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Atomistic picture of the shock to deflagration transition in a solid explosive: ultra-fast chemistry under non-equilibrium MITCHELL WOOD, MATHEW CHERUKARA, Materials Engineering, Purdue University, EDWARD KOBER, Theoretical Division, Los Alamos National Lab, ALEJANDRO STRACHAN, Materials Engineering, Purdue University — We use large-scale molecular dynamics (MD) simulations to describe the chemical reactions following the shock-induced collapse of cylindrical pores in the high-energy density material RDX. For shocks with particle velocities of 2km/s, we find that the collapse of a 40 nm diameter pore leads to a deflagration wave, resulting in the first atomic-level description of this process. Pore collapse leads to ultra-fast, multi-step chemical reactions that occur under non-equilibrium conditions. The formation of exothermic product molecules within a few picoseconds of the pore collapse prevents the nanoscale hot spot from quenching. Within 30 ps, a local deflagration wave develops which propagates at speeds of $\sim$ 0.25 km/s and consists of an ultra-thin reaction zone of only $\sim$ 5 nm, thus involving large temperature and composition gradients. These results provide insight into the initiation of detonation, which is critical to understanding the performance and safety of this class of materials.

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