#### Poster Sessions

BioRef will be a time-of-flight reflectometer complementing the monochromator based V6 reflectometer at Hahn-Meitner Institute. Combined with an in-situ infrared spectrometer it will be optimised for soft matter applications at solid-liquid interfaces. A flexible double-chopper set-up together with a wavelength band chopper will enable the selection of well defined wavelength bands at different wavelength resolutions in order to optimize measurements with regard to the given application. The selection of different distances between the first choppers allow for choosing constant resolutions of  $\delta \lambda / \lambda$  between 1% and 5%, while different frequencies of the choppers are intended to alter the used bandwidth. A width of the band of 4 Å up to 12 Å can be selected between a minimum wavelength of app. 3 Å and a maximum of 15 Å. Lower wavelength resolutions than 5% can be realised when giving up the constant resolution. A state-of-the-art 2D position sensitive <sup>3</sup>He detector will be used for the reflectivity measurements in horizontal scattering geometry. The time-of-flight mode is also chosen to realise the investigation of dynamic interface processes under shear and flow conditions. A q-range spanning 3 orders of magnitude and reflectivity measurements over 7 orders of magnitude are envisaged and their feasibility is supported by Monte Carlo simulations.

Keywords: neutron time-of-flight, neutron reflectivity, infrared spectroscopy

#### P01.08.59

Acta Cryst. (2008). A64, C189

# The new polarised hot neutron single crystal diffractometer POLI-HEiDi at FRM II

Vladimir M. Hutanu<sup>1</sup>, Martin Meven<sup>2</sup>, Gernot Heger<sup>3</sup>

<sup>1</sup>RWTH Aachen, Institut fuer Kristallographie, Aussenstelle FRM II, TU Muenchen, Lichtenbergstr. 1, Garching b. Muenchen, Bayern, 85747, Germany, <sup>2</sup>Forschungsneutronequelle Heinz Maier-Leibnitz (FRM II), TU Muenchen, Lichtenbergstr. 1, 85747 Garching Germany, <sup>3</sup>Institut fuer Kristallographie RWTH Aachen, Jaegerstr. 17-19, 52056 Aachen Germany, E-mail:vladimir.hutanu@frm2.tum.de

Polarised neutron diffraction is one of the most important tools to determine magnetic structures. One-dimensional neutron polarisation analysis is used to determine the directions of magnetic moments. In addition, the recently developed spherical neutron polarimetry (SNP) is very useful to investigate complex magnetic structures in detail. For instance, the non-diagonal terms of polarisation matrices measured in SNP give us important informations on chiralities and magnetic domains of magnetic structures. The new polarised neutron diffractometer POLI-HEiDi- currently under construction at the hot neutron source (SR 9) at FRM II -is dedicated to investigate complex magnetic structures by means of SNP. Two zero-field polarimeters, the Cryopad and the MuPAD, are available for this task and could be used with the new instrument. 3He spin filters will be used for producing and analysing the neutron polarisation. New important parts and components for the polarised neutron diffractometer POLI-HEiDi were build and tested recently. In this report we will present these new components as well as the concept and design of the whole instrument. For 2008 the commissioning of the most important components like the detector-analyser unit Decpol, the zero-field sample environment Cryopad as well as the controlling electronics software is planned. Our project is carried out by the Institut fuer Kristallogaphie, RWTH Aachen University with financial support of the German Ministry of Education and Science (BMBF).

Keywords: neutron instrumentation, polarized neutron scattering, neutron spin filtering

#### P01.09.60

Acta Cryst. (2008). A64, C189

#### Polarimetric neutron spin echo spectroscopy

<u>Catherine Pappas</u><sup>1</sup>, Eddy Lelievre-Berna<sup>2</sup>, Phillipp M Bentley<sup>1,2</sup>, Evgeny Moskvin<sup>1,3</sup>, Bela Farago<sup>2</sup>, Peter Falus<sup>2</sup>, Sergey Grigoriev<sup>3</sup>, Vadim Dyadkin<sup>3</sup>

<sup>1</sup>HMI Berlin, SF1, Glienickerstr. 100, Berlin, Berlin, 14109, Germany, <sup>2</sup>Institut Laue-Langevin, 6 rue Jules Horowitz, 38042 Grenoble, France, <sup>3</sup>PNPI, 188300 Gatchina, Leningrad District, Russia, E-mail : pappas@ hmi.de

