MM 4: Topical Session Designing Innovative Structural Materials and Steels II

Time: Monday 11:30–12:45 Location: H4

MM 4.1 Mon 11:30 H4

From atoms to materials: one billion atoms with DFT accuracy — •Tobias Kerscher[1], Stefan Müller[1], Gus Hart[2], and Quinn Snell[3] — [1]Universität Erlangen-Nürnberg, Lehrstuhl für Theoretische Physik 2, Staudtstr. 7, 91058 Erlangen, Germany — [2]Brigham Young University, Department of Physics and Astronomy, Provo UT 84602, USA — [3]Brigham Young University, Computer Science Department, Provo UT 84602, USA

We use an ab-initio-based cluster-expansion Hamiltonian (see e.g. [1]) to bridge the gap in length-scales between atomistic density-functional calculations ($\sim 10^3$ atoms at $T = 0$ K) and macroscopic materials ($\sim 10^9$ atoms at $T > 0$ K). To this end, our code UNCLE [2] comprises a weak-scaling parallel Monte-Carlo algorithm, which enables us to perform large-scale simulations with the cluster-expansion's ab-initio precision. We demonstrate the effectiveness of the algorithm by a simple 2d Ising model, and apply it on the macroscopic scale ($\sim 0.3\,\mu$m) to the ternary bulk system $Ni_{48}Al_{50}$ with one billion atomic sites.
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[1] S. Müller, J. Phys.: Condens. Matter **15** (2003), R1429
[2] D. Lerch *et al*, Modelling Simul. Mater. Sci. Eng. **17** (2009), 055003

MM 4.2 Mon 11:45 H4

From DFT via TB to BOP: Atomistic simulations with ab-initio derived bond order potentials — •Martin Reese[1,2], Matous Mrovec[1,2], Bernd Meyer[3], and Christian Elsässer[1,2] — [1]Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg — [2]IZBS, Universität Karlsruhe — [3]ICMM, Universität Erlangen-Nürnberg

Nanostructered composites of crystalline and amorphous carbides and nitrides can yield materials that reach the limit of super-hardness. These unusual properties are related to a subtle balance between the amorphous and crystalline phases and the properties of interfaces at the nanometer level. Atomistic simulations can significantly contribute to a better understanding of these complex materials provided that the employed models of atomic interactions are robust and reliable.

In this work we present a bottom-up procedure, which enables a development of ab-initio derived analytic bond-order potentials (BOPs). First, by projecting the self-consistent electronic wave functions from density functional theory onto a minimum basis of atomic orbitals we construct tight-binding models, which retain the crucial aspects of electronic structure. These are then further coarse-grained into a form of the interatomic BOPs, which describe correctly the interatomic bonding and are computationally efficient.

The procedure will be demonstrated for C-H and C-Si systems. The performance and transferability of the constructed BOPs on various complex structures will be presented.

MM 4.3 Mon 12:00 H4

Ab initio determination of the magnetic free energy contribution of metallic systems — •Fritz Körmann, Alexey Dick, Blazej Grabowski, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

An accurate prediction of the free energy is the basis to compute phase diagrams, finite temperature materials parameters, or kinetic barriers and is thus fundamental in computational materials design. One of the most challenging contributions - but crucial for many engineering materials - is the magnetic entropy. The most popular ab initio approach for the latter is the use of an effective Heisenberg model solved using classical Monte Carlo (cMC) approaches and neglecting quantum effects. We discuss the impact of the latter based on extensive model calculations where Quantum MC calculations are available. An empirical rescaling scheme is derived allowing to considerably improve the cMC. The method is applicable to strong ferromagnetic systems with magnetic frustration is absent or weak. The application and performance of the new approach is demonstrated for pure Fe.

MM 4.4 Mon 12:15 H4

Sensitivity of the stacking fault energy in FeMn alloys on the local environment: A first-principles study — •Alexey Dick, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany

An in-depth understanding of the physical processes that may influence the stacking fault energy (SFE) is necessary for a knowledge-based optimization and engineering of high-Mn-steels. We have performed a first-principles study of the SFE in austenitic FeMn-alloys, which are prototype structures for realistic high-Mn-steels. The relevant atomic configurations have been identified by combination of the cluster-expansion methodology and the concept of special quasirandom structures based on the density functional theory calculations. Employing either the axial interaction model and/or explicit calculations of the generalized SFE surfaces we show that the value of the SFE sensitively depends on type of the chemical and magnetic ordering in the system. We further show that the SFE can be changed not only by varying the composition of the FeMn-alloy or its temperature, but also by admixing different chemical elements or by controlling local strain fields.

MM 4.5 Mon 12:30 H4

DFT-based calculation of temperature-dependent stacking fault energy in the Fe-Mn alloy — •Andrei Reyes-Huamantinco[1,2], Andrei Ruban[3], Peter Puschnig[1], and Claudia Ambrosch-Draxl[1] — [1]Chair of Atomistic Modelling and Design of Materials, University of Leoben, Austria — [2]Materials Center Leoben, Austria — [3]Applied Material Physics, Royal Institute of Technology, Stockholm, Sweden

We have studied the Fe-22.5at.%Mn alloy in the temperature range between 300 and 800 K. The random alloy in the paramagnetic state was modelled by the coherent potential approximation (CPA) and the disordered local moment (DLM) approach. The DFT-calculations were carried out using the exact muffin-tin orbitals (EMTO) method. Temperature-dependent lattice parameter and local magnetic moment were used in constrained DFT-calculations. The former was obtained from measurements, while the latter was calculated through a longitudinal spin-fluctuation (LSF) Hamiltonian in combination with Monte Carlo simulations. The stacking fault energy (SFE) was expanded in terms of free energies of the fcc, hcp and dhcp structures, including electronic and magnetic entropies. We find that the SFE increases by 17 mJ/m^2 between 300 and 600 K, and that the hcp/fcc transformation temperature is 390 K, in agreement with experiments.