SYMS 2: Modern developments in multiphysics materials simulations II - Poster (joined by SYEC posters)

Time: Thursday 18:30–19:30 Location: Poster F

SYMS 2.1 Thu 18:30 Poster F

KMC studies for epitaxial growth of perovskites — Petar Petrov and •Wolfram Miller — Institut für Kristallzüchtung (IKZ), Max-Born-Str. 2, 12489 Berlin

Epitaxial layers of perovskites are of great intererest because of their piezo- and ferroelectric properties. For exploiting these properties a higher quality of the layers is needed, which requires a better understanding of the growth kinetics. For an understanding on atomic level we have developed a kinetic Monte-Carlo (KMC) method, which take into account the perovskite structure. In a first step we have studied the dynamics of the rather complex system. The mobility of oxygen and metal atoms on the surface is strongly effected by the local structure. We have performed computations with given coverage and without adsorption in order to study the surface diffusion in more detail and to obtain an effective diffusion coefficient, which might be used in a coarse-grained continuum calculation. In studies on the adsorption and growth dynamics we investigated the efficiency of adsorption and the growth velocity as a function of the ratio flux of metal/flux of oxygen.

SYMS 2.2 Thu 18:30 Poster F

Quantized density-functional theory for molecular fluids in nanoporous — •Thomas Heine[1], Sergei Yurchenko[1], Aliezer Martinez[1], and Serguei Patchkovskii[2] — [1]Institut für Physikalische Chemie und Elektrochemie, TU Dresden, D-01069 Dresden, Germany — [2]Steacie Institute for Molecular Sciences, NRC Canada, 100 Sussex Drive, Ottawa, Ontario, K1A 0R6 Canada

In this contribution we present an extension of the density functional theory of liquids to quantized liquids at finite temperatures (QLDFT). Following the Kohn-Sham partitioning of the total energy, we introduce a reference fluid of non-interacting particles obeying Boltzmann statistics. The role of the exchange-correlation (XC) functional is played by the effects of inter-particle interactions. We incorporate the effects of inter-particle interactions and deviations from Boltzmann statistics into the exchange-correlation (XC) functional. We extract the local-density approximation (LDA) expression for the XC functional from experimental data for uniform hydrogen fluids. We implemented QLDFT using real-space discretization and sparse matrix techniques. The code exhibits linear scaling with the system size and an essentially perfect parallel scaling.

We applied this theory to evaluate the hydrogen storage capacities of nanoporous materials. A promising approach to increase storage densities is adsorption of molecular hydrogen in nanoporous environments, where quantum effects may become significant, even at near-room temperatures. We show that with our simplified approach one can study a large variety of systems - both model and real - at equal footing.

SYMS 2.3 Thu 18:30 Poster F

Evolution operator method for solving the Kohn-Sham equations — Eduardo Hernandez[1], Stefan Janecek[2], •Marcin Kaczmarski[3], and Eckhardt Krotscheck[2] — [1]CSIC Institute de Ciencia de Materials de Barcelona,Campus de Bellaterra, 08193 Barcelona, Spain — [2]Institut für Theoretische Physik, Johannes Kepler Universität, Altenbergstrasse 69, A 4040 Linz, Austria — [3]Fachbereich Physik, Universitaet Osnabrueck, Barbarastrasse 7, 49076 Osnabrueck, Germany

This work deals with the problem of solving efficiently the Kohn-Sham equations. These equations constitute the famous density functional theory, which is a very successful approximation to the expensive many body description of the Fermi liquid. Density functional theory allows for very accurate determination of physical and chemical properties of materials by means of numerical calculation. Still, however, solving these equations in practice constitutes a difficult problem and many different approximations and methods at various levels of complication and efficiency have been proposed. Here, we introduce a new method relying on the application of the imaginary time evolution operator to the Kohn-Sham Hamiltonian. We try to show its conceptual simplicity and check how competitive this method could be.

Reference: E. R. Hernandez, S. Janecek, M. Kaczmarski, E. Krotscheck: Phys. Rev. B 75, 075108 (2007)

SYMS 2.4 Thu 18:30 Poster F

A Hybrid Modelling Approach for the Structural Evolution of Stepped Surfaces — •Sibylle Gemming[1], Julia Kundin[2], Chol-Jun Yu[2], Maria Radke de Cuba[2], and Heike Emmerich[2] — [1]Forschungszentrum Dresden-Rossendorf, D-01314 Dresden, Germany. — [2]Inst. f. Gesteinshüttenkunde und Center for Computational Engineering Science, RWTH Aachen, D-52064 Aachen, Germany.

