induced sponge to lamellar phase transitions in Cetylpyridinium chloride (CPCl)-hexanol-brine-sugar systems. Our measurements show a well-defined shear response that proceeds in three steps characterized by two critical shear rates: G1 and G2. At shear rates G below G1 no shear effect was observed. For $G1<G<G2$, the systems shear thin and the sponge phase is progressively transformed into a lamellar phase with the membrane normals aligned parallel to the shear gradient. The critical shear for the onset of this transformation scales as the cube of the membrane volume fraction and as the inverse of the viscosity. Above G2, the induced lamellar phase apparently collapses. This higher critical shear shows the same scaling behavior as G1 and is probably related to faster membrane diffusion processes. From SANS and rheological measurements we extract master curves giving a universal phase response for these systems under shear flow. These results disagree with previous published results.

C-65 The Temperature Dependence of the de Gennes narrowing in Liquid Rubidium

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To explain the positive dispersion effect in simple liquids there is a supposition, that icosahedral clusters will stay temporarily in the liquid above the melting process[1]. Near the structure factor maximum the quasi elastic line shows a reduction of the line width, which is called de Gennes narrowing. A coherent inelastic neutron scattering experiment on liquid Rubidium was performed to investigate the temperature dependent next neigbor diffusion process at the structure factor maximum. This parameter should give a fingerprint of possible excisting clusters. Fiveteen temperatures from the melting point up to two times the melting point have been measured. The experiment was performed at the triple axis spectrometer of the Forschungsreaktor München FRM. The experimental results will be compared with the predictions of the Enskog hard sphere theory for self diffusion. [1] Chr. Morkel, T. Bodensteiner, H. Gemperlein, Phys. Rev. E 47, 1993, 2575

C-66 A SANS Study of the Structural Evolution in Egg White Induced by Joule Heating

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The authors have been investigating the mesoscopic structural evolution of egg white during the gelation process. In the usual heat-induced gelation experiments, the specimen is heated with the thermal conduction from the heater located around the sample cell, which tends to give rise to temperature gradient in the specimens. In order to prevent such a temperature gardient, in the present study, the authors adopted a new heating technique utilizing the Joule heat of electric current which passes through the specimen, and observed the mesoscopic structural evolution of egg white during the heat-induced gelation process by the small angle neutron scattering (SANS) method. Before heating, a broad peak appeared around q=0.06Å^{-1} in the SANS profile. With the heat-induced gelation proceeded, the intensity of the broad peak gradually decreased while that around q=0 increased remarkably.

C-67 SANS studies of solutions and molecular composites prepared from cellulose tricarbanilate.

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We report on SANS measurements carried out on the instrument SANS1 (V4) at the BENSC facility on solutions and composites of cellulose tricarbanilate (CTC). This cellulose derivative exhibits lyotropic behaviour in methylacrylate (MA). The SANS data indicate that in the isotropic liquid state (up to 25wt% CTC in MA) the CTC chains behave like rods of mass per unit length (M/L). In the liquid crystalline (LC) phase (at and above 35wt% CTC in MA), the Q dependence varies from Q^{-1} to Q^{-4} probably as a result of self-assembling of the CTC chains. The general aim of our work is to prepare molecular composites, i.e. miscible blends of rigid-rod and flexible-coil polymers, from CTC solutions in polymerizable media. To establish the degree of homogeneity of the composites, we performed SANS measurements on UV-cured CTC/MA solutions. Here we compare the SANS data of CTC/monomer solutions to those of the corresponding composites.

C-68 Neutron Incoherent inelastic and quasielastic scattering of oriented oleic acid

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In order to investigate a hierarchical structure of vibrational modes we have observed neutron incoherent inelastic and quasielastic scattering of oriented oleic acid($CH_3(CH_2)_7CH=CH(CH_2)_7COOH$) in crystal and liquid states at several temperatures by using time-of-flight neutron spectrometer AGNES in JRR-3M. In the liquid and crystal phases the lattice vibration, the molecular vibration and the intermediate transition modes were assigned.

C-69 Small angle neutron scattering study in a ternary microemulsion depending on the concentration of droplet

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Small angle neutron scattering (SANS) experiment has been done in a ternary microemulsion system composed of AOT (dioctyl sulfosuccinate sodium salt), D_2O and n-decane at room temperature. With fixed water to AOT molar ratio ($[D_2O]/[AOT]=38.2$), the volume fraction of water and AOT, ϕ, was changed. The measured ϕ range was from 0.05 to 0.7 with a step of 0.05. The observed SANS profile from bulk contrast sample was changed with increasing ϕ due to the inter-droplet structure factor. The peak position of the SANS was linearly depended on ϕ. The droplet concentration dependence of SANS profile will be discussed.

C-70 Chemical effects on the crystallization dynamics: crystallization of two chemical isomers

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The crystallization dynamics of the two isomers of propanol (1- and 2-propanol) is studied by means of real-time dielectric and neutron diffraction experiments. What is interesting about these samples is that they show dielectric spectra which combine the temperature dependence of a fragile liquid with a Debye lineshape for its main relaxation [1]. Moreover what is even more intringuing is the fact that the two isomers exhibit markedly different dynamic and structural properties [2,3], and different crystallization time from the supercooled liquid to the most stable phase. These differences drove us to investigate the crystallization dynamics of the two isomers of propanol by comparing two real-time experiments (dielectric spectroscopy and neutron diffraction) in order to: i) answer the question whether the crystalline morphology influences the alpha relaxation and ii) obtain some information about the crystallization process and the possible morphology. [1] M. Jiménez-Ruiz et al., submitted to Phys. Rev. B [2] C. Talón et al., J. Non-Cryst. Solids (in press) [3] S. Kojima et al., Prog. Theor. Phys. Suppl. 126, 427 (1997)

C-71 Neutron Spin Echo Studies on the Effects of Temperature and Pressure on Amphiphilic membranes

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We have investigated dynamical features of amphiphilic membranes in a ternary complex fluids, consisting of AOT (dioctyl sulfosuccinate sodium salt), water and n-decane, using neutron spin echo spectrometer (NSE). In this study, we investigated how the rigidity of the membranes depended on temperature and pressure in a dilute droplet system by means of NSE. We obtained the bending modulus of membranes in increasing temperature or pressure by using the droplet deformation theory proposed by Milner and Safran. We present the results of these experiments, and discuss the effects of temperature and pressure to the membranes.

C-72 Soft interaction of dendrimers as investigated by SANS

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Dendrimers are synthetic molecules with a tree-like architecture. Their interaction and their radial structure is still a matter of debate. We have investigated a dendrimer of fourth and fifth generation with and without deuterated endgroups. Experimental meassured structure factors up to high concentrations shows that the interaction differs extremely from a hard sphere interaction. Recently, Likos has developed a description for the structure factor of particles with a soft density profile. With this theory, S(q) can fully determined from the radial structure of the particle without adjustable parameters. To compare this theory to our experiment, we determined also the density distribution of the dendrimers. With the help of an contrast variation experiment, we were able to show that the density distribution has the shape of a gaussian.

C-73 The Effect of Solvent Density Inhomogeneties of Supercritical Carbon Dioxide on Ultrathin Polymer Films

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The swelling and dynamics of the ultrathin polymer films (thicknesses less than 1000 Å) in CO_2 (T_c=31.3 °C, P_c=73.8 bar) were monitored by means of in situ neutron reflectivity (NR). Four kinds of the ultrathin polymer films (deuterated polystyrene (d-PS), deuterated poly(methyl methacrylate) (d-PMMA), deuterated polybudadiene (d-PB) and deuterated styrene-budadiene copolymer (d-SBR, volume fraction of d-PS:47%) were used in this study. NR results showed that (i) the swelling isotherms for the polymer films-CO_2 mixtures showed anomalous maxima at the ridge in supercritical region where the density fluctuations of CO_2 had maxima under the conditions, and (ii) the swelling maxima for rubbery polymers were much larger than those the glassy polymers. Additionally, it is found that this fluctuation-induced swelling occurs only near the CO_2-polymers surface. We will also discuss the effect of the density fluctuations on the interdiffusion of polymers and reduction of the glass transition temperature.

C-74 Neutron Reflectivity Studies of Electric Field Driven Structural Transformations of Surfractans

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We will review our recent studies of the structure of organic molecules at a solid-liquid interface. We will describe how surfactant molecules aggregate to form monolayer or bilayer films, how stable these films are in the presence of an electric field. In these studies we employed electrochemical methods together with in-situ neutron reflectometry. This allowed us to determine the surface coverage, thickness, the relative positions and the roughness of the aggregates. We found that the applied electrical field may be used to manipulate the architecture of the organic molecules: from uniform monolayers to adsorbed hemi-micelles in the studied film. These studies are expected to reveal new insight into the roles played by entropic and electrostatic forces in complex fluids or biomaterials.

C-75 Nucleated dewetting of thin polymer films

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Polymer coatings are an essential topic in industrial processing. In all applications it is important that the polymer builts up a homogenous and stable film on its substrate. A destability of the originally continous film frequently is caused by impurities inside the films. We choose polystyrene as our model system because of its broad range of applications. A smooth surface is simulated in our experiments by a silicon wafer and residues of solvent doped with dust act as nucleation grains. The dewetting process has been studied by neutron reflectometry and optical microscopy. With optical microscopy the growth of individual holes in the polymer films was observed in-situ. The growth of the hole area is described within the Kolmogorov model which is known as a common nucleation and growth formalism. The grain dimension and the time constant were extracted from fits to the data.

C-76 Diffusion and Evaporation of Plasticizer from an Aging Polymer Thin Film

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We present the first measurements of the diffusion of a plasticizer from a polymer matrix using neutron reflection. The evolution of a nitroplasticizer from Estane 5703 was determined as a function of annealing time at an elevated temperature (73°C). We found that the diffusion equations for a material traveling through the film and then evaporating into a vacuum at the free surface best describe this system. We show that the loss of plasticizer from the film is not rate limited by its passsage through the polymer, but rather by the rate of evaporation from the surface. Furthermore, we find that the rate of evaporation is consistent with the evaporative loss from a free standing surface of liquid showing that there is little interaction between the polymer host and the plasticizer.

C-77 Structure Analysis of Adsorbed Starlike Polymers with GISAS and SFM

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Changes of the architecture of polymers influences the whole behavior of polymers, like the glass temperature or dynamics. Regular starlike polymers are special classes of branched polymers which show a spread behavior depending on their functionality (number of arms) and the molecular weight of the arms. With different number of arms and molecular weight of the arms the adsorption behavior can be widely varied. Using small angle grazing incidence scattering techniques (GISAS) and scanning force microscopy (SFM) we were able to determine different dominant in-plane length scales of adsorbed starlike polymers. Typical structures are blobs which are formed from single stars or agglomerates of star polymers. Our model system consists of a mixture of fully protonated and deuterated polybutadiene star polymers with arm numbers of 15 up to 128.

C-78 Retardation of the dewetting process due to the addition of statistical copolymers at polymer-polymer interfaces

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We studied the retardation of the dewetting process due to the addition of a statistical copolymer in a polymer bilayer film. Our model system consists of fully deuterated polystyrene (PS-d) on top of an amorphous polyamide sublayer on silicon substrates. We prepared bilayer films with different content (0, 5, 10, 30% vol.) of a statistical copolymer (protonated styrene maleic anhydride acid (SMA2) containing 2% MA groups along the chain) in the topmost film. To evaluate the retardation effect reference samples of pure PS-d:PA bilayer films were prepared. The as-prepared as well as the annealed samples were investigated by neutron reflectivity (NR) experiments (ADAM beamline at ILL, Grenoble/France), scanning force microscopy (SFM) and optical microscopy (OM). From model fits of NR curves the scattering length density profiles perpendicular to the sample surface were calculated. The protonated material is located within the deuterated PS-d matrix. The surface homogeneity of the blended samples in comparison to the pure PS-d film were determined by scanning force microscopy as well as by optical microscopy.

C-79 Film thickness dependence of structure formation in ultra-thin polymer blend films

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We investigated the film thickness dependence of structure formation in ultra-thin polymer blend films prepared from mixtures. As a model system we used binary mixtures of poly-styrene-stat-para-bromostyrene copolymers dissolved in toluene as a common solvent. The ultra thin films were prepared via spin coating of the polymer solutions onto silicon (100) substrates. In total three different samples series differing in the miscibility of the blended polymers and varying film thickness were prepared. The resulting morphologies were investigated with scanning force microscopy, reflectometry and grazing incidence scattering techniques in order to obtain a picture of the sample at and below the sample surface.

C-80 Structure and Stability of Polyion-Complexed Langmuir-Blodgett films

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Spreading amphiphiles on a water surface and compressing the monolayer is one of the most important methods to prepare ordered two-dimensional organic structures. Replacement of the counterions in the solution with ionic polymers results in the formation of complex-stabilized monolayers.

These monolayers can be transferred onto solid substrates giving multilayers (LB-films). X-ray and neutron reflectivity measurements on the LB-multilayers from arachidic acid complexed with poly(allylaminehydrochloride) reveal an ordered bilayer structure of the films with a very thin polyelectrolyte layer between the headgroups. Uptake of water in these ionic regions of the layers results in a swelling of the films and some structural changes when placed in an atmosphere saturated with water. Selective deuteration and contrast changes were used to get insight to the structure of the LB-film and the dynamical processes therein.

C-81 Reflectivity studies of ionomer blends

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Preliminary results are presented of a neutron reflectivity study of the interfacial width between lithium- and zinc-sulphonated deuterated polystyrene with polycarbonate (PC). Both systems are partially miscible and exhibit an upper critical solution temperature behaviour [1]. The interdiffusion in these systems, with annealing at a temperature above the glass transition temperature of both polymers, has been measured. The interfacial profiles obtained for these systems were found to be described by symmetric Gaussian interfaces. No significant diffusion has been observed. [1] Lu, X., and R. A. Weiss. 1996. Development of Miscible Blends of Bisphenol-A Polycarbonate and Sulfonated Polystyrene Ionomers From Intrapolymer Repulsive Interactions. Macromolecules, 29: 1216-1221.

C-82 Intermolecular structure of liquid D-tert-Butanol by Neutron Diffraction data

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The neutron diffraction (ND) measurements are carried out on high-Q diffractometer for liquid D-tert-Butanol at room temperature (RT) and the data are analyzed successfully. The molecular structure of t-Butanol molecule is obtained by using an iterative method by making RDF zero at core region[1]. Analysis of x-ray diffraction data[2] tells about the dominant presence of hexamer closed chain (ring) cluster in liquid t-Butanol at RT[3] like liquid Methanol and Ethanol at RT[4]. Now we find that this average intermolecular structure having H-bonding also reproduces very well the ND data and helps to obtain intermolecular atom-atom partial pair distribution functions which are well comparable with EPSR model results[5]. [1] H. Bertagnolli et al.,Molec.Phys.32(1976)759. [2] S. Sarkar, R.N.Joarder, J.Chem.Phys.99(1993)2032,100(1994)5118. [3] A.H.Narten, S.I. Sandler,J.Chem.Phys.71(1979)2069. [4] A.K.Karmaker,S.Sarkar, R.N.Joarder,J.Phys.Chem.99(1995)16501 [5] D.T.Bowron et al., Molec.Phys.93(1998)531.

C-83 Crystallization of paraffin in decane in the presence of PEB-7 ethylene-butene random copolymers

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By SANS we studied the crystallization of $C_{24}H_{50}$ tetracosane and $C_{36}H_{74}$ hexatriacontane paraffins in decane in the presence of PEB-7 poly(ethylene-butene) random copolymers. The measurements were performed at temperatures between the single coil regime at around 80°C and the aggregate regime, far below the room temperature. Using contrast matching techniques the structures of paraffin and copolymer could be studied separately. The two paraffin-copolymer systems show different mechanisms of aggregation. In tetracosane solution the copolymer controls the aggregation behavior by forming a periodic structure of two-dimensional objects which is strengthened by the paraffin. In hexatriacontane solution well-defined two-dimensional objects and additional three-dimensional structures are formed, but the aggregation process is controlled by the paraffin which mediates the plate formation of the copolymer.

C-84 A Study on the Structure of Organic-inorganic Hybrids

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Organic-inorganic hybrids were prepared with an inorganic constituent composition of $(100-x)SiO_2.xMO_2$ (M=Ti or Zr) and an organic component of PDMS. The preparation involved sol-gel processing, to obtain high purity vitreous material at relatively low temperatures, and gamma ray irradiation, to form a pre-network of the polymer. The structure of the hybrids has been characterised using mainly Small Angle Neutron Scattering (with contrast variation) and Scanning Electron Microscopy. The present work reports the main results found in this investigation.

C-85 Micellization of PEP-PEO Block Copolymers in Water: Molecular Weight Dependence

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The micellar behaviour of the amphiphilic block copolymer poly-(ethylene-propylene)–poly-(ethylene oxide) (PEP-PEO) in aqueous solution has been studied with small-angle neutron scattering (SANS). The polymer was studied over a wide range of molecular weights, keeping the volume of the blocks equal. The low molecular weight samples were fully protonated and measured in D_2O to achieve maximum contrast. The high molecular weight copolymers were prepared with partially deuterated PEP and studied under various contrasts conditions. The scattering experiments showed that a morphological transition took place upon lowering the molecular weight. The high molecular weight block copolymers all built spherical, monodisperse micelles with large aggregation numbers. At low molecular weights long cylindrical micelles formed. An interesting intermediate case was represented by the PEP2-PEO2 system, in which a morphological transition occurs upon dilution. Mean-field theories of micellization provided a theoretical explanation of the observed trends. The micellar parameters of the spherical micelles formed by the high molecular weight samples agreed excellently with theoretical predictions. In the case of the low molecular weight systems only qualitative agreement could be obtained.

C-87 Temperature-dependent SANS-investigations of cylindrical micelles in TTABr-D_2O-NaBr systems

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Numerous studies of micellar TTABr-D2O solutions (TTABr = $C_{14}H_{29}(N(CH_3)_3^+Br^-)$ using different experimental methods revealed a strong decrease of the effective radii of spherical micelles with increasing temperature, a finding which seems to be in-compatible with the physical picture of micelles. In the present SANS-study, we in-vestigated the behaviour of micelles with cylindrical shape which are formed after the addition of electrolyte (NaBr). Even in these systems it is found that the apparent radii as determined from the cylindrical Guinier-plot ln(J(Q)Q) vs. Q^2 decrease with tem-perature from 2.46 nm at 20°C to 2.28 nm at 80°C. Possible explanations for this unexpected behaviour will be discussed.

C-88 Scattering Functions of Janus Particles

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Recent advances in polymer synthesis has produced so-called Janus micelles; tailor-made copolymer structures in which the blocks constitute separate moieties (Erhardt, R., Böker, A., Zettl, H., Kaya, H., Pyckhout-Hintzen, W., Krausch, G., Abez, V., and Müller, A. H. E., *Macromolecules*, **2001**, *34* 1069.) We present expressions for the form factors P(Q) and the radii of gyration R_g of Janus particles with spherical, cylindrical and lamellar morphology and check their validity by fitting them to Monte-Carlo simulated scattering data, from which plots of the pair distance distribution function p(r) are extracted as well. The effect of the block incompatibilities on the scattering curves is briefly investigated.

C-89 Universal Aspects of Macromolecules in Blends, Organic and Supercritical Solvents

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For two decades, SANS data from polymer blends have been analyzed via the random phase approximation (RPA), based on the assumption that the radius of gyration (Rg) remains unchanged on mixing, and thus exhibits the unperturbed (theta) dimensions. We have performed a systematic test of the RPA by measuring the Rg of polydimethyl siloxane (PDMS) in polyethyl methyl siloxane (PEMS) and shown that PEMS is a poor solvent for PDMS. However, diverging concentration fluctuations (CF) stabilize the dimensions and prevent chain collapse, so PDMS exhibits the theta-dimensions down to the critical point. We have also shown that blends of polystyrene-polyvinylmethyl ether exhibit both upper and lower theta-temperatures, which separate the poor and good solvent domains, and have developed a scaling description of the CF-correlation length, which reduces data from polymer blends and solutions onto a single master curve. Thus, the RPA remains valid over a wide range of temperatures in polymer blends, but breaks down at the edges of the phase diagram where the chains may shrink or swell beyond their unperturbed dimensions.

C-90 Solution behavior polyethylene oxide in different solvents as function of temperature and salt.

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Small-angle neutron scattering was used to study hydrosoluble polyethylene oxide. An appropriate mixture of hydrogenated and deuterated polyethylene oxide in a mixture of hydrogenated and deuterated water was used, satisfying the condition of zero average contrast in-order to measure intrachain correlations. At the same time, we used deuterated polyethylene oxide in hydrogenated and deuterated water to measure interchain chain correlations. In the following paper we will discuss the measured intra- and interchain structures of polyethylene oxide in different solvents as function of temperature and salt.

