Department of Mechanical Engineering William Maxwell Reed Seminar Series and Department of Chemical Engineering Present

Computing mass transport in crystals: Theory, computation, and applications

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Abstract: The processing of materials as well as their technologically important properties are controlled by a combination of thermodynamics--which determines equilibrium--and kinetics--how a material evolves. Mass transport in solids, where different chemical species diffuse in a material due to random motion with or without a driving force, is a fundamental kinetic process for a wide variety of materials problems: growth of precipitates in nearly every advanced structural alloy from steels to superalloys, fusing of powders to make advanced ceramics, degradation of materials from irradiation, permanent changes in shape of materials over long times at high temperatures, corrosion of materials in different chemical environments, charge/discharge cycles in batteries, migration of atoms in electric fields, and more. Mass transport is a fundamentally multiscale phenomenon driven by crystalline defects, where many individual defect displacements sum up to produce chemical distributions at larger length and time scales. State-of-the-art first principles methods make the computation of defect energies and transitions routine for crystalline systems, and upscaling from activation barriers to mesoscale mobilities requires the solution of the master equation for diffusivity. For all but the simplest cases of interstitial diffusivity, and particular approximations with vacancy-mediated diffusion on simple lattices, calculating diffusivity directly is a challenge. This leaves two choices: uncontrolled approximations to map the problem onto a simpler (solved) problem, or a stochastic method like kinetic Monte Carlo, which can be difficult to converge for cases of strong correlations. I will describe and demonstrate our new developments for direct and automated Green function solutions for transport that take full advantage of crystal symmetry. This approach has provided new predictions for light element diffusion in magnesium, "pipe diffusion" of hydrogen along dislocations cores in palladium, and the evolution of vacancies and silicon near a dislocation in nickel. I will also show our latest results for technologically relevant magnesium alloys with containing Al, Zn, and rare earth elements (Gd, Y, Nd, Ce and La), where prior theoretical models to predict diffusivity from atomic jump frequencies make uncontrolled approximations that impact their accuracy. The underlying automation also makes the extension of first-principles transport databases significantly more practical and eliminate uncontrolled approximations in the transport model.

Bio: Dallas R. Trinkle is a Willett Faculty Scholar and an Associate Professor in Materials Science and Engineering at Univ. Illinois, Urbana-Champaign. He received his Ph.D. in Physics from Ohio State University in 2003. Following his time as a National Research Council postdoctoral researcher at the Air Force Research Laboratory, he joined the faculty of the Department of Materials Science and Engineering at Univ. Illinois, Urbana-Champaign in 2006. He was a TMS Young Leader International Scholar in 2008, received the NSF/CAREER award in 2009, the Xerox Award for Faculty Research at Illinois in 2011, the AIME Robert Lansing Hardy Award in 2014, co-chaired the 2011 Physical Metallurgy Gordon Research conference, and became a Willett Faculty Scholar at Illinois in 2015. His research focuses on defects in materials using density-functional theory, and novel techniques to understand problems in mechanical behavior and transport.

Date: October 28, 2016
Time: 3:00p to 4:00p
Place: CB 106
Contact: Dr. Alexandre Martin 257-4462

Meet the speaker and have refreshments
Attendance open to all interested persons

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