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Atomistic Simulation of Orientation Dependence in Shock-induced Initiation of Pentaerythritol Tetranitrate (PETN) TZU-RAY SHAN, RYAN WIXOM, ANN MATTSSON, AIDAN THOMPSON, Sandia National Laboratories, SANDIA NATIONAL LABORATORIES TEAM — Predicting the behavior of energetic materials requires a detailed description of how chemical reactions initiate during initial stages of detonation. In this talk, the dependence of the reaction initiation mechanism of pentaerythritol tetranitrate (PETN) on shock orientation and shock strength is investigated with molecular dynamics simulations using a reactive force field and the multi-scale shock technique. In the simulations, a single crystal of PETN is shocked along [110], [001], and [100] orientations with shock velocities in the range 3-10 km/s. Major reactions occur with shock velocities of 6 km/s or stronger, and reactions initiate through the dissociation of nitro (NO_2) and nitrate (NO_3) groups from the PETN molecules. The most sensitive orientation is [110], while [100] is the most insensitive. For the [001] orientation, PETN decomposition via nitro group dissociation is the dominant reaction initiation mechanism, while for [110] and [100] orientations the decomposition is via mixed nitro and nitrate group dissociation. For shock along the [001] orientation, we find that C-NO_2 bonds initially acquire more kinetic energy, facilitating nitro dissociation. For the other two orientations, C-ONO_2 bonds acquire more kinetic energy, facilitating nitrate group dissociation.

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