MM 60: Computational Materials Modelling IX - Interfaces and Boundaries

Time: Thursday 17:15–19:00 Location: TC 006

MM 60.1 Thu 17:15 TC 006

Atomistic modelling of interfaces between cubic phases and complex phases in refractory metals — •Thomas Hammerschmidt, Miroslav Cak, Jutta Rogal, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Bochum, Germany

Topologically close-packed (TCP) phases play in important role in many modern alloys and steels. The TCP phase stability can be attributed to an interplay of bandfilling effects and differences in atomic size. In order to shed light on the precipitation of TCP phases, we study their interfaces to cubic phases. Here, we have chosen the interfaces bcc-A15 and fcc-σ due to their technological relevance in W thin films and in Ni-based superalloys, respectively. We investigate the interface formation energy by atomistic simulations with electronic structure methods at different levels of coarse-graining. On the tight-binding level, we employ simple canonical models to investigate relations between band-filling and interface structure. On the level of bond-order potentials (BOP), an approximation to the tight-binding scheme, we employ recently developed parametrisations for refractory metals. With the analytic BOPs we observe that the interface energy of a commensurate interface of multiple unit cells is minimised by a coincidence-site-lattice arrangement. We then minimise the interface energy with respect to the number of atoms by directly employing the atom-resolved binding energies of the analytic BOP. Our observation of a more densely packed interface for increased bandfilling can be attributed to a decrease in the covalent character of the bonds.

MM 60.2 Thu 17:30 TC 006

The stability of Bi-Te and Sb-Te layered structures: a first-principles study — •Kirsten Govaerts[1], Marcel H.F. Sluiter[2], Bart Partoens[3], and Dirk Lamoen[1] — [1]EMAT, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerpen, Belgium — [2]Department of Materials Science and Engineering, 3mE, Delft University of Technology, Mekelweg 2, 2628 CD, Delft, The Netherlands — [3]CMT group, Department of Physics, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerpen, Belgium

Using an effective one-dimensional cluster expansion in combination with first-principles electronic structure calculations we have studied the energetics and electronic properties of Bi-Te and Sb-Te layered systems. In order to get a fast convergence we used a (pseudo)ternary cluster expansion, which takes into account the formation of Sb or Bi bilayers after relaxation due to a Peierls distortion of the lattice. With this new method, groundstates of Bi-Te and Sb-Te can be found without making the dataset of ab initio calculated structures unreasonably large. For a Te concentration between 0 and 60 at.% an almost continuous series of (meta)stable structures is obtained consisting of consecutive X bilayers next to consecutive X_2Te_3 units, with X corresponding to Bi or Sb. Our calculations (at T = 0 K) do not show evidence for the existence of separate single phase regions. Metastable compounds with a Te concentration between 0 and 40 at.% are semimetallic, whereas compounds $(X_2)_n(X_2Te_3)_m$ $(n, m = 1, 2, ...)$ with a Te concentration between 50 and 60 at.% are semiconducting. Compounds with an odd number of consecutive X layers are metallic.

MM 60.3 Thu 17:45 TC 006

Interfaces of hybrid materials: Structure and properties of silylated TiO_2 surfaces — •Beatrix Elsner, Wolfgang Heckel, and Stefan Müller — Technische Universität Hamburg-Harburg, Institut für Keramische Hochleistungswerkstoffe, Denickestr. 15, D-21073 Hamburg

Silane coupling agents are commonly used to modify the interface properties of composite materials such as ceramic-polymer systems. The ability to control the interface stability is a key to modern materials design. Using density functional theory, we have investigated the adsorption characteristics of silane coupling agents on the low-index surfaces of rutile titanium dioxide. The resulting energetics are strongly linked to surface stability and adsorption geometry. We found that the less stable surfaces allow for higher coupling agent coverage as they contribute more dangling bonds to the adsorbate. Further the divergency from ideal silicon tetrahedral angles displays a strong influence on the binding energy. Hence a detailed knowledge of the atomic structure is crucial to understand the interface properties of hybrid systems.

MM 60.4 Thu 18:00 TC 006

Simulations of grain boundary migration via the nucleation and growth of islands — •Christopher Race, Johann von Pezold, and Joerg Neugebauer — Max-Planck-Institut fuer Eisenforschung, Duesseldorf, Deutschland

Classical molecular dynamics simulations of bicrystals have been much used to explore the motion of grain boundaries. Commonly, previous studies were designed to explore the large configurational space of possible grain boundary structures and so necessarily employed small simulation cells. In such small cells the whole area of the grain boundary is constrained to move simultaneously and so the boundary remains atomically flat. The formation of important features such as double kinks and islands is often absent.

