MATERIALS ENGINEERING
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"ROLE OF ENERGY LOCALIZATION ON CHEMICAL REACTIONS AT EXTREME CONDITIONS"

By

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Purdue MSE PhD Dissertation

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ABSTRACT

High explosives represent a class of materials known as energetic materials, in which providing an external stimulus of impact, heat, or electric shock can result in rapid exothermic reactions. Hence, there has always been a considerable research focus into the development, production, optimization, and control of these materials, aiming to increase explosive capabilities while also decreasing overall sensitivity to ignition.

The study of impact induced chemical initiation of explosives is an inherent multiscale problem that requires time and length scales not accessible by a single experiment or calculation. The work presented here provides a theoretical effort to contribute to bottom-up modeling of the physics and chemistry phenomena in reacting high explosives using molecular dynamics simulations. Focus will be placed how energy localizes in the molecular crystal TATB, an insensitive high explosive.

The idea of energy localization will focus on hotspots, which are areas of extreme temperature following interactions between a shockwave and the microstructure. To date, hotspots have been characterized and described by their temperature fields only. Here, I develop a description of the potential energy field in the hotspot, which is markedly different from the temperature field and cannot be predicted from it. This latent potential energy manifests from intra-molecular strain in which individual molecules in the hotspot become highly distorted. This strain energy is shown to be driven by plastic flow during the formation of the hotspot.

Reactive molecular dynamics calculations of shockwave induced pore collapse shows these deformed molecules react faster, follow different ensemble statistics, and undergo different first step reaction pathways. To better study these deformations under equilibrium, the Many-Bodied Steered MD method is developed in which multiple deformation modes are explored. It is shown that different deformation paths in the same molecule leads to different mechanochemical accelerations of kinetics and a different alteration of first step reaction pathways.

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