SYMS 1: Modern developments in multiphysics materials simulations I

Time: Thursday 14:00–17:00 Location: A 151

Invited Talk SYMS 1.1 Thu 14:00 A 151

Valence-dependent analytic bond-order potentials for metals and semiconductors — •D.G. Pettifor, R. Drautz, and T. Hammerschmidt — Department of Materials, University of Oxford, Oxford, United Kingdom

Valence-dependent analytic bond-order potentials (BOPs) for transition metals and semiconductors are derived by systematically coarse graining from the electronic to atomistic modelling hierarchies. First, the density functional theory (DFT) electronic structure and binding energy is simplified by introducing the tight-binding (TB) bond model whose parameters are determined directly from the DFT results. Second, this TB electronic structure is coarse grained through atom-centred moments and bond-centred interference paths, thereby predicting the analytic form of the interatomic BOP for both close-packed transition metals [1] and open-packed semiconductors [2]. The resultant BOPs are valence-dependent and provide the first interatomic potentials that predict the observed structural changes across the d-valent transition metals series and the sp-valent elements. Current development of these potentials for simulating transition metal alloys and the growth of semiconductor films is discussed.

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

[2] R. Drautz, X.W. Zhou, D.A. Murdick, B. Gillespie, H.N.G. Wadley and D.G. Pettifor, Prog. Mater. Sci. 52 (2007) 196.

Invited Talk SYMS 1.2 Thu 14:30 A 151

Modelling Fracture Processes: Macroscopic Consequences of Atomistic Details — P. Gumbsch[1,2], J.R. Kermode[3], T. Albaret[4], D. Sherman[5], N. Bernstein[6], M.C. Payne[3], G. Csányi[7], and •A. De Vita[8] — [1]IZBS, Universität Karlsruhe (TH), 76131 Karlsruhe, Germany — [2]Fraunhofer-Institut für Werkstoffmechanik IWM, 79108 Freiburg, Germany — [3]Cavendish Laboratory, Cambridge, CB3 0HE, United Kingdom — [4]Université Claude Bernard, Lyon 1, France — [5]Technion-Israel Institute of Technology, Haifa, 32000, Israel — [6]Naval Research Laboratory, Washington, DC 20375-5343, USA — [7]Department of Engineering, Cambridge, CB2 1PZ, United Kingdom — [8]King's College London, Strand, London WC2R 2LS, United Kingdom

The catastrophic failure of a brittle material is a complex, multiscale process. The applied stress at the macroscopic scale is concentrated by the sharp geometry of the crack tip. However, the way the solid fails in response to the stress concentration is determined by subtle lattice trapping and propagation instability effects which are controlled by atomic-scale chemical processes. We have investigated stability of cracks and dynamic, low speed, propagation instabilities in silicon using quantum mechanical hybrid multi-scale modelling and single-crystal fracture experiments. Our simulations reveal a tip reconstruction mechanism for a crack propagating on the (111) cleavage plane, causing a low speed instability which we observe experimentally. Conversely, propagation on the (110) plane is only stable up to a maximum speed, above which dynamical processes deflect the crack onto (111) planes as observed in experiments. So it looks as if cracks in silicon can "sink"and "stumble"as they propagate.

Invited Talk SYMS 1.3 Thu 15:00 A 151

Discovery of Novel Hydrogen Storage Materials: An Atomic Scale Computational Approach — •Chris Wolverton — Department of Materials Science and Engineering, Northwestern University, Evanston, IL USA

Practical hydrogen storage for mobile applications requires materials that exhibit high hydrogen densities, low decomposition temperatures, and fast kinetics for absorption and desorption. Unfortunately, no reversible materials are currently known that possess all of these attributes. Here we present an overview of our recent efforts aimed at developing a first-principles computational approach to the discovery of novel hydrogen storage materials. Such an approach requires several key capabilities to be effective: (i) Accurate prediction of decomposition thermodynamics, (ii) Prediction of crystal structures for unknown hydrides, and (iii) Prediction of preferred decomposition pathways. We present examples that illustrate each of these three capabilities: (i) prediction of hydriding enthalpies and free energies across a wide range of hydride materials, (ii) prediction of low-energy crystal structures for complex hydrides, [such as $Ca(AlH_4)_2$ $CaAlH_5$, and Li_2NH], and (iii) predicted decomposition pathways for $Li_4BN_3H_{10}$ and destabilized systems based on combinations of $LiBH_4$, $Ca(BH_4)_2$ and metal hydrides. For the destabilized systems, we propose a set of thermodynamic guidelines to help identify thermodynamically viable reactions. These capabilities have led to the prediction of several novel high-density hydrogen storage materials and reactions.

Invited Talk SYMS 1.4 Thu 15:30 A 151

Phase-field simulation of microstructure evolution: Linking atomistics to processes and properties — •Ingo Steinbach — RWTH-Aachen, Access e.V.

Properties of materials are determined by their atomic lattice structure and their microstructure which comprises the arrangement of microscopic defects and the mesoscopic distribution of phases and grains. This microstructure is determined by the history of the production process and may change under service conditions. The talk will focus on the phase-field method for the simulation of microstructure evolution in complex materials. Atomistic features determine the magnitude and anisotropy of important model parameter like interfacial energies and mobilities. The production process determines the boundary conditions of the simulations. Properties are derived by homogenization procedures or using heuristic arguments. Examples will be presented from casting, heat treatment and - as an outlook - in service degradation.

Invited Talk SYMS 1.5 Thu 16:00 A 151

QM/MM Studies of Biosystems — •Walter Thiel — Max-Planck-Institut für Kohlenforschung, Kaiser-Wilhelm-Platz 1, D-45470 Mülheim, Germany

In recent years, it has become possible to model chemical reactions in large biomolecules using combined quantum mechanical / molecular mechanical (QM/MM) methods. After a general outline of the theoretical background and the chosen strategy, the lecture will describe some of our recent work on biocatalysis by enzymes, in particular p-hydroxybenzoate hydroxylase (PHBH) and cytochrome P450cam. In the case of PHBH, the focus will be on methodological advances in multiscale QM/MM approaches, while P450cam will serve as an example of the chemical insights that can be provided by QM/MM calculations. The comparison between the QM/MM results for the enzyme and the QM results for gas-phase model systems allows us to assess the role of the protein environment and to gain an improved mechanistic understanding of enzymatic reactions.

Invited Talk SYMS 1.6 Thu 16:30 A 151

Error-controlled multiscale modeling approaches to surface chemistry and catalysis — •Karsten Reuter — Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin (Germany)

A materials science modeling that is based on understanding, predictive, and applicable to a wide range of realistic conditions requires to cover a wide range of length and time scales. Electronic structure theory deals with the finest scale and is thus the base for such a multiscale modeling of materials properties and functions. First-principles statistical mechanics and continuum mechanics techniques represent the next levels that build on this basis. Using examples from heterogeneous catalysis I will demonstrate the approach using density-functional theory, kinetic Monte Carlo and rate equation theory to treat the electronic, statistical and continuum levels, respectively. I will discuss the need for error-controlled links between the levels, e.g. using sensitivity analyses, as well as an approach to address binding interactions that challenge present-day exchange-correlation functionals.