MM 19: Methods in Computational Materials Modelling I: Materials Design

Time: Tuesday 10:15–11:45 Location: H 0106

MM 19.1 Tue 10:15 H 0106

Theory-guided design of high-strength superlattices containing metastable phases: example of nano-scale CrN/AlN — •Martin Friák[1,2], Darius Tytko[1], David Holec[3], Pyuck-Pa Choi[1], Philip Eisenlohr[1], Dierk Raabe[1], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, v.v.i., Brno, Czech Republic — [3]Montanuniversität Leoben, Leoben, Austria

A theory-guided materials design of nano-scaled superlattices containing metastable phases is critically important for future development of advanced lamellar composites. Our study combining theoretical and experimental methods exemplifies this approach in the case of elastic properties of AlN/CrN superlattices with a bilayer period of 4 nm in which CrN stabilizes AlN in a metastable B1 cubic phase. As B1-AlN crystals do not exist as bulk material at ambient pressure, experimental data for this phase are not available. Therefore, quantum-mechanical calculations have been applied to simulate an AlN/CrN superlattice. The ab initio predicted Young's modulus (428 GPa) in a direction perpendicular to (001) oriented interfaces is in excellent agreement with measured nano-indentation value (408 +/- 24 GPa). Aiming at a future rapid high-throughput design of superlattices, we have also tested predictions obtained within linear-elasticity continuum modeling that employs elastic properties of B1-CrN and B1-AlN phases as input. Using single-crystal elastic constants from ab initio calculations for both phases, we discuss the accuracy of this approach, too.

MM 19.2 Tue 10:30 H 0106

Big Data of Materials Science - Critical Role of the Descriptor — •Luca M. Ghiringhelli[1], Jan Vybiral[2], Sergey V. Levchenko[1], Claudia Draxl[3], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin, DE — [2]Charles University, Prague, CZ — [3]Humboldt-Universität zu Berlin, Berlin, DE

Statistical learning of materials properties or functions so far starts with a largely silent, non-challenged step: the introduction of a multidimensional descriptor. However, when the scientific relationship of the descriptor to the actuating mechanisms is unclear, causality of the trained (learned) descriptor-property relation is uncertain. Thus, scientific advancement, trustful prediction of new promising materials and identification of anomalies is doubtful. We discuss and analyze this issue and define requirements for a descriptor that is suited for statistical learning of materials properties and functions. We show how a meaningful descriptor can be found systematically, by means of compressed sensing techniques. These concepts are demonstrated for examples in materials science: prediction of the relative stability of zincblende/wurtzite vs rocksalt octet binary semiconductors, and prediction of their band gaps, by using simple atomic input for building the descriptor.

MM 19.3 Tue 10:45 H 0106

Accurate Thermal Conductivities from First Principles — •Christian Carbogno and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin

In spite of significant research efforts, a first-principles determination of the thermal conductivity at high temperatures has remained elusive. Boltzmann transport techniques that account for anharmonic effects only perturbatively become inaccurate or inapplicable under such conditions; non-equilibrium molecular dynamics (MD) methods suffer from enormous finite-size artifacts in the computationally feasible supercells. Using Green-Kubo theory [1], we overcome this limitation by performing equilibrium *ab initio* MD simulations, from which the thermal conductivity is assessed from the auto-correlation function of the heat flux (including anharmonic effects to all orders). Foremost, we introduce and discuss a first-principles definition of the heat flux using the virial theorem. We validate our approach and in particular the techniques developed to overcome finite time and size effects, e.g., by inspecting silicon, the thermal conductivity of which is particularly challenging to converge [2]. Furthermore, we investigate the thermal conductivity of ZrO_2, which is known for its high degree of anharmonicity. Our calculations shed light on the heat resistance mechanism active in this material, which eventually allows us to discuss how the thermal conductivity can be controlled by doping [3].

[1] R. Kubo, *et al.*, *J. Phys. Soc. Jpn.* **12**, 1203 (1957).
[2] Y. He *et al.*, *Phys. Chem. Chem. Phys.* **14**, 16209 (2012).
[3] C. Carbogno, *et al.*, *Phys. Rev. B* **90**, 144109 (2014).

MM 19.4 Tue 11:00 H 0106

Structure map for crystal-structure prediction of sp-d valent compounds — Arthur Bialon, •Thomas Hammerschmidt, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Germany

The prediction of the crystal structure of a material from only its chemical composition is one of the key challenges of materials design. We present a three-dimensional structure map based on experimental data for compounds that contain sp-block elements and transition metals. The map predicts the correct crystal structure with a probability of 86% and has a confidence of 98% that the correct crystal structure is among a candidate list of three crystal structures. The three order parameters of the structure map are physically intuitive functions of the number of valence electrons, atomic volume and electro-negativity of the constituent elements. We test the structure map against standard density functional theory calculations for 1:1 sp-d-valent compounds and demonstrate that our three-parameter model has a comparable predictive ability. We show that the structure map can be applied to off-stoichiometric compounds and extended to ternary crystal-structure prototypes.

MM 19.5 Tue 11:15 H 0106

Property-based *cascade* genetic algorithms for tailored searches of metal-oxide nano-structures — •Saswata Bhattacharya[1], Luca M. Ghiringhelli[1], and Noa Marom[2] — [1]Fritz-Haber-Institut der MPG, Berlin, DE — [2]Tulane University, New Orleans, LA, USA

There is considerable interest in the computational determination of structures of atomic clusters that are detected in spectroscopy experiments. It has been suggested that in photo-emission experiments performed on anions, isomers of small $(TiO_2)_n$ clusters with high electron affinity (EA) are selectively observed rather than those with the lowest energy [1]. For the theoretical modeling of these situations, searching for the energy global minimum of the potential energy surface (PES) is inefficient. By using such an approach, in fact, it is unlikely to find meta-stable isomers that have high EA or low ionization potential (IP), but energy significantly above the ground state. We present an extension to our recently developed *ab initio* cascade genetic algorithm [2], here tailored to conduct property-based (e.g., high EA, low IP) searches over the PES. The term *cascade* refers to a multi-stepped algorithm where successive steps employ a higher level of theory, and each step of the next level takes information obtained at the immediate lower level. The new algorithms are benchmarked and validated for $(TiO_2)_n$ clusters ($n = 3 - 10, 15, 20$). – [1] N. Marom *et al.* Phys. Rev. Lett. **108**, 106801 (2012) [2] S. Bhattacharya *et al.*, New J. Phys., in press (2014).

15 min. break