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Hotspot criticality in amorphous and crystalline RDX – role of thermal conduction and initial free energy[1] ALEJANDRO STRACHAN, MICHAEL SAKANO, BRENDEN HAMILTON, Purdue University — We use molecular dynamics (MD) simulations with the reactive force field ReaxFF to characterize the criticality of nanoscale hot spots and crystalline and amorphous RDX. This is motivated by the recent finding that hotspots formed from the dynamical collapse of a pore are significantly more reactive than thermally created ones with identical size and thermodynamic conditions. The increased reactivity of the dynamical hotspot can be attributed to mechano-chemistry, reactions away from local equilibrium or the fact that the material around the dynamical hotspot is disordered and, thus, possesses higher free energy and lower thermal conductivity. We studied hotspots of various sizes and temperatures and follow their evolution to determine conditions under which they transition to a deflagration wave. Our preliminary results indicate that hotspots in amorphous RDX are more reactive and, for a give size, transition to a deflagration wave at lower temperatures. We discuss the possible origins of this increased reactivity in terms of thermal transport that tends to quench the hotspot and the free energy of the initial states.

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