

MM 10: Computational Materials Modelling - Accelerated Approaches

Time: Monday 11:45–13:15

Location: IFW B

MM 10.1 Mon 11:45 IFW B

An on-the-fly parameterized redundant internal coordinate preconditioner for quasi-Newton geometry optimization in atomistic calculations — ●CHRISTOPH FREYSOLDT and JÖRG NEUGEBAUER — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

We propose a variant of quasi-Newton geometry optimization for atomistic calculations, using an approximate Hessian in terms of internal coordinates (bond lengths, bond angles) as a preconditioner for a BFGS-type cartesian-coordinate quasi-Newton scheme. The key idea is to parameterize the Hessian on the fly. By automatically classifying all interatomic bonds according to bond length and elements involved, and treating all similar bonds equal, we arrive at a very small number of parameters that can be determined from few displacements, often only one. The superior performance for supercell calculations compared to a standard cartesian-coordinate optimizer is demonstrated.

MM 10.2 Mon 12:00 IFW B

Implementation and testing of a temporal acceleration scheme for kinetic Monte Carlo simulations: The case of CO methanation on stepped metals — ●MIE ANDERSEN and KARSTEN REUTER — Theoretical Chemistry, Technische Universität München, Germany

The efficiency of kinetic Monte Carlo (kMC) simulations is limited by the disparity of the timescales for the processes included in the microkinetic model. A novel algorithm has been developed to overcome this problem by the automatic detection of fast, reversible processes and the scaling of their rate constants with respect to the slower irreversible processes [1]. We have implemented this algorithm in our in-house kMC code 'kmos' [2] and assessed its efficiency and accuracy for the case of CO methanation on stepped metals. By making use of a scaling-relation based approach, we cover the trends over the entire transition metal series, which makes for a range of different test cases for the algorithm. While the algorithm overall performs well, we point out some limiting cases where the algorithm breaks down and discuss strategies for overcoming these issues.

[1] E. Dybeck, C. P. Plaisance, M. Neurock, submitted to J. Chem. Theory Comput. (2016) [2] M. J. Hoffmann, S. Matera, K. Reuter, Comput. Phys. Comm. 185, 2138 (2014)

MM 10.3 Mon 12:15 IFW B

Defect migration in metals by atomistic-continuum coupling — ●LIAM HUBER, BLAZEJ GRABOWSKI, and JÖRG NEUGEBAUER — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Atomistic simulations provide important insight into the underlying mechanisms which control material behaviour, and are an important part of knowledge-based design for new alloys. However, experimental time- and length-scales often lie beyond the reach of classical molecular dynamics (MD), even with modern advances in computational power. One approach to extend the length-scales accessible is to couple MD to a less expensive continuum model, typically represented using finite elements (FE). We present improvements to the FE-atomic (FEAt) coupling scheme which allow the MD-domain to track the migration of planar, line, and point defects at finite temperatures. By dynamically adapting our MD/FE domain partitioning through refinement and coarsening, we keep defects fully atomistically resolved while maintaining the cost-advantage of the coupled method. We apply this method to study grain boundary migration in Al and the nucleation and motion of dislocations during Al nano-pillar compression.

MM 10.4 Mon 12:30 IFW B

Nested sampling for alloys — ●ROBERT J.N. BALDOCK¹, CHRISTOPHER SUTTON², and LUCA M. GHIRINGHELLI² — ¹Theory and Simulation of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland — ²Theory Department, Fritz Haber Institute of the Max Planck So-

ciety, Berlin, Germany

We present a new nested sampling algorithm that enables the calculation of complete composition-temperature phase diagrams of alloys in a single simulation. Multicomponent phase diagrams are obtained in both the semi-grand ensemble, and at fixed overall composition, as a simple post-processing of the same simulation. We demonstrate the method by calculating the fixed pressure phase diagram of an eutectic binary Lennard-Jones system with fully continuous configuration space and an eutectic Ising model. Finally we showcase the approach by calculating the first principles phase diagram of a prototypical transparent conducting oxide (wide bandgap) material, $(\text{Zn}_x\text{Mg}_{1-x})\text{O}$, using a lattice model derived from density functional theory.

MM 10.5 Mon 12:45 IFW B

Controlling the energy of defects and interfaces in the amplitude expansion of the phase-field crystal model — ●MARCO SALVALAGLIO¹, RAINER BACKOFEN¹, AXEL VOIGT¹, and KEN ELDER² — ¹Institute of Scientific Computing, Technische Universität Dresden, 01062 Dresden, Germany — ²Department of Physics, Oakland University, Rochester, 48309 Michigan, USA

The Phase-Field Crystal (PFC) approach describes the dynamics of local atomic probability density on atomic length and diffusive time scales. It generally requires a fine spatial discretization, which limits the application of the method to small systems. The so-called amplitude expansion of the PFC model is known to solve this issue, accounting for the slowly-varying amplitudes of periodic probability densities. However, some restrictions exist in the quantitative description of material properties. In this work, we address the tuning of the interface and defect energy within the amplitude expansion of the PFC model. We extend the standard approach by including an additional energy term accounting for changes in the order of the solid phase. Its effects are investigated by FEM calculations. First, the control of the solid-liquid interface energy is considered as well as the changes induced in the interface morphology. Then, the tuning of the energy of defects is illustrated. The influence of the additional energy term on the dynamics and annihilation of defects is also discussed. We focus here on 2D systems involving crystal lattices with triangular symmetry. The connection of the considered approach to the description of realistic materials is shown for the technology-relevant graphene structure.

MM 10.6 Mon 13:00 IFW B

Ab initio determination of phonon lifetimes at elevated temperatures — ●ALBERT GLENSKI¹, BLAZEJ GRABOWSKI¹, TILMANN HICKEL¹, JÖRG NEUGEBAUER¹, PASCAL NEIBECKER², JÜRGEN NEUHAUS², MICHAEL LEITNER², KLAUDIA HRADIL², and WINFRIED PETRY² — ¹Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany — ²Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

The experimental measurement of phonon dispersions is well established. The corresponding phonon lifetimes (i.e., inverse linewidths) are - in contrast - assessed experimentally only for a handful of materials and are usually restricted to room temperature where anharmonic effects are small. Standard theoretical methods applying perturbation theory have shown to successfully describe the underlying phonon-phonon interactions at low temperatures. However, significant discrepancies to experiment (~100%) are found at elevated temperatures where the phonon broadening due to anharmonicity becomes large [1-2]. Applying the recently developed Local Anharmonic approximation [3] we determine ab initio values for phonon lifetimes in Al for a temperature range up to melting. We discuss its performance in comparison to previous perturbative approaches and our own experimental assessments for this temperature range.

[1] J. Pang et al., PRL 110, 157401 (2013).

[2] X. Tang et al., PRB 84, 054303 (2011).

[3] A. Glensk et al., PRL 114, 195901 (2015).