MM 10: Computational Materials Modelling II - Theory/Numerics

Time: Monday 11:45–13:15 Location: IFW D

MM 10.1 Mon 11:45 IFW D

Accurate ab-initio elastic properties at 0K and above: The ElaStic tool — •Jürgen Spitaler[1], Rostam Golesorkhtabar[2], Pasquale Pavone[2], Claudia Draxl[2], and Peter Puschnig[3] — [1]Materials Center Leoben Forschung GmbH, Roseggerstr. 12, 8700 Leoben, Austria — [2]Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [3]Institut für Physik, Karl-Franzens-Universität Graz, Universitätsplatz 5, 8010 Graz, Austria

Elastic properties are a key for understanding the mechanical behavior of materials. ElaStic [1] greatly facilitates a reliably determination of elastic constants for materials with any lattice type from first-principles. Results for various materials at 0K will be presented, including systems with low symmetry. At the same time, some nuts and bolts of elastic-constant calculations will be discussed. We will show, how the formalism can be extended towards finite temperatures, either implicitly via the lattice expansion, or explicitly by fitting free energy versus strain. Its application will be demonstrated for a prototypical example.

[1] R. Golesorkhtabar, P. Pavone, J. Spitaler, P. Puschnig, and C. Draxl, Comp. Phys. Commun. 184 (2013), 1861

MM 10.2 Mon 12:00 IFW D

KKR*nano*: DFT for nano-scale systems — •Elias Rabel, Rudolf Zeller, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich

The screened KKR Green's function method has been implemented in our code KKR*nano* [1] for all-electron DFT calculations of unit cells containing thousands of atoms. KKR*nano* has been successfully applied in the study of phase-change materials and dilute magnetic semiconductors. The KKR method considers multiple scattering of partial waves up to a maximal angular momentum $\ell_{\max}$. Motivated by the idea that at long-range low ℓ-components dominate the scattering, we employ a distance dependent angular momentum cut-off of the Green's function to reduce the effective matrix size with little compromise in accuracy. The special case of neglecting all partial waves scattered from reasonably large distances leads to an $O(N)$-scaling method. Combining this approach with the capacities of present day supercomputers, DFT calculations of more than 100000 atoms become technically feasible. The question of attaining sufficiently accurate, self-consistent solutions has to be addressed. We present extensions of the program for calculations of amorphous structures and structural relaxations.

[1] A. Thiess et al., Phys. Rev. B **85**, 235103 (2012).

MM 10.3 Mon 12:15 IFW D

Large scale supercell calculations for forces around substitutional defects in NiTi — •Rudolf Zeller — IAS-3, Forschungszentrum Jülich GmbH

Density functional calculations are used to investigate the force field arising from substitutional Ni and Cu defect atoms on Ti sites in the shape memory alloy NiTi. The forces for the unrelaxed atomic positions are calculated by the Korringa-Kohn-Rostoker (KKR) Green-function method for the experimentally found monoclinic B19' ground state structure. The force pattern in the vicinity of the defect atoms is markedly different between 32-atom and 256-atom supercells while it is nearly the same between 256-atom and 2048-atom supercells. This difference is explained by symmetry arguments and its possible implication on the concentration dependence of the transition from the high temperature B2 phase to the low temperature B19' or strain glass phases is discussed.

MM 10.4 Mon 12:30 IFW D

Analytic Bond-Order Potential for Fe and Fe-C — •Sebastian Schreiber, Thomas Hammerschmidt, and Ralf Drautz — Ruhr-Universität Bochum, Universitätsstr. 150, 44801 Bochum

The analytic bond-order potential (BOP) is an interatomic potential, that provides a linear scaling solution to the tight-binding (TB) energy. It includes itinerant magnetism and charge transfer explicitly and may be viewed as a systematic extension of second-moment models (e.g. Finnis-Sinclair) to include higher moment contributions. In the analytic BOPs the bond-order, the density of states, the atomic magnetic moments and charges adjust self-consistently according to the atomic environment. The analytic BOP also provides exact derivatives of the energy for calculating forces and stress.

Here, we demonstrate the transferability of recently developed TB models for Fe and Fe-C to the analytic BOP formalism. We present BOP simulations for core structures and Peierls barriers of a/2[111]-screw-dislocations in α-Fe. We also discuss the interaction of these line-defects with carbon impurity atoms and its impact on plastic deformation.

MM 10.5 Mon 12:45 IFW D

Efficient implementation of analytic bond-order potentials — •Thomas Hammerschmidt[1], Sebastian Schreiber[1], Bernhard Seiser[2], Michael Ford[2], David Pettifor[2], and Ralf Drautz[1] — [1]ICAMS, Ruhr-Universität Bochum, Germany — [2]MML, University of Oxford, United Kingdom

The bond-order potentials (BOPs) are based on tight-binding (TB) models that are derived from density-functional theory. The BOPs provide an approximation to the TB energy that can be systematically improved by increasing the number of moments considered in the expansion. At the lowest level of two moments, the BOPs are equivalent to the Finnis-Sinclair potential and the closely related embedded-atom method. By taking into account higher moment contributions a systematic convergence to the TB energy is observed. We present an efficient implementation of analytic BOPs in close connection to a review of the BOP methodology. We will particularly discuss the fast identification of self-returning hoppings paths, the linear-scaling implementation of analytic forces and the performance of different self-consistency schemes. We will present recent results for several materials to illustrate the application to large-scale simulations.

MM 10.6 Mon 13:00 IFW D

Self-energy electronic structure renormalization effects in first-principles calculations of solids — •Alberto Marmodoro[1], Arthur Ernst[1], Paolo Trevisanutto[2], and Leonid Sandratskii[1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle — [2]Istituto Italiano di Tecnologia, Lecce

We report on a first-principles KKR-DFT calculation scheme for the evaluation of finite relaxation time and general bands structure renormalization effects for electrons in a solid. These are expressed in terms of an ad-hoc self-energy term on top of a reference hamiltonian, to which higher order corrections may be added. The case of substitutional disorder represents a well-known possible mechanism that gives raise to such phenomenology, here further pursued in the particular direction of including low-lying excitations above the globally colinear magnetic ground state of a magnetic material.