α-RDX

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Molecular dynamics study of shock loading followed by release in (100)-oriented ANDREY PEREVERZEV, University of Missouri, NITHIN MATHEW, E.M. KOBER, Los Alamos National Laboratory, TOMMY SEWELL, University of Missouri — Molecular dynamics simulations were used to study shock loading and release in (100)-oriented α-RDX. A reverse-ballistic configuration was used where the sample, initially at 300 K, impacts onto a rigid, stationary piston at an initial velocity of either 1 km/s or 2 km/s, generating a supported shock wave. Failure is induced by allowing the simulations to continue through the release process from the maximum compression out to some final sample length that is about 1.5 times the starting value. The material response to the shock compression differs significantly for the 1 km/s and 2 km/s impacts. In the former case, extended, intersecting shear bands oriented at approximately 45 to the shock direction form fill the [010] zone of the sample. For the latter case, a high density of localized translational defects develop but these do not grow or glide, presumably because they are formed immediately at the shock front and are "locked in" due to their very high density and interactions. These qualitatively differing states exhibit decidedly different behaviors during release, namely failure mediated by the shear bands in the weaker shock case and cavitation in the case of the stronger shock. Efforts to characterize these phenomena and draw contrasts with what is typically observed for spall in metals will be discussed.

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