Computational Protocol to Predict Sensitivity:

Validation for PETN

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Abstract

To understand its orientation-dependent shock sensitivity, pentaerythritol tetranitrate (PETN) explosive single crystal has been thoroughly studied using molecular dynamics (MD) simulations with reactive force field (ReaxFF). Based on our preliminary results and J. J. Dick’s steric hindrance theory, a compress-and-shear protocol is designed to test high energy materials’ shock sensitivity. Tests on various slip systems for pre-compressed single crystal are found to have different resolved shear stress and distinguishable stress evolvement in shearing, from which we can decide the possible active slip systems for a given shock and how sensitive it will be. Our analysis shows good agreement with the available experimental results. For most high energy materials without much experimental results, this protocol provides not only a rigorous and simple way to predict its shock sensitivity, but also some useful hints to aid the explosive design and improvement.