The Burton-Cabrera-Frank (BCF) model describes the structural evolution of vicinal surfaces in terms of an incoming particle flux and concentration-dependent desorption and surface diffusion terms. A continuum formulation of the BCF scheme given by a phase-field implementation for the moving-boundary problem yields the long-term evolution of the step structure during a step-flow growth mode. A particle-based Ising-type approach with a Metropolis-Monte-Carlo kinetics additionally provides nucleation processes in a temperature-controlled manner and on a shorter time and length scale. We have integrated both approaches in a hybrid algorithm, which describes adsorption, nucleation, and structure evolution processes at solid-liquid and solid-gas interfaces on both time and length scales. The short-term nucleation is resolved by the Monte-Carlo generated dynamics of an anisotropic Ising model, whose interaction parameters stem from first-principles calculations. The long-term microstructure dynamics is calculated by the phase-field method. Several growth modes are distinguished: In addition to step-flow growth the nucleation processes on the terraces can lead to roughening or an epitaxial layer-by-layer growth controlled by temperature and by flux.

SYMS 2.5 Thu 18:30 Poster F

Error-propagation in multi-scale approaches to the elasticity of polycrystals — •Martin Friák and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Strasse 1, 402 37, Düsseldorf, Germany

The fundamental elements of many state-of-the-art multi-scale strategies are coarse-graining and inverse-mapping methods for the inter-scale parameter transfer. What has received only little attention recently is the fact that the parameter values determined on one scale may not be processed and transferred to another scale as infinitely precise. The crucial aspects that must be taken into account are then (i) limited precision of the single-scale parameter determination and (ii) frequently non-linear character of the actual multi-scale methodology employed. In our paper the multi-scale error propagation is addressed in case of the ab-initio based homogenization approaches to the elasticity of polycrystalline metallic materials. The problem is illustrated on three widely used schemes of (i) Voight, (ii) Reuss, and (iii) Hershey and Dahlgren [1]. The reliability and error-bars of the approaches are cross-validated against the experimental data for a few selected systems [2].

[1] A. V. Hershey and V. A. Dahlgren, *J. Appl. Mech.* **9**, 49 (1954).
[2] D. Raabe, B. Sander, M. Friák, D. Ma and J. Neugebauer, *Acta Mater.* **55**, 4475 (2007).

SYMS 2.6 Thu 18:30 Poster F

Novel multi-descriptive approach to crystal plasticity of textured β-Ti alloys — •Duancheng Ma, Martin Friák, Jörg Neugebauer, and Dierk Raabe — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 402 37, Düsseldorf, Germany

The (thermo-)mechanical treatment constitutes a back-bone processing step in many industrial production routes. The crystal plasticity finite element method (CP-FEM) is an excellent *continuum*-based method to predict the changes in texture and mechanical properties of polycrystals induced by e.g. cold-rolling. The methodology is based on (i) a detailed understanding of the deformation behavior of crystals as well as (ii) a number of input material parameters that are in most cases difficult to access and measure experimentally. First principle calculations, that take into account a *discrete* character of matter on the atomic scale, provide an alternative way to investigate the materials with respect to the mechanical properties both quantitatively and qualitatively without any empirical parameters. We thus introduce a new multi-descriptive concept that is based on (i) the extraction of the input data from the density-functional (DFT) calculations and (ii) the

up-scale transfer of the parameters into the CP-FEM simulations. The method is exemplified on texture β-Ti alloys intended for bio-medical applications.

SYMS 2.7 Thu 18:30 Poster F

Massive multi-phase-field simulations: An efficient algorithm to compute large grain systems in 3D — •Mathias Reichardt, Michael Selzer, and Britta Nestler — Institute of Computational Engineering, Karlsruhe University of Applied Sciences

In the last few years, there has been fast progress in phase-field simulations of microstructures. By the attempt of incorporating more and more physical effects, the complexity of the model formulations has become computationally extremely intense. The hardware requirements for conducting large scale simulations in reasonable time has increases in the same manner.

In applications to polycystalline materials such as grain growth and grain coarsening processes, it is necessary to run simulations with a large number of different order parameters. Recently, it has been discussed that the number of phase states simultaneously present at the same place is limited to approximately six in three space dimensions. By using this fact, we demonstate that it is possible to radically reduce memory requirement and computing time. This technique in combination with parallel algorithms on multiprocessor machines allows the 3D simulation of an unlimited number of grain orientations keeping memory and computation time constant. This is traced back to the fact, that there are several optimizations regarding data representation, quantity of numerical operations and data storage.

SYMS 2.8 Thu 18:30 Poster F

Valence dependent analytic bond-order potential including magnetism — •Ralf Drautz and David Pettifor — Department of Materials, University of Oxford, Oxford, United Kingdom

We recently derived an analytic interatomic bond-order potential (BOP) that depends explicitly on the valence of the transition metal element [1]. This analytic potential predicts the structural trend from hcp $\rightarrow$ bcc $\rightarrow$ hcp $\rightarrow$ fcc that is observed across the non-magnetic 4d and 5d transition metal series. In this talk we discuss how the analytic BOP may be extended to include magnetic contributions to the binding energy. We show that the resulting magnetic potential describes the experimental trend from antiferromagnetism to ferromagnetism across the 3d transition metal series.

[1] R. Drautz and D.G. Pettifor, Phys. Rev. B 74, 174117 (2006).