

## MM 48: Topical session: X-ray and neutron scattering in materials science I - Coherent X-ray Diffraction Imaging of Excitations in Metal Nanoparticles

Time: Thursday 10:15–11:30

Location: BAR 205

MM 48.1 Thu 10:15 BAR 205

### Structural study of CuZr and Cu<sub>50</sub>Zr<sub>45</sub>Al<sub>5</sub> metallic glasses in relation to their GFA and mechanical properties —

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In this work we investigate the atomic structure of CuZr and Cu<sub>50</sub>Zr<sub>45</sub>Al<sub>5</sub> metallic glasses in view of their glass-forming ability and mechanical properties. Using a combination of the state-of-the-art experimental techniques (synchrotron X-ray diffraction and absorption spectroscopy and neutron diffraction), reverse Monte-Carlo simulation and Molecular Dynamics modelling we have obtained partial pair distribution functions, coordination numbers and bond lengths for the glasses studied. Remarkable differences are found for the total as well as for the partial pair distributions in the CuZr and Cu<sub>50</sub>Zr<sub>45</sub>Al<sub>5</sub> metallic glasses, especially for the Cu-Cu and Zr-Zr pairs at the second and higher coordination shells, suggesting important role of the medium-range order in the glass formation and in the mechanical behaviour.

MM 48.2 Thu 10:30 BAR 205

### Static atomic displacements of Fe-27 at.% Pt in the Invar regime —

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X-ray diffuse scattering from a single crystalline Fe-27.1 at.% Pt Invar alloy was measured at room temperature and close to the Curie temperature. The sample was set up in a short-range ordered state by quenching from 1120 K. As expected due to the nearby located L<sub>12</sub> ordered structure, diffuse maxima are seen close to the X position. Separation of the diffuse scattering into short-range order scattering and displacement scattering was performed by the method of Georgopoulos and Cohen. The short-range order parameters remain nearly unchanged for both measurements and yield effective pair interaction parameters that properly reproduce the order-disorder transition temperature. On the other side, differences are observed in the species-dependent static atomic displacements of the first two coordination shells for both measurements. This change close to the Curie temperature is compared with literature data in Ni-Fe where two measurement temperatures were chosen well below the Curie temperature.

MM 48.3 Thu 10:45 BAR 205

### Hydrogen desorption pathway of Mg(BH<sub>4</sub>)<sub>2</sub> probed by in-situ X-ray Raman scattering —

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With a hydrogen density of 14.9 wt% the complex hydride Mg(BH<sub>4</sub>)<sub>2</sub> is considered as a solid-state hydrogen storage material. Identifying

the amorphous boron-containing species during the desorption process provides essential information about the decomposition pathway of Mg(BH<sub>4</sub>)<sub>2</sub>. Unlike diffraction, X-ray Raman scattering allows investigating the local atomic and electronic structure and hence quantitatively estimating the amounts of different amorphous constituents. By modelling the X-ray Raman spectra from the possible constituents we unveiled the reaction pathway and determined the role of boron within.

MM 48.4 Thu 11:00 BAR 205

### Hydrogen absorption in Mg-Ti multilayers studied by neutron re<sup>\*</sup>ectometry —

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Mg-Ti thin film alloys have large H-storage capacities, fast kinetics of hydrogen absorption and desorption and are structurally stable. These qualities stem from a short-range ordered distribution of the Mg and Ti atoms. In order to study the influence of short-range order on the hydrogen sorption properties of Mg-Ti systems, we artificially engineered chemical segregation by depositing a Ti/Mg multilayer with 10 repetitions of Ti(2 nm)/Mg(4.4 nm). On exposure to H<sub>2</sub> a two-step hydrogenation process occurs with the Ti layers forming the hydride before Mg. In-situ, time resolved Neutron Reflectometry (NR) allows an accurate determination of the out-of-plane expansion associated with each hydrogenation step. The volume expansion expected for the hydrogenation of both Ti and Mg is transferred completely in the vertical direction, indicating that large plastic deformations have to occur upon hydrogen absorption. Owing to the large negative neutron scattering length of hydrogen, NR proves to be an excellent technique for the in-situ characterization of the hydrogen absorption properties of thin films.

MM 48.5 Thu 11:15 BAR 205

### Electrode Lithiation in Lithium-Ion Batteries Investigated by In-Operando Neutron Reflectometry —

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Lithium-ion batteries are widely developed and used as rechargeable power sources for portable electronic devices and will be essential in the field of automotive transportation. One of their major advantages is their low weight, and therefore the high energy density available. Kinetic processes and interface phenomena at electrodes during charging and discharging cycles play a key role for optimization of these batteries (e.g. for charging times and power density). As negative electrode material, amorphous silicon has become a promising candidate for future Li-ion battery applications due to its high theoretical specific capacity of about 4 Ah/g.

We present in-operando neutron reflectometry experiments on the lithiation of amorphous silicon electrodes during galvanostatic charging or during cyclic voltammetry. Such studies allow to monitor the modification of Li content and the corresponding volume expansion/contraction of the electrode during lithiation on the nanometer scale. Possible lithiation mechanisms are discussed.

B. Jerliu et al. Phys. Chem. Chem. Phys., 15 (2013) 7777.