MM 31 Symposium Materials Modelling I

Time: Thursday 10:15–13:00											Room: IFW A

Keynote Talk									MM 31.1 Thu 10:15 IFW A

Metallic nanoparticles: Challenging objects for computer simulations — •KARSTEN ALBE — TU Darmstadt, Fachbereich Material- und Geowissenschaften, Petersenstr. 23, D-64287 Darmstadt

Metallic nanoparticles play an important role in many functional devices and can also be used as building blocks for nanocrystalline materials. Because of their finite size they exhibit peculiar structural, thermodynamic and functional properties that are not fully understood and in many cases difficult to reconcile with perceptions established for bulk materials. At this point computer simulations can serve as a valuable tool for gaining a better understanding of particle structure and properties as well as processing conditions. Although continuum models that include particle size as additional variable are applicable in some instances, atomic scale models appear to be the more appropriate choice for computer simulations of such finite objects. Nanoparticles, however, typically consist of several thousands of atoms and therefore are computationally too demanding for nowadays quantum mechanical methods. In this talk I will briefly present strategies how efficient, yet reliable, hamiltonians can be derived from first principles, that make atomic scale modelling feasible. Then a number of results obtained from molecular dynamics simulations on nanoparticle formation in the gas phase and nanoparticle-surface interactions will discussed. Finally, I will show lattice Monte-Carlo simulations that help to gain insights into the thermodynamics and kinetics of binary nanoalloys.

MM 31.2 Thu 10:45 IFW A

A Multi-lattice kinetic Monte Carlo study on the activation enthalpies for the interface mobility and interphase boundary diffusion in a massive transformation in iron — •CORNELIS BOS, FERDINAND SOMMER, and ERIC-JAN MITTEMEIJER — Max Planck Institute for Metals Research, Heisenbergstrasse 3, D-70569 Stuttgart

Multi-lattice kinetic Monte Carlo simulations of lateral growth of ferrite in a massive austenite to ferrite transformation in iron were performed with a variable jump specific activation energy taking the local surroundings of the jumping atoms into account. From the simulations the activation enthalpy for the interface mobility and the migration activation enthalpy for interphase boundary diffusion were determined. It is shown that, depending on the interface structure the interface migration activation enthalpy can be larger or smaller than the migration activation enthalpy for boundary diffusion.

MM 31.3 Thu 11:00 IFW A

Ordering and correlation of cluster orientations in CaCd$_6$ — •PETER BROMMER[1], FRANZ GÄHLER[1], and MAREK MIHALKOVIČ[2] — [1]Unversität Stuttgart, Institut für Theoretische und Angewandte Physik, 70550 Stuttgart, Germany — [2]Slovak Academy of Sciences, Institute of Physics, 84511 Bratislava, Slovakia

Cadmium and Calcium form a wide variety of complex alloy phases up to an icosahedral quasicrystal. The 1/1 approximant, a bcc arrangement of multi-shelled clusters, shows an order-disorder transition at around 100 K, probably caused by reorientation of the innermost, tetrahedral shell. We use molecular dynamics and EAM potentials generated by force matching to study this transition. Firstly, we isolated the 48 optimal locations for the tetrahedron atoms, out of which four are occupied. We then determined the ground state of a single cluster. From experiment it is known that the tetrahedron orientation in neighbouring clusters is correlated. By developing an effective cluster bond Hamiltonian we can explain the ordering and correlation of the cluster orientations in CaCd$_6$.

Keynote Talk									MM 31.4 Thu 11:45 IFW A

Atomic-scale modelling of austenitic stainless steel — •HANS L. SKRIVER — CAMP, Technical University of Denmark

We have determined the stability of a ternary alloy of Fe, Cr, and Ni in the austenitic γ-FeNi phase including interstitial nitrogen and carbon by a variety of computational methods and approximations: the full charge density Exact Muffin-tin Orbitals (EMTO) method for accurate determination of formation energies, the order-N Locally Self-consistent Green Function (LSGF) method for efficient treatment of large supercells with a single interstitial nitrogen atom, and the Linear Muffin-Tin Orbitals (LMTO) method in conjunction with the Coherent Potential Approximation (CPA) and the Generalized Perturbation Method (GPM) for the calculation of the effective cluster interactions used in Monte Carlo simulations.

We find that the stability of nitrogen and carbon in the octahedral sites depends mainly on the number of Cr atoms in the first coordination shell. The calculated relative solution energies of nitrogen in γ-FeNi as a function of the local octahedral configuration and the abundance of the different octahedral configurations obtained in the Monte Carlo simulations as a function of temperature form the basis for a discussion of the experimental uptake curves for nitrogen in stainless steel.

Keynote Talk									MM 31.5 Thu 12:15 IFW A

Bond-Order Potentials: Bridging the electronic-atomistic modeling hierarchies in materials science — •RALF DRAUTZ and DAVID PETTIFOR — Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, United Kingdom

Quantum mechanical ab-initio methods are restricted to small numbers of atoms. Classical interatomic potentials, such as Tersoff, embedded atom (EAM), or Finnis Sinclair (FS) can simulate large numbers of atoms but their empirical character can render them inaccurate. In this talk we outline the derivation of interatomic bond-order potentials (BOPs) for sp-valent systems and d-valent transition metals by two well defined approximations within density functional theory. The resulting BOPs include a systematic variation of the bond order with valence [1] and are therefore applicable to a wide range of sp-valent and non-magnetic d-valent multicomponent systems. We demonstrate that the BOPs contain the Tersoff and EAM/FS potentials at the lowest order of approximation. [1] Drautz et al., Phys. Rev. B 72, 144105 (2005).

MM 31.6 Thu 12:45 IFW A

Effective potentials and dynamic fracture: C15 NbCr$_2$ — •FROHMUT RÖSCH and HANS-RAINER TREBIN — Universität Stuttgart, Institut für Theoretische und Angewandte Physik, 70550 Stuttgart

As fracture is ultimately determined by the breaking of bonds, an understanding of the fundamental mechanisms is required on the atomic level. To study such processes we perform molecular dynamics simulations on the Friauf-Laves phase C15 NbCr$_2$. For the interatomic interactions we match effective potentials to ab-initio data for the compound. Potentials for the elemental metals from the literature are also used for comparison. Ab-initio and experimental data indicate that our potentials are reliable and outperform available potentials making predictions on crack propagation reasonable. Fracture behaviour for the different potentials is discussed.