MM 59: Phase Transitions I

Time: Thursday 14:00–15:15 Location: H5

MM 59.1 Thu 14:00 H5

The Phase Diagram of Iron Clusters: A molecular Dynamics Study — •Denis Comtesse[1], Ralf Meyer[2], and Peter Entel[1] — [1]Universität Duisburg-Essen, 47048 Duisburg, Germany — [2]Laurentian University, Sudbury, Ontario, P3E 2C6 Canada

The stability of phases at finite temperatures is given by the free energy. But the fact that it is not expressible in terms of ensemble averages over functions of position and velocity coordinates, complicates its determination in atomistic simulations. In order to overcome this problem, thermodynamic integration methods are used. This method is not limited to thermodynamic paths which can be followed in experiments. Often artificial paths along which the inter-particle interaction is switched off, lead to much better results.

Here we calculate the free energy of iron nano clusters along a thermodynamic path starting from the embedded atom model and ending up in a set of three dimensional harmonic oscillators. The results allow to arrange the various morphologies in a phase diagram of temperature and number of atoms. The phase boundaries, which are normally hidden in between hysteresis loops, can be determined very accurately from the intersection of the free energies of the competing morphologies. As examples, we analyse three common morphologies, namely the icosahedron, the cuboctahedron with fcc structure and its Bain transformation to the bcc structure. Additionally the new shellwise Mackay transformed morphology reported in Phys. Rev. Lett. **99** 083402 is taken into account.

MM 59.2 Thu 14:15 H5

Bulk and near-surface microstructure of Ni-23 at.% Pt — •Markus Engelke[1], Bernd Schönfeld[1], and Andrei Ruban[2] — [1]LMPT, Department of Materials, ETH Zurich — [2]KTH Stockholm, Sweden

Diffuse x-ray scattering was taken from bulk single-crystalline Ni-23.2 at.% Pt. The sample was aged at 923 K to set up a state of thermal equilibrium. Using separation techniques, short-range order and static atomic displacements were determined. In comparison with a previously performed study from the same sample to characterize the near-surface microstructure by grazing incidence diffraction, differences are noted: they mainly refer to the static atomic displacements, being smaller in magnitude in the bulk than in the near-surface region. Effective pair interaction parameters show a dominant nearest-neighbor parameter, larger than that on the Pt-rich side. This is reflected in different order-disorder transition temperatures for Ni with 25 and 75 at.% Pt ($L1_2$ structure). First-principles electronic structure calculations support these findings.

MM 59.3 Thu 14:30 H5

Bonding in boron: building high-pressure phases from boron sheets — •Jens Kunstmann[1], Lilia Boeri[2], and Jens Kortus[3] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, Germany — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany — [3]Institute for Theoretical Physics, TU Bergakademie Freiberg, Germany

We present the results of a study of the high pressure phase diagram of elemental boron, using full-potential density functional calculations. We show that at high pressures (P > 100 GPa) boron crystallizes in quasi-layered bulk phases, characterized by in-plane multicenter bonds and out-of-plane unidimensional sigma bonds. These structures are all metallic, in contrast to the low-pressure icosahedral ones, which are semiconducting. We show that the structure and bonding of layered bulk phases can be easily described in terms of single puckered boron sheets [1]. Our results bridge the gap between boron nanostructures and bulk phases. [1] Kunstmann et al., Phys. Rev. B 74, 035413 (2006).

MM 59.4 Thu 14:45 H5

Memory Effects in Confined Fluids via Diffusion Measurement — •Sergej Naumov, Rustem Valiullin, and Jörg Kärger — Universität Leipzig, Fak. Phys, u. Geowiss., Linnestr. 5, 04105, Deutschland

The detailed knowledge about the molecular transport in nanoporous materials is of enormous importance for the industrial applications. The transport of molecules in the nanopores can be affected by gas-liquid phase transitions. The latter are often accompanied by adsorption hysteresis, i.e., the concentration of the molecules inside the pores depends not only on the external parameters like gas pressure or temperature, but also on the history how the external parameters have been varied. The evolution of the fluid state may be probed by means of Pulsed Field Gradient NMR which can trace the amount adsorbed simultaneously with the self-diffusion coefficients of the molecules [1]. The thus obtained self-diffusivities are found to depend not only on fluid concentration, but also on the history how a particular concentration has been attained [2].

[1] Naumov, S.; Valiullin, R.; Monson, P. A.; Kärger, J., Langmuir, 2008, 24, 6429-6432

[2] Valiullin, R.; Naumov, S.; Galvosas, P.; Kärger, J.; Woo, H.; Porcheron, F.; Monson, P. A. Nature, 2006, 443, 965-968

MM 59.5 Thu 15:00 H5

Microstructure simulations of porous media, of cell motion in flow fields and the interaction with structured surfaces — •Britta Nestler, Ali Aksi, Michael Selzer, Marcus Jainta, and Frank Wendler — Institute of Materials and Processes, Karlsruhe University of Applied Sciences, Karlsruhe, Germany

A Lattice-Boltzmann method for modelling fluid flow is coupled with the dynamic equations of a phase-field model for phase transformations and microstructure evolutions in multiple order parameter systems. The model contains a formulation for phases with preserved volume fractions and an extension for considering pressure differences in the various phase regions. The combined approach is applied to dry and wet foams and to computationally evaluate the permeability and microporosity in porous media. At the phase boundaries, we employ a smooth formulation of a bounce-back condition related to the diffuse interface profile. Simulations of fluid flow in static porous media with stationary non-moving interfaces and in microstructures performing a dynamic evolution of the boundaries are presented. We further study the motion of particles in a shear flow and measure the effective viscosity of the fluid for different particle distributions, channel geometries, volume fractions and properties of the fluid. The method is also capable to investigate the behaviour of liquid droplets on top of structured surfaces. The results are compared with experiments related to the Lotus effect for different surface energies and contact angles in the presence and absence of fluid flow.