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Phase-field modeling of shock-induced α-γ phase transformation of RDX[1] - RAHUL, SUVRANU DE, Rensselaer Polytechnic Institute — A thermodynamically consistent continuum phase field model has been developed to investigate the role of shock-induced α-γ phase transition in the sensitivity of RDX. Dislocations and phase transformations are distinguished and modeled within a crystal plasticity framework. The Landau potential is derived for the finite elastic deformation analysis. The response of the shock loaded RDX crystal is obtained by solving the continuum momentum equation along with phase evolution equation using a Helmholtz free energy functional, which consists of elastic potential energy and local interfacial energy that follows from the Cahn–Hilliard formalism. We observe that the orientations for which there is a resolved shear stress along the slip direction, the material absorbs large shear strain through plastic deformation, allowing it to be less sensitive as less mechanical work is available for temperature rise. Therefore, plastic slip should be associated with greater shear relaxation and, hence, decreased sensitivity. For elastic orientations, large shear stress arises from steric hindrance that may provides much more mechanical work to increase the temperature and hence more sensitive to detonation. Our simulations suggest that the α-γ phase transformation in RDX may be associated with the increased temperature rise and hence the shock sensitivity.

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