Mesoscale Modeling of Thermo-Mechanical Response: Constant-Energy Dissipative Particle Dynamics Simulations

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ABSTRACT

Nanocomposites such as energetic materials (EMs) are inherently heterogeneous, containing several species types of disparate shapes and sizes. EMs are often comprised of micro-sized crystallites (or grains) held together by a small amount of polymer binder, and in some instances contain metal nanoparticles. Accordingly, mechanical stimulation (e.g., shock or shear) of these materials can incite responses over a wide range of spatial and temporal scales. For example, localized regions of elevated thermal energy, or hot spots, often occur near microscale defects in the material such as voids and grain boundaries; however the energy transfer processes are atomistically governed. While modeling and simulation of such phenomena can offer fundamental insight, it is computationally challenging. Computing power and resources continue to grow, but there still exists much behavior that cannot be studied using atomistic simulation techniques. Moreover, field-based mesoscale modeling techniques have fidelity limitations with respect to gaining a fundamental understanding.

To address these issues, we recently embarked on a study of the thermo-mechanical response of crystalline nanocomposites using a particle-based mesoscale modeling technique, namely, the constant-energy Dissipative Particle Dynamics method (DPDE) [1, 2]. A constant energy approach is required since materials subjected to mechanical stimuli will inevitably respond via energy exchange and transfer processes. In contrast to the standard Dissipative Particle Dynamics method [3, 4] that conserves only momentum, the DPDE method conserves both momentum and energy. The DPDE method assigns an internal energy to each particle, allowing particles to exchange both momentum and thermal energy. This particle internal energy is included as a separate equation of motion along with the equations of motion for the particle's position and momentum. The atomic degrees-of-freedom are explicitly resolved or coarse-grained into the particle internal energy, and included in the simulation in an averaged way.

A number of modeling challenges exist for nanocomposites, including the development of an accurate mesoscale model that can capture the following known thermo-mechanical responses: (i) phase transitions (solid↔liquid↔vapor); (ii) structural rearrangements (plastic deformation, shear banding); and (iii) chemical decomposition reactions. Furthermore, models must be for multiple species types such that these phenomena can occur at different thermodynamic conditions for each species present. And finally, the model parameters should be physics-based so that direct links to real material properties or higher resolution modeling are possible. The standard DPD model [5] likely cannot capture such features, fortunately though, promising alternatives exist which we will assess in this study [6-8]. Technical challenges also exist for such studies. Since while numerical integrator algorithms work quite satisfactorily for DPD [5] and DPDE [8] simulations under normal conditions, at extreme conditions such as high

densities, much shorter integration timesteps are required to maintain numerical stability. In order to maintain a reasonable timestep that allows for the simulation of mesoscale events, higher quality integrators will be explored.

In this work, we will present the status of this ongoing project, including progress on nanocomposite model development, mesoscale simulation of phase transitions, and improved integrator algorithms. To date, progress has been encouraging, where we find the DPDE method to be a viable tool for simulating the thermo-mechanical response of crystalline nanocomposites to mechanical stimuli.

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