C-91 Magnetic structure of the ternary carbides HoMoC$_2$ and ErMoC$_2$

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The magnetic structures of the orthorhombic carbides HoMoC2 and ErMoC2 have been investigated by neutron powder diffraction between 1.6 K and 20 K. The magnetic Ln atoms are on the Wyckoff position 4c of the space group Pnma: (1) x, $\frac{1}{4}$, z; (2) -x, $\frac{3}{4}$, -z; (3) $\frac{1}{2}$ - x, $\frac{3}{4}$, $\frac{1}{2}$ + z; (4) $\frac{1}{2}$ + x, $\frac{1}{4}$, $\frac{1}{2}$ - z. We use here the notation of Ref. [1] for the following sequences of + and - signs: F(+ + + +), G (+ - + -), C(+ + - -) and A(+ - - +). In the case of HoMoC2 a non-collinear ferrimagnetic structure has been found, where the magnetic moments are turned out of the orthorhombic ac-plane by an angle of 32(2)°. The magnetic structure of HoMoC$_2$ can be described with the basis functions [Cx - Fz] and [- Cy -] resulting in a reducible representation with the basis function [Cx Cy Fz]. The antiferro- and ferromagnetic components along the a- and c-axis are mexp = 1.2(3) mB and mexp = 5.1(2) mB, respectively. The moment along the b-axis is mexp = 3.3(2) mB. In ErMoC$_2$ the erbium moments are ordered antiferromagnetically with a moment direction parallel to the b-axis and the magnetic structure can be described with the basis function [- Cy -]. The lanthanoid moments in HoMoC$_2$ and ErMoC$_2$ reach an experimental magnetic moment of mexp = 6.2(1) mB and mexp = 6.5(1) mB, respectively. These values are somewhat smaller than the theoretical values ms = g J mB of the free Ho^{3+} (ms = 10.0 mB) and Er^{3+} ion (ms = 9.0 mB). From the temperature dependence of the reflection 001 it could be seen that the magnetic intensity disappears in HoMoC$_2$ at the Curie temperature T_C = 7.0(5) K, while in the case of ErMoC$_2$ it disappears at the surprisingly larger Néel temperature T_N = 9.0(5) K.

C-92 Magnetic signature of charge ordering in Li[Mn$_{1.96}$Li$_{0.04}$]O$_4$ and Li$_{0.2}$[Mn$_{1.96}$Li$_{0.04}$]O$_4$

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The stoichiometric compound LiMn$_2$O$_4$ is known to show charge ordering with well-defined Mn^{3+} and Mn^{4+} sites just below RT. Above RT the electrons are hopping rapidly between sites. For lithium insertion batteries the material Li[Mn$_{1.96}$Li$_{0.04}$]O$_4$ is technological relevant. Due to the small amount of Li on the Mn site, the low T regular ordering of the Mn charge appears to be destroyed completely as is evidenced by neutron diffraction in the magnetically ordered state. However, the charges are still fixed in an irregular fashion as can be deduced from ^{7}Li nuclear magnetic resonance measurements. In the lithium extracted compound Li$_{0.2}$[Mn$_{1.96}$Li$_{0.04}$]O$_4$ predominantly Mn^{4+} is present. Neutron diffraction in the magnetically ordered state shows a well-defined antiferromagnetic ordering, with doubling of the unit cell in three directions. Clearly (a trivial type of) charge ordering occurs now, since almost only Mn^{4+} is present.

C-93 Magnetic order in CeI$_2$

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CeI$_2$ is a halide with metallic conductivity according to the formula (Ce^{3+})(I$^-$)$_2$(e$^-$). The conduction electrons mediate the magnetic interactions and make them significantly stronger than for insulating rare-earth halides. CeI$_2$ crystallizes in the MoSi$_2$ layer-type structure with space group I4/mmm and lattice parameters of a = 3.8721(1) Åand c = 13.8646(2) Åat 15 K. At T_N = 10.0(2) K a phase transition to a 3D antiferromagnetically ordered state occurs with an incommensurate extbfk-vector of (0, 0.2761(1), 1). The **k**-vector is temperature dependent and, as the sublattice magnetization, reaches saturation below 4 K. CeI$_2$ has one magnetic sublattice with moments parallel to the a-axis. The amplitudes are sine-modulated along the b-axis and amount to 1.87(2) μ_B per Ce^{3+}. The crystal field slightly reduces the ordered moment below the $^2F_{5/2}$ free-ion value of g·J = 15/7 for Ce^{3+}.

C-94 Magnetic ordering in $(La_{0.653}Dy_{0.347})_{0.7}Ca_{0.3}MnO_3$ perovskite

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We have investigated the nature of magnetic ordering in the Dy substituted $(La_{0.653}Dy_{0.347})_{0.7}Ca_{0.3}MnO_3$ perovskite by carrying out ac susceptibility, neutron diffraction and neutron depolarization measurements. Low temperature neutron diffraction study shows the absence of long-range magnetic ordering. AC susceptibility and neutron depolarization measurements confirm the spin glass phase with the spin glass freezing temperature T_{sg} = 46.5K. Detailed neutron diffraction structural study gives the microscopic origin (in terms of crystal structure parameters such as Mn-O-Mn bond angles, bond distances etc.) of the observed magnetic phase.

C-95 Magnetic structure of tetragonal TmB$_2$C$_2$

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RB$_2$C$_2$ (R=rare earth) system which includes the antiferroquadrupolar (AFQ) ordering materials, DyB$_2$C$_2$ and HoB$_2$C$_2$, shows characteristic magnetic properties due to coexistent of AFQ and antiferromagnetic (AFM) orderings. In this work, we report magnetic properties of TmB$_2$C$_2$, especially its magnetic structure, and compare it with those of the other compounds. The magnetic structure of TmB$_2$C$_2$ below T_N=16.5K is a simple AFM one with k=[1 0 1/2] and magnetic moments parallel to c axis. The results and our previous works indicate that the ground states of RB$_2$C$_2$ shows various magnetic couplings due to competition between AFQ and AFM interactions: a ferromagnetic one in R=Ce, k=[1 0 0] type ones in R=Nd, Gd, Dy, Ho, Er, and [1 0 1/2] type one in R=Tm and Tb.

C-96 Structural and magnetic disorder in $Nd_{90-x}Fe_xAl_{10}$ glassy hard magnets

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The specific microstructure of Nd-Fe-(Si,Al) bulk amorphous alloys, supposed to consist in exchange coupled Fe-Nd magnetic clusters, determines coercivities as high as 550 kA/m at 200 K [1]. Total structure factors have been measured for $Nd_{90-x}Fe_xAl_{10}$ (x = 35 - 50) melt-spun ribbons with thicknesses of 25 and 120 μm at temperatures between 15 and 300 K by powder neutron diffraction using the SLAD diffractometer at the Studsvik Neutron Research Laboratory. The split first peak and the pronounced structure at higher angles present in the total structure factor patterns could be explained by a dense random packing of Fe and Nd atoms. From the calculated pair correlation function, g(r), obtained by Fourier inversion of the diffraction patterns, we estimated the dominant nearest neighbors as being Fe-Fe and Fe-Nd. The magnetic structure is predominantly ferromagnetic at all temperatures, in agreement with the static magnetic measurements indicating about 475 K for T_C. The data have been used to simultaneously model the atomic and magnetic structures using the reverse Monte Carlo (RMC) method in order to prove the existence of the magnetic clusters. [1] H. Chiriac and N. Lupu, Physica B (2001), accepted for publication.

C-97 Neutron Diffraction Study of YFe$_2$D$_{4.2}$

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Hydrogen absorption in YFe_2, leads to the formation of several hydride phases, which present various structures derived from the C15 cubic structure. These structural changes influence the magnetic properties of the hydrides. YFe_2 is ferromagnetic with Tc=540 K and a moment of 1.8μ_B/Fe. From $YFe_2H_{1.2}$ to $YFe_2H_{3.6}$, the hydrides remains ferromagnetic, with a linear decreases of the Curie temperature, and an increase of the Fe moment at 4.2 K. Rhombohedral $YFe_2H_{4.2}$ displays a more unusual effect, since a weak ferromagnetic behaviour is observed down to 110 K. Below this temperature a field dependant transition is observed with a sharp incrase of the magnetization. Neutron diffraction study has been performed in LLB to identify the origin of this transition, in complement of high magnetic fields and ^{55}Fe Mössbauer experiments. The data analysis shows the existence of an intermediate magnetic phase between 60 and 140 K, with a maxima at 90 K, accompanied with a large magnetovolume effect.

C-98 Characterisation of magnetic phases of DyNi$_2$B$_2$C in an applied magnetic field

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DyNi$_2$B$_2$C with the space group $I4/mmm$ shows superconductivity (T_C=6.1 K) in the antiferromagnetically ordered state (T_N=10.5 K). The magnetic phase diagram was investigated by magnetisation and magnetostriction measurements. The magnetic structures were characterized by temperature and magnetic field dependent neutron scattering experiments on D23 at ILL Grenoble. At zero field the propagation vector is (001). For an applied field along [110]-direction metamagnetic phases MM2 and MM4 with propagation vectors (00 3/4) and (0 0 2/3) are determined. For applied fields along [100]-direction the phases MM1 and MM3 with propagation vectors (0 7/8 0) and (3/5 00) exist. To investigate the hysteresis effects at low temperatures the neutron scattering experiments were extended to temperatures down to 50 mK. The diffraction pattern measured on E4 at HMI Berlin show clearly, that the depression of superconductivity at low tempertures in zero field after field cooling are originated by the existence of the metamagnetic phase MM1.

C-99 Magnetic structural studies of the two polymorphs of Li$_3$Fe$_2$(PO$_4$)$_3$: analysis of the magnetic ground state from super-superexchange interactions

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The nuclear and magnetic structures of the monoclinic (P21/n, A-LFP) and rhombohedral (R-3, B-LFP) forms of Li$_3$Fe$_2$(PO$_4$)$_3$ have been solved using powder neutron diffraction at room temperature and 1.5K on polycrystalline samples. Both structures are built on [Fe$_2$(PO$_4$)$_3$] ”lantern units” that are connected in a different way for each form. SQUID measurements reveal a global antiferromagnetic behavior with ordering temperatures of 25 and 23 K for the A and B forms, respectively. Both magnetic structures, determined from symmetry analysis and Rietveld refinements of neutron diffraction data recorded at 1.5 K are collinear. The Fe atoms are oriented antiparallel within the [Fe$_2$(PO$_4$)$_3$] ”lantern units” while parallel orientation takes place between Fe atoms that do not belong to the same ”lantern unit”. Using numerical calculations we have established a magnetic phase diagram and determined the necessary constraints to be satisfied by the values of the exchange interactions in order to obtain the observed magnetic structures as the ground state.

C-100 Magnetism in superconducting ErNi$_2{}^{11}$B$_2$C

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ErNi$_2{}^{11}$B$_2$C shows coexistence between weak ferromagnetism and superconductivity below T_{WFM}=2.75K. We have performed magentization measurements and unpolarized neutron diffraction experiments on a ^{11}B substituted large single crystal. When the system enters a weak ferromagnetic state, a strong incommensurate SDW peak locks in to a commensurate position q=0.55a*. In addition to this strong peak, small magnetic peaks appear at every 1/20a* positions. In the present paper, we report detailed magnetic structures and a magentic (H-T) phase diagram of this material.

C-101 Low-Temperature Incommensurate Magnetic Order in R_2BaCoO_5 (R=Rare Earth)

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R_2BaCoO_5 oxides have been studied by means of neutron powder diffraction. The compounds where R= Pr-Er present orthorhombic symmetry (S.G. $Immm$) and they are isostructural with the Haldane system Y_2BaNiO_5. The oxides with smaller rare earths, $i.e.$ R=Tb-Lu, crystallize in the green phase structure type R_2BaCuO_5 (S.G. $Pnma$) related with the $YBaCuO$ HTSC. The existence of polymorphism in some range of R^{3+} cation size (Tb-Er) is pointed out. The oxides belonging to the $Immm$ family show AF order of both R^{3+} and Co^{2+} sublattices at fairly high temperatures ($T_N \sim$ 100K) but 1D magnetic correlations in Co chains (S=3/2) are still present at rather higher T than T_N. By contrast, $Pnma - R_2BaCoO_5$ develop 3D magnetic order at T<10K involving complex phase transitions between commensurate (C) and incommensurate (I) magnetic structures. It is worth noting as the most striking cases those of R_2BaCoO_5 with R= Er, Tm, Lu and Y. The former remains as an I-magnetic structure down to T=40mK and the latter shows the coexistence of both C and I structures in the vicinity of a Lifshitz point. Both facts are quite uncommon. Devil's staircase behaviour in helimagnetic Tm_2BaCoO_5 is observed at 1.4K<T<2.5K. A sudden collapse of a sine-wave modulation of Co moments to a C-magnetic structure is evidenced in Lu_2BaCoO_5 at T=2.5K.

C-102 Exchange interactions and magnetic structure of $CuFe_2(P_2O_7)_2$

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The compound $CuFe_2(P_2O_7)_2$ crystallises in the monoclinic system with space group P21/n. The crystal structure is characterised by the presence of centrosymmetric Fe-Cu-Fe trimers with intra-trimer superexchange interactions. The magnetic interactions between trimers occur through super-super-exchange paths consisting of PO4 groups connecting the FeO6 octahedra and the square planar group CuO4 that form the trimers. Susceptibility measurements indicate an anti-ferromagnetic behaviour at low temperature. Neutron powder diffraction confirms this and the determined Néel temperature is T_N=16.6(5) K. The propagation vector of the magnetic structure is k=(0.5, 0, 0.5), the ions inside a trimer are coupled ferromagnetically and the magnetic moments are all oriented along the b axis. The value of the staggered moments at 1.5K are 0.76(6) and 4.18(4) μ_B for Cu^{2+} and Fe^{3+} ions respectively. The conditions to be satisfied by the exchange interactions in order to get the observed magnetic structure as the stable ground state are discussed.

C-103 Influence of the real structure on the magnetic properties of $FeNbO_4$

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Potential applications for some types of ABO_4 oxides, e.g. $FeNbO_4$, $FeTaO_4$ and $FeWO_4$, in gas sensors, as catalysts and in photo detector technology have given rise to an intensive study of these materials within the last decades. Special topics of interest are the electrical and magnetic properties as well as new routes of synthesis. Fundamental for the understanding of the physical properties of these materials is a detailed knowledge of the underlying structure. Based on the determined realstructure, neutron powder diffraction was used to investigate its influence on the magnetic ordering of the system.

C-104 Low Temperature Neutron diffraction studies of Sr_2FeMO_6 (M=Nb, Sb)

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The magnetization of Sr_2FeNbO_6 and Sr_2FeSbO_6 showed a maximum at 20 and 35.5 K, respectively. Field-cooled and zero-field cooled magnetic susceptibility of Sr_2FeNbO_6 showed a hysteresis below 20 K. Crystal structures and magnetic properties of these two materials were studied by low temperature neutron powder diffraction. By Rietveld analysis above the magnetic transition temperatures, Sr_2FeNbO_6 has an orthorhombic unit cell with a space group of Pbnm and Sr_2FeSbO_6 has a monoclinic unit cell with a space group of $P2_1/n$. The six-coordinate site of Sr_2FeNbO_6 was randomly occupied by Fe and Nb and this site of Sr_2FeSbO_6 was orderly occupied by Fe and Sb. The diffraction pattern of Sr_2FeNbO_6 showed no evidence of a magnetic order down to 2.3 K, whereas Sr_2FeSbO_6 showed some antiferromagnetic Bragg peaks below 35.5K. We conclude that Sr_2FeNbO_6 has a simple perovskite structure and transforms to a spin-glass state below 20K.

C-105 Neutron diffraction and muSR Studies of $La_{1-x}Sr_xCoO_3$ magnetic structure

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Neutron diffraction and muSR studies of $La_{1-x}Sr_xCoO_3$ with different x values have been carried out over a temperature range from 10 to 300 K. A ferromagnetic transition have been found at low temperature for $x \geq 0.15$. Values of magnetic moments are in agreement with those, reported from other measurements. No any spin-glass transition have been found for all x concentrations.

C-106 The structural and magnetic properties of the $Nd_{n+1}Co_{3n+5}B_{2n}$ compounds investigated by neutron diffraction

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The crystal and magnetic structures of $Nd_{n+1}Co_{3n+5}B_{2n}$ (n=1,2 and 3) have been studied by high resolution powder diffraction at the ILL. The results are compared to magnetisation measurements and analysed in the light of earlier measurements on isotype $Y_{n+1}Co_{3n+5}B_{2n}$. The neutron diffraction analysis shows that the magnetic moments are ferromagnetically ordered. The anisotropy of the Nd sub lattice is found to play a major role in determining the easy magnetisation direction lies in the basal (a,b) plane of the hexagonal structure whatever the temperature is. The magnetic structures of $Nd_3Co_{11}B_4$ and $Nd_2Co_7B_3$ confirm the large variety of cobalt magnetic moments obtained in these compounds. The magnetic behaviour of the Co(2c) atoms is not significantly affected by the substitution of boron for cobalt. Cobalt atoms with significantly reduced magnetic moments are found on the 3g and $6i_2$ sites in both $Nd_3Co_{11}B_4$ and $Nd_2Co_7B_3$.

C-107 Investigation of the magnetic properties of solid ^{3}He by neutron diffraction

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The condensed isotope ^{3}He is a fermion system with spin $\frac{1}{2}$ where, dependent on density and temperature, a wealth of physical phenomena is observed. Embedded in a complex phase diagram of liquid and solid additional co-operative phenomena are found. They range from the suprafluid liquid phases to the observation of magnetic order in solid phases.. The low mass of ^{3}He leads to strong zero point fluctuations. One consequence is that it solidifies only under high pressure in the bcc - phase, further increase of pressure then leads to the hcp phase. Due to the high delocalisation of the 3He atom the exchange of particles on adjacent sites is a very likely. These processes, which involve 2,3, and more particles, also dominate the magnetic behaviour. They lead to a direct magnetic exchange interaction which at temperatures around 1mK also induces magnetic order. At present, solid ^{3}He is the only system known for such a direct exchange interaction. The possibility of a magnetic structure investigation on solid ^{3}He was investigated and found feasible at short neutron wavelength. Consequently, at the HMI now a new diffractometer is constructed for a neutron study of solid ^{3}He. We present the experimental concept and the first results obtained with the new spectrometer on crystal growth at high temperatures.

C-108 Neutron Diffraction Studies of a Cr+0.88at%Ga Alloy Single Crystal

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A discrepancy exists between the calculated and measured signs of dT_{IC}/dp from magnetoelastic measurements on a Cr+0.88at.%Ga single crystal [1]. A neutron diffraction study is reported to provide additional information on its magnetic phases. The temperature dependences of rocking curves through (010) reveal an incommensurate SDW phase for T<278K and commensurate there above to the Néel temperature T_N. The integrated intensities show anomalies at T_{IC}=278K, corresponding to a weak minimum in the α-T curve, and at 80K taken as the spin-flip transition from longitudinal to transverse polarisation upon heating. Above T_{IC} the intensity drops off linearly tending to zero around 500K. Magnetoelastic measurements observed T_N=335K. The long tail in the neutron intensity above T_N is ascribed to strong spin fluctuation effects persisting to temperatures well above T_N. [1] A.R.E. Prinsloo, H.L. Alberts and P. Smit, J. Phys.: Condensed Matter **9** (1997) 9961.

C-109 Symmetry and magnetic structures determination: developments in refinement techniques

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Group Theory techniques can aid greatly the determination of magnetic structures. The integration of their calculations into new and existing computer programs is an ongoing development. This paper presents an overview of the practical application of symmetry analysis to the determination of magnetic structures. Details are given of the different programs that perform these calculations and how refinement can be carried out using their results. Examples are presented that show how such analysis can be important in the interpretation of magnetic diffraction data, and to our reasoning of the causes for the observed ordering.

C-110 Neutron Diffraction Study on Magnetic Structure of GdB_2C_2

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There are two purposes in this study. One is to see performance of our powder neutron diffractometer, HERMES, for very heavy neutron absorber. The other is to see the magnetic structure of GdB_2C_2 as a compound of tetragonal RB_2C_2 family in which antiferroquadrupolar and magnetic interactions are competing. A typical compound of this family is DyB_2C_2 which takes so called ”rectangular structure” at the low temperature because of the competing of these two interactions. In the present study we pick up GdB_2C_2 to clarify purely magnetic interaction in this system because Gd ion lacks quadrupolar moment. We got the diffraction data using reflection geometry and concluded the magnetic interaction is antiferromagnetic in the c-plane and ferromagnetic along the c-axis.

C-111 Neutron diffraction study of metamagnetism in $HoRu_2Ge_2$

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The ternary compound $HoRu_2Ge_2$ shows antiferromagnetism below T_N=13.5 K. At low temperatures a two-step metamagnetic magnetization process appears in the c-axis process; There are two magnetic phases below a field-induced ferromagnetic phase. To determine the magnetic structures, neutron diffraction study on a single crystal compound has been carried out under non magnetic field and magnetic fields as well. It is confirmed that the antiferromagnetic structure at H=0 is characterized by the propagation vector Q_1=(0.219, 0.011, 0). The field-induced intermediate phase is a double-Q structure having Q_2 =(0.219, 0, 0) and Q_3=(0, 0.219, 0).

