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Grain Scale Simulations of Hot Spot Initiation of TATB* MICHAEL HOWARD, Lawrence Livermore National Lab, FADY NAJJAR, Lawrence Livermoer National Lab, LAURENCE FRIED, Lawrence Livrmoer National Lab — High-energetic (HE) material consists of large-sized grains with micronsized embedded impurities and pores. Under various mechanical/thermal insults, these pores collapse generating high-temperature regions leading to ignition. A computational study has been performed to investigate the mechanisms of pore collapse and hot spot initiation in TATB crystals, employing the thermo-hydrodynamics arbitrary-Lagrange-Eulerian code ALE3D. This initial study includes non-reactive dynamics to isolate the thermal and hydrodynamical effects. Two-dimensional highresolution large-scale meso-scale simulations have been undertaken. We study an axisymmetric configuration for pore radii ranging from 0.5 to $2\mu m$, with initial shock pressures in the range from 3 to 11 GPa. A Mie-Gruneisen Equation of State (EOS) model is used for TATB, and includes a constant yield strength and shear modulus; while the air in the pore invokes a Livermore Equation of State (LEOS) model. The parameter space is systematically studied by considering various shock strengths, pore diameters and material properties. We find that thermal diffusion from the collapsed pores has an important effect in generating high-temperature hot spots in the TATB.

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