Neutron Spin Echo spectroscopy (NSE) uses polarized neutrons and in turn polarization analysis is an intrinsic feature of NSE. However, the multifaceted dynamics of antiferromagnets and hellimagnets ask for more than the classical Neutron Spin Echo set-up (NSE). In these systems the magnetic interaction vector is complex and the neutron beam polarization is not necessarily flipped upon scattering but can rotate at any angle around or towards a specific direction. The only way to access the components of the scattered polarization that are transverse to the incoming polarization is to implement a zero-field area around the sample position. Here we present the feasibility test and first results of the Polarimetric NSE, a powerful technique which combines a variant of the Intensity Modulated NSE (IMNSE) and the Cryopad. The Cryopad is a zero-field polarimeter based on Meissner shields and mu-metal screens able to do the most generalized polarization analysis experiments measuring all theoretically possible pair-correlation functions at any point of the reciprocal space. On the other side, IMNSE is a powerful variant of NSE that disconnects completely the sample area from the precession area at the price of some intensity losses due to the addition of polarizer and analyzer devices. This new technique was successfully developed on the wide angle NSE spectrometer SPAN at the HMI and then implemented on IN15 at the ILL, where new results on the magnetic relaxation in MnSi, a reference hellimagnet were obtained.

Keywords: neutron spin echo, neutron polarization analysis, chirality

### P01.08.61

Acta Cryst. (2008). A64, C189-190

### The study of thermal diffuse scattering measured by pulsed neutron diffraction

Kaoru Shibata<sup>1</sup>, Nobuaki Takahashi<sup>1</sup>, Itaru Tsukushi<sup>2</sup>, Kenji Nakajima<sup>1</sup>, Masatoshi Arai<sup>1</sup>

<sup>1</sup>J-PARC Center, Japan Atomic Energy Agency, shirakata-shirane 2-4, Tokai-mura, Naka-gun, Ibaraki-ken, 319-1195, Japan, <sup>2</sup>Department of Physics, Chiba Institute of Technology, 275-0023, Japan, E-mail : shibata. kaoru@jaea.go.jp

In this presentation, we will report the experimental results of the

thermal diffuse scattering (TDS) around strong Bragg peaks in some analyzer crystals measured by pulsed neutron diffraction technique at near back scattering conditions and discuss the comparison of those experimental results with theoretical predictions. We measured the thermal diffuse scatterings around some analyzer crystals Bragg peaks; pyrolitic graphite PG(002),



perfect silicon Si(111) and natural green mica: Mica(006) at near back scattering condition;  $2qB \sim 160$ . deg. using the diffraction counter bank on LAM-80: the indirect geometry crystal analyzer time of flight (TOF) spectrometer installed at KENS; a pulsed neutron source in KEK, Japan. At several offset angles from some Bragg conditions, we observed clear TDS peaks due to some acoustic phonon branches in the time of flight (TOF) diffraction spectrum.

Keywords: thermal diffuse scattering, time-of-flight diffraction, pulsed neutron scattering

#### P01.09.62

Acta Cryst. (2008). A64, C190

# Simultaneous thermogravimetric and neutron diffraction characterization of hydrogen stores

Martin M Jones<sup>1</sup>, William I. F. David<sup>1,2</sup>, Marco Sommariva<sup>2</sup>, Peter P Edwards<sup>1</sup>

<sup>1</sup>University of Oxford, Inorganic Chemistry Laboratory, South Parks Road, Oxford, Oxon, OX1 3QR, UK, <sup>2</sup>ISIS Facility, Rutherford Appleton Laboratory, Chilton, Oxon, OX11 0QX, UK, E-mail:martin.jones@chem. ox.ac.uk

We have developed apparatus that allows us to perform simultaneous thermogravimetric and neutron diffraction measurements on the GEM and HRPD diffractometers at ISIS as a function temperature, pressure and/or time. This apparatus, the Intelligent Gravimetric Analyzer for Neutrons (IGAn), was constructed as a collaborative effort between the Rutherford Appleton Laboratory and the University of Oxford. Dynamic neutron diffraction allows us to follow the transformation of materials on hydrogenation and dehydrogenation. Simultaneous thermogravimetric measurements permit these transformations to be correlated to the key kinetic and

thermodynamic processes. In this way, we can fully characterize the hydrogenation and dehydrogenation profile of hydrogen storage materials and thus obtain a fuller understanding of the critical processes involved. Initial benchmarking experiments on the Mg/MgD<sub>2</sub> system have identified the potential of this approach, and we report here the results of deuterium absorption / desorption cycling experiments for the Li<sub>3</sub>N -Li2ND - LiND2 system.



