

## MM 53: Topical session: X-ray and neutron scattering in materials science II - Atomic migration studies ranging from neutrons to coherent X-rays

Time: Thursday 11:45–13:15

Location: BAR 205

**Topical Talk** MM 53.1 Thu 11:45 BAR 205

**Atomic migration studies ranging from neutrons to coherent X-rays** — ●BOGDAN SEPIOL<sup>1</sup>, MARKUS STANA<sup>1</sup>, MANUEL ROSS<sup>1</sup>, and MICHAEL LEITNER<sup>1,2</sup> — <sup>1</sup>Universität Wien, Fakultät für Physik, Boltzmannngasse 5, 1090 Wien, Austria — <sup>2</sup>Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

Numerous properties of materials can be attributed to the movement of single atoms. Understanding the processes involved in atomic transport is therefore of great importance for improving both the fabrication and the stability of materials. Studies of diffusion mechanisms on the atomic scale are, however, particularly challenging. Just a few methods are sensitive to movements on the atomic scale but they are limited to a restricted number of suitable isotopes. Due to these limiting factors it is very difficult or even impossible to apply these methods for studying metastable systems like glasses or nanocrystalline materials on the atomic scale. The advent of modern synchrotron sources opened the way for a new experimental technique which is not subject to these restrictions. I will follow in my talk the development of atomic migration studies ranging from quasielastic neutron scattering, quasielastic Mössbauer spectroscopy, nuclear resonant scattering until the most advanced method for studying dynamics in solid state materials called atomic-scale X-ray photon correlation spectroscopy.

This work was financially supported by the Austrian Science Fund (FWF) P-22402.

MM 53.2 Thu 12:15 BAR 205

**Hydrogen motion in LiBH<sub>4</sub> across the structural phase transition** — ●LUCA SILVI and WIEBKE LOHSTROH — Forschungsneutronenquelle Heinz Maier-Leibnitz FRM II, Lichtenbergstrasse 1, 85747 Garching, Germany

Lithium Borohydride (LiBH<sub>4</sub>) has an intense research activity due to its high hydrogen content (18.4 mass% H<sub>2</sub> and 121.3 kg/m<sup>3</sup> of gravimetric and volumetric hydrogen density). The slow sorption kinetics and the high temperatures required for hydrogen exchange are major obstacle for everyday-life applications. In LiBH<sub>4</sub>, hydrogen is bonded covalently to a central Boron atom forming a (negatively charged) tetrahedron, and the BH<sub>4</sub> unit bonds ionically to Li ion. By means of Quasielastic Neutron Scattering (QENS), the localized hydrogen motions were investigated as a function of temperature, across the phase structural transition at 380 K. QENS have been performed at the direct time-of-flight neutron spectrometer TOFTOF at FRM-II, and the Elastic Incoherent Structure Factor (EISF) could be determined in a momentum transfer-range up to 4 Å<sup>-1</sup>. The large dynamical range is essential for the discrimination of different kind of rotational modes. At temperature below the phase transition, 120° rotations occur around the C<sub>3</sub> symmetry axis of the BH<sub>4</sub> unit. As the phase transition is approached, the dynamic of the BH<sub>4</sub> unit changes continuously. At an intermediate state, a tumbling motion of the tetrahedron is observed, while at 413K the hydrogen motion is best described as a diffusion on a surface of a sphere. The results confirm that the structural phase transition is closely linked with the dynamic of the BH<sub>4</sub> units.

MM 53.3 Thu 12:30 BAR 205

**Study of Slow Dynamic processes with Depth Resolution** — ●OXANA IVANOVA<sup>1</sup>, OLAF HOLDERER<sup>1</sup>, and MICHAEL MONKENBUSCH<sup>2</sup> — <sup>1</sup>Jülich Centre for Neutron Science, Forschungszentrum Jülich, Aussenstelle am MLZ, Garching, Germany — <sup>2</sup>JCNS-Jülich Centre for Neutron Science, Forschungszentrum Jülich, Jülich, Germany

Neutron spin-echo (NSE) spectroscopy is a scattering technique where the spin precession of polarized neutrons in magnetic field is used to achieve the highest energy resolution for measuring tiny velocity changes of the neutron during the scattering process. Unlike

the other inelastic scattering techniques, such as time-of-flight spectroscopy, NSE measures the intermediate scattering function  $S(Q,t)$  in reciprocal space and time directly. Microscopic to macroscopic time range on large and intermediate length scales are covered.

