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Shear-strain Sensitivity of Energetic Crystals and the Origin of Hot-spots MAIJA KUKLJA[1], Division of Materials Research, National Science Foundation, SERGEY RASHKEEV[2], Center for Advanced Modeling & Simulation, Idaho National Laboratory — Simulation of shear-induced chemical reactions of decomposition of crystalline FOX-7 and TATB is performed by means of Density Functional Theory and First Principles Molecular Dynamics. It is shown that the shear-strain deformation plays a crucial role in defining the sensitivity of explosive crystals to initiation and strongly depends on the shape of crystalline layers constituting the materials. Energetic barriers for FOX-7 decomposition are found to decrease due to shear while those for TATB are not affected by this deformation. We discuss possible mechanisms of chemistry in hot spots, associated with the local shear-strain deformation. This work made possible to provide specific recommendations for synthesis of insensitive energetic materials.

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