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Micron-scale Reactive Atomistic Simulation of Void Collapse and Hotspot Growth in PETN[1] AIDAN THOMPSON, TZU-RAY SHAN, Sandia National Laboratories — Material defects and heterogeneities such as dislocations, grain boundaries, and micro-porosity play key roles in the shock-induced initiation of detonation in energetic materials. Non-equilibrium molecular dynamics simulations (NEMD) with the ReaxFF force field (ReaxFF) in LAMMPS were performed to explore the effect of nanoscale voids on hotspot growth and initiation in pentaerythritol tetranitrate (PETN) crystals under weak shock conditions. Previously, we have performed reactive NEMD simulations of weak shocks in a $(20nm)^3$ PETN crystal containing a spherical void. We observed hotspot formation and an exothermic reaction zone. To observe growth of the hotspot, we have now greatly extended the time and lengthscale of the simulation. We created a cylindrical pore in a $0.3 \times 0.2 \times 0.001\mu m^3$ crystal. Once the shockwave reached the free surface we continued the simulation using the shock-front absorbing boundary condition. Results show steadily increasing axial and lateral spatial extent of the hotspot and a complex coupling of exothermic chemistry to hotspot growth.

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