C-112 Contribution of neutron and X-ray Laue scattering to the investigation of domains and magnetic phenomena by new recording

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Neutron diffraction has the potential to provide information deep below the surface of real materials. Magnetic, mechanical and thermal loading are considered. Firstly an experimental set up to realise the uniaxial stress is described. Samples of NiO and alpha-uranium are submitted to an external uniaxial stress that gives complementary information in neutrons and X-rays scattering. Reversible or displacive phase transformations take place reversibly through the transition. Finally for high spatial resolution stress it is necessary to use high energy X-ray facilities optimising effectively the stress rig. At ILL on the S42 instrument, dedicated to quality tests and alignment facilities, progressively is set up an updated tool offering rapid data collection with optimised detectors to be tested.

C-113 Neutron Scattering Image of the Spin Ice State in $Dy_2Ti_2O_7$

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$Dy_2Ti_2O_7$ is a rare magnetic material that has a zero point entropy. On the basis of bulk measurements it has been suggested to be a ”spin ice” material, with a frozen and disordered low temperature structure analogous to that of water ice. We have now used the PRISMA spectrometer at ISIS to investigate the magnetic disorder in isotopically enriched $Dy_2Ti_2O_7$ at millikelvin temperatures. The results establish the basic ice-like nature of the disordered correlations, and show that it can be described by a ”dipolar” spin ice model. This result resolves a controversy as to whether $Dy_2Ti_2O_7$ has qualtatively the same or different behaviour to that of its relative $Ho_2Ti_2O_7$ and provides an important test of alternative theoretical methods of treating dipolar sums.

C-114 Neutron diffraction studies of the ferrimagnetic $Cu_{1-x}Fe_xCr_2S_4$.

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The neutron diffraction studies of the spinel $Cu_{1-x}Fe_xCr_2S_4$ have shown that the $Cu_{0.5}Fe_{0.5}Cr_2S_4$ has the 1:1 type of ordering of Cu^+ and Fe^{3+} in A-site(Sp.gr. F43m), and the calculations for the magnetic moments of Fe3+ are 3.06(0.17) and for Cr^{3+} are 2.76(0.22)μ_B. In the $CuCr_2S_4$ (Sp.gr.Fd3m), Cu does not have the magn. moment and the m(Cr^{3+})=2.30(0.03)μ_B. Hence, Cr has two valency states Cr^{3+} and Cr^{4+}. The neutron diffraction of the $Cu_{0.5}Fe_{0.5}Cr_2S_4$ at 14K up to P=43kbar does not show the change of the ferrimagnetic type ordering. From measuring the neutron diffraction up to pressure 94kbar at 300K of the $Cu_{0.7}Fe_{0.3}Cr_2S_4$,we determined the compressibility (DV/V0=0.91 at P=94kbar) in accordance with the equation of the state of Birch-Murnagan type with the parameters B_0=76.8GPa and B'=4.

C-115 Program for the representation analysis of magnetic structures

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The representation analysis of magnetic structures has been known as a general purpose and a mathematically elegant method, which exploits space group symmetries of the underlying crystal structure. However, it is also a complicated method requiring knowledge of representation of space group. This, unfortunately, inhibits many people from applying it to neutron diffraction experiments. Its difficulty is caused by the complicated procedure to obtain possible magnetic structures, i.e., basis vectors of the representation. In order to solve this problem and to make the method much easier to use, we wrote a Fortran program which calculates possible magnetic structures from information of the space group and the modulation vector. The procedure of the program and a few applications to magnetic structure determinations are reported.

C-116 Magnetic structure of $Sr_3Fe_2O_{7-\delta}$

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It is well known that $Sr_3Fe_2O_7$ shows charge disproportionation, $2Fe^{4+} \rightarrow Fe^{3+} + Fe^{5+}$. However extensive studies have been carried out for this compound by various authors, the crystal or magnetic structure is still poorly understood. In this work, we carried out neutron powder diffraction measurements for powder samples of $Sr_3Fe_2O_{7-\delta}$ with different oxygen contents. Moreover, we succeeded to synthesize the single crystal of $Sr_3Fe_2O_{7-\delta}$ with $\delta \approx 1$ and performed magnetic susceptibility measurements. From these results, we determined the magnetic structure of $Sr_3Fe_2O_{7-\delta}$ with $\delta \approx 1$. We also observed that magnetic structures of $Sr_3Fe_2O_{7-\delta}$ drastically change with changing the oxygen-deficient.

C-117 Polarised Neutron Scattering Studies Of the Antiferromagnetic Pyrochlore $Tb_2Ti_2O_7$

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We have carried out extensive polarised neutron scattering studies on the pyrochlore antiferromagnet $Tb_2Ti_2O_7$. This insulating material belongs to a family of rare earth titanate pyrochlores, whose magnetic rare earth ions reside on a network of corner sharing tetrahedra. Such a local geometry is known to give rise to geometrical frustration in the presence of antiferromagnetic interactions. Earlier studies have shown $Tb_2Ti_2O_7$ to be an Ising system with large moments constrained to point along local [1,1,1] directions; that is into and out of the tetrahedra. It displays a co-operative paramagnetic or spin liquid state at low temperatures, with neither long range Néel order, nor spin glass ordering at temperatures as low as 0.07 K. Polarised inelastic scattering measurements on a single crystal samples show five excitations at least 3 of which are magnetic in origin. These results will be discussed in terms of recent crystalline electric field calculation.

C-118 SANS study of slow dynamics in reentrant spin glasses

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In order to probe the microscopic mechanism of slow dynamics in spin glasses, time-resolved small-angle neutron scattering (SANS) experiments on concentrated spin glass alloys, $Fe_{65}(Ni_{0.866}Mn_{0.134})_{35}$ and $Fe_{70}Al_{30}$, were made. Measurements were made utilizing the SANS-J spectrometer installed at the JRR-3M reactor of JAERI-Tokai. The momentum-transfer range of $0.03 < Q < 2nm^{-1}$ was covered with the incident-neutron wave length 0.65nm. The time variation of the magnetic diffuse scattering pattern arising from magnetic clusters after being quenched into the reentrant spin glass phase was measured up to 20 hours. The time evolution of magnetic clusters will be discussed.

C-119 Neutron study of the magnetic interactions in frustrated Laves hydrides

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In $\mathrm{RMn_2}$ compounds (R is a magnetic rare earth) the pyrochlore-like Mn sublattice is topologically frustrated and the Mn-Mn first-neighbor distance is just above the critical value, below which the magnetic moments become delocalized. We have studied the influence of applied pressure and hydrogen doping (acting also as a negative pressure) on their magnetic properties [1]. In $\mathrm{R(Mn,Al)_2H}_x$, H disorder induces a short-range magnetic order [2]. We present here new results obtained in these compounds by diffraction and inelastic scattering. The spin freezing temperature coincides with the temperature where the static correlations appear. Under an applied pressure of 8.3 GPa the Mn moments vanish and a long-range order is recovered, simply controlled by the ferromagnetic interactions inside the R sublattice. [1] I.N. Goncharenko et al, PRB 59, 9324 (1999) [2] I. Mirebeau et al, PRB 62, 9493 (2000)

C-120 Field induced transitions in the highly frustrated magnet Gadolinium Gallium Garnet - long or short range order?

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In Gadolinium Gallium Garnet (GGG) the antiferromagnetically interacting Gd ions are located on two corner-sharing triangular sublattices. The magnetic system is therefore highly frustrated and does not order in a zero field, while AF order can only be induced by the application of an external magnetic field. We have measured the magnetic diffraction pattern of a single crystal of GGG at temperatures between 50 mK and 0.9 K in fields of up to 4 T. These experiments reveal that the H-T phase diagram has a much more complicated nature than previously assumed. Three groups of magnetic Bragg peaks were found: strong ferromagnetic peaks, saturating in fields above 2.5 T; strong AF peaks with maximum intensity at the lower-field phase boundary around 0.6 T; weak AF peaks which have a maximum intensity at the upper phase boundary around 1.5 T. The widths of the strong AF peaks are limited by the instrument resolution only in the vicinity of the lower phase boundary.

C-121 Fe Moment instability in $\mathrm{Ti}_{1-x}\mathrm{Sc}_x\mathrm{Fe}_2$ Laves Phases Compounds

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The magnetic properties of the pseudo-binary Laves phases compounds $\mathrm{Ti}_{1-x}\mathrm{Sc}_x\mathrm{Fe}_2$ were investigated by means of magnetisation and high resolution powder neutron diffraction techniques. For $x < 0.2$ a transition from antiferromagnetic state to a canted one with a ferromagnetic component in the basal plane, while for $0.2 < x < 0.27$, the transition is from a collinear ferromagnetic state along the c-axis to a canted one. For $x \sim 0.3$, an additional first order transition is observed at low temperature accompanied by a large magnetovolume anomaly due to the increase of the intrinsic moment of the Fe atoms at the 2a site. Most of the magnetic ground states in this system can be discussed within the Moriya's theory for itinerant electron systems where ferromagnetic and antiferromagnetic spin fluctuations coexistent. However, Fe moment instability in frustrated lattice should be considered to interpret the first order transition.

C-122 Observation of Linear SpinWave Dispersion in Re-entrant Spin Glass $\mathrm{Fe}_{0.7}\mathrm{Al}_{0.3}$

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$\mathrm{Fe}_{0.7}\mathrm{Al}_{0.3}$ is a reentrant spin glass, which undergoes a transition from a paramagnet to a disordered ferromagnet at Tc 500K and at a lower temperature the spins progressively freeze and it exhibits spin glass like behavior. The spin dynamics of this system has been extensively studied at small angles around $Q = q = 0$ where $Q = q + \tau$, with $\tau = 0$ [1,2]. In the FM phase spin waves with a q^2 dispersion are observed at small q, which broaden rapidly and become diffusive [2] beyond a critical wave-vector q$_($0). On cooling the spin waves also disappear and a strong elastic central peak develops. For measurements around the (1,1,1) Bragg peak, a new sharp excitation is observed which has a linear dispersion behavior. It disappears above T $_c$, but persists throughout the spin glass phase. It is not present in the stoichiometric $\mathrm{Fe_3Al}$ material. Possible origin of this excitations related to the disorder will be discussed. [1] K. Motoya et al., Phys. Rev. B28, 6183 (1983). [2] W. Bao et al., Phys. Rev. Lett. 82, 4711 (1999).

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C-123 2-Dimensional magnetic correlations in the kagome spin-glass $D_3OCr_3(OD)_6(SO_4)_2$. A neutron spin-polarisation study.

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The temperature dependence of the magnetic correlation in the quasi 2-dimensional kagome spinglass material $(D_3O)Cr_3(OD)_6(SO_4)_2$ has been studied using the 3-direction (xyz) neutron spin-polarisation technique in the temperature range 0.1–15 K. A broad magnetic responce is observed around $Q \sim 1.1$Å^{-1}. A very small temperature dependence is present above the spin-freezing temperature at $T_{sf} \sim 1.8$ K. The inplanar magnetic correlatation length above T_{sf} is approximately 11Åover the temperature range covered. Below T_{sf}, the increasing importance of the interlayer interaction become noticable in an increasing neutron depolarisation behaviour below 1K. This behaviour indicates a ferromagnetic interlayer coupling similar to the one observed in the ordered Cr-kagome system $KCr_3(OD)_6(SO_4)_2$.

C-124 Correlation Length of Charge Ordering in $La_{1-x}Sr_xMnO_3$

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As a study object the single crystals of the $La_{1-x}Sr_xMnO_3$ (x=0.15, 0.23) compound has been chosen. The experiments on elastic scattering of thermal neutrons have been carried out using the multidetector neutron diffractometer. The neutron scattering patterns have been obtained in symmetry planes of the crystal lattice of manganites. The fact that diffraction patterns at relatively high temperature (close Curie temperature) contain the ferromagnetic superlattice diffusion maxima appeared to be one of the main and new result of the present work. The correlation length of charge ordering at manganites was determined from those neutron data. The work was partially supported by SSTP(No 107-19-(00)-D01)

C-125 Neutron and X-ray diffraction studies of bulk and powdered $La_{0.7}Sr_{0.3}MnO_3$ ceramics

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A bulk and powdered $La_{0.7}Sr_{0.3}MnO_3$ ceramic samples were investigated by neutron diffraction in the temperature range from 80K to 280K and in a magnetic field up to 4.5T. The neutron diffraction was performed with λ=1.798Å and λ=2.443Å. X-ray measurements were carried out for a bulk ceramic and for a thick layer on MgO substrate using Co-K$_\alpha$ (λ=1.7908Å). The bulk ceramic sample had a rhombohedral structure with lattice constants a=5.520Å and c=13.332Å. The powdered ceramic consisted of about 70% of the rhombohedral phase and 30% of an orthorhombic contribution with lattice constants a=5.592Å, b=5.510Å and c= 7.757Å. The layered ceramic had only the orthorhombic phase. The crystallographic and magnetic structures were analyzed by Rietveld method. A temperature dependence of the unit-cell parameters and the magnetic moments was determined both for the bulk and the powdered ceramics.

C-126 Investigation of magnetic structure evolution in the substitutional solid solution $Sc_xLu_{(1-x)}MnO_3$

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The hexagonal structures (space group P6$_3$cm) AMnO$_3$ (A = Lu, Sc) phases are excellent model systems for the investigation of magnetic frustration due to nearest neighbour antiferromagnetic exchange on the edge sharing triangular magnetic sublattices. At low temperatures the Mn$^{3}+$ sublattices of the above compounds form a 120 degree magnetic long range ordered state. In LuMnO$_3$ (T_N=96K) the magnetic moments are in the ab-plane and perpendicular to the hexagonal axis, whereas ScMnO$_3$ (T_N=129K) undergoes an in-plane spin-reorientation transition below T = 70K. Powder neutron diffraction experiments for the solid solution $Sc_xLu_{(1-x)}MnO_3$ ($0.0 \leq x \leq 1.0$) show the evolution of the spin-reorientation transition for Sc rich compositions. Based on the comparison of structural and magnetic details an explanation of the nature of the low temperature transition is proposed.

C-127 Effect of Ga substitution on the magnetic properties of $La_{0.67}Ca_{0.33}Mn_{0.75}Ga_{0.25}O_3$

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The effects of 25 at.% Ga substitution on the Mn site in the ferromagnetic $La_{0.67}Ca_{0.33}MnO_3$ perovskite (T_C = 265K) have been studied by ac susceptibility, dc magnetization, neutron diffraction (ND) and neutron depolarization (NDP) techniques. ND study shows a complete absence of any long range magnetic ordering in the substituted sample. However, the presence spin clusters (with net moments) at it T<48 K is confirmed from the NDP study. Under external fields, spin clusters are found to persist at it T>48 K. Temperature independent cluster size and moment are prominent at T≤25 K. Above 35 K (blocking temperature), superparamagnetic relaxation is evident. Anisotropy is seen to play a major role at $T < 10$ K.

C-128 Low Energy Excitation in $La_{1-x}Ca_xMnO_3$ single crystals with $0.05 \leq x \leq 0.20$

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Inelastic neutron scattering measurements were carried out to study the spin dynamics of $La_{1-x}Ca_xMnO_3$ single crystals with x = 0.15 and x = 0.20. We observed a spin gap at 1.0 meV with x = 0.15 and 0.9 meV with x = 0.20 at Q = 1/2 0 1/2. The gap was only observed in the ferromagnetic region and disappearing in the paramagnetic region. The spin-wave stiffness constant D was calculated from the relation of D = 2JSa2, where a is the lattice constant. The J value is estimated to be 0.41 meV and 0.43 meV for x = 0.15 and x = 0.20, respectively. The spin gap is discussed in conjunction with a single ion anisotropy term in the Heisenberg Hamiltonian. The study of single crystal sample with x=0.05 is now in progress.

C-129 Structure and magnetic order in perovskite manganites $Y_{1-x}Ca_xMnO_3$(x=0.3 and 0.5)

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The $Y_{1-x}Ca_xMnO_3$ orthoperovskites exhibit an extreme tilting of the MnO_6 octahedra. The Mn-O-Mn angles is as low as 148^o for x=0.3 (151^o for x=0.5). As a result, the ferromagnetic double exchange interactions are weakened and the tendencies to the 3d electron localization and orbital polarization become dominant. The sample with x=0.3 displays a cooperative Jahn-Teller ordering (MnO_6 axes ratio of 1.055). Manganese spins are largely frustrated with some short range antiferromagnetic correlations. Relatively large net magnetization can be induced by external magnetic field. The sample x=0.5 exhibits at 300 K the Mn^{3+}/Mn^{4+} (1:1) charge ordering, which is followed at 115 K with the CE antiferromagnetic transition.

C-130 Diffuse magnetic scattering in quasi-2D $La_{1.2}Sr_{1.8}Mn_2O_7$

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We have measured diffuse magnetic scattering above the ordering temperature T_C from the quasi-2D bilayer manganite $La_{1.2}Sr_{1.8}Mn_2O_7$ which shows colossal magnetioresistance (CMR) behaviour. Rod-like diffuse scattering parallel to $\vec{c}^\star$ in the $(h0l)$ plane has been observed. The modulation of the diffuse scattering intensity parallel to the rod shows that the two ferromagnetic Mn planes in the bilayer are ferromagnetically correlated. By fitting the experimentally measured intensity distribution of the diffuse scattering in the $(h0l)$ plane to a model mean-field calculations we have been able to determine the exchange interactions between the Mn ions in the individual planes of hte bilayer and also that between the two planes of the bilayer. The exchange interactions so derived agree well to those obtained from spin wave dispersions at low temperature.

C-131 Charge Ordering in $Ca_{2-X}Pr_xMnO_4$ (x<0.25)

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These last years, a renewed interest stimulated studies of layered metal oxides with the K_2NiF_4 or related structures. The crystal and magnetic structures of $Ca_{2-x}Pr_xMnO_4$ (0<x<0.25) compounds have been studied by neutron powder diffraction and electron microscopy. Magnetisation and magnetoresistance measurements have also been made in connection with the structural studies. These experiments evidence charge and magnetic orders depending on the x values. For instance, for the $Ca_{1.75}Pr_{0.25}MnO_4$ compound, we observe charge ordering below 280K and an antiferromagnetic structure below 150K. Below the charge ordering temperature, the electron diffraction study of this compound shows extra reflections corresponding to superlattice due to alternating Mn^{4+}/Mn^{3+} stripes (3:1) with a wave vector qco = (0 0 $\frac{1}{4}$) for T<280K. Neutron diffraction patterns refinements show a structural transition from Cmca (RT) to C2/c (LT) at the charge ordering temperature, but no crystalline change at the Néel temperature.

C-132 Magnetic Short-Range Order in $La_{0.9}Sr_{0.1}MnO_3$

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The colossal magneto-resistance (CMR) effect in the hole-doped $La_{1-x}Sr_xMnO_3$ compounds is connected with a magnetic double-exchange interaction between the manganese ions. We are studying the magnetic interaction in these compounds by diffuse neutron scattering. Experiments were done with a single crystal of $La_{0.9}Sr_{0.1}MnO_3$, kindly provided by Martine Hennion from LLB (Saclay). We used the E2 Flat-Cone diffractometer (HMI Berlin) with a wavelength of 2.39Åand studied a temperature range between 1.5K to 300K. With the banana-type multidetector complete layers of reciprocal space were recorded. We determined in the paramagnetic phase, above $T_C = 140K$, the magnetic correlation and interactions from the diffuse scattering distributions. The domain distribution was determined from the orthorhombic nuclear reflections. This is important for the evaluation of the diffuse scattering with a mean-field theory. A total scale factor can then be fitted with the software *TVtueb* (J.-U. Hoffmann and R. Schneider) using the constant relative scale factors of the domain distribution. The interaction parameters were determined using a renormalized temperature. This is equivalent to a correction of the meanfield theory by an Onsager reaction field.

C-133 Polarised Neutron Scattering Study of Magnetic Correlations and Spin Dynamics in $La_{0.875}Sr_{0.125}MnO_{3+\delta}$

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The rhombohedral $La_{0.875}Sr_{0.125}MnO_{3+\delta}$ compound exhibits colossal magnetoresistance in the vicinity of the ferromagnetic transition, T_c (∼250 K). From neutron polarisation analysis measurements, the scattering peak in the forward direction above T_c ($T_c > T > 1.6T_c$), showed a Lorentzian-type q dependence, with magnetic correlation lengths (Ornstein-Zernike form) in the range 11-14 Å. This forward scattering peak has both neutron spin-flip and non-spin-flip components and our measurements demonstrate that we have simultaneously observed the lattice and magnetic components of polarons above T_c. From the energy scale of the observed diffusive fluctuation in this compound, the polarons were determined to have mobility of $\sim 2.5 \times 10^{-11}$ cm^{2}s^{-1} at room temperature.

