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Multiscale Simulation of Hot Spot Ignition LAURENCE FRIED, 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. The simulations were performed with mesh sizes as fine as 10 nm in 2 dimensions with axisymmetric symmetry. We find that thermal transport does not significantly change void shape during the compression phase before chemistry begins. On the other hand, temperatures are dramatically affected by thermal transport.

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