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.