C-134 Magnetic alignment of the RE-sublattice in REMnO$_3$

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The occurrence of multiple phase transitions is one of the interesting phenomena of condensed matter. A good example is found in the hexagonal compounds of formula REMnO$_3$ in which the coexistence of ferroelectricity with magnetic ordering is not well understood yet. The rare earth and yttrium manganites, REMnO$_3$, with RE = Ho, Er, Tm, Yb, Lu, Y, crystallize in the space group P6$_3$cm, with an antiferromagnetic transition around 100K and a ferroelectric one at about 800K. We report our neutron diffraction data on ErMnO$_3$, TmMnO$_3$ and LuMnO$_3$ below the Mn magnetic transition ($T < T_N$) and the role of the RE alignment in this temperature range. Mn^{3+} has one crystallographic site and lies in the basal plane in a triangular lattice where the spins are 120^0 with respect to each other while the RE have two different crystallographic sites. Our neutron data show that in LuMnO$_3$ the Mn spins are arranged differently than in YMnO$_3$ and that we can transit from one arrangement to the other one by changing the lattice parameters due to the lanthanide contraction. We will discuss the alignment of the RE^{3+} spins due to their coupling with the already aligned Mn-sublattice based on our thermodynamic, magnetic and the present neutron diffraction measurements.

C-135 Neutron Diffraction Studies of YMnO$_3$

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Hexagonal structure YMnO$_3$ is a rare example of electromagnet materials, which shows the coexistence of ferroelectric and magnetic order parameters below T_N = 75 K. Bulk properties display a strong anomaly at T_N, suggesting that the two order parameters should be strongly coupled. In order to understand the proposed coupling between the ferroelectric and the magnetic order parameters, we have measured detailed neutron diffraction measurements from room temperature to 10 K. Our analysis of the data shows that the magnetic structure of YMnO$_3$ can be described equally well by the Γ_1 and Γ_3 representations of the space group P63cm. In order to study the high temperature structure of YMnO$_3$, we also made neutron diffraction measurement from room temperature to 1200 K. These high temperature measurements show that there is a gradual change in the structure.

C-136 Magnetic Structure Studies of ErMnO$_3$

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ErMnO$_3$ forms in the hexagonal structure of P63cm. Unlike manganites of orthorhombic symmetry, it has a ferroelectric transition at 830 K and an antiferromagnetic transition at 80 K, i.e. a ferroelectromagnet where ferroelectric and magnetic order parameters coexist at low temperatures. In order to understand the magnetic structure of ErMnO$_3$, we made neutron diffraction measurements from room temperature to 10 K. From the neutron diffraction data, we find that it undergoes an antiferromagnetic transition due to Mn moments ordering at 80 K. According to our analysis using a magnetic group theory, the magnetic structure of ErMnO$_3$ can be described by two representations of the space group P63cm: Γ_2 and Γ_4.

C-137 Magnetic ordering in $La_{0.7}Sr_{0.3}Co_{1-x}Mn_xO_3$

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The structure and magnetic order of the distorted perovskite $La_{0.7}Sr_{0.3}Co_{1-x}Mn_xO_3$ (x=0.1, 0.5, 0.9) has been studied by neutron diffraction and magnetization measurements. The samples crystallize in the rhombohedral structure (R -3C). The unit cell volume and ferro-paramagnetic transition temperature increases with x. The Co-O bond length increases with x while bond angles do not show appreciable change. On substituting Co with Mn (x=0.1) the moment is significantly lowered to $0.7\mu_B$ at 4.5T from $1.89\mu_B$ reported for x=0. Low angle Bragg reflections and Arrott plot do not indicate long range FM order for x=0.1. This is attributed to increase in $Co^{3+} - O - Mn^{4+}$ interaction and reduction in $Co^{3+} - O - Co^{4+}$ DE interaction. With increase in Mn ($x \geq 0.5$) the FM state is stabilized and the moment increases to $\sim 3\mu_B$ for x=0.9 indicating a dominance of $Mn^{3+} - O - Mn^{4+}$ DE mechanism.

C-138 Suppression of antiferromagnetic order in Y substituted $La_{0.5}Ca_{0.5}MnO_3$

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The evolution of structural charecteristics on reducing the A-site ionic radii $< r_A >$ have been studied in charge ordered antiferromagnet (AFM) $La_{0.5-x}Y_xCa_{0.5}MnO_3$ (x=0, 0.1, 0.18) using neutron diffraction technique. The samples have orthorhombic $GdFeO_3$ structures. The CE-type AFM order observed in x=0 is completely suppressed by partial replacement of La with Y (x=0.1). The low temperature phase of x=0.1 concentration was found to be ferromagnetic ($T_C \approx 100K$). In x=0.18, no long range magnetic order is observed. This result is in contrast to the reported observation of CE-type AFM order in $Nd_{0.5}Ca_{0.5}MnO_3$ with the same A-site ionic radii. On reducing $< r_A >$, the volume and $< Mn - O - Mn >$ bond angle decreases while the Mn-O bond length increases. This results in decreasing of one electron band width thus influencing the magnetic order.

C-139 The Magnetic Structure of $HoMnO_3$ and $YMnO_3$

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$YMnO_3$ and $HoMnO_3$ have both the acentric space group $P6_3cm$ which supports ferroelectricity, and ferroelectric order has been found in these compounds below $T \sim 800, K$. The simultaneous occurence of magnetic ($T_N \sim 70K$) and ferroelectric order, together with the coupling between the two order parameters has triggered recently a number of investigations about optical, magnetic and electric properties [1]. We have taken Neutron (E2/HMI, Berlin, $\lambda = 1.21$ Åand 2.396Å) and high resolution X-ray powder data (Tübingen). The data are compatible with two models, an incoherent superposition of two kinds of domains having the magnetic space groups $P6_3'c'm$ and $P6_3'cm'$ or a coherent model with reduced symmetry of $P6_3'$. [1] M. Fiebig, D. F. Fröhlich et al., Phys. Rev. Lett. **84**, 5620-5623 (2000)

C-140 FM Magnetisation in Electron-doped $CaMnO_3$: Role of Phase Separation Between Competing AFM States

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The colossal magnetoresistive (CMR) perovskite $La_{1-x}Ca_xMnO_3$ has been relatively neglected in high-x region. Magnetic susceptibility measurements suggest the presence of small FM clusters in the crossover region between the Type-C (x∼0.75-0.90) and Type-G (x∼0.90-1.00) AFM states. A phase transition intimately associated with the C-AFM (but not G-AFM) state has allowed us to determine with which AFM phase the FM clusters are associated, via a combination of synchrotron XRD, SANS, polarised neutron powder diffraction and in-field neutron powder diffraction. The high-symmetry phase contains a FM component in addition to G-AFM, but the low-symmetry phase contains no FM component in addition to C-AFM. Furthermore, there is evidence that below T_N(G), the low-symmetry phase associated with C-AFM is slowly colonized by G-AFM, as observed in our recent study of the analogous pseudo-2D system $La_{2-2x}Sr_{1+2x}Mn_2O_7$. By combining these different powder scattering methods, we have mapped out the phase separation process between competing AFM states, placing the induced FM component in context, and giving us greater insight into the nature of this FM.

C-141 Evolution of the local atomic structure as a function of temperature in oxygen isotope substituted samples of $Pr_{0.175}La_{0.525}Ca_{0.3}MnO_3$

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We have studied the local atomic structure using the pair distribution function (PDF) obtained from pulsed neutron diffraction of two oxygen isotope substituted samples of $Pr_{0.525}La_{0.175}Ca_{0.3}MnO_3$ with ^{16}O and ^{18}O as a function of temperature. The sample with ^{16}O undergoes a insulator-metal (IM) transition at 110 K while the sample with ^{18}O remains insulating at all temperatures. We find from the PDF that the MnO_6 octahedra change abruptly from being locally elongated due to a Jahn-Teller distortion to regular below the IM transition. The same effect is not seen in the ^{18}O sample.

C-142 Neutron scattering study of the magnetic coupling in the insulating and metallic ferromagnetic phases of the CMR manganites.

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Inelastic neutron scattering has been utilized to study the spin excitations in ferromagnetic $\mathrm{La}_{1-x}\mathrm{Ca}_x\mathrm{MnO}_3$ (LCMO) as a function of the hole-doping x (0.2, 0.25 and 0.30), and in ferromagnetic $\mathrm{Pr}_{0.70}\mathrm{Ca}_{0.3}\mathrm{MnO}_3$ as a function of external magnetic field. The evolution of the magnetic coupling in these materials as they undergo a metal-to-insulator transition is both surprising and inconsistent with existing models for these materials such as Heisenberg ferromagnetism, double-exchange or modified double-exchange. These results will be discussed.

C-143 Low Energy Magnetic Excitations in the Invar $\mathrm{Fe}_{65}(\mathrm{Ni}_{1-x}\mathrm{Pd}_x)_{35}$ and $\mathrm{Fe}_3\mathrm{Pt}$ Alloys.

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The energy analysis of small-angle neutron scattering in the polycrystal $\mathrm{Fe}_{65}(\mathrm{Ni}_{1-x}\mathrm{Pd}_x)_{35}$ (x=0; 0.5) and $\mathrm{Fe}_3\mathrm{Pt}$ alloys at different (fixed) angles of scattering and temperatures being both lower and higher the Curie points was carried out on a triple-axis spectrometer. This analysis was made only by the method $(\theta - 2\theta)$ of analyser. In all the above alloys the energy analysis spectra, obtained by this method, represent maxima of the magnetic inelastic neutron scattering, which are located at approximately equal distances from the zero energy point. The maxima have a small value of energy (E≤1meV.) and a weak dependence of energy from a wave vector at the fixed temperature. If the energies of maxima at a fixed temperature are plotted against a wave vector, they do not coincide with the corresponding dispersion curves of spin waves. It is assumed that in these invar ferromagnetic alloys besides spin waves there exists some other type of low energy magnetic excitations.

C-144 INS Study of Molecular Magnetic Clusters

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Recent INS experiments on molecular magnetic clusters have been able to determine with high accuracy the relevant anisotropy parameters that drive the so-called quantum tunneling effect of the magnetization vector in ”Single Molecular Magnets”. More generally, spectroscopic methods like INS or high-field EPR are able to access the microscopic details in a unique way which will be illustrated by recent results.

C-145 The impact of fourth-order exchange interactions on spin dynamics, order parameters and critical magnetic behaviour

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An experimental study of magnets with pure spin moments is presented showing that the spin dynamics is different for integral and half-integral spin quantum number. This is attributed to fourth-order exchange interactions, i.e., biquadratic, three-spin and four-spin interactions which usually are nearly as strong as second-order (Heisenberg) interactions. Not only the exponent in the low temperature power law of the order parameter is different for integral and half-integral spins but also the critical magnetic behaviour. For isotropic interactions we propose Heisenberg critical behaviour for integral spins but mean field critical behaviour for half-integral spins.

C-146 Spin dynamics at the magnetic instability in $\mathrm{Cr}_{1-x}\mathrm{V}_x$

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The Néel temperature of the antiferromagnetic order in $\mathrm{Cr}_{1-x}\mathrm{V}_x$ decreases linearly with V doping x and vanishes at $x_c = 0.04$. We report on inelastic neutron scattering to determine the energy response in critical $\mathrm{Cr}_{1-x}\mathrm{V}_x$ $(x = 0.04)$. The fluctuations in $\mathrm{Cr}_{0.96}\mathrm{V}_{0.04}$ show compared to Cr a larger splitting from the commensurate positions similar to $\mathrm{Cr}_{0.95}\mathrm{V}_{0.05}$ with a typical energy scale $\omega_{\mathrm{SF}} = 45$ meV at low T, roughly a factor of 2 smaller than for $x = 0.05$. Surprisingly no magnetic intensity is observed at low energies and temperatures for $x = 0.04$, i.e. at the magnetic instability, indicating a possible pseudo-gap.

C-147 The Generalized Susceptibility of FCC Mn(38%Ni) Alloy

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Essential differences in spin dynamics between Mn-Ni and Mn-Fe alloys motivated the extended studies of these systems. Within this program the uniaxial anisotropy of the critical scattering found earlier in the fcc Mn(38%Ni) alloy suggested the investigation of the anisotropy of the spin wave (SW) velocity in this alloy. The detailed measurements ware performed by 3-axis neutron spectrometer in LLB, Saclay in a wide energy transfer range. The values of SW velocities at 13 K were 140, 210 and 170 meVA for the SW vector parallel, perpendicular and at 45 degrees to Q0, correspondingly. An indication of a small anisotropy of the SW velocity was found in our earlier study of magnetic excitations in the fct Mn(18%Cu) alloy. The present data give the first clear evidence of such an anisotropy for an itinerant system with the full crystal and magnetic cubic symmetry.

C-148 Spin Excitations in Mn- and $\mathrm{Ni(dca)}_2$ [dca = $\mathrm{N(CN)}_2^-$] Probed by Neutron Scattering

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Molecular magnets based on dicyanamide (dca) such as $\mathrm{M(dca)}_2$ M=Mn, Ni have shown interesting bulk magnetic properties that prompted more detailed inelastic neutron scattering (INS) studies. While the Mn^{2+} center is isotropic based on the S=5/2 configuration, the isostructural Ni analog is S=1 and demonstrates marked single ion anisotropy. $\mathrm{Mn(dca)}_2$ is a canted AFM below 16K, however, $\mathrm{Ni(dca)}_2$ is a FM below 21 K. In the case of the Mn system, INS reveals a spin wave excitation that develops gradually from critical fluctuations upon cooling. Prominent in the low-energy spectrum of Ni(dca)$_2$ are spin excitations whose position, intensity and momenta transfer vary below T$_c$. These studies clarify the microscopic origins of the magnetism.

C-149 Spin Waves in the Intermetallic Compound MnNi

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Intermetallic compound MnNi with fct structure, the highest, among the 3d metal alloys, value of the Neel temperature (T$_N$ ≈1080 K) and magnetic moment 3.8 μ_B presents a unique case for a study of 3d alloy antiferromagnets. Its highly anisotropic arrangement of spins and high value of T$_N$ suggests a strong anisotropy of various properties and high spin wave (SW) velocity (v), correspondingly. The present study was performed with the 3-axis neutron spectrometer in LLB, Saclay at 300 K in the energy transfer range from 20 to 84 meV. The derived values of the parameters of the SW dispersion relation are: v≈300 meVÅ, Eg = 2.5 meV and damping parameter ≈20 meVÅ. Neither the expected high value of the SW velocity nor its anisotropy is confirmed. The very small value of the SW damping parameter is in strong contrast to the heavy damping found in our data for the polydomain MnNi and with high damping found in all γ-Mn alloys.

C-150 Fincher-Burke Excitations in Single-Q Chromium

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The low energy excitations of incommensurate antiferromagnetic Cr have been investigated by means of high-resolution, inelastic neutron scattering with unpolarized, cold neutrons within an energy range -1.5 meV $< E <$ 9 meV. In agreement with previous measurements by other groups we observe excitations in the transverse spin density wave phase that appear between the unresolved spin wave peaks at the incommensurate positions $Q^{\pm} = (1 \pm \delta 00)$. In contrast to previous measurements that indicate excitations with a dispersion curve $E = c \cdot q$ that is similar to that of the longitudinal acoustic phonon we do not find clear evidence that these excitations (Fincher-Burkes modes) follow a linear dispersion curve. In contrast, the major part of the scattering is concentrated in the range 4 meV $< E <$ 8 meV.

C-151 Spin-wave dynamics in invar $Fe_{65}Ni_{35}$ studied by small-angle polarized neutron scattering

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The spin dynamics in invar $Fe_{65}Ni_{35}$ alloy has been studied below $T_C = 485$ K in the magnetic fields 0.05 - 0.5 T by the left-right asymmetry in Small-Angle Polarized Neutron Scattering for momentum transfers of q<0.05Å^{-1}. The spin wave stiffness D and the damping Γ were obtained from a fit of the theoretical spin-wave contribution to the measured intensities. The effect of the spin lattice coupling on the spin dynamics is observed. The temperature dependent spin stiffness D decreases as $(T/T_C)^{5/2}$. The extrapolated spin wave stiffness at $T = 0$ K is $D = 121 \pm 0.5$ meV Å^2 which is somewhat smaller than the spin wave stiffness obtained by triple-axis spectroscopy for $q > 0.1$ Å^{-1}.

C-152 Magnetic Excitations in the antiferromagnetic phase of NdCu$_2$

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Neutron spectroscopy on single crystals was used to measure the magnetic excitations in the antiferromagnetic phase of NdCu$_2$ [1]. In MF-RPA the dispersion of the magnetic excitations has been calculated using exchange parameters, which have been determined by neutron spectrocopy in the ferromagnetically aligned phase in a magnetic field of 3 Tesla parallel to b [2]. For the calculation the program package *McPhase* http://www.physik.tu-dresden.de/iapd was used. [1] M.Loewenhaupt, T.Reif, P.Svoboda, S.Wagner, M.Waffenschmidt, H.v.Loehneysen, E.Gratz, M.Rotter, B.Lebech and T.Hauss, Z. Phys. B 101 (1996) 499 [2] M.Rotter, M.Loewenhaupt, S.Kramp, T.Reif, N.M. Pyka, W.Schmidt and R.Kamp, Europ. Phys. J. B 14 (2000) 29

C-153 Spin dynamics and magnetic order near the field-induced quantum critical point in Pr$_2$CuO$_4$

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We have studied the magnetic order and the spin dynamics of Pr$_2$CuO$_4$ under a magnetic field applied along (110). Pr$_2$CuO$_4$ is a non-collinear antiferromagnet made of strongly coupled CuO$_2$ AF planes with spin direction at right angle in adjacent planes. Neighbouring planes are loosely coupled along the c-axis through pseudo-dipolar exchange interactions. When a magnetic field is applied along (110), the direction of the staggered magnetization of both types of planes gradually moves towards the direction perpendicular to the field up to a second order transition line H$_c$(T) which ends at the quantum critical point (H$_c$, T=0). We have found that one of the magnetic order parameter with k$_1$=(1/2 1/2 1) vanishes at the quantum critical point (H$_c$,0) with a non-classical critical exponent. We have shown that, at Q=(1/2 1/2 1), the gap Δ_0 of the acoustic magnetic excitation also vanishes at H$_c$. These results will be discussed in the light of recent theoretical predictions.

C-154 Observation of a continuumpart ofthe spin excitation spectrum of a Haldane spin chain

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The spin excitation continuum, expected to dominate the low-energy fluctuation spectrum in the Haldane spin chain around the Brillouin zone center, q=0, is directly observed by inelastic magnetic neutron scattering in the S=1 quasi-1D antiferromagnet $CsNiCl_3$. Employing two complementary ”next generation” experimental setups of the SPINS triple axis cold neutron spectrometer at NIST Center for Neutron Research which take full advantage of the large-area PG(002) segmented crystal analyser we achieved a tremendous increase in the data collection rate without relaxing the instrument resolution. This was vital for the success of our measurement, as the structure factor for the spin fluctuations in an isotropic Haldane antiferromagnet vanishes on approaching q=0.

C-155 Comparison and complementarity of the $\omega(q)$ and $\sigma(\theta)$ methods of neutron scattering in spin wave measurements

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The spin wave (SW) stiffness D, that is a coefficient in the dispersion law $\epsilon = Dq^2$, and SW damping may be obtained in two methods, mentioned in the title. The quadratic dispersion law causes the spherical distribution of scattering intensity in $\omega - \theta$ space, where radius of the sphere is $k_0(1+\theta_0)\theta_0$ and θ_0 is a cut-off angle. We see a complementarity of both methods in the fact that the $\omega(q)$ method can cover only limited q-range (q ¿ 0.05 $Å^{-1}$), while the $\sigma(\theta)$ one (based on antisymmetric SANS of polarized neutrons) can include very small q at rather high luminosity. The different levels of modeling are requested for these two methods. The example of the application of both methods to the same sample will be shown.

C-157 Magnetic excitations in single crystal PrNiSn

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We have made a detailed study of the low energy magnetic excitations in single crystal PrNiSn using the triple-axis spectrometer V2 at HMI, and observed modes centred around energies of 0.5, 2.5 and 3.5 meV. Magnetic susceptibility measurements on PrNiSn show a strong anisotropy, but no sign of magnetic ordering above 2K. We attribute the modes to crystal field excitations: there is a significant dispersion of the 3.5 meV excitation. A crystal field level scheme has been deduced to explain our results.

C-158 Magnetic field effect on spin waves in $La_{1-x}Ca_xMnO_3$, x=0.1, 0.08, close to the transition towards the insulating ferromagnetic state.

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Spin waves have been measured under applied magnetic field (H=1-5 Teslas) in $La_{1-x}Ca_xMnO_3$, x=0.08 and 0.1, close to x=0.125. For x<0.125 and H=0, two distinct spin wave branches were observed, ω_1(q) with a large gap, reflecting the spin dynamics of the AF layered structure (AF stacking along (001)) and ω_2(q) with a small gap, reflecting the ferro (F) coupling induced by bidimensionnal F clusters *through* the AF ordering (bending at (00.5)) [1]. Applying a field along (100), yields a transfer of spin wave intensity from the large-gap ω_1(q) spin wave, to a gapless dispersed spin wave around the AF (001) zone center, in perfect continuity with ω_2(q). This effect is larger for x=0.1 than for x=0.08. Since the field is expected to increase the hole mobility, this finding could be related, in some aspects, to the F magnetic state observed at x=0.125 and H=0 (Ref. 1), where the large-gap spin wave branch disappears and a disordered orbital state is suggested from the decrease of the orthorhombicity. [1] G. Biotteau et al Cond.-matter/0101414

C-160 Quantitative Multiphase Analysis of Archaeological Bronzes by Neutron Diffraction

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The diagnostic techniques usually employed in archaeometry to characterize bronze artifacts in terms of alloy compositions, metallographic structures, and corrosion products are, to some extents, destructive. Furthermore, since the material analyses are usually performed on a few small samples removed from the archaeological artifact, the generalization of the characterization data to the whole artifact or to its elements is in many cases quite arbitrary. In the present work we investigated the possibility to analyze archaeological bronzes by time-of-flight neutron diffraction. This diagnostic approach can represent, other than a complement to conventional archaeometry, a powerful tool to investigate the large number of archaeological pieces where any sampling is impracticable. The present feasibility study was performed on artificial samples, simulating typical compositions and working processes of ancient bronzes, as well as on two original Etruscan pieces. Quantitative multiphase analysis by Rietveld refinement was successfully demonstrated in all cases, while other important archaeometric potentials were suggested by observed peak shapes.

