

Abstract Submitted  
for the SHOCK19 Meeting of  
The American Physical Society

**Hotspot formation due to crack in HMX crystals**<sup>1</sup> CHUNYU LI, ALEJANDRO STRACHAN, Purdue Univ — The shock to detonation transition in composite high energy density materials results from the complex interplay between the propagating wave and microstructural features that lead to the formation of hotspots and the exothermic reactions in these hotspots. We report on large-scale molecular dynamics simulations of the formation of hotspots due to the interaction of a shockwave and internal flaws and pores in crystalline HMX. We characterize the effect of size and orientation of elliptical cracks on the resulting hotspots. Comparing non-equilibrium shock propagation simulations with equilibrium Hugoniotstat simulations for identical shock strength enables us to separate the contribution of different mechanisms to the overall temperature and size of the resulting hotspot. Specifically, we focus on the role of jetting, expansion and recompression, friction and viscous pore collapse.

<sup>1</sup>This work was support by the US Office of Naval Research, Multidisciplinary University Research Initiatives (MURI) Program, Contract: N00014-16-1-2557.

Chunyu Li  
Purdue University

Date submitted: 19 Mar 2019

Electronic form version 1.4