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**Shock response of single crystal and nanocrystalline pentaerythritoltetranitrate: Implications to hotspot formation in energetic materials**
YANG CAI, University of Science and Technology of China, SHENG-NIAN LUO, The Peac Institute of Multiscale Sciences (PIMS) — We investigate shock response of single crystal and nanocrystalline pentaerythritol tetranitrate (PETN) with a coarse-grained model and molecular dynamics simulations, as regards mechanical hotspot formation in the absence or presence of grain boundaries (GBs). In single crystals, shock-induced plasticity is consistent with resolved shear stress calculations and the steric hindrance model, and this deformation leads to local heating. For regular-shaped hexagonal columnar nanocrystalline PETN, different misorientation angles lead to activation of different/same slip systems, different deformation in individual grains and as a whole, different GB friction, different temperature distributions, and then, different hotspot characteristics. GB friction alone can induce hotspots, but the hotspot temperature can be enhanced if it is coupled with GB-initiated crystal plasticity, and the slip of GB atoms has components out of the GB plane. The magnitude of shearing can correlate well with temperature, but the slip direction of GB atoms relative to GBs may play a critical role. GB-related friction and plasticity induce local heating or mechanical hotspots, which could be precursors to chemical hotspot formation related to initiation in energetic materials, in the absence of other, likely more effective, means for hotspot formation such as void collapse.

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