MM 30: Topical Session: Thermodynamics at the nano scale III - Novel experimental and theoretical approaches

Time: Tuesday 15:45–17:45 Location: BAR 205

MM 30.1 Tue 15:45 BAR 205

Efficient evaluation of thermoelectric and electronic transport properties in a maximally-localized Wannier-function basis using the BoltzWann code — •Giovanni Pizzi[1], Dmitri Volja[2], Boris Kozinsky[3], Marco Fornari[4], and Nicola Marzari[1] — [1]Theory and Simulation of Materials, EPFL (CH) — [2]Department of Materials Science and Engineering, MIT (USA) — [3]Robert Bosch LCC Research and Technology Center, Cambridge (USA) — [4]Dept. of Physics, Central Michigan University (USA)

The calculation of thermoelectric and electronic transport properties of extended systems requires extremely dense Brillouin-zone samplings together with the evaluation of band derivatives, that are however difficult to converge using standard finite-difference methods in systems where band crossings are present. We address both issues in our BoltzWann code [1] by adopting a maximally-localized Wannier function basis set. This allows both to interpolate the bands with very high accuracy thanks to the strong localization of the Wannier functions, and to calculate band derivatives analytically giving precise results also in the case of band crossings. BoltzWann then solves the semiclassical Boltzmann transport equations in the constant relaxation-time approximation to obtain transport properties (conductivities, Seebeck coefficient). We apply the code to some relevant systems like the $CoSb_3$ and $CoGe_{3/2}S_{3/2}$ skutterudites. BoltzWann is freely distributed as a module within the Wannier90 2.0 code [2].

[1] G. Pizzi *et al.*, Comp. Phys. Comm. 185, 422 (2014)
[2] www.wannier.org

MM 30.2 Tue 16:00 BAR 205

Gaussian Approximation Potential: an interatomic potential derived from first principles Quantum Mechanics — •Albert Bartók-Pártay and Gábor Csányi — Department of Engineering, University of Cambridge, Trumpington Street, CB21PZ, Cambridge, UK

We present a method that allows the exploration of the DFT Born-Oppenheimer potential energy surface by interpolating between precomputed values at a set of points in atomic configuration space. The resulting model does not have a fixed functional form and hence is capable of modelling complex potential energy landscapes. In order to achieve this, we developed an invariant representation of the atomic environment. The potential is systematically improvable with more data. The accuracy of this interpolated PES is remarkable for a wide variety of systems, including semiconductors, metals and polarisable crystals.

MM 30.3 Tue 16:15 BAR 205

Ab initio prediction of solvus lines in Al alloys: The importance of anharmonic contributions — •Albert Glensk, Blazej Grabowski, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung, Düsseldorf

The prediction of alloy phase diagrams without any experimental input is a major challenge in materials science. First-principles studies including temperature effects in the harmonic approximation have already demonstrated to provide a qualitative agreement with CALPHAD phase diagrams, but truly quantitative predictions are rare. Recent first-principles calculations on point defects have shown that a highly accurate computation of formation free energies is possible up to the melting temperature, if all excitation mechanisms, in particular anharmonic excitations, are taken into account [1]. Applying these methods, we have studied the solvus line of Si in Al, giving access to the Al-rich region of the Al-Si phase diagram. We will discuss the methodological challenges and the unexpectedly large impact of anharmonic lattice excitation on these results.

[1] B. Grabowski et al, PRB 79, 134106 (2009)

MM 30.4 Tue 16:30 BAR 205

Low temperature specific heat of pure titanium made nanocrystalline by severe plastic deformation — •Martin Peterlechner[1], Jochen Fiebig[2], and Gerhard Wilde[1] — [1]Institute of materials physics, WWU Münster, Germany — [2]Department of Chemical Engineering and Materials Science, UC Davis, USA

In the last decades it was shown that severe plastic deformation can be used to obtain bulk nanostructured materials. In the present work, pure titanium was processed by equal channel angular pressing and subsequently annealed to obtain fairly dislocation free bulk nanostructured samples. The arising structures were analyzed using electron microscopy. Specific heat measurements using the two-tau method were conducted in the temperature range between 1.9 and 300 K, to obtain data sets of nanocrystalline titanium and its coarse grained counterpart. Using the Debye model for the lattice-vibrational contribution to the low temperature specific heat (<5K), and using the Sommerfeld model for the contribution of the electrons to the specific heat a function g*T+a*T^3 was fitted to obtain the Sommerfeld coefficient g and the Debye temperature. It is concluded, that in nanocrystalline titanium the contribution of electrons to the specific heat is increased due to the high number of grain boundaries. There is an indication that the Debye temperature slightly decreases and, moreover, the total enthalpy of the nanocrystalline phase increases. Based on the results thermodynamic properties of grain boundaries are deduced, and the limits of the applied models are discussed.

15 min break

Topical Talk MM 30.5 Tue 17:00 BAR 205

Soft Matter in Hard Confinement: Molecular Assemblies confined in Nanoporous Solids — •Patrick Huber — Materials Physics and Technology, Hamburg University of Technology, D-21073 Hamburg

The advent of tailorable nanoporous solids, such as porous silicon and alumina, allows one to explore the equilibrium and non-equilibrium properties of condensed matter in well-defined, nanostructured geometries. In my talk I will present selected experiments on kinetic and thermodynamic phenomena, ranging from spontaneous imbibition, capillary condensation and glass formation to nematic ordering and crystallization in pores a few nanometers across. Depending on the nature of the basic building block of the molecular assemblies investigated (rare gas molecules, water, liquid crystals, linear hydrocarbons, polymers and proteins) and the mean pore diameter of the porous host a remarkable robustness, however, also substantial deviations from the macroscopic bulk behaviour can be observed, both with regard to the equilibrium and non-equilibrium behaviour.

MM 30.6 Tue 17:30 BAR 205

Polarization discontinuities in two-dimensional honeycomb lattices — •Marco Gibertini, Giovanni Pizzi, and Nicola Marzari — Theory and Simulation of Materials, École Polytechnique Fédérale de Lausanne, Switzerland

The unprecedented and fascinating phenomena taking place at oxide interfaces such as $LaAlO_3/SrTiO_3$ have recently triggered the search for their two-dimensional analogues. In this respect, honeycomb lattices seem to offer a rich playground, both for their versatility and the fundamental experimental developments that ensued from the discovery of graphene. In this talk we would like to emphasize, with the help of atomistic first-principles simulations, how to achieve polar discontinuities across interfaces between honeycomb lattices, elucidating the key physical processes that occur and their possible practical applications.