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An abundance of mechanisms for plastic flow in an extremely brittle material: dislocations and phase transformations in RDX

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Orientation-dependent anisotropies in the initiation sensitivity of PETN can be rationalized elegantly by the availability and activity of dislocation slip systems for a given crystallographic orientation of the shock propagation direction. The true power of the resulting steric hindrance model is that it provides a framework for predicting anisotropies in the initiation sensitivity of any pristine energetic molecular crystal once its slip systems have been identified and characterized rigorously. I will present a review of recent molecular dynamics simulations and experiments that demonstrate that the energetic molecular crystal RDX is a rather plastic material under compression owing to a surprising number of mechanisms for plastic flow and stress relaxation. I will focus on the homogeneous nucleation of dislocations under shock compression and surface indentation, complex patterns of spatially localized melting and flow during void collapse, and the discussion of two shock-induced phase transformations in oriented RDX single crystals.