MM 8: Computational Materials Modelling II - Methods

Time: Monday 11:45–13:00 Location: TC 006

MM 8.1 Mon 11:45 TC 006

Discontinuous epitaxial Bain paths and consequences for coherent epitaxial growth — •Stephan Schönecker, Manuel Richter, Klaus Koepernik, and Helmut Eschrig — IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

Strained coherent epitaxy is a valuable mean to influence structural, electronic, magnetic and optical properties of bulk-like films as a function of symmetry and in-plane lattice spacings of the substrate. A remarkable example are 50 nm thick films of body centred tetragonal (BCT) $Fe_{70}Pd_{30}$, whose ferromagnetic properties, e.g. magnetic moment and magnetic anisotropy, can be tuned by the choice of the substrate (Buschbeck *et al.*, PRL **103**, 216101 (2009)). This tuning extends over a wide range of tetragonal distortion in the film, $1.09 \leq c/a \leq 1.54$ (Kaufmann-Weiss *et al.*, PRL **107**, 206105 (2011)).

From the point of theory, an epitaxial Bain path (EBP) models the bulk part (i.e. the interior) of films in BCT structure coherently grown on substrates with four-fold symmetry by establishing a relationship between the substrate lattice parameter, a, and the out-of-plane lattice parameter of the film, c (Alippi *et al.*, PRL **78**, 3892 (1997)). We show in this contribution using several examples of the transition metal family, that c need not be a continuous function of a, hence the c/a ratio in BCT films of these elements cannot continuously be adjusted giving rise to a discontinuous EBP. Calculations of the electronic structure in the framework of density functional theory were carried out in the implementation of the full potential local orbital program package FPLO (www.fplo.de).

MM 8.2 Mon 12:00 TC 006

An evolution strategy for crystal structure prediction — •Silvia Bahmann, Thomas Gruber, and Jens Kortus — TU Bergakademie Freiberg, Institute for Theoretical Physics, Leipziger Str. 23, 09596 Freiberg, Germany

The crystal structure determines many physical properties. For materials design of new systems with a given chemical composition one therefore needs the ability to predict possible crystal structures. The challenge in this prediction lies in the facts that it is a global search in a search space that grows exponentially with the number of atoms per unit cell and the unknown energy landscape containing several minima.

Our evolutionary strategy uses the main features of natural evolution - recombination, mutation, selection and the survival of the fittest - to global search. The crystal structures represent the individuals in this picture whereas their fitness value is determined by calculating the free energy of the individual using electronic structure programs. The individual having the minimal free energy in the whole search space is considered to be the most stable structure. The combination of the effective local optimisation already implemented in electronic structure programs with stochastic elements of the evolution strategy ensures an efficient search.

We present the developed evolution strategy designed for general 3D crystal structure prediction that also features the search of 2-dimensional structures. As an application we focus here on the search for 3D structures of lithium-silicides that are promising for new electrode materials for lithium ion batteries.

MM 8.3 Mon 12:15 TC 006

Fingerprinting defects and structures in atomistic simulations — •Thomas Schablitzki, Jutta Rogal, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Bochum, Deutschland

Employing atomistic simulations to investigate structural phase transformations in solids is a challenging task. A prerequisite for analysing the simulation results is the ability to locally identify structures and structural features. It is then possible to find point and extended defects and to track e.g. the movement of an interface between two structures during a phase transformation. To address this problem we have implemented a polyhedron analysis method. Within our approach we analyse the local coordination polyhedra around each atom and establish a fingerprint that reflects the arrangements of polyhedra within the polyhedron network. The distribution of polyhedra in a structure together with the fingerprint then provides sufficient information to classify a given structure.

The polyhedron analysis method is based on the distinct geometrical features of complex phases that form in metal alloys. The formation and growth of such complex phases is of particular interest since they can significantly influence the materials properties. Insight on the atomistic level provides valuable information on the underlying microscopic processes. We have applied our polyhedron analysis in molecular dynamics and adaptive kinetic Monte Carlo simulations, to track vacancies, monitor phase growth, identify interfaces and follow their motion.

MM 8.4 Mon 12:30 TC 006

Transferable tight-binding description of the Fe-C interaction — •Nicholas Hatcher, Georg K. H. Madsen, and Ralf Drautz — ICAMS Ruhr-Universität Bochum, Stiepeler Strasse 129, 44801 Bochum, Germany

A coherent transferable tight-binding (TB) parameterization including magnetism has yet to be developed for the Fe-C interaction. Although interatomic potentials have been obtained for this system, recent findings show that the results from these potentials are inconsistent with DFT calculations and do not give an accurate portrayal of chemical bonding in the system. Using dual DFT grid and LCAO calculations within GPAW, we obtain one electron wave functions expanded in a multiple-ζ LCAO basis. This is then down-folded onto an optimal minimal basis, giving a continuous and transferable description of Fe-C bonding. By constructing a TB energy functional using these bond integrals and a parameterized interatomic repulsion, we show how an accurate description of the energy hierarchy of interstitial carbon in Fe-structures can be achieved. Furthermore, we use the model to calculate elastic properties and energies of a variety of Fe-carbides, defects, and carbon diffusion paths. This simple model based on physical insights may be used to study systems containing thousands of atoms.

MM 8.5 Mon 12:45 TC 006

A novel minimum search method for complex optimization problems — •Julian Hirschfeld and Hans Lustfeld — Forschungszentrum Jülich, IAS-1 and PGI-1, Jülich, Germany

Optimization is essential in many scientific and economical areas, as well as in the development of products. In many cases the optimization problem is too complex to be tackled by simple straight forward calculations or by trial and error. The reason is the too large phase space of the optimization problem and a rough potential surface with too many local minima. To find the global minimum, or at least a representative one, there are methods like simulated annealing, which has the chance to escape local minima, or the genetic algorithm, which changes the configurations by combining subsets of different deep minima. The chance to get stuck in a local minimum or to escape is proportional to the depth of the minimum in these methods.

Here we present a new method, which is complementary to the established ones. The chance to get stuck in a local minimum or to escape is independent of the minimum's depth but depends on the minimum's attractor size. Therefore, it can overcome local minima and high barriers equally well. Even though it does not get stuck in local minima of small attractor size, it is especially advantageous when searching for a minimum with a small basin of attraction. We successfully applied the method to find the ground states of the phosphorus P_4 and P_8 molecules as well as the arsenic As_4 and As_8 molecules. In the case of P_8 we were able to find a new stable configuration.