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Influence of Combined Normal and Shear Loading on the Hotspot Criticality¹ MD MAHBUBUL ISLAM, MICHAEL SAKANO, ALEJANDRO STRACHAN, Purdue University — We are interested in understanding hotspot (HS) formation and criticality in energetic materials. The pore collapse is thought to be the dominant HS formation mechanism, and the process consists of expansion, compression, jetting, and shearing of the materials involved. Given the significant molecular disorder during the formation of hotspots, we contrast the criticality of hotspots in amorphous and crystalline RDX and observe that structural effects are relatively insignificant. Using ReaxFF molecular dynamics simulations, we further characterize how different types of mechanical loading affect the formation and criticality of the HS in RDX. We choose an initial planar configuration of the pore to independently control the relative contributions of the normal and shear loadings and investigate their role on the HS criticality. We evaluate how energy input to the HS, in the form of PV work and interfacial friction due to the impact and shear, respectively, regulates the HS temperature and chemical kinetics. We also elucidate the loading type dependency on the reaction initiation pathways and evaluate the role of dynamic loading and non-equilibrium states towards the HS criticality.

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