

Abstract Submitted  
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**Coupling crystal plasticity and phase-field damage to simulate  $\beta$ -HMX-based polymer-bonded explosive under shock load** NICOLO GRILLI<sup>1</sup>, AKSHAY DANDEKAR, MARISOL KOSLOWSKI, Purdue University — The development of high explosive materials requires constitutive models that are able to predict the influence of microstructure and loading conditions on shock sensitivity. In this work a model at the continuum-scale for the polymer-bonded explosive constituted of  $\beta$ -HMX particles embedded in a Sylgard matrix is developed. It includes a Murnaghan equation of state, a crystal plasticity model, based on power-law slip rate and hardening, and a phase field damage model based on crack regularization. The temperature increase due to chemical reactions is introduced by a heat source term, which is validated using results from reactive molecular dynamics simulations.

An initial damage field representing pre-existing voids and cracks is used in the simulations to understand the effect of these inhomogeneities on the damage propagation and shock sensitivity. We show the predictions of the crystal plasticity model and the effect of the HMX crystal orientation on the shock initiation and on the dissipated plastic work and damage propagation. The simulation results are validated with ultra-fast dynamic transmission electron microscopy experiments and x-ray experiments carried out at Purdue University.

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