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Dependence of hotspot criticality on molecular structure: amorphous vs. crystalline RDX MICHAEL SAKANO, BRENDEN HAMILTON, MD MAHBUBUL ISLAM, ALEJANDRO STRACHAN, Purdue Univ — Recent large-scale molecular dynamics (MD) simulations showed that hotspots resulting from the dynamical collapse of a void are significantly more reactive that nominally identical ones (in terms of size and thermodynamic conditions) but created under equilibrium conditions. In this work we assess whether the molecular disorder caused by the pore collapse is the main culprit for the increased reactivity of the dynamical hot spot. We use MD with the reactive force field ReaxFF to characterize the kinetics of decomposition of crystalline and amorphous RDX and to characterize the criticality of cylindrical hotspots in both materials. The simulations indicate negligible differences in the reactivity between the two structures when subjected to homogeneous heating. We also studied the chemical decomposition and reaction of cylindrical hotspots of various sizes and temperatures in the two structures. Our preliminary results indicate that hotspots in amorphous RDX are more reactive and, for a given size, transition to a deflagration wave at lower temperatures. We will discuss the possible origin of these surprising observation, including differences in thermal conductivity, temperature-induced structural transformations and the difference in exothermicity between the two systems..

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