Atomistic Predictions of Thermo-Mechanical Properties of Explosives

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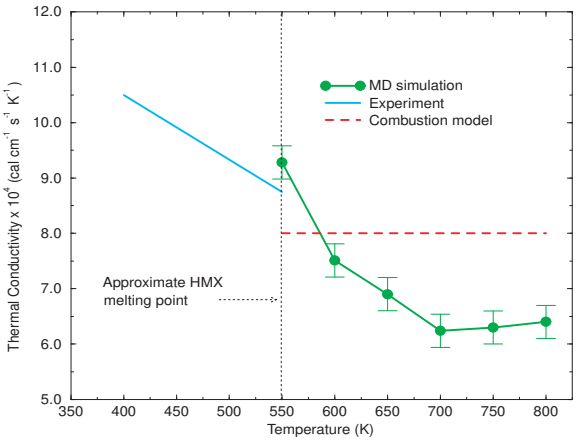
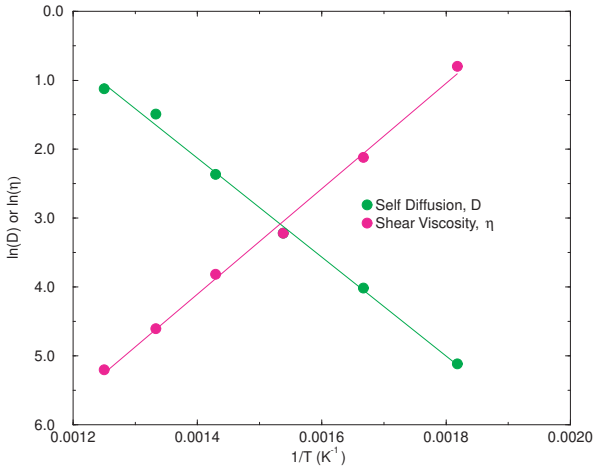
Plastic-bonded explosives (PBXs) are highly loaded composite materials comprised of high-explosive (HE) grains suspended in a polymeric binder. When a PBX is subjected to an abnormal external stimulus such as a weak shock, the ultimate outcome of the event is dependent on a complicated interplay among several processes including the intensity and rate of energy input, dissipative mechanisms that convert shock energy to heat and control its delocalization and, of course, chemical kinetics.

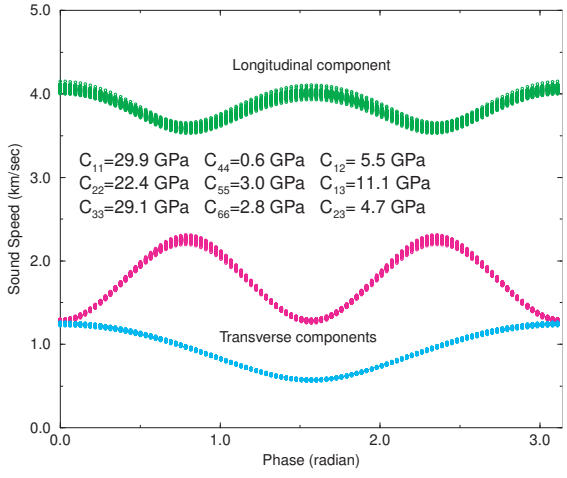
As the completeness of the physics incorporated into mesomechanical models improves, there is an ever greater need for reliable values of the physical parameters that appear in their formulation.

Since the HE grains used in a typical PBX formulation are ca. 10-100 microns in diameter, structural heterogeneities in the composite are readily apparent on a millimeter spatial scale. These heterogeneities complicate matters since they lead to a distribution of stresses and temperatures in the material; localized regions can have temperatures hundreds of degrees in excess of the spatially averaged value. These extreme temperature excursions correspond to 'hot spots' where chemical reaction rates are extremely fast. If the size and/or spatial density of these hot spots is sufficiently high, isolated initiation events can coalesce and ultimately lead to detonation.

Mesomechanical simulation techniques in which the heterogeneities in a PBX are explicitly resolved are increasingly used to understand, in a statistical sense, the response of high explosives to imposed stress waves, and to aid in the construction of constitutive laws or sub-grid physics models for use in engineering-scale hydrodynamic codes. As the completeness of the physics incorporated into mesomechanical models improves, there is an ever greater need for reliable values of the physical parameters







that appear in their formulation. Examples of what is needed include elastic constants, transport coefficients, and chemical reaction rates for the isolated constituents, as well as information concerning the interactions among them. More details about mesomechanical and sub-grid models as applied to HE can be found in articles by Menikoff (p. 143) and Dienes (p. 155) in this issue.

Unfortunately, there are little or no data for many of the properties needed for mesoscopic descriptions for explosives; and, in many cases, their direct experimental determination is very difficult, if not impossible, due to the extreme reactivity of the explosive across large regions of the relevant thermodynamic parameter space. Increasingly, however, some of the gaps in our knowledge can be filled through judicious application of atomistic simulation tools to appropriate problems.

An effective, ASCI-based collaboration involving Thomas D. Sewell at Los Alamos and the Smith Group at the University of Utah (home of a Level One ASCI/ASAP University Alliance) is producing information about some of the thermophysical and mechanical parameters mentioned above. In particular, we are using multi-nanosecond, equilibrium and non-equilibrium classical molecular dynamics simulation methods in conjunction with a recently published, quantum chemistry-based potential-energy surface [1] to compute pressure- and temperature-dependent liquid transport coefficients [2,3] and anisotropic crystal elastic properties for octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX), which is the energetic component in several important PBX formulations. These quantities, or others derived from them, can be directly incorporated into mesomechanical modeling formulations, thereby serving the dual purposes of successfully bridging, in part, the atomistic-mesoscopic spatial scale and reducing the number of "free" parameters appearing in the mesoscale models.

[1] G. D. Smith and R. K. Bharadwaj, *J. Phys. Chem. B* **103**, 3570 (1999).

[2] D. Bedrov, G. D. Smith, and T. D. Sewell, "Temperature Dependent Shear Viscosity Coefficient of HMX. A Molecular Dynamics Simulation Study," *J. Chem. Phys*. (in press).

[3] D. Bedrov, G. D. Smith, and T. D. Sewell, "The Thermal Conductivity of Liquid Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX) from Molecular Dynamics Simulations," *Appl. Phys. Lett.* (submitted).

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