DEPARTMENT OF MECHANICAL ENGINEERING

TOWARDS PREDICTIVE MODELING OF MOLECULAR MATERIALS AT EXTREMES

Friday, October 12, 2018 | 1:30 p.m.
2164 Martin Hall, DeWALT Seminar Room

Guest Speaker
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ABSTRACT

Understanding material response under extreme conditions is critical for developing informed multi-scale, multi-physics models, but many properties and processes are beyond the current resolution of experiments. Molecular dynamics can predict mechanics and transport in molecular materials, but direct simulation of dynamic processes is often encumbered by competing needs in computational efficiency and physical accuracy required to capture features on multiple time and length scales. We are developing multiple methods to push the envelope on these constraints and gain insight into fundamental material anisotropy. Recent examples on shock mechanics and heat transport in energetic materials will be discussed, highlighting their interconnected nature in predicting material responses at extremes and the roles of various modeling techniques in pursuit of this larger goal. A generalized crystal-cutting method (GCCM) is outlined that overcomes many limitations for simulating low-symmetry materials in 3D-periodic cells and gives direct access to orientation-dependent properties. The GCCM is applied to characterize the anisotropic shock response of TATB single crystals and grain boundaries, revealing new deformation mechanisms and modes for energy localization (e.g., hot spot formation). Applicability of continuum transport models is quantified by scale bridging with molecular dynamics predictions for inherently anisotropic and hierarchical energy transport processes. Parameterization and validation of a phonon Boltzmann transport equation model for graphene is outlined and applied to understand transient responses to localized heat. Implications for modeling the dynamic response of low-symmetry energetic materials at various levels of coarse graining are discussed.

BIO

Matthew (Matt) Kroonblawd is a staff scientist in the Reaction Dynamics Group at Lawrence Livermore National Laboratory (LLNL). He holds a BA in Physics from the University of Minnesota - Morris (2012) and a PhD in Chemistry from the University of Missouri - Columbia (2016), where he studied with Prof. Tommy Sewell. Nominally a physical chemist by training, his work is focused broadly on using computational approaches to understand thermomechanical response and chemistry in molecular materials under dynamic, highly nonequilibrium conditions. One of his ongoing research interests is in the development and application of generalized simulation methods to understand anisotropic (directionally dependent) properties of low-symmetry crystalline materials.

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