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Micron-scale Reactive Atomistic Simulation of Void Collapse and Hotspot Growth in PETN[1] AIDAN THOMPSON, TZU-RAY SHAN, RYAN WIXOM, Sandia National Laboratories — Material defects and other heterogeneities such as dislocations, micro-porosity, and grain boundaries play key roles in the shock-induced initiation of detonation in energetic materials. We performed non-equilibrium molecular dynamics simulations to explore the effect of nanoscale voids on hotspot growth and initiation in micron-scale pentaerythritol tetranitrate (PETN) crystals under weak shock loading (Up = 1.25 km/s; Us =4.5 km/s). We used the ReaxFF potential implemented in LAMMPS. We built a pseudo-2D PETN crystal with dimensions 0.3 μm x 0.22 μm x 1.3 nm containing a 20 nm cylindrical void. Once the initial shockwave traversed the entire sample, the shock-front absorbing boundary condition was applied, allowing the simulation to continue beyond 1 nanosecond. Results show an exponentially increasing hotspot growth rate. The hotspot morphology is initially symmetric about the void axis, but strong asymmetry develops at later times, due to strong coupling between exothermic chemistry, temperature, and divergent secondary shockwaves emanating from the collapsing void.

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