

## MM 28: Topical Session Electron Theory III

Time: Wednesday 15:45–17:15

Location: IFW A

MM 28.1 Wed 15:45 IFW A

**Parameterization of bond-order potentials from first principles** — MARTIN REESE<sup>1,2</sup>, ●MATOUS MROVEC<sup>2,1</sup>, CHRISTIAN ELSÄSSER<sup>2,1</sup>, ALEXANDER URBAN<sup>3</sup>, and BERND MEYER<sup>3</sup> — <sup>1</sup>IZBS, Karlsruhe Institut of Technology, Karlsruhe, Germany — <sup>2</sup>Fraunhofer IWM, Freiburg, Germany — <sup>3</sup>ICMM and CCC, University of Erlangen-Nürnberg, Erlangen, Germany

Bond-order potentials (BOPs) provide a real-space semi-empirical description of interactions between atoms based on the chemically intuitive tight-binding approximation for the electronic structure. The BOP approach offers two key advantages that are crucial for a successful modeling of extended crystal defects in covalent materials and transition metals. First, due to its quantum mechanical character it conveys a physically sound description of chemical bonding rather than ad hoc functional forms, which are common to classical empirical interatomic potentials. Second, its real space parameterization and computationally linear scaling enables to carry out computer simulations of large and complex systems, which are usually inaccessible to rigorous first-principles density-functional-theory (DFT) methods. We will present a recently developed atomic-orbital-projection approach that enables to construct BOPs for transition metals and their compounds in a rigorous manner from DFT results via tight-binding models. The success of these BOPs will be demonstrated on studies of extended defects, in particular lattice dislocations and grain boundaries.

MM 28.2 Wed 16:00 IFW A

**Bond-Order Potentials for bcc Transition Metals Niobium and Tungsten** — ●MIROSLAV ČAK, THOMAS HAMMERSCHMIDT, and RALF DRAUTZ — ICAMS, Ruhr Universität Bochum

Bond-order potentials (BOPs) are derived from the tight-binding approximation by expanding the density of states in local moments contributions. The BOPs provide comparable accuracy as tight-binding at less computational cost and a better scaling behavior. While the previously developed BOPs involve numerical evaluation of the response (Green's) function, the expressions for the bond energy and related interatomic forces are analytical within the formalism of the analytic BOPs. In this contribution, we present the parametrisation of analytic BOPs for the bcc transition metals Niobium and Tungsten. The parameters were optimised for the equilibrium bcc structure and extensively tested for atomic environments far from equilibrium that have not been considered in the fitting procedure. These tests include structural energy differences for competing structures; tetragonal, trigonal, hexagonal and orthorhombic deformation paths; formation energies of point defects and phonon dispersion relations. Comparison of these calculations with corresponding calculations using density-functional theory and numerical BOPs demonstrates a very good transferability of our analytic BOPs to atomic structures of experimentally relevant complexity.

**Topical Talk**

MM 28.3 Wed 16:15 IFW A

**Hydrogen in metals, atomic defects in crystals, and wetting phenomena. - The benefit of using density functional theory** — ●LOTHAR SCHIMMELE — Max-Planck-Institut für Metallforschung, Stuttgart, Germany

Examples from three different research areas will be discussed in order to demonstrate how ab-initio electron theory can contribute to a quantitative understanding of complex physical behaviour of materials if it is used in combination with theoretical models, statistical mechanics, and experiment.

For a proper description of hydrogen in solids quantum effects on the nuclear motion have to be included in the modelling. Some methods and simple results are presented.

In order to quantify, e.g., concentrations of atomic defects a statistical theory of defect equilibria is required.

Finally some ideas as to a systematic route from ab-initio investigations to a mesoscopic and macroscopic description of capillarity are presented.

MM 28.4 Wed 16:45 IFW A

**First-principles simulations of H interstitials within  $\Sigma 3$  and  $\Sigma 5$  grain boundaries in bcc Fe** — ●YAOJUN DU, JUTTA ROGAL, and RALF DRAUTZ — ICAMS, Ruhr-Universität, Bochum, Germany

Hydrogen impurities in steels can degrade the mechanical properties of the host material. Due to the complex nature of hydrogen-embrittlement (HE), the underlying HE mechanism has not been fully understood. One possible cause is that H impurities may weaken the bonding of Fe atoms near the grain boundaries, leading to an embrittlement of the bulk material. In this work, we study the interaction of H interstitials with  $\Sigma 3$  and  $\Sigma 5$  grain boundaries (GBs) in bcc Fe, and investigate the migration processes of H within the GBs, using density functional theory. Our results indicate that the GBs that we studied provide energy traps of 0.4-0.5 eV for H interstitials, and these trapped H interstitials may facilitate the crack growth at the GB interface. For the  $\Sigma 5$  bcc Fe GB we find that the fast diffusing H within Fe bulk region can be readily trapped to the GB interface with an escape barrier of 0.6 eV. On the other hand, the trapped H interstitial can perform a relatively slow migration within the interface with a diffusion barrier of 0.25 eV. We are now carefully computing the transition rates among inequivalent H sites within the  $\Sigma 5$  bcc Fe GB. These results will serve as input for a lattice kinetic Monte Carlo model to study the dynamics of H diffusion in the vicinity of the GB.

MM 28.5 Wed 17:00 IFW A

**Effect of H on homogeneous dislocation nucleation: Consequences for hydrogen embrittlement** — ●JOHANN VON PEZOLD and JÖRG NEUGEBAUER — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

The embrittlement of modern high-strength steels is commonly explained by the HELP (Hydrogen-Enhanced Local Plasticity) mechanism. In its original form this mechanism attributes the embrittlement to a localized increase in plasticity resulting from a hydrogen-induced shielding of the stress fields of pre-existing dislocations. Recent in situ electrochemical nano-indentation experiments [1] suggest that H also reduces the critical shear stress for the homogeneous nucleation of dislocations in a range of metals. The observed reduction in the critical shear stress was correlated to a H-induced decrease in the stacking fault energy and/or shear modulus of the host material, as well as an increased dislocation core radius. In this study the model is evaluated using density-functional theory. In particular, the effect of H on the shear modulus and the stacking fault energy in Al, Ni and Cu was determined. Preliminary results indicate a significant reduction in the shear modulus and a moderate reduction in the stacking fault energy with increasing H content, in line with the originally proposed model. Whether or not the observed reduction in the critical shear stress for the dislocation nucleation can be explained by this model will depend on the H solubility under the elevated H chemical potential conditions in the in situ nano-indentation experiments.

[1] A. Barnoush and H. Vehoff, Acta. Mat. 58, 5274 (2010).