MI 2: Analytical Transmission Electron Microscopy and Atom Probe Tomography

Time: Monday 12:00–13:15 Location: EMH 225

MI 2.1 Mon 12:00 EMH 225

Imaging Phase Transition of LiMn2O4 Nanowire Battery by in-situ TEM — •Soyeon Lee[1,3], Yoshifumi Oshima[2,3], and Kunio Takayanagi[1,3] — [1]Tokyo Tech., Tokyo, Japan — [2]JAIST, Ishikawa, Japan — [3]JST-CREST, Tokyo, Japan

In order to understand mechanism of phase transition in the electrode and transport of lithium ions, a nano model battery with a single LiMn2O4 (LMO) nanowire as positive electrode was developed specially for in-situ transmission electron microscope (TEM) observation. The LiMn2O4 (LMO) nanowire was free standing, contacted with ionic liquid electrolyte (ILE) on a Li4Ti5O12 negative electrode by one side of the wire. The nanowire battery was charged and discharged by cyclic voltammetry in the range of 2.7-5.2 V (vs Li/Li+) at high charge rate (fully charged within 24 minutes) in TEM. The local structure change of LMO was successfully imaged by TEM imaging and transmission electron diffraction (TED) at the position far from LMO/ILE interface by about 50 μm: The phase transition region from lithium rich phase to poor phase was observed. The transition region moved continually during whole charge-discharge cycle by changing local structure. The two domains had different orientation: Li-rich phase, (100); Li-poor phase, (11-1). Interestingly, the domain orientation of one phase was also changed into that of the other. Our developed nanowire battery worked reversibly without capacity fading for high-rate charge/discharge operation. The reversible cycle without capacity fading is considered that the transition region acted as a mediator between two phases.

MI 2.2 Mon 12:15 EMH 225

In-situ Transmission Electron Microscopy Study of Ge(8-n)Sn(n)Sb2Te11 — Dietrich Häussler[1], •Torben Dankwort[1], Lorenz Kienle[1], Christine Koch[2], Wolfgang Bensch[2], and David C. Johnson[3] — [1]Institut für Materialwissenschaft, CAU Kiel — [2]Institut für Anorganische Chemie, CAU Kiel — [3]University of Oregon, Eugene, USA

(GeTe)x(Sb2Te3)y - known as phase change materials (PCM) - are of large interest for applications in data storage devises like blu-ray discs. We report on a novel type of short range ordering phenomena for Ge(8-n)Sn(n)Sb2Te11 (n=2, n=4). Amorphous, stoichiometric thin films of such compositions and with thicknesses <40 nm were directly deposited on carbon coated Ni grids using molecular beam epitaxy. In-situ heating TEM experiments revealed an exceptional growth of large grains with sizes >500 nm starting at 130°C. Furthermore, diffuse scattering was observed in electron diffraction patterns, which implies short range order phenomena unknown for PCMs so far. In-situ heating experiments indicate that close to 150°C diffuse scattering is altered to an ordered superlattice structure. This is in accordance with the resistance-temperature behavior, which is characterized by a remarkable additional resistance drop at ~150°C (heating rate of 5 K/min). Possibly, these results suggest that the diffuse scattering is an indication for a new intermediate phase.

MI 2.3 Mon 12:30 EMH 225

Exploring the properties of individual nanomagnets: EMCD on FePt nanocubes — •Sebastian Schneider[1,2], Darius Pohl[1], Thomas Schachinger[3], Stefan Löffler[3], Peter Schattschneider[3,4], and Bernd Rellinghaus[1] — [1]IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, D-01171 Dresden, Germany — [2]TU Dresden, Institut fur Festkörperphysik, D-01062 Dresden, Germany — [3]Vienna University of Technology, USTEM, A-1040 Vienna, Austria — [4]Vienna University of Technology, Institute of Solid State Physics, A-1040 Vienna, Austria

Electron magnetic chiral dichroism (EMCD) is the electron wave analogue of X-ray magnetic circular dichroism (XMCD). It offers the possibility to study magnetic properties at the nanoscale in a transmission electron microscope (TEM). In a 'classical' EMCD setup, the sample is illuminated with a plane electron wave and acts as a beam splitter. Although this method is meanwhile well established, only very few EMCD spectra were so far obtained from individual nanoparticles. We report on EMCD measurements on individual FePt nanocubes with a size of roughly 30 nm and compare our experimental findings with simulations. The dichroic signals at the L_3 and L_2 edges are expected to be as small as 10 % of the total scattering intensity. Our experiments are supported by simulations utilizing the WIEN2k program package, based on which FePt cubes with a thickness, that should provide maximal EMCD signals, are chosen for the experiments. The experiments indeed reveal a small but reproducible dichroic signal that agrees well with the results of the theoretical calculations.

MI 2.4 Mon 12:45 EMH 225

How electrostatic simulations improve the understanding of APT measurement results — •Christian Oberdorfer, Daniel Beinke, and Guido Schmitz — Institute of Materials Science, University of Stuttgart, Germany

Simulations represent a complementary approach to atom probe experiments. By flexible electrostatic modeling, the field evaporation and the ion trajectories are calculated. Important insights into the presence and the origin of measurement artifacts may be revealed in this way.

Numeric treatment is rigidly based on the representation of atoms by Wigner-Seitz cells. Field evaporation is assumed to be induced by polarization forces acting on the atomic cells. Evaluation of the force represents an essential cornerstone to a more realistic prediction of the field evaporation sequence.

Investigated trajectory aberrations show a decisively limited resolution of the computed 3D reconstruction if the standard protocol based on geometric back-projection is followed. The applied point-projection neglects important information of the detailed surface field and fails for this reason.

MI 2.5 Mon 13:00 EMH 225

Accurate volume reconstruction by numerical calculation of trajectories — •Daniel Beinke, Christian Oberdorfer, and Guido Schmitz — Institute of Materials Science, University of Stuttgart, Germany

A new approach for the reconstruction of atom probe data is presented. It is based on the calculation of realistic trajectories of evaporated ions. To this end, a Voronoi tessellation of the simulation space is used in order to bridge several orders of magnitude in distance. Compared to other reconstruction techniques, the order of reconstruction is inverted, which means that last detected atoms are reconstructed first. Consequently the emitter shape is known at each reconstruction step.

Based on numerical model emitters with particles or layers of heterogeneous evaporation threshold, we demonstrate that this new concept has indeed the natural potential to overcome artifacts of local magnification, such as depleted zones at interfaces or distorted particle shapes. Still issues in detail, scoping with the finite detection efficiency, finite aperture size, and the limitation in computing resources have to be resolved before practical application to experimental data sets.