Tuesday Afternoon, November 11, 2014

Accelerating Materials Discovery for Global Competitiveness Focus Topic
Room: 302 - Session MG-TuA

Multi-scale Modeling in the Discovery of Advanced Materials

Moderator: Alberto Roldan, University College London, Veena Tikare, Sandia National Laboratories

2:20pm **MG-TuA1 Search for Substitutes of Critical Materials with Targeted Properties by Scale-Bridging and High-Throughput Modelling and Simulation**, ***Christian Elsässer***, Fraunhofer Institute for Mechanics of Materials IWM, Germany **INVITED**

In this lecture three case studies will be addressed on how sustainable substitutes for materials, which have outstanding functionalities but also constraining criticalities, can be discovered and developed efficiently by employing multi-scale-coupling and high-throughput-screening concepts.

In the first case, a multi-scale chain from atomic-level first-principles theory to microstructure-level phase-field theory for ferroelectric piezoelectrics is set up for the still best material $Pb(Zr,Ti)O_3$ (PZT), which contains the biomedically health-critical element Pb, and then transferred to $(K, Na)NbO_3$ (KNN), which is a potential substitute for PZT. [1]

The second case is on the modelling of structure-property relationships for transparent and conductive oxides (TCO), which are free of the geologically ressource-limited element Indium and therefore potential substitutes for the still best TCO material Indium Tin Oxide (ITO) for front electrodes on, e.g., smart phones or solar cells. [2]

In the third case, a combinatorial high-throughput-screening approach is employed to search for crystal structures and chemical compositions of intermetallic phases of transition-metal (TM) and rare-earth (RE) elements, which have sufficiently good intrinsic ferromagnetic properties for permanent magnets but contain less amounts of the geopolitically supply-critical RE elements than, e.g., the still best permanent magnets based on $(Nd,Dy)_2Fe_{14}B$. [3]

References:

[1] B. Völker, P. Marton, C. Elsässer, and M. Kamlah, *Multiscale modeling for ferroelectric materials: a transition from the atomic level to phase-field modelling*, Contin. Mech. Thermodyn. **23**, 435-451 (2011); S. Körbel and C. Elsässer, *Alignment of ferroelectric polarization and defect complexes in copper-doped potassium niobate*, Phys. Rev. B **88**, 214114 (2013).

[2] W. Körner, P. Gumbsch, and C. Elsässer, *Analysis of electronic subgap states in amorphous semiconductor oxides on the example of Zn-Sn-O systems*, Phys. Rev. B **86**, 165210 (2012); W. Körner and C. Elsässer, DFT study of stability and subgap states of crystalline and amorphous Zn-Sn-O, Thin Solid Films **555**, 81-86 (2014).

[3] N. Drebov, A. Martinez-Limia, L. Kunz, A. Gola, T. Shigematsu, T. Eckl, P. Gumbsch, and C. Elsässer, *Ab-initio screening methology applied to the search for new permanent magnetic materials*, New J. Phys. **15**, 125023 (2013).

3:00pm **MG-TuA3 Monte Carlo Simulations of Nanoscale Focused Electron Beam Induced Etching**, *R. Timilsina*, ***Philip Rack***, The University of Tennessee Knoxville, *K. Wolff, M. Budach, K. Edinger*, Carl Zeiss SMS, Germany

Focused beam (electron-ion-photon) induced processing has long been utilized as a micro-/nano-scale direct synthesis method for both additive (via deposition) and subtractive (via etching) machining for a variety of editing and prototyping applications. Nanoscale lithography mask editing is one critical area which is pushing the limits for these beam induced processing methods. Beam damage associated with liquid gallium and the recently developed gas field ion source limits their utility in lithography mask repair due to the stringent optical requirements. Thus, electron beam induced processing for mask repair of both clear and opaque defects is the method of choice. To understand the fundamental electron-solid-precursor interactions, a Monte Carlo electron-solid simulation has been developed with a dynamic precursor gas routine which emulates adsorption/desorption, surface diffusion and electron stimulated reactions. The simulation was recently modified to handle electron beam induced etching. The electron beam induced etching of silicon dioxide is studied at low and high energies, short and long dwell times and various etch precursor gas conditions to elucidate important rate limiting regimes. Furthermore, the temporal behavior of the high-aspect ratio etch process is demonstrated. In this presentation we will overview the Monte Carlo simulation and will illustrate how various parameters affect the resolution and etch rate of the electron beam stimulated etch process. We will demonstrate how beam parameters (beam energy, current, and dwell and refresh time) precursor parameters (flux, residence time, surface diffusion coefficient, dissociation cross-section) and material (secondary electron yield, density) all contribute to the nanoscale etching process.

4:20pm **MG-TuA7 Advances in Multiscale Mathematical Modeling of Materials: From Phase Diagrams to Interface Dynamics**, ***Maria Emelianenko***, George Mason University **INVITED**

This talk will survey recent developments in two areas critical for advancing materials design. First is the mesoscale kinetic modeling of polycrystalline materials, focused on the task of understanding how statistical distributions develop in the process of coarsening of materials microstructure and how these distributions in turn relate to materials properties. The challenges here include the design of reliable benchmarks for curvature-driven growth, vertex and Monte Carlo grain growth simulation codes, as well as the development of coarse-grained kinetic theories capable of capturing realistic materials behavior. These and other questions will be discussed in the context of nonlocal evolution theory and particle gas dynamics, and unexpected connections with other fields of science will be revealed. The other part of the talk will be concerned with phase diagram calculation methods, where robust and accurate numerical optimization methods are required to prevent costly mistakes. A universal Gibbs energy minimization formulation will be discussed that allows to link traditional Calphad codes and databases to state-of-the-art optimization engines, paving the road to a more intelligent automated phase data exploration.

5:00pm **MG-TuA9 Discrete All-Atom Simulations: Predicting Fit-for-Purpose Properties of Fuels**, *M.T. Knippenberg*, High Point University, ***BarbaraL Mooney***, *J.A. Harrison*, United States Naval Academy

Hydrotreated renewable fuels are complex blends of hydrocarbons produced by catalytic treatment of oils from such materials as corn, algae, and tallow. These fuels are of potential interest to the US Navy for use in their fleet, but due to their complexity it is not obvious which blends are suitable, and which are not. To this end, we use computational modeling for the prediction, based upon chemical composition, of the fit-for-purpose (FFP) properties of these alternative fuels. Low-cost, high-throughput assessment of fuel space from molecular dynamics (MD) simulation accelerates fuel discovery by: 1) identifying suitable candidate fuels out of a large phase space of possible fuel mixtures and environmental conditions; 2) providing an informed starting point for experimental investigations; and 3) reducing waste by eliminating the need to perform expensive, time-consuming measurements on unviable candidates. We are able, through MD with the modified-AIREBO potential, to obtain excellent agreement with experimental measurements of density, enthalpy of vaporization, and bulk modulus for a range of example surrogates containing up to 12 hydrocarbon components, as well as for binary mixtures of the straight-chain alkane *n*-dodecane with the branched 2,2,4,4,6,8,8-heptamethylnonane over the full range of mole fractions.

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