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Compressive shear reactive dynamics to evaluate the anisotropic sensitivity of single-crystal energetic materials[1] SERGEY ZYBIN, California Institute of Technology, PENG XU, YI LIU, WILLIAM GODDARD III, California Institute of Technology — Complex coupling between mechanical, thermal, and chemical effects are at the heart of many important but not understood phenomena, including the shock sensitivity of materials to detonation. We propose a general protocol (Compressive Shear Reactive Dynamics, CS-RD) for predicting the mechanic, thermal, and chemical processes and show that this protocol predicts correctly the relative sensitivities observed experimentally for single crystal PETN [C(CH2ONO2)4]. We find that sensitive directions lead to close molecular contacts (steric hindrance) resulting in severe deformation that leads to large stress overshoots and increases in temperature that results in bond-breaking processes whereas insensitive directions exhibit little distortion or stress overshoot, delayed temperature increases and less dissociation. This insight that a planar shock fails because of shear in a plane oblique from the shock direction and that the essential features controlling the failure mechanisms must be sought in this shear phenomena should be useful in elucidating the mechanisms for more complex multigranular multicomponent systems including defects and it may be useful for other complex collision phenomena.

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