Meso-scale Modeling of Heterogeneous Energetic Materials

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Heterogeneous energetic materials like plastic bonded explosives (PBX), pressed explosives, etc., have very detailed and non-uniform microstructure. In PBX, the heterogeneities are mainly because of the presence of energetic crystals embedded in polymer binder matrix. Also, manufacturing defects often creates pores and cracks in the material. In pressed explosives, grain boundaries, micro-cracks, pore defects, etc., are the major form of heterogeneities. Shock interaction with these heterogeneities leads to the formation of local heated regions known as hot spots. It is widely accepted that these hot spots are predominantly responsible for the triggering of chemical reaction and eventually ignition in energetic materials. There are various physical phenomenon through which hot spots can be created such as pore collapse, formation of shear bands because of plastic dissipation, inter-granular friction between the energetic crystals, debonding between crystals and binder, damage and fracture of crystals, etc. Meso-scale analysis of heterogeneous explosives demands modeling of all the necessary physical processes that governs the formation of hot spots. The modeling of the various hot spot formation mechanisms is dependent on the accurate representation of the microstructural heterogeneities. In the current work, a general framework is established to perform meso-scale simulations of heterogeneous explosives. To obtain accurate representation of the microstructure, image processing algorithms are employed on the experimentally obtained XCMT/SEM images of PBX and pressed explosive microstructures. The image processing framework is built up with a massively parallel level set based Eulerian hydrocode SCIMITAR3D. The focus of the current work is to analyze the importance of the mentioned hot spot formation mechanisms on the relative sensitivity of different samples of PBX and pressed explosives. Pore collapse, intergranular friction between the crystals, debonding between the crystals and binder and damage of energetic crystals are modeled in the current analysis to understand the shock initiation behavior of energetic materials.