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Multiscale Simulation of Hot Spot Ignition LAURENCE FRIED, Lawrence Livermore National Lab, FADY NAJJAR, W. MICHAEL HOWARD, M. RIAD MANAA, SORIN BASTEA, Lawrence Livermore National Laboratory —
High explosive shock sensitivity is controlled by a combination of mechanical response, thermal properties, and chemical properties. How these properties interplay in realistic condensed energetic materials is not well understood. In this paper, we use a multiscale approach to achieve a realistic simulation of hot spot (void) ignition in a single crystal of the explosive 1,3,5-triamino-2,4,6-trinitrobenzene (TATB). The smallest length scale (¡ 10 nm) of the multiscale model was treated quantum mechanically. We have conducted multiple simulations of the decomposition of the explosive TATB using density functional tight binding molecular dynamics (DFTB-MD). Nanoscale continuum simulations were performed of void ignition using the ALE3D hydrodynamic/thermal/chemical code. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

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