Multiscale Modeling of Energetic and Armor Materials

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This presentation will be an overview of current research efforts underway at the Army Research Laboratory focusing on creation of a predictive, quantum mechanically informed, multiscale modeling and simulation capability for energetic and armor materials. The development and application of an atomistic model of the two component explosive formulation Composition A3 Type II, which consists of the cyclotrimethylene trinitramine (RDX) energetic and polyethylene plasticizer, will be described and efforts to experimentally validate the model will be discussed. Application of the model in multi-million atom molecular dynamics simulations of shock compression will be presented and the development of a coarse grained representation of the atomistic model, to extend its range of applicability to the mesoscale, will be demonstrated. Finally, quantum mechanically based research efforts to improve the performance of the boron carbide (BC) armor ceramic will be discussed. The effect of stoichiometry on the shock response of BC will be demonstrated and a recently developed method to accelerate convergence of extended system molecular dynamics methods used for rapid determination of material states lying on the Hugoniot locus will be presented.