We have therefore studied the motion of a symmetric tilt boundary in system sizes large enough to accommodate the nucleation and growth of stable islands of migrated crystal volume. We consider the effect of the driving force for grain boundary motion on the size of a critical island nucleus and on the energy barrier for its formation. Based on our results we identify two distinct regimes of mesoscale migration mechanism (island-based vs. flat) in terms of driving force and system size. We consider the implications of this insight for the interpretation of results of typical grain boundary simulations.

MM 60.5 Thu 18:15 TC 006

Hydrogen diffusion in Fe grain boundaries: A kinetic Monte Carlo study — •Yaojun A. Du[1], Jutta Rogal[2], and Ralf Drautz[2] — [1]Fakultät für Physik, Universität Duisburg-Essen, Lotharstraße 1, 47048 Duisburg, Germany — [2]ICAMS, Ruhr-Universität Bochum, 44780 Bochum, Germany

Hydrogen embrittlement in iron and steels is a complex problem that is still not fully understood. Structural defects in the material such as vacancies, grain boundaries, and dislocations can trap hydrogen and a local accumulation of hydrogen at these defects can lead to a degradation of the materials properties. An important aspect in obtaining insight into hydrogen embrittlement on the atomistic level is to understand the diffusion of hydrogen in these materials.

In our study we employ kinetic Monte Carlo (kMC) simulations to investigate hydrogen diffusion in bcc iron including the effect of different microstructures. All input data to the kMC model, such as available sites, solution energies, and diffusion barriers are based on *ab initio* calculations. In particular we consider an idealised cubic grain structure exhibiting bulk and interface sites, an idealised layered structure and a more realistic model of the $\Sigma5[001](310)$ grain boundary in bcc-Fe. We find that hydrogen mainly diffuses within the interface region with an overall diffusivity that is lower than in pure bcc-Fe bulk. To describe the macroscopic diffusion behaviour we derive an analytic expression as a function of hydrogen concentration and temperature which is in excellent agreement with our numerical results.

MM 60.6 Thu 18:30 TC 006

Interfacial layering of a room-temperature ionic liquid thin film on mica surfaces — •Daniele Dragoni[1], Nicola Manini[2], and Pietro Ballone[3] — [1]Theory and Simulation of Materials, École Polytechnique Fédérale de Lausanne — [2]Dipartimento di Fisica, Universitá degli Studi di Milano — [3]Atomistic Simulation Centre, Queen's University Belfast.

We investigate the structure of a thin (4 nm) [bmim][Tf_2N] film on mica by molecular-dynamics simulations using an empirical force field. Interfacial layering at $T = 300$ K and at $T = 350$ K is investigated by determining the number- and charge-density profiles of [bmim][Tf_2N] as a function of distance from mica, and by computing the normal force F_z opposing the penetration of the ionic liquid film by a hard nanometric tip, represented by a spherical particle interacting with [bmim][Tf_2N] atoms by a short range potential. The results show that layering is important but localized within ~ 1 nm from the interface. The addition of a surface charge on mica, globally neutralised by an opposite charge on the [bmim][Tf_2N] side, gives rise to low-amplitude charge oscillations extending through the entire film. However, outside a narrow interfacial region, the resistance of the [bmim][Tf_2N] film to penetration by the mesoscopic tip is only marginally affected by the charge at the interface. The results obtained here for [bmim][Tf_2N]/mica are similar to those obtained using the same method for the [bmim][Tf_2N]/silica interface, and agree reasonably well with experimental force-distance profiles measured on this last interface at ambient conditions.

MM 60.7 Thu 18:45 TC 006

Dispersive and Covalent Interactions Between Graphene and Metal Surfaces from the random phase approximation —

•Thomas Olsen — Technical University of Denmark

The potential energy surfaces for graphene adsorbed on Cu(111), Ni(111), and Co(0001) have been calculated using density functional theory and the Random Phase approximation (RPA) (PRL 107 156401). For these adsorption systems covalent and dispersive interactions are equally important and while commonly used approximations for exchange-correlation functionals give inadequate descriptions of either van der Waals or chemical bonds, RPA accounts accurately for both. It is found that the adsorption is a delicate competition between a weak chemisorption minimum close to the surface and a physisorption minimum further from the surface.