Symposium Modern developments in multiphysics materials simulations (SYMS)

jointly organized by
Surface Science Division (O),
Semiconductor Physics Division (HL), and
Metal and Material Physics Division (MM)

Jörg Neugebauer
MPI für Eisenforschung
Max-Planck-Straße 1
40237 Düsseldorf
neugebauer@mpie.de

Mark Asta
University of California
3098 Bainer Hall
Davis, California
mdasta@ucdavis.edu

Overview of Invited Talks and Sessions

(lecture rooms A 053 and A 151; Poster F)

Invited Talks

SYMS 1.1	Thu	14:00–14:30	A 151	**Valence-dependent analytic bond-order potentials for metals and semiconductors** — •D.G. Pettifor, R. Drautz, T. Hammerschmidt
SYMS 1.2	Thu	14:30–15:00	A 151	**Modelling Fracture Processes: Macroscopic Consequences of Atomistic Details** — P. Gumbsch, J.R. Kermode, T. Albaret, D. Sherman, N. Bernstein, M.C. Payne, G. Csányi, •A. De Vita
SYMS 1.3	Thu	15:00–15:30	A 151	**Discovery of Novel Hydrogen Storage Materials: An Atomic Scale Computational Approach** — •Chris Wolverton
SYMS 1.4	Thu	15:30–16:00	A 151	**Phase-field simulation of microstructure evolution: Linking atomistics to processes and properties** — •Ingo Steinbach
SYMS 1.5	Thu	16:00–16:30	A 151	**QM/MM Studies of Biosystems** — •Walter Thiel
SYMS 1.6	Thu	16:30–17:00	A 151	**Error-controlled multiscale modeling approaches to surface chemistry and catalysis** — •Karsten Reuter

Sessions

SYMS 1.1–1.6	Thu	14:00–17:00	A 151	**Modern developments in multiphysics materials simulations I**
SYMS 2.1–2.8	Thu	18:30–19:30	Poster F	**Modern developments in multiphysics materials simulations II - Poster (joined by SYEC posters)**
SYMS 3.1–3.11	Fri	10:15–13:00	A 053	**Modern developments in multiphysics materials simulations III**

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.

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 → bcc → hcp → 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).

SYMS 3: Modern developments in multiphysics materials simulations III

Time: Friday 10:15–13:00 Location: A 053

SYMS 3.1 Fri 10:15 A 053

A Neural Network Representation of High-Dimensional Potential-Energy Surfaces for Solids — •Jörg Behler[1], Davide Donadio[2], Roman Martonak[3], and Michele Parrinello[4] — [1]Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, Germany — [2]Department of Chemistry, UC Davis, USA — [3]Department of Experimental Physics, Comenius University, Bratislava, Slovakia — [4]Department of Chemistry and Applied Biosciences, ETH Zurich, USI-Campus Lugano, Switzerland

We present a generalized neural network scheme for the representation of high-dimensional density-functional theory (DFT) potential-energy surfaces of bulk materials. The neural network is several orders of magnitude faster to evaluate than the underlying DFT energies, while the accuracy of the potential-energy surface is essentially maintained. The method enables long-term molecular dynamics and metadynamics simulations of large systems and is applicable to crystalline and amorphous structures, as well as to the melt. The method is illustrated by studies on the pressure-induced phase transitions in silicon. The obtained results are in excellent agreement with experiment and density-functional theory.

SYMS 3.2 Fri 10:30 A 053

Cluster-Expansion formalism for arbitrary lattices — •Daniel Lerch[1], Ole Wieckhorst[1], Gus Hart[2], and Stefan Müller[1] — [1]Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen — [2]Department of Physics and Astronomy, BYU, N283 ESC, Provo, UT 84602

In the past decades the cluster-expansion (*CE*) has evolved to an important tool for the modelling of multi-scale problems for both bulk and surface systems. However, up to now CE studies have been limited to primitive lattices (e.g. *fcc, bcc, sc*). We present a CE formalism implemented in our program package UNCLE, which can expand systems with up to three components based on arbitrary non-primitive lattices (e.g. *hcp*). In the two-dimensional case this formalism allows furthermore the treatment of surface systems such as multi-site adsorption (e.g. *H on Ir(100)-5x1-H*) or alloy surfaces. The included groundstate search has been designed to minimize not only computing time but also user-interference in order to achieve correct predictions independent of chemical intuition. This makes these predictions from ab-initio studies more reliable.

