MM 43: Materials Design I

Time: Wednesday 14:45–16:00 Location: H5

MM 43.1 Wed 14:45 H5

Prediction by means of an evolutionary algorithm and stability of boron sheet structures — •Silvia Schumann and Jens Kortus — TU Bergakademie Freiberg, Institute for Theoretical Physics, Leipziger Str. 23, 09596 Freiberg, Germany

There is great interest in designing new nano materials which drives theory and experiment. Similar to carbon nanotubes and graphene there are some theoretical efforts investigating boron sheets and nanotubes. So far there are no boron sheet structures found in experiment but several sheets are suggested by theory.

We present additional work in the field of predicting boron sheets as a pre-stage to boron nanotubes. Additional to analysing already known structures we used an evolutionary algorithm reproducing those structures or discovering new boron sheets. This algorithm produces a randomly chosen population of sheets which are evaluated using pseudopotentials and plane waves to compute the free energy of each boron sheet. The more stable (lowest free energy) sheets are allowed to recombine and are mutated to form the sheets of the next generation. Promising sheets were treated with conventional structure relaxation to encounter slow convergence rates of evolutionary algorithms close to minima. We further investigated the found local minima in the energy landscape with respect to their stability by phonon calculations.

MM 43.2 Wed 15:00 H5

Stability and properties of Fe/ZrO_2 interfaces — •Jürgen Kutzner — TU Bergakademie Freiberg, Leipziger Str. 23, 09596 Freiberg

The stability of the Fe/ZrO_2 interface was investigated by means of density functional theory. In order to estimate surface energies we carried out calculations on pure phases of iron and ZrO_2 for several surface orientations and phases. Further, we compared total energies and mechanical properties of different possible interface structures to predict the most stable interface structure. In order to investigate the influence of chemical composition on these properties we replaced then the pure components to simulate a simplified steel and MgO stabilized ZrO_2.

We would like to thank the DFG for financial support within SFB 799: TRIP-Matrix-Composite.

MM 43.3 Wed 15:15 H5

Ab initio study of nano-precipitate nucleation and growth in ferritic steels — •Natalie Tillack, Tilmann Hickel, Dierk Raabe, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung, Düsseldorf

The hardness of metallic alloys can be substantially improved by inducing the formation of nano-precipitates having dimensions of only a few nm. To realize such structures, chemical compositions and process conditions have to be identified that lead to a spontaneous (self-organized) formation of such structures.

For the example of ferritic alloys we have therefore studied nucleation and growth of such nano-particles combining ab initio calculations and kinetic Monte Carlo simulations. As example we consider the alloy systems Fe-Ni-Mn and Fe-Cu-Si. Using density functional theory and two supercell approaches we determine in a first step formation and interaction energies of Ni, Cu, and Si atoms in an FeMn or an Fe matrix. Our calculations reveal a repulsive interaction for pairs of Ni atoms and Si atoms, whereas the Cu-Cu and the Cu-Si interaction is attractive.

The physical origin for the different behaviour has been investigated, with a particular focus on the charge distribution and relaxation effects in the considered supercells. In a second step the ab initio determined energies are used to construct the Master equation which is solved by a Monte Carlo approach. These simulations provide a very direct insight into the formation and size distribution of the nano-precipitates as function of alloy composition, temperature and the calculated energies.

MM 43.4 Wed 15:30 H5

Epitaxial Bain Path in Transition Metals — •Stephan Schönecker, Manuel Richter, Klaus Koepernik, and Helmut Eschrig — IFW Dresden, Helmholtzstrasse 20, 01069 Dresden, Germany

Epitaxial films grown pseudomorphically on substrates provide a way to stabilise non-equilibrium structures of materials. Obviously, there always is a certain lattice misfit between substrate and film material in its bulk equlilibrium structure. In the pseudomorphic regime, this misfit can either lead to the growth of films in a strained bulk structure or even yield structures that are not stable in the bulk. Large misfits do not necessarily imply large lateral stress. Theory can help to predict e.g. geometry, stress and magnetic properties of pseusomorphically grown metal films. In this work, we considered the fcc-bcc epitaxial Bain path (see Marcus *et al.*, PRB **66**, 064111 (2002)) of 3*d*, 4*d*, and 5*d* transition metals, which provides a reasonable description of tetragonally distorted films on substrates. We carried out density functional calculations in the implementation of the full potential local orbital program package FPLO (*www.fplo.de*). Emphasis is put on similarities among the transition metals.

MM 43.5 Wed 15:45 H5

On the Process of Structure Formation — •Peter Häussler — Chemnitz University of Technology, Institute of Physics, Thin Film Group, 09107 Chemnitz, Germany

While the formation of molecules is well understood the path crystalline matter gets formed is not. Liquid and amorphous systems are intermediate states. The fundamental processes causing their structural features may help us to understand the formation of long ranging crystalline order.

For elementary systems, irrespective wether they get formed from molecular or noble gases, from polyvalent elements, from elements with 3d- or even f-states at E_F, we could show, all along the Periodic Table, that structural features of the liquid state are formed under the influence of resonances between global subsystems as there are all the electrons as one, and the forming static structure as the other one. Both mutually adjust their internal parameters, causing medium-ranging spherical periodic order (SPO) in the mean around any atom.

We discuss resonances based on momentum exchange as the driving force, causing anti-bonding (non-equilibrium) as well as bonding (equilibrium) states, with a gap or pseudogap at E_F in-between, with all the conseqences on phase stability and electronic transport. We discuss the importance of the creation of entropy whenever the system transfers to the bonding state. Instead of a thermodynamical description only we apply General Dynamics, able to describe the formation of distances and angles, the indispensable ingredients of any description of structure formation.