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Modeling pore collapse and chemical reactions in shock-loaded HMX crystals[1] RYAN AUSTIN, NATHAN BARTON, WILLIAM HOWARD, LAURENCE FRIED, Lawrence Livermore National Laboratory — The collapse of micron-sized pores in crystalline high explosives is the primary route to initiating thermal decomposition reactions under shock wave loading. Given the difficulty of resolving such processes in experiments, it is useful to study pore collapse using numerical simulation. A significant challenge that is encountered in such calculations is accounting for anisotropic mechanical responses and the effects of highly exothermic chemical reactions. In this work, we focus on simulating the shock-wave-induced collapse of a single pore in crystalline HMX using a multiphysics finite element code (ALE3D). The constitutive model set includes a crystal-mechanics-based model of thermoelasto-viscoplasticity and a single-step decomposition reaction with empirically determined kinetics. The model is exercised for shock stresses up to $\sim$10 GPa to study the localization of energy about the collapsing pore and the early stages of reaction initiation.

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