C-161 Microstructural SANS - Studies on Hydrating Tricalcium Silicate (C3S)

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According to the typical composition of cement powder the cement clinker phases tricalcium silicate (C3S) is of high importance for the formation of the hydration products in cement paste. - This presentation exemplarily discusses results of SANS investigations to study the effect of different parameters on the microstructure of hydrating C3S. Here all samples were made of C3S with a varied water-solid ratio. In addition the samples were stored for a given time in various climatic conditions (CO_2 content of the ambient air). Simulating a very high degree of carbonation (3.00 vol-% in air) microstructural changes are most evident. It is shown that an increasing water-solid ratio causes increased carbonation effects in the micro-structure of C-S-H-phases.

C-162 Age Dependent Dynamics of Water in Hydrated Cement Paste

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We investigate diffusional dynamics of water molecules in hydrated tricalcium silicate, a major component in ordinary Portland cement, as functions of temperature, aging and additive. Spectra of incoherent quasi-elastic neutron scattering from hydrogen atoms were measured with a resolution of 28 μeV. The spectra were analyzed with an explicit dynamical model taking into account the existence of two types of water: ”immobile water”, and ”glassy water”. The model fits very well all normalized spectra in an absolute scale over a range of spectrum covering an energy transfer of ± 300 μeV. We deduced three important parameters: a Q-independent fraction of the immobile water p; a Q-independent stretch exponent b and the Q-dependent average relaxation time of the glassy water, as functions of temperature, aging and additive. From trends of the age dependence of the first parameter, we obtain a quantitative picture of the kinetics of the curing process. From the other two parameters, age dependence of the dynamics of structural relaxation in glassy water has been established for the first time. We found that the additive has a dramatic effect on slowing down the curing process of the cement.

C-163 In Situ Hydration of Portland Cement Monitored by Neutron Diffraction

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Ordinary Portland Cement (OPC) was mixed with Deuterium Oxide with a water/cement ratio of 0.6 to monitor the hydration in situ, while acquiring diffraction patterns every 2.5 minutes. Two different experiments were carried out under different heating conditions. In one case, the temperature was uniformly risen from room temperature to 130°C at a heating rate of 12°C/hr. In the second case, the heating was performed with intermediate plateaux at 40, 60 and 80°C. The disappearance and appearance of relevant anhydrous and hydrated phases was quantified by measuring the diffraction intensities. The information obtained by this in-situ technique has allowed improving the existing knowledge on the phenomena that take place when hydrating OPC at moderately high temperatures, which is of technological importance to the manufacture of steam-curing of concretes.

C-164 Characterization of Thermal-Spray Metallic NiCrAlY Deposits by Multiple Small-Angle Scattering

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The technique of multiple small-angle neutron scattering (MSANS), so far successfully applied to thermal-spray ceramics [1], has now been extended to thermal-spray metallic deposits. The samples under investigation are technologically relevant Ni based NiCrAlY coatings manufactured by different spraying techniques (atmospheric and water-stabilized plasma spraying and flame spraying). MSANS measurements were made in directions parallel and perpendicular to the surface plane. Based on empirical considerations and the analysis of SEM micrographs of coating cross sections, the complex microstructures were modelled allowing for three distinct void systems. Employing the most recent MSANS formalism, the experimental beam broadening as a function of incident wavelength was used to derive the model parameters under the constraints of MSANS anisotropy, total measured porosity, and total surface area. The surface area was obtained from SANS analysis in the Porod regime. Relationships to macroscopic coating properties such as wear behaviour [2] are discussed. [1] A.J. Allen, J. Ilavsky, G.G. Long, J.S. Wallace, C.C. Berndt, H. Herman, Acta Mater., in press (2001). [2] T. Keller, W. Wagner, J. Ilavsky, N.Margadant, S. Siegmann et. al, submitted to the Proc. ITSC 2001.

C-165 First Principles Calculations to Guide and Interpret Neutron Spectroscopy of Materials

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We will present several projects at the NIST Center for Neutron Research that exemplify the power of neutron scattering when combined with first-principles calculations. Systems that we will discuss include new 40 K superconductor MgB_2, solid cubane, protonic-conducting oxides, and the negative-thermal-expansion material ZrW_2O_8. The measured structural and dynamical properties and their temperature dependencies are compared with those obtained from first-principles calculations. In most cases, impressive agreement was obtained even for systems as diverse as van der Waals molecular solids and ionic oxides. Therefore, the first-principles computational method with its predictive power should be considered as an indispensable tool for the analysis of neutron scattering data.

C-166 Phason disorder in icosahedral AlPdMn quasicrystals

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Diffuse scattering from large single grains of icosahedral AlPdMn has been studied in situ. The anisotropy of the diffuse scattering is well described by phason disorder according to the elasticity theory of Jaric and Nelson. The variation of the diffuse scattering with temperature can be related to a phason softenting along 3-fold symmetry directions at lower temperatures, which is due to the closeness of one of the possible phason instabilities predicted by Widom. Temperature dependent absolute phason coupling constants are determined from the calibrated neutron diffuse intensities and new models of the icosahedral structure. Possible effects due to phason-phonon coupling are discussed.

C-167 Structure analysis of the disordered high-temperature modification I of $KLiSO_4$

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The two high-temperature modifications of $KLiSO_4$, phase II (708-949 K, orthorhombic $Pcmn$) and phase I (949-989 K, hexagonal $P6_3/mmc$), were studied by neutron and X-ray diffraction experiments on heated single crystals. The results obtained with both experimental techniques and the reliabilities concerning the description of the disordered oxygen atoms are compared. Both high-temperature modifications are characterized by extremely disordered SO_4 and LiO_4 tetrahedra and high ionic conductivity. Modification I shows the strongest decrease of Bragg intensities for higher diffraction angles and reqires the longest measuring times for sufficient statistics. Important diffuse scattering intensities were observed.

C-168 Temperature Evolution of Structure of KLTN Single Crystals

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Results of neutron scattering study of $K_{1-x}Li_xTa_{1-y}Nb_yO_3$ (KLTN) single crystals are reported. Earlier the giant relaxation peak of dielectric permittivity and formation of reentrant dipole-glass state were reported for these crystal. Temperature evolution of lattice parameter and the width of Bragg peaks was measured using HRFD (JINR). No indication of the transition to the tetragonal state, expected for such composition, was found. Observed behavior can be attributed to the formation of glassy phase or slightly distorted rhombohedral ferroelectric phase. Measurements of the temperature evolution of diffuse neutron scattering were performed; the results are under evaluation. Work was supported by the RFBR (grants 99-02-18074, 00-02-16875), NATO Linkage grant SA (PST. CLG. 977348) 5941 and Russian program "Neutron researches of Solids"

C-169 Structure and ionic conductivity in doped $LaGaO_3$

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$LaGaO_3$ doped with lower valence cations creating vacancies on the oxygen lattice is a promising material for technical applications due to its excellent oxygen-ionic conductivity, e.g. in fuel cells. E.g. $La_{0.9}Sr_{0.1}Ga_{0.8}Mg_{0.2}O_{2.85}$ shows a higher conductivity than the commonly used yttria stabilised zirconia and allows lower operating temperatures. In order to understand the conduction mechanism and its temperature dependence neutron powder data have been collected between 2 K and 1273 K on instrument E9/HMI-Berlin. Various anomalies including a phase transition from a monoclinic to a rhombohedral distorted perovskite structure were found which can be related to anomalies in the conductivity curve. Although these distortions are small and no splitting of the reflections is directly observable, the profile refinement technique allows a reliable determination of the monoclinic cell. Diffusion pathways and disorder are derived from an analysis of the atomic displacement parameters.

C-170 Reorientation of anions in ion conducting sodium phosphate, a Reverse Monte Carlo study of neutron diffraction data

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Many solids containing anion groups line SO_4^{2-} or PO_4^{2-} have high temperature phases where the anions have rotational disorders. Coupling between the rotating anions and cations (paddle effect) could give an increasing conductivity of cations in the solid. Neutron diffraction measurement on sodium phosphate in the high conducting phase T = 648 K were performed. A model of the structure were obtained with the Reverse Monte Carlo technique.

C-171 Structure and Li positions in novel Manganese Oxide cathode compounds

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The spinel $\mathrm{Li[Ni_{0.5}Mn_{1.5}]O_4}$ (space group Fd3m) is a well known high-voltage cathode material (4.7 V vs. $\mathrm{Li/Li^+}$) that can be used in advanced lithium ion batteries. A new series of Mg doped materials has been synthesized with the compositions $\mathrm{Li[Mg}_y\mathrm{Ni}_{0.5-y}\mathrm{Mn}_{1.5}\mathrm{]O_4}$ $(0 < y < 0.15)$. Mg was chosen to increase the electronic conductivity of the material. In order to assign the cation distribution ($\mathrm{Li^+}$, $\mathrm{Mg^{2+}}$, $\mathrm{Ni^{2+}}$ & $\mathrm{Mn^{4+}}$) neutron and X-ray diffraction as well as structure refinement have been performed. Li was found to reside on the 8a tetrahedral positions while the 8b,f and 16c positions were not occupied. The Mg, Ni and Mn show to be located on the expected 16d positions.

C-172 Anion and cation dynamics in ion conducting sulfates and phosphates

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Some cubic high-temperature phases of simple inorganic salts combine dynamic rotational disorder of their polyatomic anions with fast cation conductivity. The challenge here is to examine cation and anion dynamics, their interaction and the strongly disputed possible enhancement of cation conductivity by anion rotation ("paddle-wheel mechanism"). We report new results from quasielastic neutron scattering experiments on several ion conducting rotor phases, viz, $x, \mathrm{Na_2SO_4} \cdot (1-x), \mathrm{Na_3PO_4}$ $(x = 0.0, 0.1, 0.5)$, $\mathrm{Li_2SO_4}$, and $\mathrm{LiNaSO_4}$. In the phosphate system the linewidths due to anion reorientation and cation hopping differ by up to three orders of magnitude, allowing for a complete characterization of both types of motion in backscattering and time-of-flight measurements. The situation in $\mathrm{Li_2SO_4}$ and $\mathrm{LiNaSO_4}$ is completely different: here both types of motion have a similar time scale, and time-of-flight experiments reveal both diffusional and reorientational contributions to the quasielastic scattering.

C-173 Deep Inelastic Neutron Scattering on $\mathrm{LiMn_2O_4}$

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We measured with the TOSCA spectrometer (ISIS) the inelastic neutron spectrum of a $\mathrm{LiMn_2O_4}$ powder for energies between 5 and 500 meV, and at temperatures between 10 and 50 K. For all temperatures we observe a sharp inelastic peak at 13 meV with a weak repetition at 26 meV, while the remaining spectrum is featureless. Most likely these peaks arise from local excitations of the manganese spins in the sample.

C-174 Time-evolution of phonon spectra during the decomposition in ionic crystals

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Real-time inelastic neutron scattering has been used to characterise the mechanism of decomposition in silver-alkali halides. The chemical demixing process is associated with a splitting of acoustic phonon branches which is observed to take place within some 100 s. Interestingly, the Bragg reflections exhibit a completely different time-behaviour: The adaptation of the equilibrium lattice parameters occurs on a much longer time-scale which is strongly temperature-dependent. Hence, decomposition is governed by large coherency strains which persist over a long period of time. The relaxation of these strains leads to an additional shift of the phonon frequencies of the product phases.

C-175 Quasielastic neutron scattering study of silver selenium halides

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Both silver chalcogenides ($\mathrm{Ag_2S}$, $\mathrm{Ag_2Se}$, and $\mathrm{Ag_2Te}$) and silver halides (AgCl, AgBr, and AgI) are known to be fast-ion solids in which the silver atoms can diffuse quickly in a sublattice formed by the other atoms. The present work aims at clarifying whether mixtures of these materials (such as $\mathrm{Ag_3SeI}$) possess comparable properties and whether a systematic dependence on the cation-to-anion ratio can be observed. Some of these mixtures have been studied by quasielastic neutron scattering both in the solid and liquid phases. Preliminary results, obtained from Bayesian as well as maximum-likelihood fits, are presented.

C-176 Structure and Temperature Dependence of the Lattice Dynamics of the Superionic Conductors $\mathrm{CaF_2}$ and $\mathrm{LaF_3}$

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The fluoride crystals CaF_2 and LaF_3 are superionic conductors with a strong increase of fast ionic conductivity at 1430 K and 1150 K, respectively. We compare the structural and dynamical properties determined with the help of *ab initio* calculations with results from inelastic neutron scattering experiments. Phonon dispersion curves reflect the structure of a material. Moreover, in the case of superionic conductors additional information for a deeper insight into the mechanism of fast ionic conductivity is hoped to be provided. Powder (TOF) and single crystal (TAS) inelastic neutron scattering studies have been carried out to investigate the temperature dependence of the lattice dynamics of these systems.We observed an anomalous softening of one phonon mode in CaF_2 which is attributed to oscillations in the fluorine sublattice. In contrast, for LaF_3 we have detected a shift to higher frequencies for one mode assigned to fluorine vibrations with increasing temperature. The line widths of these modes increase enormously with temperature. alculated frequencies reasonably agree with experimental data. The temperature dependence will be calculated by means of *ab-initio* molecular dynamic simulations.

C-177 Characterization of the Intermediate-range Order in new Superionic Conducting Ag_2S-AgI-$AgPO_3$ Glasses by Neutron Diffraction

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Superionic conducting glasses are of considerable technological interest because of their usein batteries, sensors, and displays. We have investigated the new ternary systems AgI-Ag_2S-$AgPO_3$ with the ratio of AgI:Ag_2S is 1:1. The new system AgI-Ag_2S-$AgPO_3$, for AgI+Ag_2S fraction less than 82 mol%, yields glasses. We have used neutron diffraction technique to obtain the total scattering structure factor of this system at room temperature by using a HIT, spectrometer at High Energy Accelerator (KEK), Tsukuba, Japan. As for AgI-$AgPO_3$ glasses, the S(Q) shows an anomalously low Q in the range 0.6 to 0.9 $Å^{-1}$. This peak is not observed in the corresponding glass Ag_2S-$AgPO_3$ or the pure $AgPO_3$. The prepeak depends strongly on the dopant salts. Its intensity increases as the amount of (Ag_2S+AgI) increases and the peak position shifts to lower Q as x increases. The prepeak intensity decreases also proportionally to number densities of the glasses. This peak can be associated with an intermediate structure of particles lying inside a continuouos host with the interparticle distance between 8 and 10Å[1]. [1] J. Swenson, A. Matic, C. Gejke, and L. Borjesson, Phys. Rev. B 60 (1999)12203

C-178 SANS study of concentration effect in ferrofluids

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The effect of magnetic particle concentration on the structure of three- and four-component ferrofluids (the magnetite and oleic acid in benzene, the magnetite and two modifications of dodecylbenzenesulphonic acid in heavy water) was investigated by small-angle neutron scattering (SANS). A decrease in the width of surfactant shells covering magnetic particles with increase in the particle concentration was observed. In the case of the four-component ferrofluids a significant relative contrast between inner and outer surfactant shells was revealed, which can be explained by the fact that changes in the structure of only the outer shell (surfactant interlacing, as well as solvent penetration) take place.

C-179 Neutron Small Angle Scattering on Liquid Helium in the Temperature Range 1.5-4.2 K

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The small angle neutron scattering from liquid helium at saturated vapour pressure in the temperature range from 1.5 to 4.2 K was measured with the instrument D22 of the ILL Grenoble at a wave length of 4.6Åand 8Å. The zero angle cross section is monotonically decreasing with decreasing temperature and does not show any singularity at the lambda-point. On the other hand, we observe a change of the slope of the temperature dependence of the second momentum of the pair correlation function (correlation length) at the lambda-point that reflects the transition of liquid to the superfluid state. The comparison of the static structure factor with X-rays data ia also presented.

C-180 The structure and dynamic properties of liquid phosphorus oxychloride $POCl_3$ from neutron scattering experiments

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The structure and microdynamics of liquid phosphorus oxychloride $POCl_3$ are investigated by neutron diffraction and inelastic neutron scattering. The structure results are in agreement with that, obtained by X-ray diffraction and demonstrate the wide peculiarity, connected with intermolecular interactions. The analysis of inelastic scattering experiment is performed, basing on simplified approaches and phenomenological models. In the frame of this approach it was discovered the quasielastic peaks could be described by two-Lorentzian representation, corresponding to superposition of coherent and incoherent components of quasielastic scattering. The Q-dependence of half-widths at half maximum for quasielastic peaks reveals the seldiffusion in liquid $POCl_3$ proceeds like jump one. From analysis of inelastic neutron scattering results the generalized frequency distribution of chlorine atoms was extracted and its intermolecular region represented as superposition of vibration and libration molecular modes. In the limits of our experimental conditions the existence of collective mode in liquid $POCl_3$ was not observed.

C-181 Thermodynamic Functions of Liquid Potassium from Slow Neutron Frequency Spectrum

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The generalized frequency spectrum of liquid potassium at the temperature range 340 K - 550 K was obtained by means of inelastic neutron scattering [1]. First link to thermodynamics was performed by evaluation of the isochoric specific heat Cp [2]. Following the single harmonic oscillator formalism developed in [3] and integrating through the whole frequency region we calculated free energy A, internal energy E and entropy S. Satisfactory agreement with reference data [4] is achieved. An attempt to broad this technique to the potassium-oxygen system (1.8, 5.1 and 8.5% at of oxygen) is presented as well. [1] M.V. Zaezjev, M.N. Ivanovsky, A.G. Novikov, V.V. Savostin and A.L. Shimkevich, Russian J. Phys.Chem. (New York, Plenum) 68, p. 240 (1994). [2] M.V. Zaezjev, A.G. Novikov, V.V. Savostin, J. Non-Cryst. Solids 250-252, p.120 (1999) [3] D.A. Zichi and P.J. Rossky, J.Chem.Phys.84 (5), p.2823 (1986). [4] Handbook of Thermodynamic and Transport Properties of Alkali Metals, ed. R W Ohse (Blackwell, Oxford, 1985), p 753.

C-182 Phonon dispersion in austenitic stainless steels

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Ultrasonic studies of austenitic stainless steel allowed the determination of elastic constants and engineering elastic moduli. These investigations reveal the complicated interplay of alloying elements and interstitial nitrogen on the elastic properties, in disagreement with model calculations based on continuum mechanics. We report on phonon dispersion measurements of austenitic stainless steel Fe-18Cr-12Ni-2Mo and Fe-18Cr-16Ni-10Mn. Data are analysed by model calculations based on Born - von Karman theory, using least squares fit procedures to evaluate the interatomic force constants, elastic constants and engineering elastic moduli. Previous investigations show in general good agreement between model calculations and experimental data. Elastic constants of Fe-18Cr-12Ni-2Mo obtained by least squares fitting of the linear part of dispersion branches agree well with previous predictions, based on ultrasonic measurements of elastic moduli.

C-183 Disorder Type and Degree Effect on Vibrational Spectra of Complex Perovskites.

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Generalized density of the vibrational states G(E) of a number of complex perovskites has been studied as a function of temperature using KDSOG-M spectrometer (JINR, Dubna). The measurements were carried out at the range of 10 K - 290 K. Obvious correlation of the anomalous temperature dependences of G(E) and dielectric permeability of these compounds was observed. In the report we will discuss these features for

$PbMg_{1/3}Nb_{2/3}O_3$ (PMN), $PbSc_{1/2}Ta_{1/2}O_3$ (PST), $PbMg_{1/3}Ta_{2/3}O_3$ (PMT) and $BaMg_{1/3}Ta_{2/3}O_3$ (BMT) compounds. Disorder effect on Raman light spectra of these compounds will be considered.

C-184 Neutron and Raman scattering studies of $[K_{1-x}(NH_4)_x]_3H(SO_4)_2$ mixed crystals

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Neutron powder diffraction (NPD), inelastic incoherent neutron scattering (IINS) and Raman scattering (RS) of $[K_{1-x}(NH_4)_x]_3H(SO_4)_2$ are carried out for x=0.0, 0.1 and 0.7 at 300 and 10 K. RS spectra show noticeable changes in widths of nu1 and nu3 inner modes of SO4 ions and splitting of the modes, related with H-bond in energy region 480-560 cm^{-1}, with cooling the temperature for x=0.0 and 0.1. H-bond mode for sample with x=0.7 is not observed, nui, (i=1, 2, 3, 4) inner modes of SO4 are split at 300K and the splitting of these modes are increased at low temperature. The NPD spectra don't expose phase transition with cooling the temperature for x=0.0 and 0.1, but show change of diffraction spectra for x=0.7 for account of phase transition. The IINS spectra are in accordance with Raman spectra.

