SHOCK05-2005-020012

Abstract for an Invited Paper
for the SHOCK05 Meeting of
the American Physical Society

Atomistic and mesoscale modeling of the response of high energy materials to dynamical loading[1]

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The mechano-chemical response of high energy density materials to dynamical loading involves a variety of complex processes that remain to be characterized at the molecular level. For example the translational kinetic energy of the shock-wave is transformed into intra-molecular excitations; the shock-wave leads to plastic deformation in the material, and defects (such as voids) and interfaces interact with the propagating wave causing energy and temperature localization (hot spots) that play a crucial role in the initiation and propagation of detonation. I will describe recent reactive and un-reactive MD simulations using accurate interatomic potentials designed to characterize the chemical decomposition and plastic response of various HE materials under dynamical loading. Non-equilibrium shock simulations enable the characterization of the induced plastic deformation and the initial chemical events while equilibrium simulations at various temperatures and densities enable us to follow the reactions to completion. While providing a very detailed description, all-atom MD has a serious limitation: being based on classical mechanics it leads to classical (rather than quantum) statistical mechanics. This results in a significant overestimation of the specific heat in molecular crystals for the temperatures relevant in HE materials. To address this shortcoming we have recently developed a new mesodynamical method (where a single particle describes groups of atoms) that enables a thermodynamically accurate description of energy transfer between mesoparticles (molecules in this case) and their internal degrees of freedom (DoFs). The thermal properties of the implicit DoFs are described via their specific heat. The mesodynamics results are in excellent agreement with all-atom MD simulations when a classical expression for the specific heat is used but also enables the accurate quantum mechanical-based treatment of the thermal role of the implicit DoFs.

[1]LA-UR-05-2701