High energy resolution, low background and high stability of the Jülich Neutron Spin-Echo spectrometer (J-NSE) at Heinz Maier-Leibnitz Zentrum (MLZ) makes the instrument suitable for grazing incidence technique. Along with conventional NSE spectroscopy, which enables the measurements in bulk, grazing incidence NSE spectroscopy (GINSES) can be used as dynamic analog to GISANS in order to resolve depth dependent near surface motions. Typical applications of J-NSE include dynamics in soft matter systems (polymers in solution and under confinement, microemulsions, blends, microgels, proteins, membranes, nano-composites) or paramagnetic properties of e.g., spin glasses. Some examples of the recent experiments will be presented.

MM 53.4 Thu 12:45 BAR 205

**Microscopic structure of supercooled water studied by x-ray Compton scattering** — ●JURI NYROW<sup>1</sup>, FELIX LEHMKÜHLER<sup>2</sup>, MIKKO HAKALA<sup>3</sup>, THOMAS BÜNING<sup>1</sup>, INGO STEINKE<sup>2</sup>, AGNIESZKA POULAIN<sup>4</sup>, THOMAS BUSLAPS<sup>4</sup>, METIN TOLAN<sup>1</sup>, and CHRISTIAN STERNEMANN<sup>1</sup> — <sup>1</sup>Fakultät Physik/DELTA, Technische Universität Dortmund, 44221 Dortmund, Germany — <sup>2</sup>Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — <sup>3</sup>Department of Physics, University of Helsinki, FI-00014 Helsinki, Finland — <sup>4</sup>ESRF, 38043 Grenoble Cedex 9, France

The structure of the hydrogen bond network of water at ambient and in supercooled conditions is controversially discussed, e.g. with respect to a mixture of two phases, LDW (low density water) and HDW (high density water). HDW and LDW phases differ fundamentally in respect of the local structure, with the high density phase showing a highly disturbed OH bonding network and the low density phase showing a nearly tetrahedral coordinated water network. Recently inelastic neutron scattering studies reported a disturbance of the water network at slight supercooling. We investigated changes in the local molecular structure in supercooled water for temperatures down to 256 K by x-ray Compton scattering and found evidence for structural changes which will be discussed on the basis of different structure models.

MM 53.5 Thu 13:00 BAR 205

**Mechanical properties of mesocomposite silk fibres: viscoelasticity, structural and molecular origin** — ●IGOR KRASNOV<sup>1</sup>, TYLO SYDLE<sup>2</sup>, MICHAEL M. KOZA<sup>2</sup>, MANFRED BURGHAMMER<sup>3</sup>, and MARTIN MÜLLER<sup>1</sup> — <sup>1</sup>Helmholtz-Zentrum, Geesthacht, Germany — <sup>2</sup>ILL, Grenoble, France — <sup>3</sup>ESRF, Grenoble, France

To study the response of silk to a mechanical perturbation we monitor the changes of the microscopic structure of silk as well as the molecular dynamics of the amorphous phase. In order to achieve this goal *in situ* scattering experiments were performed: synchrotron radiation X-rays and cold neutrons were used as probes of the structure and dynamics, respectively. Much attention was devoted to the temporal evolution. Generally, a link between the macroscopic viscoelastic behaviour and the mechanism at the molecular length scales has been established. With our experimental techniques and analyses we could separate the mechanical properties of the crystalline region of silk from those of the amorphous part, as well as show their interplay [1]. Interesting novel results were also obtained concerning the long-time mechanical relaxation of silk and molecular diffusion processes. Both phenomena exhibit definitive memory effects and can be well described by the models based on fractional calculus. Despite the fact that these phenomena belong to very different temporal and spatial levels the fractional characteristics of these phenomena are very similar.

[1] Krasnov I., et al. PRL **100**, 048104 (2008)