Support of this work by the *Studienstiftung des deutschen Volkes* is gratefully acknowledged.

SYMS 3.3 Fri 10:45 A 053

Conformational hierarchies of weakly bonded systems: Accuracy of dispersion corrected DFT — •Alexandre Tkatchenko, Volker Blum, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

It is well known that long-range dispersion interactions, important for stabilization of, e.g., molecular crystals, biomolecules and physisorption, are badly described by state-of-the-art *xc* functionals in DFT, but naturally included in post-HF or empirically in force field simulations. We have implemented a semi-empirical C_6/R^6 correction [1,2] in the numeric atom-centered orbital based code FHI-aims [3] and obtained correction parameters by fitting to a database of high quality *ab initio* calculations [2], improving on previous results due to the more accurate basis set (0.5 kcal/mol average error for binding energies using PBE+C_6). We assess the accuracy and impact of the correction for a completely different class of systems; rather than testing the average properties of a database, we focus on conformational energy *hierarchies* of (i) $(H_2O)_n$ clusters (n=2-6), (ii) Ala_2 and Ala_4, and (iii) infinite polyalanine conformers, comparing to published post-HF results for (i) and (ii). Even though the relative energies are not changed for small H_2O clusters and Ala_2 compared to DFT-GGA, the impact of dispersion on the conformation hierarchy of larger systems is surprisingly large, reaching ∼1-4 kcal/mol for different polyalanine conformers. [1] S. Grimme, J. Comput. Chem. 25, 1463 (2004) [2] P. Jurecka et al., J. Comput. Chem. 28, 555 (2007) [3] V. Blum et al., FHI ab initio molecular simulations (FHI-aims) project.

SYMS 3.4 Fri 11:00 A 053

Magnetic Bond-order Potential: Application to Defect Behavior — •Matous Mrovec[1,2], Duc Nguyen-Manh[3], Christian Elsaesser[1,2], Peter Gumbsch[1,2], and David Pettifor[4] — [1]IZBS, University of Karlsruhe, Kaiserstr. 12, 76131 Karlsruhe — [2]Fraunhofer-Institute for Mechanics of Materials IWM,Wöhlerstr. 11, 79108 Freiburg, Germany — [3]EURATOM/UKAEA Fusion Association, Culham Science Centre, Abingdon, OX14 3DB, United Kingdom — [4]Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, United Kingdom

Development of reliable interatomic potentials for simulations of structural defects in iron and iron-based materials presents a significant challenge. Energetics and structural stability of magnetic materials is strongly influenced by magnetic effects and details of the Fermi surface. These materials are therefore described rather poorly by the embedded-atom-method or Finnis-Sinclair-type potentials, which are only density dependent. We present a bond-order potential (BOP) for iron, which is based on a tight-binding bond representation. The model is able to capture the directional character of bonds present in transition metals and includes a description of magnetic effects within the Stoner model of tinerant magnetism. The constructed BOP is applied in studies of point defects, dislocations, and grain boundaries in ferromagnetic iron.

