Abstract Submitted
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**Computational Study of 3-D Hot-Spot Initiation in Shocked Insensitive High-Explosive**[1] F.M. NAJJAR, W.M. HOWARD, L.E. FRIED, LLNL — High explosive shock sensitivity is controlled by a combination of mechanical response, thermal properties, and chemical properties. The interplay of these physical phenomena in realistic condensed energetic materials is currently lacking. A multiscale computational framework is developed investigating hot spot (void) ignition in a single crystal of an insensitive HE, TATB. Atomistic MD simulations are performed to provide the key chemical reactions and these reaction rates are used in 3-D multiphysics simulations. The multiphysics code, ALE3D, is linked to the chemistry software, Cheetah, and a three-way coupled approach is pursued including hydrodynamics, thermal and chemical analyses. A single spherical air bubble is embedded in the insensitive HE and its collapse due to shock initiation is evolved numerically in time; while the ignition processes due chemical reactions are studied. Our current predictions showcase several interesting features regarding hot spot dynamics including the formation of a "secondary" jet. Results obtained with hydro-thermo-chemical processes leading to ignition growth will be discussed for various pore sizes and different shock pressures. LLNL-ABS-471438.

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