C-185 Inelastic neutron scattering and lattice dynamical studies of BaFCl

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The matlockite structured compounds (e.g. BaFCl) on dilute-doping with rare earth ions are of technological importance for its X-ray image storage properties. The knowledge of their thermodynamic properties would be useful in designing new and improved materials. We report the measurement of phonon density of states for BaFCl using the triple axis spectrometer at Trombay. A rigid ion lattice dynamical model is used for the interpretation of the experimental results. The model is then exploited for the calculation of high pressure and temperature thermodynamic properties of BaFCl.

C-186 Phonon dispersion relations in andalusite and sillimanite, Al_2SiO_5

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The minerals andalusite and sillimanite find extensive applications in geothermometry and geobarometry. Studies of the phonon spectra of minerals are important for a microscopic understanding of their thermodynamic properties. We report measurements of the phonon dispersion relations of andalusite and sillimanite along various high symmetry directions using the Dhruva reactor, India and the ORNL facility. The planning of the experiments and their analysis was based on a lattice dynamical shell model. The model has been successfully used to derive the high pressure-temperature thermodynamic properties like the equation of state, specific heat and thermal expansion.

C-187 Lattice dynamics in rhodochrosite, $MnCO_3$

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Phonon dispersion curves along the threefold axis [111] and the phonon density of states of the external modes in rhodochrosite, $MnCO_3$ have been measured by inelastic neutron scattering employing the triple axis spectrometer at Dhruva reactor, Trombay. Lattice dynamics computations based on a transferable potential model reveal the differences in the phonon properties of the isostructural minerals, calcite and rhodochrosite and their manifestations in various thermodynamic quantities. The calculated dispersion curves and phonon density of states are in good agreement with experiments. The obtained results provide a strong experimental basis to validate the potential model.

C-188 Fine structure of phonon dispersion curves in lead

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Lead is the first metal where the Kohn anomalies on phonon dispersion branches were identified but so far the full picture of the anomalies of electron-ion interaction in this metal is missing. Here we present the detailed measurements the phonon dispersion curves in principal symmetry directions of the crystal lattice of lead. The derived wave vector dependencies of the phonon group velocities exhibit a number of irregularities which cannot be all described in the approximation of the spherical Fermi surface. It is shown that the superconducting phase transition does not affect the shape and strength of the observed anomalies while the BCS parameters of lead would anticipate some measurable changes. In the high-resolution measurements of the low-frequency part of the TA(111) phonon branch we have found a pronounced non-symmetric line shape of the one-phonon resonances in the neutron scattering cross-section. This effect is not visible in lower-resolution runs. The phonon line shape remains largely unchanged when measured in different Brillouin zones. The asymmetry gradually diminishes at larger phonon wave vectors. There are no irregularities detected in the phonon line shape for the TA(110) branch. A charge-fluctuation model, derived earlier for transition metals, is attempted to describe the phonon spectrum of lead.

C-189 Anomalous Phonon Behaviour in V_3Si

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In earlier studies of phonons in V_3Si, a gradual softening of the TA hh0 mode was observed and attributed to the martensitic transition in this compound, which precedes the onset of superconductivity by a few degrees K. In this work, the temperature dependence of this mode was studied ingreater detail and it is shown that while the TA hh0 mode starts to soften at relatively high temperatures ($>$200K), an anomalous softening, which is rather localized in q, occurs just beloe T$_c$. The intensity of this peak correlates well with the order parameter as a function of temperature and applied field. Similarities between this and the borocarbide superconductors suggests the existence of a common mechanism for the superconducting transition.

C-190 Observation of the Gap-Modes in Interstitial Alloys

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In paper the experimental spectra of N and C impurity atoms vibrations in interstitial phases on the basis of V and Nb are presented. In spectra of inelastic scattering of neutrons well defined singularities in a gap between optic modes and spectrum of host atoms were observed (eps=45 meV and eps= 35 meV for phases on the basis of V and Nb respectively). There is no clear answer on a question about a nature of these oscillations. These modes may concern to quasi-molecular vibrations (we means the vibrations of host matrix atoms which are the nearest neighbors to impurity), or may be determined by vibrations of pairs of interstitial atoms, or to have another nature. Possible mechanisms of gap-modes formation in the metal-impurity interstitial alloys are discussed. The present research is supported by Russian Foundation of Basic Research, grant No. 01-03-96009.

C-191 γ formation and growth in the Nickelbase superalloy SC16.

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An in-situ study of the kinetics of the formation and growth of the γ-phase in the single crystal Ni-base superalloy SC16 was carried out by means of Neutron Diffraction. This alloy has got both industrial applications (turbine blades for power generation) and scientific interest because of its modelling properties (small number of components). On cooling from the solvus temperature (1250°C) the γ-precipitate phase reappears and the different stages formation, growth and concurrent coarsening could be followed by means of a superstructure reflection. Results show that at every temperature T$<$ 1200°C an increasing volume fraction of γ can be found with decreasing temperature, till a saturation around 800°C occurs. An Avrami-like growth law is applicable at every temperature and the isothermal reaction rates have got a maximum around 1050°C, where the competing processes find equilibrium. This explains the pseudo-Arrhenius behaviour which does not agree with a pure coarsening Lifschitz-Slyozov-Wagner time law.

C-192 Neutron Diffraction Study of $(Mo,W)Si_2$ Prepared by Self-Propagating High-Temperature Synthesis

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Neutron diffraction study of $(Mo,W)Si_2$ powders prepared by self-propagating high temperature synthesis was carried out to investigate the effect of tungsten addition on the phase stability and formation mechanism. The powder neutron diffraction patterns from 5 to 155 were measured at room temperature using the 32-detector high resolution powder diffractometer (HRPD) at KAERI. 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). The lattice parameter of the Si_2Mo phase was obtained from the Rietveld refinement as followings : a=0.3204 nm, c=0.7844 nm. As tungsten contents increases, a and c values of the lattice parameters changes into 0.3207 nm and 0.7839 nm. The microstructural and chemical analysis of the final products by electron microscopy and neutron diffractometry indicated that the formation of $(Mo,W)Si_2$ occurs via dissolution of Mo and W into Si melt followed by silicide precipitation.

C-193 Neutron Diffraction Analysis of Titanium Carbide Fibers Formed by Self-propagating High Temperature Synthesis Reaction

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Neutron diffraction analysis was carried out to study the relationship between the non-stoichiometric number of titanium carbide and its microstructural development during self-propagating high temperature synthesis reaction. The final morphology of the titanium carbide was controlled by the processing parameters such as mixing media, pressure, initial powders size and compositions to have different shapes of powders, fibers and whiskers. Titanium carbide fibers with 80 μm in diameter and whiskers with less than 0.3 μm in diameter and fine powers were achieved through the SHS reaction. Neutron diffraction analysis showed that the non-stoichiometric numbers of the titanium carbide fiber, whiskers and powders were 0.68, 0.89 and 0.91, respectively. The microstructural observation and measurement the reaction temperature revealed that the formation mechanism is related to a liquid-solid reaction including the diffusion process of carbon atom into liquid titanium.

C-194 SANS experiments on Nb(C,N) and MnS precipitates in HSLA steel

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The size distribution of precipitates in high-strength low-alloy (HSLA) steels has been studied using small-angle neutron scattering (SANS) at high temperatures. Three samples with different niobium concentrations (0.00, 0.05, and 0.10 wt.%) were slowly heated from a temperature of 910 to 1200°C. With increasing temperatures, the scattered intensity strongly decreases as the precipitates gradually dissolve or coarsen. A comparison between the overall particle size distributions of the 3 different materials indicate two different contributions: Nb(C,N) precipitates with a radius of about 5 nm and MnS precipitates with a radius around 20 nm.

C-195 Polarized SANS study of microstructural evolution in a martensitic steel for fusion reactor

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Owing to their good resistance to radiation effects, ferritic/martensitic steel are currently considered as attractive candidates for the construction of future fusion reactors. This contribution presents the results of a polarized SANS study carried out on modified martensitic steel DIN 1.4914 (MANET) originally developed for the Next European Torus (NET) project. The measurements were carried out by the PAPOL instrument al Laboratoire Léon Brillouin (CEA-CNRS, Saclay) with the aim of investigations Cr redistribution phenomena in the martensitic matrix following different thermal treatments. In fact, as it is known by previous microstructural investigations and mechanical tests such phenomena play a crucial role in ductile-to-brittle transition changes under irradiation. The nuclear-magnetic interference term and the size distributions obtained considering separately the nuclear and magnetic SANS components show that the Cr-rich aggregates present immediately after quenching dissolve even for short tempering treatments with consequent changes in precipitate composition. These results are discussed with reference to material stability in service conditions.

C-196 In-situ SANS investigation of precipitate microstructure at elevated temperatures in Re-rich Ni-base superalloy

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Investigation of the gamma prime (gp) precipitate microstructure in Ni-base superalloys at high temperatures is an important task not only from the scientific but also from the technological point of view. E.g., a precise knowledge of the gp-solution window (homogenizing temperature in single phase gamma region) is needed to eliminate harmful segregation in cast alloys. SANS is a reliable method for in-situ test at extreme conditions and is thus suited for the observation of gp-precipitate dissolution. SANS was employed for observation of the gp dissolution in Re-rich superalloys. Temperature dependence of the volume fraction and the size distribution of precipitates, as well as other parameters were determined from the measured anisotropic scattering curves.

C-197 SANS examination of precipitate microstructure in Ni-base superalloys

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Ni-base superalloys are suited for high-temperature applications. Their excellent mechanical properties originate in two-phase microstructure: ordered gamma prime (gp) precipitates embedded in gamma-phase matrix. SANS had been used for investigation of precipitate morphology in single-crystal as well as polycrystalline alloys for many years in HMI. An overview of applications of the method to the research of these materials is presented. Along with the size and distance of precipitates, their shape can be examined for single-crystal specimens. In special cases, SANS is able to detect low volume fraction of oriented phases other than gp. Evolution of microstructure at high temperatures can be investigated in situ. Selected examples (creep exposed specimens, dissolution of gp at high temperatures, long-time thermally exposed alloy) are presented to demonstrate the possible output of SANS studies.

C-198 Structure Investigations on Russian Reactor Pressure Vessel Steels by Small Angle Neutron Scattering

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The effect of radiation embrittlement has high safety significance for Russian VVER reactor pressure vessel steels. Heats of base and weld metal of the as-received state, irradiated state (up to fluence of 10^{20} n/cm^2) and post-irradiation annealed state were investigated by SANS to get insights about the microstructural features caused by neutron irradiation. The SANS intensities increase in the momentum transfer range between 0.8 and 3 nm^{-1} for all material compositions in the irradiated states. The size distribution function of the irradiation-induced defects has a pronounced maximum at a radius of 1 nm. Their volume content varies between 0.1 and 0.7 vol.% depending on material composition and increases with the neutron fluence. The comparison of nuclear and magnetic scattering indicates that the defects differ in their composition. Thermal annealing reduces volume fraction of irradiation defects.

C-199 Microstructural Changes in Long-time Thermally Exposed Ni-base Superalloy studied by SANS

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The presented Small-Angle Neutron Scattering (SANS) experiment was a crucial part of a broader investigation of a long-time structural stability of polycrystalline nickel base superalloy and its effect on the subsequent creep characteristics. The results of testing have shown that long-time isothermal exposure at temperature of 430°C up to 25 000 hours changed the alloy creep deformation behaviour and creep life decreased with prolonged time of thermal exposure. While structure analyses (TEM) showed no evidence on morphological and/or dimensional gamma prime change the SANS technique has reveal significant changes of the gamma prime morphology already after the shortes thermal exposition. The SANS experiment contributed to the clarification of the above discrepancy and collected data covered the scattering vector magnitude range suitable for determination of the precipitate sizes. The resulting parameters on size, distribution, mean distance and mean size among the precipitates made the evidence that both the size and the distance increase in the bulk of the alloy with the increasing thermal exposure.

C-200 SANS investigation on precipitation hardening of two-phase gamma-TiAl alloys

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Two-phase titanium aluminide alloys are being considered as light weight materials to replace nickel-based superalloys in some high temperature aero-engine applications. However, at an intended service temperature of 700°C the strength and creep resistance of the titanium aluminides are inferior to those shown by superalloys. Therefore, precipitation hardening treatments using carbon additions were tested for an improvement of the strength. As revealed by transmission electron microscopy (TEM), ageing of a Ti-48.5 at% Al-0.4 at% C alloy for 24 h at 750°C leads to the formation of perovskite type precipitates, significantly improving the high temperature strength. The size distribution and volume fraction of the perovskite precipitates were measured using small-angle neutron scattering (SANS). The results after extended ageing periods will be discussed in connection with the corresponding yield stresses and creep behaviour of the material.

C-201 The Precipitation of NbC on Dislocations in Austenite

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The precipitation of NbC in austenite is a key step in the production of microalloyed steels as well as several important grades of stainless steel. In the present investigation, SANS was utilized to study the precipitation kinetics in a model austenitic alloy with a high SFE (69.2%Ni, 29.7%Fe, 0.851%Nb and 0.114%C). The kinetics were determined at 973 K for a non-deformed sample as well as samples deformed by 20 and 30%. The effect of deformation is to increase the rate of precipitation and to reduce the precipitate particle size. We were able to detect precipitate volume fractions as small as 0.1%. In addition, we were able to extract information on the evolution of particle shape and distribution. This information is particularly valuable because the traditional techniques of extraction replicas and HRTEM are unable to reliably measure particles that are smaller than 3 nm in diameter.

C-202 Effect of Nitrogen on SANS in Fe-Cr-Mn-Ni-N Austenite

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Our previous study of SANS in the Fe-18%Cr-10%Mn-16%Ni-0.5%N austenite has shown that there are inhomogeneities of colloid size in the steel after solution treatment which are characterized by fractal like structure [1]. We assumed that fractal properties are associated with the effect of Ni and N on atomic distribution and magnetic structure. To check this assumption the SANS (q = 0.006 - 0.25) was measured in the steels with different nitrogen content (0.06, 0.17, 0.5%N). It was shown that differential cross-section of neutron scattering in austenite is changed with the nitrogen concentration. The SANS curves were treated within the Porod approximation and the data were compared with the previous observations [1]. [1] V.M. Nadutov, L.A. Bulavin, V.M. Garamus, Mater. Sc. Eng. A264 (1999) 286-290.

C-203 Orbital, Charge and Spin Ordering in $\mathrm{Bi}_{1-x}\mathrm{Ca}_x\mathrm{MnO}_3$ (x>0.5): Implications for Phase Segregation

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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 $\mathrm{Bi}_{1-x}\mathrm{Ca}_x\mathrm{MnO}_3$ ($0.5 \leq x < 1$) 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.

C-204 Porosity and Grain Structure of Nanophase YSZ Films Grown on Polycrystalline $\mathrm{AL}_2\mathrm{O}_3$ Substrates

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Thin films of yttria-stabilized zirconia (YSZ) grown on alumina ($\mathrm{AL}_2\mathrm{O}_3$) substrates were characterised with regard to structure, grain morphology and porosity. The present study shows that the deposition of YSZ films onto polycrystalline $\mathrm{Al}_2\mathrm{O}_3$ substrates by MOCVD under the given deposition conditions leads to nanostructured film morphologies with grain sizes in the range 10 to 14 nm when the substrate temperature is kept between 450 and 550°C. Small Angle Neutron scattering (SANS) was applied to analyse the void structure in the nanometer range, revealing that the films have a pronounced, very fine dispersed porosity. For substrate temperatures ranging from 425 to 500°C the average void diameters are found between 0.7 and 1 nm. For higher substrate temperatures, the size increases, reaching up to 9 nm in average for 650°C substrate temperature.

C-205 Competitive Adsorption of Binary Mixtures of Alkyl Species on Graphite

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Recently we have developed a combination of neutron scattering and sensitive calorimetry techniques in to investigate the structure, composition and dynamics of monolayers adsorbed from the liquid or solution to solid surfaces. These adsorbed layers are a central feature of many industrial and academic problems, however, due to the ?buried? nature of these interfaces very little detailed information is available. Here we present calorimetry, incoherent elastic neutron scattering and neutron diffraction results on the adsorption of binary mixtures of linear alkanes, and other alkyl species, adsorbed onto the surface of graphite, from the liquid hydrocarbons and their binary mixtures. These techniques allow us to determine the phase diagram of the adsorbed layer, identify the coexistence of more than one crystalline material in a single solid layer and to determine absolute composition of such mixed monolayers. In particular neutron diffraction results are presented that provide a structural basis for the apparent "odd"-"even" variation in monolayer melting points of the simple alkanes and quantitative rules for the identification of mixing or eutectic behaviour of monolayers adsorbed from their binary mixtures.

C-206 Bending stresses in plasma sprayed coatings measured by neutron diffraction

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Results of stress measurements in plasma sprayed coatings obtained by x-ray diffraction measurements are often ambiguous and difficult to interpret. The neutron diffraction method was used to determine the residual and applied stresses during a four-point bending and compared with results obtained previously by X-ray diffraction. The volume- and surface-effective Young's modulus was calculated from applied force and lattice deformation, respectively. The obtained results are discussed from the point of view of the behavior of cracks during tensile and compressive loading.

C-207 Investigation of the Formation of the Bi-2223 Phase in Multifilamentary $(\mathrm{Bi;Pb})_2\mathrm{Sr}_2\mathrm{Ca}_2\mathrm{Cu}_3\mathrm{O}_x$/Ag Superconducting Tapes by in situ High Temperature Neutron Diffraction

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Results of in-situ high temperature neutron diffraction experiments for the investigation of multifilamentary (Bi,Pb)$_2$Sr$_2$Ca$_2$Cu$_3$O$_x$ (Bi-2223)/Ag superconducting tapes are reported. The aim is to characterise the formation of the Bi-2223 phase from a multi phase precursor with the changes in the main and secondary phases assemblage under real reaction conditions in an oxygen containing atmosphere. Furthermore, the mechanism of the evolution of a fibre texture of the superconducting phases Bi-2212 and Bi-2223 are discussed. The results of the in-situ diffraction experiments will be related to microstructural characterisations of quenched specimens and results of thermal analyses. Finally, a reaction model of the formation of the Bi-2223 phase will be discussed being a heterogeneous nucleation and growth beginning in a transient liquid phase.

C-208 Dynamic features of hydration water interacting with hydrophobic molecules

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We have studied the hydration properties of trimethylamine-N-oxide (TMAO) and t-butyl alcohol (TBA) performing a QENS investigation on H_2O/TMAO and H_2O/TBA mixtures at different co-solvent molar fractions (x, 0-0.04), and at T=20°C. We analyse the QENS spectra in terms of a random jump model. On increasing x, the diffusion coefficient, D, and the residence time, τ, change in a way similar to pure water on decreasing T: water dynamics slows down. A marked difference is observed in the shape of the D- and τ- vs. x curves for TMAO and TBA. In the former case D and τ vary almost linearly, while in the latter they show a change in slope at about 2.5mol%, where previous studies evidence the onset of a self-aggregation process among TBA molecules.

C-209 Temperature Dependence of the Chemical Structure of $K_2Na[Ag(CN)_2]_3$

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As a basis to understand essential variations of optical properties, the layer compound $K_2Na[Ag(CN)_2]_3$ [1] was investigated by means of high-resolution powder neutron diffraction on HRPT at SINQ in the temperature range from 9 K to 300 K. Sample oscillation during the measurements reduced preferred orientation problems essentially. As a function of temperature the crystal structure corresponding to space group C 2/m is found by means of profile analysis and rigid-body constraints to change continuously with small reorientations (mainly the angle $|\ \theta_c\ |$: 26°, 28° at 9 K, 300 K) of two approximately linear N-C-Ag-C-N groups, resulting in an anomalous increase of the c-lattice parameter with decreasing temperature. [1] C. L. Larochelle et al., Solid State Commun.**114**, 155 (2000)

C-210 Order-Disorder Transition in Pyridinium Iodide: QENS Study

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Reorientational motion of pyridinium cation in pyridinium iodide across the phase transition (T_c=247K) temperature has been studied using high-resolution LAM80-ET spectrometer at KEK, Japan. A clear evidence of the order-disorder transition with respect to the pyridinium ion reorientation is observed. Above T_c, pyridinium ions are found to undergo a 6-fold jump rotation around the axis perpendicular to its plane. Below T_c, pyridinium ions are found to be frozen. However, a weak quasielastic broadening was observed in the high Q-range indicating presence of some residual disorder. Reorientational time and activation energy of rotation are also obtained in the high temperature phase.