Keywords: neutron diffraction techniques, thermogravimetry, hydride compounds

#### P01.08.63

Acta Cryst. (2008). A64, C190

# Boost of multiple reflection effects - a new challenge for high-resolution neutron experiments

Pavol Mikula<sup>1</sup>, Miroslav Vrana<sup>2</sup>, Volker Wagner<sup>3</sup>

<sup>1</sup>Nuclear Physics Institute v. v. i., Academy of Sciences of the Czech Republic, Neutron Physics Department, Husinec-Rez, Rez near Prague, Czech, 25068, Czech Republic, <sup>2</sup>Nuclear Physics Institute v. v. i., Academy of Sciences of the Czech Republic, Rez near Prague,Czech

Republic, <sup>3</sup>Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany, E-mail:mikula@ujf.cas.cz

An enormous excitation of the multiple reflection (MR) effects achieved by bending the perfect single crystals is reported. These MR-effects (often called as Renninger effects) can be observed when more than one set of planes are simultaneously operative for a given wavelength i.e. when more than two reciprocal lattice points are at the Ewald sphere. Using a bent perfect crystal, the MR-effect can be considered as a two step process when primary reflection represented by (h1k111)-planes is simulated by successive reflections realized on the lattice planes (h2k2l2) and (h3k3l3) which are mutually in dispersive diffraction geometry. The luminosity corresponds to the volume of the phase space element of the monochromatized beam represented by the very narrow wavelength spread and the divergence as well. Therefore, the dispersive double-crystal reflections can provide very high angular and wavelength resolution without use of any collimators with a possible application namely at the high flux neutron sources. In relation to the value of the bending radius, the obtained doubly reflected beam has, a narrow wavelength band-width of 10<sup>-4</sup> -10<sup>-3</sup> and the collimation of the order of minute of arc. In NPI Rez we are building neutron optical bench employing such dispersive MR-monochromator which will operate at the neutron wavelength lambda of 0.16 nm. The bench could be used e.g. for some neutron optics testing, for investigation of structure quality of real single crystals and high resolution neutron radiography. First preliminary results will be presented.

Acknowledgement: Bragg diffraction optics investigations are supported by the grants GA-CR (No. 202/06/0601), AV0Z10480505 and MSM2672244501.

Keywords: neutron diffraction, Bragg diffraction optics, multiple reflections

### P01.08.64

Acta Cryst. (2008). A64, C190

# Transmission neutron monochromator and coherent neutron scattering images

#### Masayoshi B. Tamaki

TAMAKI Memorial Institute, Preparatory Room, Kuboshin-machi 2, Komaki, Aichi, 485-0006, Japan, E-mail:a40507a@cc.nagoya-u.ac.jp

Transmission neutron monochromator(TNM) is of a combination of single crystals. Through Bragg-cut-off and anti-Bragg-cut-off filters, a white neutron beam is changed to a narrow-band [1]. To cut off shorter wavelength neutrons, long pass filter is used. It is of a Bragg cut-off wavelength  $\lambda_1$ . To cut off longer one, short pass filter is used. It is of an anti-Bragg cut-off filter with  $\lambda_2$ . Here,  $\lambda_1 < \lambda_2$ . The transmitted neutron has spectrum from  $\lambda_1$  to  $\lambda_2$ . Using graphite single crystals, the TNM set-up is shown in a following figure. When a pair of single crystals was set in the white beam by diffraction angles of  $\theta + \Delta \theta$  and  $\theta - \Delta \theta$ , it was changed into spectrum with two depletions. Increasing number of the pairs of single crystals, a sharp peak is remained due to that other wavelengths were diffracted. It is monochromatic. The proposed and prepared TNM, installed together with neutron velocity selector and spectrometer, was successfully verified to be intrinsic function as neutron monochromator. Applications were tested for coherent scattering imagings of anisotropic structure of welded iron, of nickel single crystal, and of neutron polarizer.

[1] M. Tamaki, NIM A 542,32(2005).

Keywords: neutron imaging, transmission monochromator, coherent scattering