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Shock Waves and Defects in Energetic Materials, a Match Made in MD Heaven.[1] MITCHELL WOOD, DAVID KITTELL, COLE YARRINGTON, AIDAN THOMPSON, Sandia National Labs — Shock wave interactions with defects, such as pores, are known to play a key role in the chemical initiation of energetic materials. In this talk the shock response of Hexanitrostilbene (HNS) is studied through large scale reactive molecular dynamics (RMD) simulations. These RMD simulations provide a unique opportunity to elucidate mechanisms of viscoplastic pore collapse which are often neglected in larger scale hydrodynamic models. A discussion of the macroscopic effects of this viscoplastic material response, such as its role in hot spot formation and eventual initiation, will be provided. Through this work we have been able to map a transition from purely viscoplastic to fluid-like pore collapse that is a function of shock strength, pore size and material strength. In addition, these findings are important reference data for the validation of future multi-scale modeling efforts of the shock response of heterogeneous materials. Examples of how these RMD results are translated into mesoscale models will also be addressed.

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