C-211 Neutron Powder Diffraction Study of the Disordered Structure for $Sr_{18.6}Ni_{2.4}(PO_4)_{14}$

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The crystal structure of $Sr_{18.6}Ni_{2.4}(PO_4)_{14}$ was analyzed by the Rietveld method with RIETAN-2001T using TOF neutron powder diffraction data taken on Vega at 300 K and on Sirius at 10 K. This phosphate is structurally related to β-$Ca_3(PO_4)_2$, crystallizing in space group R-3m with lattice parameters of a = 10.6092(2) Å and c = 19.6674(3) Å at room temperature. In β-$Ca_3(PO_4)_2$, the M6 site is vacant whereas the M4 site is 50% occupied by Ca^{2+} ions. On the other hand, atomic positions corresponding to the M4 and M6 sites in β-$Ca_3(PO_4)_2$ are equivalent and occupied by $0.1Ni^{2+} + 0.15Sr^{2+}$ in $Sr_{18.6}Ni_{2.4}(PO_4)_{14}$. Disordering of O atoms bonded to P1 and Sr^{2+} ions at the M3 site was observed in $Sr_{18.6}Ni_{2.4}(PO_4)_{14}$ at both temperatures. The reason for such disorder is considered on basis of structural features of this compound.

C-212 Short range structure of molten MCl_2(M=Sr, Ba)-ACl(A=Na, K) analyzed by T-O-F pulsed neutron diffraction

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The short range structure of molten $xMCl_2$(M=Sr, Ba)-(1-x)ACl(A=Na, K) systems with x=0.125, 0.250, and 0.375 has been investigated by time-of-flight (TOF) pulsed neutron diffraction using the High Intensity Total scattering spectrometer (HIT-U) in High Energy Accelerator Research Organization (KEK) in Japan. In order to refine structural parameters, such as the correlation distances, the coordination numbers, and the temperature factors of M-M, M-Cl, Cl-Cl, and A-Cl ionic pairs, the non-linear least squares fitting was applied to the correlation method [1]. [1] Y. Iwadate et al, J. Chem. Phys., 99 (1983) 6890.

C-213 Study of the Macroporosity of Vycor Porous Glass by Combining Scattering and Permeability Techniques

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Vycor 7930 porous glass was studied by adsorption in conjunction with small angle scattering and by relative permeability. Analysis of the spectra showed that at late stages of the adsorption process the Kelvin radius is related to the mean curvature of a more complicated shape than a simple geometrical one. By applying the effective medium approximation model on relative permeability data, a pore connectivity value of $\sim$3 was deduced. At a pore junction of this type, the formation of void pockets prescribed by an adsorbed film having opposite radii of curvature is possible. When this is the case, a delay on the condensation process will occur and if not taken into account may erroneously be interpreted as macropores.

C-214 Phase transition II-III study in $(NH_4)_3H(SO_4)_2$ by neutron scattering

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Crystal structure studies of phases II and III of $(NH_4)_3H(SO_4)_2$ (TAHS) are carried out for the determination of NH4 ions orientational motion. The inelastic incoherent neutron scattering spectra of TAHS measured at 290 K (phase II) and 152 K (phase III) show the contribution of quasielastic incoherent neutron scattering which can be explained by orientational disorder of NH_4 ions in these phases. The determination of NH_4 ion disorder type is established by single crystal diffraction carried out at 290 and 160 K. Diffraction data sets at these temperatures are used for difference fourier synthesis analysis and it is shown that NH_4(I) and NH_4(II) of TAHS in phase II accomplish reorientations about crystal and molecular axes but NH_4 ions in phase III do it only about molecular axes.

C-215 Neutron diffraction studies of some simple molecular systems: Si_2Cl_6, CBr_3D and CD_3I

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Neutron diffraction experiments on liquid silicon-hexachloride, deuterated bromoform and iodo-methane have been performed at the Budapest Research reactor, using the PSD medium resolution powder diffractometer. Following subtraction of the background and container scattering and correction for the detector efficiency, the MCGR programme was used for obtaining the total structure factor which was then modelled using the Reverse Monte Carlo technique. It was found that in each case, the molecular geometry determines much of the intermolecular correlations in these liquid systems.

C-217 Binary and ternary Zintl phases with NaTl-type structure

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LiAl- and LiIn-alloys belong to the 7 binary Zintl phases, which crystallize in the NaTl-structure type (B32). Up to 50% of Al or In can be replaced by Ag without dramatic changes in the crystal structure. This class of compounds is characterized by a unique hybrid bonding with covalent, metallic, and ionic contributions. Recently, LiAl is studied as a potential anode material in intercalation lithium batteries. We report on our investigations of compounds within the series LiAl-Li(Al,Ag) and LiIn-Li(In,Ag), focussed on structural aspects like defects in the Li sublattice and phase transitions. For example, LiIn transforms translationengleich from the cubic phase into a tetragonal phase with space group I41/amd at about 170 K. The cubic phase can be stabilizied by partially replacing In with Ag in Li(In,Ag).

C-218 Density effects on the intermolecular structure factor of chlorine and the interaction potential

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The density behavior of the intermolecular structure factor of dilute chlorine at 405 K has been investigated by means of neutron diffraction over an extended momentum transfer range, down to approximately 1.5 nm^{-1}. The zero-density contribution to the structure factor has thus been experimentally derived. A comparison with existing experimental and theoretical results reported in the literature is presented and discussed.

C-219 Galloalunite - a neutron diffraction study

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Some basic gallium sulphates [1] adopt the structure of alunite $KAl_3(OH)_6(SO_4)_2$ [2], with Ga replacing Al. This substition should induce changes in the structure of the octahedral MO_6 units and of the hydrogen bond system. A neutron diffraction study of galloalunite-d_6 $KGa_3(OD)_6(SO_4)_2$ should answer part of these questions. Rietveld analysis [3] of neutron powder data was done in $R\overline{3}m$ ($Z = 3$; $a = 712.8(1), c = 1719.5(1)$ pm) with the starting parameters from alunite-d_6 [2]. The centrosymmetric GaO_6 octahedra with two independent Ga-O distances are more elongated than in alunite-d_6, tilting of the octahedra towards the *c*-axis is similar. For the OD groups bridging two Ga atoms longer O-D bonds and shorter, *i e* stronger hydrogen bonds to the terinal O1 atoms of the SO_4 groups than in alunite-d_6 [2] are found, consistent with lower frequencies ν(OH/D) in IR and Raman spectra of galloalunite than in alunite. [1] J. E. Dutrizac, T. T. Chen, *Can. Metall. Q.*, **2000**, *39*, 1, and references therein. [2] H. Schukow, D. K. Breitinger, T. Zeiske, F. Kubanek, J. Mohr, R. G. Schwab, *Z. Anorg. Allg. Chem.*, **1999**, *625*, 1047, and references therein. [3] B. Hunter, Rietica 1.67a, a Rietveld program package, **2000**.

C-220 Jahn-Teller oxide spinels investigated by neutron powder diffraction

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Due to the Jahn-Teller effect the structure of some oxide spinels deviates from the ideal cubic spinel structure. Depending on the species of the Jahn-Teller ion at room temperature a tetragonal structure with the axis ratio c/a<1 (for CuRh/Cr_2O_4) and c/a>1 (for NiRh/Cr_2O_4) results, respectively. The first part of the work is focused on the deep temperature behaviour of $CuCr_2O_4$ investigated by neutron powder diffraction. The studies showed that the Jahn-Teller effect gets stronger with decreasing temperature. Further the results of current investigation of mixed compounds Cu_xNi_{1-x}Cr2O4 and Cu_xNi_{1-x}Rh2O4, where the presence of two different Jahn-Teller ions cause a rhombohedral crystal structure distortion, will be presented.

C-221 The structure of the orientationally ordered phase III of solid methane

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For many years there were only unsuccessful efforts of solving phase III of solid methane. Now, on the basis of powder diffraction data from the instrument HRPD at ISIS, a structure within the orthorhombic spacegroup Cmca (Z = 16) was determined. The departure from the teragonal cell is only 0.06%. While the carbon atoms in the centres of the CD_4 tetrahedra are located on a slightly distorted fcc lattice, all molecules are orinetationally ordered with two different site symmetries (m and 2). The sublattice structure is in agreement both with former and recent measurements of rotational tunneling.

C-222 Template-Induced Crystal Growth

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Using complementary contrasts available from x-ray and neutron reflectometry we have studied surfactant template induced growth of highly crystalline silicate films at the air/water interface. This process closely resembles the ”mineralisation” in biology which leads to the great diversity of inorganic structures based on silica or calcium carbonate. The composite structures produced in our system mimic biology. In all cases a molecular or self-assembled ”template” species has been identified as the promoter of the crystallisation of the new structure. The work described here shows how premonitory phases develop at the interface which, depending upon temperature and solution composition, may transform into new templating phases to give solid films. Data are presented both from neutron reflectivity, x-ray laboratory reflectivity and synchrotron x-ray grazing incidence diffraction where the crystallinity of the growing films is explored and an insight into the mechanism of the film growth obtained from the diffuse scattering around developing Bragg spots.

C-223 Inelastic neutron scattering (INS) studies on chloro and bromo derivatives of phenol

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Pentachlorophenol, pentabromophenol, 2,4,6-trichlorophenol, 2,4,6-tribromophenol and their OD deuterated analogues were studied by using the INS technique, IR and Raman spectra as well as by theoretical calculations. A particular attention was paid to the low frequency vibrations (below 1200 cm^{-1}). From the point of view of INS technique of particular interest seemed to be the out-of-plane C-H and O-H deformation vibrations and these in which the proton cooridinates are involved. The simulations of INS spectra performed by means of the DFT method on the BLYP/6-31G* level reproduce very well the experimental spectra if the frequency scaling factor greater than unity is applied. In the present paper there are considered the problems such like the appearance in INS spectra of overtones and summation modes and the contribution to the INS spectra of vibrations of Cl and Br atoms. The comparision of the results of INS studies with IR and Raman spectra show the advantages of this technique in complementary studies on dynamics of complex molecules such as halogenophenols.

C-224 Quasielastic incoherent neutron scattering study of NH_3 dynamics in $Mg(ND_3)_2Cl_2$

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Incoherent quasielastic neutron scattering (IQNS) is a very powerful tool to study the dynamics of molecular groups, especially such as NH_3. We investigated the behaviour of the NH_3 groups in $Mg(NH_3)_2Cl_2$ by IQNS using the SINQ-spectrometer FOCUS. Scans were performed in the temperature range from 35 K (in order to determine the instrumental resolution) up to 300 K. We observe an Arrhenius type behavior of the FWHM of the incoherent quasielastic broadening in $Mg(NH_3)_2Cl_2$ over a wide temperature range. The activation energy E_a was found to be $E_a = 44.55$ meV for the NH_3 reorientations in $Mg(NH_3)_2Cl_2$.Previous neutron powder diffraction experiments on $Mg(ND_3)_2Cl_2$ revealed uniaxial orientational order-disorder behavior of the ND_3 groups as a function of temperature. At ambient temperatures the ND_3 groups are disordered with respect to a rotation about the bond Mg-N. The D atom density is well described by a fourfold split position, each D ”site” connecting an N with a Cl atom. The orthorhombic crystal structure (Cmmm, $a = 8.1828(6)$ Å, $b = 8.2007(6)$ Å, $c = 3.7543(2)$ Å) comprises of chains of octahedra $[Mg(NH_3)_2Cl_4/2]$ where the c axis corresponds to the direction of the chains.

C-225 auntie-CLIMAX

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Modern ab-initio programs calculate chemical structures remarkably well and spectra with fair accuracy. A new data treatment program using ab-initio output and based on established approximations has been written, a-CLIMAX. The INS spectrum for TOSCA-like instruments is calculated within the harmonic approximation. Anisotropic Debye-Waller effects are available to the 4-quantum level, with 10 orders of phonon wings. The program will be fully outlined. We have used a-CLIMAX to generate INS spectra from GAUSSIAN98 and DMOL3 output. For benzene the data could be adjusted to yield reasonable approximations of the INS spectra. Their failure to agree without adjustment was thought to stem from the different molecular environments; solid phase for the INS and isolated molecules in the calculations. This hypothesis is re-examined.

C-226 INS Study of Vibrational Spectra of NH_4I At Very High Pressures

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Vibrational spectra of NH_4I have been studied by means of incoherent inelastic neutron scattering at pressures up to 8 GPa using high pressure cell of ”Toroid” type with WC anvils. Libration (L) and transverse optical (TO) modes frequencies as functions of pressure were obtained. Both frequencies increase with the pressure increase. Surprisingly, the difference between L and TO mode frequencies decreases in the pressure range up to 5 GPa and starts to increase at $P>5$ GPa. Such a behavior suggests the hybridization of L and TO modes at high pressure. This effect may lead to the phase transition in NH_4I at high pressure. The work was supported by RFBR, grant 00-02-17199.

C-227 Structural phase transition and methyl dynamics in solid mesitylene

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Combined neutron powder diffraction (NPD) and inelastic incoherent neutron scattering (IINS) investigations of mesitylene-D9, (1,3,5-$(CD_3)_3C_6H_3$), and mesitylene-D3, (2,4,6- $D_3C_6(CH_3)_3$), were performed on the NERA spectrometer at the IBR-2 pulsed reactor of JINR in Dubna. Structural phase transitions were detected between (90 and 100) K for mesitylene-D3 and (100 and 110) K for mesitylene-D9. Stochastic reorientations of methyl groups that cause quasielastic scattering (QNS) even in the low temperature phase change significantly at phase transition. Two strong modes observed at 155 and 188 cm^{-1} for mesitylene-D3 at 20 K whose intensity change significantly with increasing temperature and that disappear completely above the phase transition temperature should be assigned as librational modes of methyl groups in the low temperature phase. Thus, the assignment of low frequency internal modes observed at low temperature in solid mesitylene based on quantum chemistry calculations of free molecule vibrations [1] must be revised. [1] L.Cser, K.Holderna-Natkaniec, I.Natkaniec, A.Pawlukojc, Physica B 276-78 (2000) 296-297.

C-228 Tunnelling transitions and librational modes of ammonium in $Rb_{1-x}(NH_4)_xI$ mixed salts

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IINS studies of $Rb_{1-x}(NH_4)_xI$ were performed on the time of flight spectrometers IN6 at HFR-ILL in Grenoble and NERA at the IBR-2 pulsed reactor in Dubna over a wide range of concentrations (x = 0.01, 0.02, 0.06, 0.16, 0.29, 0.40 and 0.66). At 5K, the tunnelling transitions at 0.56, 1.21 and 1.75 meV are well observed for small ammonium concentrations (x = 0.01 - 0.06). Above 20K, the tunnelling transitions become overdamped with thermally activated jumps of NH4 ions over the rotational barrier. The IINS spectra measured at 20K on the inverted geometry NERA spectrometer and at 150K on IN6 in the energy gain mode allow us to obtain the generalised phonon density of states. The ammonium dynamics in the disorder phase is characterised by excitation bands at 10, 20 and 29 meV. A narrow band at 10 meV, which may be interpreted as librations around the axis of the induced dipole moment of the NH4 ion, decreases in intensity and broadens with increasing ammonium concentration. The smoothing of this band in the density of states correlates with disappearance of tunnelling transitions and formation of orientational glass in $Rb_{1-x}(NH_4)_xI$ mixed salts.

C-229 Methyl rotational excitations and lattice dynamics of o-, m- and p-xylene using transferable pair potentials

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On the basis of the recently determined low temperature crystal structures of o-, m- and p-xylene [1-3] lattice dynamics calculations have been performed using transferable pair potential (TPP) parameter sets within the model of semirigid molecules. In combination with the lattice dynamics rotational potentials of the methyl groups have been calculated for various parametrizations of the TPP and compared with potentials derived from experiment [4] (tunnelling and librational transitions). The results demonstrate that none of the TPP can describe the measured density of states and the rotational modes exactly. The best results obtained use a modified atom-atom potential set of type IVa given by Williams. It was possible to get a consistent picture even for all isomers simultaneously. [1] R. M. Ibberson, W. I. F. David, S. Parsons M. Prager, K. Shankland, J. Mol. Struct. 524, 121-128 (2000) [2] M. Prager, W. I. F. David, M. Ibberson, J. Chem. Phys. 95 (4)(1991) [3] R. M. Ibberson, C. Morrison, M. Prager, Chem. Commun. 2000, 539-540 [4] M. Prager, R. Hempelmann, H. Langen, W. Müller-Warmuth, J. Phys.: Condens. Matter 2, 8625 (1990)

C-230 Neutron spectroscopy and model calculation of librational modes of ammonium in monoclinic phase of NH_4SCN

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The temperature dependence of the inelastic incoherent neutron scattering (IINS) and quasielastic incoherent neutron scattering (QINS) are carried out on NERA-PR spectrometer and by backscattering on this spectrometer respectively from NH_4SCN for ammonium dynamics studies. The identification of the translational and librational modes in generalised phonon density of states (GPDOS) is accomplished using the IINS spectra measured from ND_4SCN. Librational energies for 0-1 and 0-2 transitions are calculated for a tetrahedron in a crystalline field of C1 symmetry of monoclinic crystal structure of NH4SCN. The appearance of QINS above 200 K related with reorientation of ammonium ions is accompanied by broadening of librational peaks and by their merging in one broad maximum on GPDOS.

C-231 Temperature Dependence of Dynamic Scattering Function in Glycerol Studied by Quasielastic Slow Neutron Scattering

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The dynamic scattering function S(Q,E) of the glycerol has been studied by quasielastic slow neutron scattering at various temperatures between 50 - 400 K. Measurements performed at NEAT spectrometer of BENSC are reported in the kinematic region corresponding to the range of momentum transfers from 0.33(1/Å) to 2.31(1/Å) and to the energy transfer E = 0-21.74 meV. The topic presented here concerns the temperature dependence of the low energy features in glycerol under various states: liquid, supercooled and glassy. Intersections of the dynamic scattering function for constant momentum transfers between 1.6 (1/Å) and 2.3(1/Å) show a well resolved peak located at low but finite energy as E = 2.4 - 4.0 meV for all investigated temperatures. The position of this feature is continuously decreasing as a function of temperature from about 4 meV at 50 K to 2.4 meV at 400 K.

C-232 Librations of ferrocene rings in an Y-type zeolite studied by inelastic neutron scattering and density functional theory

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We have recently determined the location of ferrocene $\mathrm{Fe(C_5H_5)_2}$ in an Y-type zeolite. From this we calculate the rotational potential of the cyclopentadienyl $\mathrm{C_5H_5}$ rings of a ferrocene molecule in an Y-type zeolite with respect to each other using density functional theory. We compare this potential with the rotational potential of the rings in a single ferrocene molecule and with the rotational potential of the whole ferrocene molecule in an Y-type zeolite. The barrier for rotation of the rings of a ferrocene molecule in an Y-type zeolite, 2.1 kcalmol^{-1}, is twice as high as the barrier in a single ferrocene molecule, indicating a weak interaction between the ferrocene molecule and the zeolite. The results agree with the measured low-frequency inelastic neutron spectrum of ferrocene in an Y-type zeolite.

C-233 The Rotational Barrier for Methyl Group Dynamics in Trihydrate and dried Sodium Acetate

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The temperature dependence of methyl group dynamics in trihydrate and dried sodium acetate has been investigated by neutron scattering. The experimental results can be explained in both cases in terms of a single-particle threefold rotational potential. It is found that methyl groups are more strongly hindered in the dried sample.

C-234 Molecular Dynamics and Phase Transitions in Thiourea Intergrowth Crystals

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In thiourea organic intergrowth crystals, thiourea molecules, by means of an extensively hydrogen-bonded arrangement, form a host sub-structure constituted of infinite and parallel channels, in which suitable guest molecules can be included. Our aim is to elucidate the phase transition mechanisms and the molecular dynamics in these commensurate composite crystals. The methodology used is based on a multi-technique approach including Molecular Dynamics simulations (MD) and Incoherent Quasi-elastic Neutron Scattering (IQNS) techniques. In this paper, we present the combined MD-IQNS investigations of the guest molecules dynamics in the chlorocyclohexane/thiourea and the cyclohexane/thiourea intergrowth crystals.

C-235 Phase III of methane: crystal structure and rotational tunneling

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Phase III is the structure of methane CD_4 at $T < 22.1K$, of CH_4 under pressure $p \geq 600at$, of partially deuterated and mixed systems at concentrations $c_D \geq 0.2$. The crystal structure of phase III was solved only recently. The unit cell contains 2 types of molecules at sites with twofold symmetry and with a mirror plane. On the basis of these two rotor subsystems high resolution tunneling spectra of 1.5% CH_4 in CD_4, spectra of CH_4III under pressure and spectra of pure CD_4III can consistently be described, the latter only if a contamination by CD_3H is taken into account. An analysis based on tunneling matrix elements yields a 5% increase of the octopole moment of methane with deuteration. Thus the mixed system shows significant inhomogeneous line broadening due to positional disorder.