SYMS 3.5 Fri 11:15 A 053

Valence-dependent Bond-Order Potentials for Modeling Ni-based Superalloys — •Thomas Hammerschmidt, Ralf Drautz, and David Pettifor — Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, UK

The creep properties of Ni-based superalloys degrade with time due to precipitation of topologically close-packed (tcp) phases. We have compiled a structure map of the occurrence of tcp phases for binary transition-metal (TM) compounds from experimental databases. The structure map highlights the well-known role of the average d-band filling for the stability of tcp phases. Atomistic modelling of tcp stability requires extending the second-moment approximation to the electronic density of states (DOS) by including up to at least the sixth moment. We have developed an analytic bond-order potential (BOP) that systematically takes into account higher moment contributions to the DOS and depends explicitly on the valence of the TM elements. By including up to sixth-moment terms the analytic BOP is able to reproduce the structural trend across the non-magnetic 4d and 5d TM series. For the parameterization of the new BOP, we performed extensive density functional theory (DFT) calculations of the elemental and binary compound phases of Ni, the technologically important alloying element Cr, and the refractory metals Mo, Re, and W. In particular, we investigated the tcp phases A15, C14, C15, C36, μ, σ, and χ for the Ni-Cr, Re-W, Mo-Re, and Mo-W binary systems. We will discuss the structural trends of the DFT calculations and compare to the predictions of the analytic BOP within the canonical d-band model.

SYMS 3.6 Fri 11:30 A 053

Numerical Implementation of a 3D-Continuum Theory of Dislocations — •Stefan Sandfeld[1,3], Thomas Hochrainer[1,2], Peter Gumbsch[1,2], and Michael Zaiser[3] — [1]University Karlsruhe, IZBS, Karlsruhe, Germany — [2]Fraunhofer IWM, Freiburg, Germany — [3]University Edinburgh, U.K.

The growing demand for physically motivated continuum theories of plasticity led to an increased effort on continuum descriptions based on dislocations. For simplified systems of straight edge dislocations in a single slip configuration a 2-dim. theory is available (Groma 2003).

However, all attempts to transfer this method to 3-dim. systems of curved dislocations failed due to the lack of a dislocation density measure being able to reflect all dislocations as line like objects. The reason is that the Kroner tensor, as a measure for geometrically necessary dislocations (GND), comprises only a fraction of all dislocations, while the scalar density of statistically stored dislocations (SSD) contains no directional information.

This deficiency can be remedied by a recently introduced continuum theory of dislocations (Hochrainer 2006), which utilizes a generalized definition of the dislocation density tensor. Within this theory the differentiation between GND and SSD becomes dispensable. We explore this theory by a numerical implementation for the 2-dim. case of a single glide system. The effect of dislocation pile-ups at impenetrable boundaries is studied and compared to alternative approaches (e.g. Sedlacek 2003). We will show, that our method can treat arbitrary distributions of dislocation loops insinde the plastic slip channel.

SYMS 3.7 Fri 11:45 A 053

An ab-initio study of the hydrogen-bond network in crystalline α-chitin — •Michal Petrov, Martin Friák, Liverios Lymperakis, Dierk Raabe, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Strasse 1, 402 37, Düsseldorf, Germany

Light, resistant and poly-functional α-chitin is the second most abundant biological polymer. Learning/understanding how nature achieves these properties is crucial to design novel bio-inspired materials. The hydrogen-bond network formed during the crystal packing plays a key role to understand the physical properties of the material such as solubility or elasticity. A deeper understanding of chitin's unique properties has been long hindered by the lack of detailed ground-state structure information. We have therefore studied the atomic structure of crystalline α-chitin with a special focus on conformational possibilities in the hydrogen bond network. In order to properly address the full complexity of the α-chitin structure a hierarchical multischeme approach has been employed: The configurational space is first searched using force field based molecular dynamics and tight binding calculations. The most promising atomic configurations thus identified are then refined within accurate ab-initio methods. The properties of the hydrogen bond network within the rotational conformational phase space of the side chains and the influence to the energetics of α-chitin are investigated. Analyzing these results the stability of the ground-state structure as well as its strong elastic anisotropy is explained in terms of an intricate interplay between covalent and the hydrogen bonds.

