MM 51: Materials Design II

Time: Friday 11:45–13:00 Location: H 0111

MM 51.1 Fri 11:45 H 0111

High strength conductors: CuAg tapes — •Jens Freudenberger, Julia Lyubimova, and Ludwig Schultz — IFW Dresden, Institute for Metallic Materials; PO-Box 270116; D-01171 Dresden

Conductor materials with a high mechanical strength and a high electrical conductivity are required for a number of applications. There especially is a growing interest in tapes and strips for connectors. CuAg tapes, prepared by conventional casting, heat treatment and rolling, show the beneficial combination of high electrical conductivity and high mechanical strength. A combination of 60%IACS and 1.2GPa is achieved and referred to the microstructure of the material.

MM 51.2 Fri 12:00 H 0111

Formation of complex 3D networks of anisotropic colloidal nanocrystals — •Stefan Kudera[1], Isabella Franchini[2], Joachim P. Spatz[1], and Liberato Manna[2] — [1]Max Planck Institut für Metallforschung, Heisenbergstraße 3, 70569 Stuttgart, Germany — [2]National Nanotechnology Laboratories of CNR-INFM, Via Arnesano, 73100 Lecce, Italy

Semiconductor nanocrystals can be synthesised in a variety of different shapes. There are standard procedures for the production of spheres and anisotropic nanorods. Additionally it is possible to introduce branching points into the structures in order to obtain objects of a more complicated shape such as bumerang shaped dipods or tetrapods.

Here, we will present a possibility to interconnect colloidal nanocrystals into complex networks. These networks are formed in a solution and they are stable for a certain amount of time, during which they might be deposited on any kind of substrate. Generally the time available for the treatment of the networks is of the order of few minutes. A metallic domain acts as linker between the individual nanocrystals.

As the networks are formed of semiconductor materials they are of interest for the production of solar cells. When embedded into a hole transporting polymer, the nanocrystal network might enable an efficient electron transport towards the anode. Thus, while providing a good electronic contact with the electrode, the network still offers a large surface, on which the charges could be separated.

MM 51.3 Fri 12:15 H 0111

Probing the rattling mode scenario in nano-cage based thermoelectric materials — Andreas Leithe-Jasper[1], Yuri Grin[1], Walter Schnelle[1], Romain Viennois[1], Hannu Mutka[2], Lucia Capogna[2], Mark Robert Johnson[2], and •Michael Marek Koza[1,2] — [1]MPI-CPfS, Noethnitzer Strasse 40, D-01187 Dresden — [2]ILL, 6 Rue Jules Horowitz, F-38042 Grenoble

The direct conversion of waste heat into electrical power in thermoelectric devices is believed to contribute substantially to future power supply and sustainable energy management. Nanocage-based crystalline structures like filled skutterudite systems XFe4Sb12 (X = Ca, Cs, Ba, La, Ce, Yb, Nd, ...) and clathrate materials like BaGe and BaSi have attracted some scientific interest as they are sought to be excellent thermoelectric materials. Their applicability for an efficient conversion of thermal into electrical energy is based on the opportunity of tuning appreciably the heat transport through the sample leaving the electron transport rather unaffected.

We will give some examples of our experimental work comprising neutron scattering techniques and bulk spectroscopies, e.g. specific heat measurements, on filled skutterudite systems and pyrochlore osmates XOs2O6 (X = K, Rb, Cs). We will present a new approach based on ab initio lattice dynamics calculations towards the interpretation of experimental data particularly dedicated to polycrystalline systems. We will show that the apparently established picture of rattling modes, i.e. decoupled dynamics of guests X and host Fe4Sb12 is not correct.

MM 51.4 Fri 12:30 H 0111

Ab initio up to the melting point: Influence of vacancies and explicit anharmonicity — •Blazej Grabowski, Lars Ismer, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck Str. 1, 40237 Düsseldorf, Deutschland

A recent study [1] on an extensive set of elementary metals showed that a wide variety of thermodynamic properties can be excellently reproduced within the quasiharmonic approximation. An exception is the heat capacity which shows a clear deviation from experiment at temperatures above 70% of the melting temperature.

To clarify the origin of the nonlinear increase, we have investigated two potential candidate mechanisms being debated controversially in the literature. On the one hand, we have calculated the contribution of monovacancies to the free energy. We have included the vibrational entropy of the vacancy using the full volume dependent dynamical matrix (quasiharmonic approximation). On the other hand, we have calculated the contribution of the volume dependent explicit anharmonicity (of the pure crystal) to the free energy. For this purpose, we have employed thermodynamic integration. We find that both contributions are of equal magnitude and correct the quasiharmonic results when compared to experiment.

[1] Grabowski B., Hickel T., and Neugebauer J., PRB 76, 024309 (2007).

MM 51.5 Fri 12:45 H 0111

Scalable molecular dynamics simulations of oxides — •Peter Brommer and Franz Gähler — Institut für Theoretische und Angewandte Physik, Universität Stuttgart, 70550 Stuttgart, Deutschland

Due to polarisable oxygen atoms and long-range ionic interactions, molecular dynamics (MD) simulations of oxides usually scale unfavourably with the system size. By using the direct summation technique described by Wolf *et al.* [1] with a slightly increased interaction cut-off radius, contributions in reciprocal space can be neglected, and the simulation scales linearly with the system size. Additionally, direct summation methods can be used within the framework of an existing MD programme, including parallelisation algorithms and freedom in the choice of boundary conditions. We present an implementation of the silica interaction potential of Tangney and Scandolo [2] using Wolf summation. This model treats the oxide atoms as polarisable, and the dipole strengths are determined in a self-consistency loop. We demonstrate the scaling properties and discuss the validity of using Wolf summation for this potential.

[1] Wolf *et. al*, J. Chem. Phys. **110**, 8254 (1999)
[2] Tangney and Scandolo, J. Chem. Phys. **117**, 8898 (2002)