Potential Development for Atomistic Modeling of Energetic and Protection Materials

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In order to revolutionize the design, development, and acquisition of novel armament and weapon systems, the Army Research Laboratory has invested in the development of a multi-scale, physics-based, modeling and simulation capability that has as its foundation quantum mechanics, which is the only computational technique enabling a rigorous, non-empirical description of material properties. However, due to current computational limitations, material properties gleaned at the quantum mechanical level must be upscaled into classical potentials that, with proper design, retain the description of the underlying quantum mechanical treatment but at a reduced computational cost. This presentation will give an overview of classical potentials that have been developed enabling multiscale descriptions of an energetic formulation, Composition A3 Type II comprised of 91% cyclotrimethylene-trinitramine (RDX) energetic and 9% polyethylene plasticizer. The interfacial energies and stresses will be shown to be in good accord with experimental force-distance spectroscopy measurements. Additionally, a classical potential of Tersoff form that has been developed for modeling of the boron carbide armor ceramic will be presented and shown to reproduce the structure, pressure response, and mechanical properties of the $B_{13}C_2$ boron carbide structure. The classical description of the shock Hugoniot will also be discussed and large scale atomistic simulations of BC subjected to flyer plate impact will be presented.