MM 2: Computational Materials Modelling I - Multiscale: Fundamentals

Time: Monday 10:15–11:45 Location: TC 006

MM 2.1 Mon 10:15 TC 006

FHI-aims becomes embedded: full-potential QM/MM-approach — •Daniel Berger[1], Volker Blum[2], and Karsten Reuter[1] — [1]TU München — [2]Fritz-Haber Institut der MPG

Photoelectrochemical processes like water splitting add to the wide range of applications for which a computationally most efficient description of (possibly locally charged) semiconducting systems is required. Properly accounting for long-range electrostatics without getting troubled with spurious interactions with periodic images, embedded cluster models are an appealing option to this end. Here, we present a corresponding implementation for the full-potential FHI-aims package [1]. In order to prevent electron leakage into the Coulomb singularities, we describe the linking atoms at the QM/MM-boundary at the level of norm-conserving pseudopotentials. The fully non-local form of the employed Kleinman-Bylander pseudopotentials allows for fast evaluation of the interaction integrals, especially in combination with FHI-aims' efficient atom-centered basis sets. We demonstrate the high accuracy and computational efficiency of this approach with applications to TiO_2(110)-supported metal clusters.

[1] V. Blum *et al.*, Comp. Phys. Commun. **180**, 2175 (2009).

MM 2.2 Mon 10:30 TC 006

Atomistic and continuum regions: Effects of coupling — •Frohmut Rösch and Hans-Rainer Trebin — Universität Stuttgart, Institut für Theoretische und Angewandte Physik, 70550 Stuttgart

Molecular dynamics simulations are a standard technique in computational materials modelling. The size of investigated solid structures, however, is limited to about the micrometer length scale. Finite element methods are less restricted in this respect but lack the atomistic description of matter. Obviously, this leads to the idea to couple both methods. The region of interest then is treated in an atomistic fashion and connected to a linear elastic continuum outside.

In this talk, fundamental effects are presented that arise in dynamic multiscale hybrid simulations due to the interface region. The scheme and procedures are illustrated, which are required to connect the two methods. In a simple setup aluminium has been chosen as a test case. In the numerical experiments, one domain determines the displacement boundary conditions for the other. The results show that the corresponding fixed boundaries influence relaxation. The decomposition into two parts also leads to a sort of asynchronism in time. In the case of strong excitations, it is observed that the anharmonic contributions lead to a deviation from linear elasticity, which is used in the continuum. Furthermore, depending on the spatial resolution of the FE mesh, short-wavelength phonons are reflected backwards into the atomistic domain.

MM 2.3 Mon 10:45 TC 006

A Two Scale Approach to Model the Freeze Casting Process — •Frank Wendler[1,2], Marcel Huber[2], and Britta Nestler[1,2] — [1]IMP, Karlsruhe University of Applied Sciences, Karlsruhe — [2]IAM-ZBS, Karlsruhe Institute of Technology, Karlsruhe

In the last years the freeze casting process has been adapted to a broad variety of materials with open porosities between 10 and 90 % (ceramics, polymers, metals). The crystallization kinetics of ice into an aquaeous colloidal suspension leads to the rejection of dispersed ceramic particles from the growing ice front and results in complex lamellar patterns, commonly explained by a Mullins-Sekerka instability of the constitutionally supercooled ice-colloid interface.

For a quantitative prediction of macro- and microscopic process variables (freezing conditions, solid fraction, particle size, colloidal interaction) on the microstructure, we simulate the free boundary problem using a multi phase-field model based on a thermodynamic free energy formulation on two different length scales: At the particle scale (50 μm) the inert particles are resolved and interact with each other and the ice front. We briefly show how the model parameters (interface tensions + mobilities, higher order potential, interface width) represent capillary properties of the colloid. At a large scale (1000 μm) the osmotic pressure of the colloid as a function of the solid particle fraction is integrated into the free energy formulation, from which diffusion coefficients are derived. We determine the limiting velocities for particle pushing and the transition from lamellar to isotropic growth from simulations, and compare them to an experimental system (ZrO2/water).

MM 2.4 Mon 11:00 TC 006

Molecular Dynamics Simulations of Laser Ablation in Metals: Parmeter Dependence, Double Pulses, and Extended Models — •Johannes Roth, Johannes Karlin, Marc Sartison, Armin Krauss, and Hans-Rainer Trebin — ITAP, Universität Stuttgart

Femtosecond laser ablation of metals depends on three parameters: electron heat conductivity, electron heat capacity and electron-phonon coupling. With respect to these parameters all metals can be devided into classes. Keeping the interaction and the crystal structure fixed we have varied the parameters within the experimentally observed range. We find that the heat capacity plays a minor role whereas the other parameters are equally important.

In a second part we have studied the melting behavior and ablation properties of Al under the influence of non-Gaussian and double pulses at a certain time interval. In general we find that a simple Gaussian pulse is the most effective method to ablate material.

The ablation by femtosecond laser pulses is a process dominated by the free electrons of the metal. To model the process correctly, one uses the two-temperature-model (TTM) with separete temperatures for the electrons and the lattice. The model still neglects a finite electron relaxation which is treated in an extended TTM. We show numerically and by simulations that the simple TTM leads to satisfactory results for Al and Nb, but that the extended TTM should be applied for example for Cu or Pb.

MM 2.5 Mon 11:15 TC 006

Computing Raman and infrared frequencies of nanostructures — •Felix Zörgiebel[1], Jens Kunstmann[1], Daijiro Nozaki[1], and Gianaurelio Cuniberti[1,2] — [1]Insitute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany — [2]Division of IT Convergence Engineering and National Center for Nanomaterials Technology, POSTECH, Pohang 790-784, Republic of Korea

We developed a method to compute Raman and Infrared frequencies of nanostructures of arbitrary dimension. Our method is based on molecular dynamics simulations and a symmetry analysis of the structure of interest. The calculation of electric properties like the polarizability and dipole moment is not required, which makes our method usable with existing molecular dynamics software. Raman peak shifts for bulk silicon were calculated for different temperatures and lattice constants and showed good agreement with experimental observations. Additionally we calculated the dependence of the Raman peak shift of silicon nanowires on the wire diameter and on surface stress.

MM 2.6 Mon 11:30 TC 006

Fast, stable convergence of electronic structure calculations for nanomaterials — •Philip Hasnip — University of York, York, UK

Ab initio materials modelling methods have become essential tools for condensed matter physicists in a wide variety of fields. The advent of more and more powerful computers has allowed larger, more complex systems to be simulated and the dramatic improvements in both experimental growth and characterisation methods have allowed the length scale of theoretical simulations and experimental studies to coincide at the nanoscale.

Whilst there has been undoubted success in the modelling of nanostructures and materials, the approach is not without its problems. As the size of the simulation system is increased to the nanoscale, the conventional algorithms used to find the electronic groundstate often show poor convergence, and for large or complex systems they may fail to converge at all. We first discuss the root cause of these problems, and then present an alternative algorithm which is not only robust, but also faster for nanomaterials simulation.