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Molecular Dynamics Simulations of Rapidly Heated RDX MARK ELERT, RYAN LE, U. S. Naval Academy, SAMUEL EMERY, PAUL GIANNUZZI, DANIEL MCCARTHY, Naval Surface Warfare Center Indian Head Explosive Ordnance Disposal Division, IGOR SCHWEIGERT, U. S. Naval Research Laboratory
— As part of a study of the possible use of explosively generated plasmas to induce deflagration in energetic materials, we have investigated the short-time dynamics of rapidly heated RDX using a version of the ReaxFF reactive potential model optimized for energetic materials simulations. For an RDX crystal heated at one end, we have examined the propagation of energy and reactivity as a function of time. We have also performed MD simulations on a uniformly heated RDX crystal at a range of temperatures up to 8000 K, to investigate the temperature vs. time profile and the detailed kinetics of the deflagration process.

Mark Elert
U. S. Naval Academy

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