C-236 Dipolar interaction in partially deuterated $(NH_4)_2PtCl_6$: rotational tunneling spectroscopy

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At 10% deuteration ammonium hexachloroplatinate stays in its cubic phase $Fm3m$ at all temperatures. NH_4 and NH_3D tunneling transitions observed at temperatures $T \geq 18K$ show energies and intensities in agreement with a statistical occurrence of ammonium isomers in a tetrahedral environment. Below $T = 18K$ there is no unusual change of the NH_4 lines while the NH_3D tranition broadens. This is interpreted as dynamical average over the manifold of orientational configurations of statistical NH_3D defects caused by long range dipolar coupling. The resharpened spectrum observed at $T \leq 12K$ is explained as due to conversion into minimum energy configurations. A dipole moment of $0.05D$ is derived from the difference of tunnel splittings assigned to NH_3D monomers and dimers.

C-237 Dynamics of the Water Molecule in Potassium Oxalate Monohydrate as Studied by Single Crystal Inelastic Neutron Scattering

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We have measured the INS spectra for a powder sample and three differently oriented single crystals of $K_2C_2O_4.H_2O$ on the TFXA spectrometer at the ISIS facility. The crystal structure consists of oxalate ions hydrogen bonded by the water molecules into infinite linear chains which are held together by electrostatic interactions with the K^+ ions. The H_2O molecules are isolated from each other. The vibrations can then be separated into internal and external vibrations. The single crystals were cut and oriented so as to separate the rocking, twisting and wagging modes as much as possible. The rocking mode appears at 656 cm^{-1} (overtone at 1278 cm^{-1}. A band at 746 cm^{-1} with strong overtones at 1448 and 2099 cm^{-1} is assigned to the twisting mode, and the band appearing on its shoulder at 760 cm^{-1} is attributed to the wagging mode. The translational modes are found at 210, 97 and 215 cm^{-1}, respectively. A normal co-ordinate analysis of the INS profiles is in progress using the program CLIMAX.

C-238 The vibrational spectrum of ferrocene in KY zeolite by means of inelastic neutron scattering

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We measure the vibrational spectrum of ferrocene $Fe(C_5H_5)_2$ in the supercages of KY zeolite. We compare this with the vibrational spectrum of solid ferrocene and with an ab-initio calculation of the internal vibrations of a single ferrocene molecule using density functional theory (without free parameters). Due to the good agreement between the experimental and calculated spectra we can assign each vibrational mode to each observed peak in the neutron spectrum. The influence of the zeolite framework on the internal vibrations of a ferrocene molecule is small.

C-239 Inelastic neutron scattering on jarosites

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IR and Raman spectra of jarosite-type compounds (representative $KFe_3(OH)_6(SO_4)_2$) were reported [1,2] but assignment problems persist. Therefore, inelastic neutron scattering (INS) on jarosites was performed (TOSCA, ISIS RAL). Factor group analyses [1,3] were executed as basis for interpretation of all vibrational spectra, including INS. In addition to all vibrations of hydrogen also motions of iron nuclei (scattering cross section 11.6 barn) should produce observable INS signals. Dominating INS features with $KFe_3(OH)_6(SO_4)_2$) are assigned to δ(OH) and γ(OH) modes (1025 and 560 cm^{-1}) in the Fe-OH-Fe fragments (only partly observable in IR and Raman), weaker ones (750 and 670 cm^{-1}) to Fe-OH valence vibrations. Low-energy transfer INS signals down to below 100 cm^{-1} have counterparts in far IR and/or Raman spectra. [1] C.J. Serna, C. Parada Cortina, J.V. Garcia Ramos, *Spectrochim. Acta,* **1986**, *42A*, 729, and references therein. [2] D. K. Breitinger, J. Mohr, H. Schukow, R. G. Schwab, in A.M. Heyns(Ed.), *ICORSCape Town '98, XVIth Intern. Conf. on Raman Spectrosc., Suppl. Vol.*, Cape Town,**1998**, 86. [3] D. K. Breitinger, R. Kriegelstein, A. Bogner, R. G. Schwab, Th.H. Pimpl, J. Mohr, H. Schukow, *J. Mol. Struct.*, **1997**, *408/409*, 287.

C-240 Neutron spectroscopy and computer simulation dynamics of crystalline urea

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Inelastic neutron scattering experiment on the polycrystalline samples of urea, $CO(NH_2)_2$ and $CO(ND_2)_2$, were performed at 20 K on the NERA spectrometer at the IBR-2 pulsed reactor in Dubna. The neutron scattering low and the experimental densities of phonon states $G(\omega)$ were determined for the vibrational frequencies up to 2000 cm^{-1}. Combined *ab initio* direct method and the generic force field method were used for computer simulation of the lattice and internal dynamics of crystalline urea. The partial and total vibrational density of states and neutron scattering cross-sections were calculated and compared with the experimental spectra. A satisfactory agreement was obtained between the calculated and experimental spectra in the range of the lattice vibrations up to 200 cm^{-1}. These spectra are very little dependent on deuteration of the urea molecule. The significant isotopic shifts were observed for the internal vibrations in the frequency range from 300 to 1500 cm^{-1}. The frequencies of these vibrations are in a worse agreement with experiment than lattice vibrations. However, the calculated intensities of internal modes and their isotopic shifts permit a reliable interpretation of the experimental spectra and assignment of the low frequency internal modes.

C-241 Application of a isotopic contrast method for investigation of atomic dynamics of polyatomic compounds.

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In standard experiment on inelastic neutron scattering on a polycrystalline sample, the information about of atomic dynamics of compound can be obtained only at a level of averaged on all atoms of a neutron-weighted vibrational spectrum G(E). The method of isotopic contrast allows to obtain the more detail data (at a level of partial vibration spectra of atoms of different chemical elements) about atomic dynamics. The method based on difference of neutron scattering cross-sections for different isotopes of the same chemical element and allows to select the contribution of this element in G(E). The analysis of capabilities of the method in researches of atomic dynamics of condenced matter is carried out. On an example of binary oxide CuO the experimental implementation of this method is demonstrated. The partial vibrational spectra for Cu and O atoms and phonon spectrum of the oxide have been recovered. Researches of the dynamical behaviour of atoms of some chemical elements in HTSC and related compounds are discussed.

C-242 Mixed Lattice and Electronic States in High-Temperature Superconductors

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Inelastic neutron scattering measurements are presented which show the abrupt development of new oxygen lattice vibrations near the doping-induced metal-insulator transition in $\mathrm{La}_{2-x}\mathrm{Sr}_x\mathrm{CuO}_4$. A direct correlation is established between these lattice modes and the electronic susceptibility (as measured by photoemission) inferring that such modes mix strongly with charge fluctuations. This electron-lattice coupling can be characterized as a localized one-dimensional response of the lattice to short-ranged metallic charge fluctuations.

C-243 Neutron Diffraction Investigation of Structural Transitions in HTSC Compounds Induced by Fast Neutron Irradiation

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Using the method of neutron diffraction, structural changes in HTSC compounds disordered by fast neutrons at liquid nitrogen temperature were investigated. The experiments were carried out without samples reheating above 80 K (cold transfer of samples from nitrogen to nitrogen, measurement temperature 80 or 65 K). The defects emerging under irradiation with fast neutrons and structural distortions following neutron irradiation were determined. A relation between such changes and changes in the SC parameters was found. For the first time phase transition from rhombohedral to tetragonal symmetry was detected in YBCO at total oxygen concentration in a cell equal to 7 (!). At irradiation fluence increase, amorphous state (second-order transition) is realized in HTSC compounds. The kinetics of recovery of the initial structural state in the annealing temperature range between 80 to 800 K was studied. Work supported by State Contracts of RF No. 107-1(00)-I (Contract No. 07/01), No. 107-19(00)-, Program of State Support to Leading Scientific Schools of RF No. 00-15-96581, and RFBR Grant No. 01-02-16877.

C-244 Structural and magnetic aspects of the metal-insulator transition in $\mathrm{Ca}_{2-x}\mathrm{Sr}_x\mathrm{RuO}_4$

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We have studied the phase diagram of $\mathrm{Ca}_{2-x}\mathrm{Sr}_x\mathrm{RuO}_4$ over the whole region of x by neutron scattering on powder and single-crystalline samples. The experiments reveal antiferromagnetic order and structural distortions of the ideal $\mathrm{K}_2\mathrm{NiF}_4$ structure type characterised by tilts and rotations of the RuO_6 octahedra. Our results strongly suggest that the structural distortions of the isovalent samples tune the magnetic as well as the electronic behaviour. In particular we observe for low Sr concentration ($x < 0.2$) characteristic changes of the Ru-O bonds and tilt angles which are associated with a metal-insulator transition and AFM ordering. Further the suppression of the tilt distortion, observed for $x \sim 0.5$, is accompanied by a critical increase of low-temperature susceptibility. Additionally we discuss the phonon dispersion and the magnetic excitations as a function of Sr content x.

C-245 Stripe order in $\mathrm{La}_{1.875}\mathrm{Ba}_{0.125-x}\mathrm{Sr}_x\mathrm{CuO}_4$

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We have carried out systematic elastic neutron scattering experiments on single crystals of $\mathrm{La}_{1.875}\mathrm{Ba}_{0.125-x}\mathrm{Sr}_x\mathrm{CuO}_4$. In the LTT or Pccn phase for $x \leq 0.08$ charge ordering peaks from the so-called parallel stripe order are clearly observed in addition to magnetic incommensurate peaks. In the LTO phase for $x > 0.08$, on the other hand, only the magnetic peaks are detected. The observed close relation between the charge ordering and superconductivity in this system is a direct evidence of strong suppression of superconductivity triggered by charge localization in the LTT or Pccn structure.

C-246 Phonon Softening in HTSC Cuprates from Lattice Coupling of a Correlated Model

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Inelastic neutron scattering experiments on phonons in HTSC Cuprates (Pintschovius, Braden) show anomalous softening of a copper oxygen bond stretching mode upon doping. We calculate by numerical diagonalization of a highly correlated model the dependence of energies and correlation functions on in plane oxygen displacements for different dislocation patterns. An estimate of the electronically caused frequency reduction of the bond stretching phonon at $q = (0.5, 0, 0)$ upon doping is given, exceeding even the experimental value. A further theoretical result is some Peierls dimerization, that means new oxygen equilibrium positions in doped areas.

C-247 A SrBPO$_5$:Eu^{2+} storage phosphor for neutron imaging

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A storage phosphor material such as SrBPO$_5$:Eu^{2+} has been investigated for 2-dimensional imaging using pulsed-neutron source. This phosphor shows photostimulated luminescence (PSL) by illumination of 632 nm laser light after X-ray or alpha particle irradiation. The PSL intensity was proportional to the irradiation time. The spectral characteristics of the phosphor are similar to those of BaFBr:Eu^{2+}. One of the most important features of this phosphor is that it has a low density compared to that of BaFBr:Eu2+. It is favorable for discriminating neutron signal from gamma-ray signal under irradiation of pulsed-neutron. In addition, we found that this phosphor itself shows PSL for neutron irradiation without adding any neutron sensitive materials such as Gd. The PSL intensity per neutron flux was proportional to E$^{-0.5}$, where E is neutron energy. The neutron sensitivity was increased by using enriched boron instead of natural boron.

C-248 Design and Performance of the Spallation Neutron Source Backscattering Spectrometer

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When the Spallation Neutron Source is operational in 2006 at Oak Ridge National Laboratory, it will provide the most intense pulsed neutron beams in the world for research. This paper describes the expected performance of the near backscattering, crystal-analyzer spectrometer designed to provide extremely high energy resolution at the elastic peak (ΔE=2.2-2.7μeV, varying with sample dimension). The design requires a long initial guide section of 84 m from moderator to sample in order to achieve the requisite timing resolution. The design is optimized for quasielastic scattering but will provide 0.1% resolution in energy transfer, E, up to E=18 meV. This spectrometer will provide an unprecedented dynamic range near the elastic peak of -258μeV¡E¡258μeV. For experiments that require the full dynamic range available at comparable reactor based instruments (or greater), we expect this spectrometer to have an effective count rate 100 times that of the current best spectrometers.

C-249 A Chopper Spectrometer for the Spallation Neutron Source

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A high-resolution, direct-geometry spectrometer is being designed for the Spallation Neutron Source currently under construction in the US. An elastic resolution as low as 1% (FWHM) will be achieved with incident energies from 10 meV to over 1 eV. The instrument will view the ambient-temperature water moderator. Preliminary calculations show that tapered neutron guides in the primary flightpath from moderator to sample will increase the flux on the sample by up to a factor of 10 for the lowest energies. Sample rotation and tilt stages will enhance capabilities for single crystal research, and an oscillating radial collimator will cut background from complex sample environment equipment. The detector array, composed of linear position-sensitive He detectors, will span at least one steradian of solid angle, almost twice that of any existing chopper spectrometer. Areas of science covered by this instrument include magnetic systems, molecular and lattice dynamics, superconductivity and quantum fluids, for example.

C-250 Proposal for a chopper spectrometer with very high energy resolution

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We propose very high energy resolution chopper spectrometers for the Joint Project in Japan. Using a chopper spectrometer with a double Fermi chopper system, one can control energy resolution function arbitrarily, and obtain very high energy resolution. Results of simulation calculation by McStas indicate that $\Delta\varepsilon/E_{mi}$ of 0.2% must be feasible. Because of its large $Q-\omega$ space, very high resolution chopper spectrometers become powerful tool for study in wide scientific fields.

C-251 High counting rate 2-dimensional neutron imaging method using rectangular scintillators with WLS fibers

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We have developed a 2-dimensional neutron imaging method using rectangular scintillators with WLS fibers for neutron scattering experiments in a next-generation high-intense pulsed-neutron source. In the method, rectangular scintillators are arranged at longitudinal direction and transverse direction and WLS fibers are arranged on the four sides of these scintillators. Luminescences generated in the scintillator are absorbed by the four fibers and wavelength-shifted luminescences are detected by multi-channel photomultipliers. The position of incident neutron is decided by coincidence of the four signals. By preliminary experiments using 5 mm x 5 mm x 2 mmt ^{6}Li glass scintillators and 0.5 mmf WLS fibers, it was concluded that detection efficiency for thermal neutron was 13% and the maximum counting rate for each pixel was 3 Mcps with the coincidence time of 200ns.

C-252 MC simulations of reflectometers at reactor and spallation sources

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We simulated spectra of reflectometers installed on pulsed sources as they are planned for the ESS (5 MW 50 Hz short pulse, 1 MW 10 Hz short pulse, and 5 MW 16.7 Hz long pulse); for each of the sources a coupled moderator was used. For comparison of spallation and reactor sources, we simulated an instrument with equivalent parameters installed on a reactor source with a neutron flux of the ILL. For comparability of the data, constant wavelength and angular resolutions (of 3% and 8%) were used for all instruments. The intensity at the detector was determined as a function of the momentum transfer for a virtual sample of total reflectivity and for deuterated water. Finally it was calculated how long it takes for each source to measure the entire spectrum with a given statistical accuracy. Best results were obtained at the 50 Hz short pulse source and the long pulse source, while the 10 Hz source performed worse. The measuring time calculated for the reactor source was the longest.

C-253 VULCAN, a dedicated engineering diffractometer at the SNS

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VULCAN, the SNS engineering diffractometer, is designed to tackle a broad range of problems in engineering materials. The primary use of the instrument is for stress-related studies, including mapping of residual stress distribution in components and the study of materials response under applied load. For mapping experiments, the measurement time with a sampling volume of 1 mm^3 will be minutes. This will make possible parametric studies of components subjected to different fabrication or operating conditions. To enable in-situ loading studies, load-frame and furnaces will be an integrated part of the instrument. With its high flux and a large detector array, VULCAN is also ideally suited for determination of texture and transformation kinetics. A 2D position-sensitive detector placed downstream will enable small angle neutron scattering measurements providing information of the microstructure. When the diffraction and SANS data are collected together, this instrument will be a great tool to understand the intricate interplay between stress, texture, and microstructure in engineering materials.

C-254 Low-frequency dynamical response of confined water in normal and supercooled region by IINS

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We analysed IINS spectra on water in a nanoporous Gelsil matrix. The obtained $Z(\omega)$, the one-phonon amplitude-weighted proton vibrational density of states, shows, in the region 0-150 meV, the translational and rotational (librational) hindered collective modes, for confined water in the T-range $+40^{\circ}\mathrm{C} \div 35^{\circ}\mathrm{C}$. These modes are relative to intermolecular vibrations H-bond imposed and, varying the hydration percentage N/N$_0$ from 100% to 5%, we quantify, for the first time, the evolution of the three librational bands with T and N/N$_0$, revealing that the libration connected with the lowest moment of inertia increases enormously when N/N$_0$ is lowered, whereas the bond-bending and -stretching modes become more and more attenuated, indicating that the C_{2v} tetrahedral symmetry is lost in water tightly bonded to surface. A critical comparison with other spectroscopic and MD results is presented.

C-255 Short-range and medium-range Order in molten Ga-Tl Alloys

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The molten phase of Ga-Tl alloys was investigated by neutron small- and wide-angle scattering around the miscibility gap which occurs in the liquid state of this binary system. For the alloys containing 35, 40 and 45 at.% Tl an increase of the small-angle scattering intensity was observed as the temperature is decreased and approaches the temperature at the binodal curve. This behaviour is regarded as a result of fluctuations in concentration and the Ornstein-Zernike formalism was applied on the scattering intensity at small momentum transfer Q. A temperature-dependent correlation length was derived and values for the critical exponents gamma and u were estimated. The wide-angle neutron scattering intensity of the alloy with 40 at.% Tl shows, however, no temperature-dependent behaviour in the considered temperature range near the binodal curve.

C-256 Quantification of thermal motions in the Purple Membrane

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Local atomic motions in Bacteriorhodopsin (BR), the membrane protein in Purple Membranes of *Halobacterium salinarum* were studied by incoherent neutron scattering. The analysed sample consisted of fully deuterated Purple Membranes with BR containing H-retinal, H-tryptophan, and H-methionine. These labelled groups are present in the retinal binding pocket and the extracellular part of BR. By using incoherent neutron scattering on two different backscattering instruments at the ILL we determined the mean square displacements of small and large amplitude motions as a function of temperature for labelled as well as completely hydrogenated PM samples at different hydration states. We showed that the dynamics of this labelled selected part is more rigid and influenced by temperature and hydration in a different way than the membrane globally.

C-257 Neutron reflectivity study of biofunctional assemblies at lipid interfaces through recombinant spherical bacterial protein Lumazine Synthase

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A novel strategy to construct biomimetic assemblies of bio macromolecules to phospholipid membranes is presented. It is based on the surface anchoring of 15 nm capsids of bacterial lumazine synthase (LuSy) which are coupled to phospholipids exhibiting different functional headgroups like biotin and Ni chelator complexes. In this feasibility study we probe the adsorption dynamics of LuSy molecules under different binding conditions. We used LuSy functionalised with different key-lock like binding mechanisms. We also studied the dependency of the adsorption process on the concentration of a lipopolymer (phospholipid with polyethyleneglycol headgroup called PEG) at the interface.

C-258 The Mockup Tests of Cylindrical Annulus Type Moderator Cell for Developing TRR-II CNS

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The Taiwan Research Reactor modified project (TRR-II) with a vertical Cold Neutron Source (CNS) is carrying out at the Institute of Nuclear Energy Research (INER). A two-phase thermosiphon loop consists of a cylindrical annulus moderator cell, a single moderator transfer tube and a condenser. A cylindrical annulus moderator cell consists of an outer shell and an inner shell of which a bottom part is open. An inner shell is expected to contain only hydrogen vapor and an outer shell to contain boiling liquid hydrogen at 1.2 bar and 20.7 K for giving an optimum moderation for cold neutrons. A full-scale mockup test facility with liquid nitrogen as a working fluid was designed and made of glass for verifying the conditions to get the state mentioned above. The electrical heaters are used for simulating nuclear heat load of a moderator cell including hydrogen moderator, and the liquid level in the inner shell was measured directly as a function of the heater input. The results regarding the visualization of the two-phase flow patterns in the cylindrical annuls and the void distribution in the liquid nitrogen of the outer shell against variations of heat load will be presented. It is reported also how to control the state in which the inner shell contains only hydrogen vapor and the outer shell liquid hydrogen in the practical TRR-II CNS facility.

C-259 Dynamics of proteins at low temperatures: Fibrous vs. globular

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We have measured quasielastic neutron scattering from H_2O-hydrated collagen (Charolais calves) and haemoglobin (human) between 80 and 270 K, using the focusing t.o.f. spectrometer FOCUS at PSI and the backscattering spectrometer IRIS at ISIS. The data consist of sets of nearly elastic peaks showing (i) Q,T-dependent decreases in window-integrated intensities $S_{qe}(Q,T)$ proportional to effective Debye-Waller factors, and (ii) small lineshape changes due to various types of proton motions with characteristic times in the ns to 10 ps region. Relative to haemoglobin, the 200 K dynamic transition is shifted upwards by 20-25 K in collagen, and the T-dependence of m.-sq. proton displacements derived from $S_{qe}(Q,T)$ suggests that in triple-helical systems there may be three rather than two regimes: one region up to 120 K (probably purely harmonic), an intermediate quasi-harmonic region with a linear dependence up to 240 K, followed by a steeper nonlinear rise similar to that in globular proteins. Lineshape analyses show that small ”core” broadenings are observable already around 100 K, distinct from wing broadenings which consist of low-intensity but much wider shoulders developing above 210 K.