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**Examining the effects of microstructure and loading on the shock initiation of HMX with mesoscale simulations** H. KEO SPRINGER, CRAIG TARVER, SORIN BASTEA, Lawrence Livermore National Laboratory — We perform reactive mesoscale simulations to study shock initiation in HMX over a range of pore morphologies and sizes, porosities, and loading conditions in order to improve our understanding of structure-performance relationships. These relationships are important because they guide the development of advanced macroscale models incorporating hot spot mechanisms and the optimization of novel energetic material microstructures. Mesoscale simulations are performed using the multiphysics hydrocode, ALE3D. Spherical, elliptical, polygonal, and crack-like pore geometries 0.1, 1, 10, and 100 microns in size and 2, 5, 10, and 14% porosity are explored. Loading conditions are realized with shock pressures of 6, 10, 20, 38, and 50 GPa. A Cheetah-based tabular model, including temperature-dependent heat capacity, is used for the unreacted and the product equation-of-state. Also, in-line Cheetah is used to probe chemical species evolution. The influence of microstructure and shock loading on shock-to-detonation-transition run distance, reaction rate and product gas species evolution are discussed. This work performed under the auspices of the U.S. DOE by LLNL under Contract DE-AC52-07NA27344. This work is funded by the Joint DoD-DOE Munitions Program.

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