SYMS 3.8 Fri 12:00 A 053

Boron-chain alloys to carry hydrogen? — •Aleksey Kolmogorov, Ralf Drautz, and David Pettifor — Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, United Kingdom

We use *ab initio* calculations to explore the hydrogen storage potential of boron-chain Li-B alloys. Analysis of the available experimental data on the boron-chain Li_xB_{1-x} compound ($x \approx 0.53$) and a high-throughput search for its most stable hydrogenated derivatives have allowed us to identify two possible LiBH (5.4 wt. % H) and $LiBH_2$ (10.2 wt. % H) phases. We suggest a synthesis route to obtain the new hydrides and discuss the possibility of adjusting the heats of reactions for hydrogen storage applications.

SYMS 3.9 Fri 12:15 A 053

Engineering materials-design parameters of the Mg-Li alloys from ab initio calculations — •William Art Counts, Martin Friák, Dierk Raabe, and Jörg Neugebauer — Max-Planck-Institute für Eisenforschung GmbH, Max-Planck Str. 1, D-40237, Düsseldorf, Germany

Ab initio calculations are becoming increasingly useful to engineers interested in designing new alloys because these calculations are able to accurately predict basic material properties only knowing the atomic composition of the material. In this paper, fundamental physical properties (like formation energy and elastic constants) of 11 bcc Mg-Li compounds are calculated using density-functional theory (DFT) and compared with available experimental data. These DFT-determined properties are in turn used to calculate engineering parameters like (i) specific Young's modulus (E/ρ) or (ii) bulk over shear modulus ratio (B/G) differentiating between brittle and ductile behavior. These engineering parameters are then used to identify alloys that have optimal mechanical properties needed for a light weight structural material. It was found that the stiffest bcc magnesium-lithium alloys contain about 70 at.% Mg while the most ductile alloys have 0-20 at.% Mg. The specific modulus for alloys with 70 at.% Mg is equal to that of Al-Mg alloys and slightly lower than that of Al-Li alloys.

SYMS 3.10 Fri 12:30 A 053

A Lattice-Boltzmann Model to simulate the growth of three dimensional microstructures under the influence of fluid flow — •Marcus Jainta, Michael Selzer, and Britta Nestler — Institute of Computational Engineering, Karlsruhe University of Applied Sciences

The effect of fluid flow on crystal growth structures is a phenomenon with particular relevance in three dimensions where solute is transported in the spatial domain and around the growing crystals. From experiments, it is well known that fluid flow dramatically alters the solidification structure during a casting process. The presence of flow admits the possibility of instabilities due to the flow itself, in addition to the well known morphological instabilities found in crystal growth. Hence, flow has an important influence on the process conditions and on the resulting material properties during the solidification from a melt. A Lattice-Boltzmann model for fluid flow is formulated and coupled with a phase-field model for multicomponent and multiphase material systems. The influence of convection on the growth process is modelled by introducing an advective term in the concentration diffusion equations. The model can be applied to multiple liquid phases with different viscosities. We discuss the numerical method and apply the parallel solver to investigate the effect of a flow field on the evolution of dendritic and eutectic solidification microstructures in two and three dimensions.

SYMS 3.11 Fri 12:45 A 053

Ab initio analysis of the carbon solubility limits in various iron phases — •Olga Kim, Martin Friák, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Strasse 1, 402 37, Düsseldorf, Germany

The solubility limits of carbon in various iron phases are of critical importance for many steel-industry applications. The actual values are difficult to measure accurately in ferrite and they have so far not be determined theoretically from first principles in austenite. The solubility limits of carbon in α-, β-, γ- and δ-iron have been thus determined employing density functional theory calculations over the entire temperature range. The results show excellent agreement with experiment.

The two-orders-of-magnitude higher solubility of carbon in austenite than in ferrite has been quantitatively analyzed and a complex interplay between two distinct phenomena has been found. First, the number of first nearest neighbors is higher in the fcc structure than in the bcc structure and the carbon atom is consequently more strongly bound, and secondly, the strain energy between the C-interstitial and the surrounding iron matrix is lower in the fcc lattice. The details of the actual magnetic state have not been found as important as the above mentioned two mechanisms.