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Simulation of Initiation in Hexanitrostilbene[1] AIDAN THOMPSON, TZU-RAY SHAN, COLE YARRINGTON, RYAN WIXOM, Sandia National Laboratories — We report on the effect of isolated voids and pairs of nearby voids on hot spot formation, growth and chemical reaction initiation in hexanitrostilbene (HNS) crystals subjected to shock loading. Large-scale, reactive molecular dynamics simulations are performed using the reactive force field (ReaxFF) as implemented in the LAMMPS software. The ReaxFF force field description for HNS has been validated previously by comparing the isothermal equation of state to available diamond anvil cell (DAC) measurements and density function theory (DFT) calculations. Micron-scale molecular dynamics simulations of a supported shockwave propagating in HNS crystal along the [010] orientation are performed (u_p = 1.25 km/s, U_s =4.0 km/s, P = 11GPa.) We compare the effect on hot spot formation and growth rate of isolated cylindrical voids up to 0.1 m in size with that of two 50nm voids set 100nm apart. Results from the micron-scale atomistic simulations are compared with hydrodynamics simulations.

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