Abstract Submitted
for the SHOCK19 Meeting of
The American Physical Society

Hot spot ignition through shear banding in TATB single crystals shocked to detonation pressures MATTHEW KROONBLAWD, LAURENCE FRIED, Lawrence Livermore National Laboratory — Detonating high explosives exhibit different reaction responses than those undergoing shock initiation. Shear banding in the bulk crystal, as opposed to void collapse, is a plausible mechanism for ignition that could become significant at higher shock pressures. Using all-atom molecular dynamics simulations, we demonstrate the dynamic formation of shear bands in TATB single crystals shocked to 30 GPa, which corresponds to the steady detonation pressure. Structural analysis reveals that shear bands in TATB develop and grow as regions of amorphous material that are substantially hotter than the crystalline bulk surroundings. Through scale-bridging with semi-empirical quantum-based molecular dynamics, we show that the amorphous shear bands are more chemically reactive than the bulk. An Arrhenius kinetics analysis of multiple simulations reveals that increases in shear band reactivity manifest as a simultaneous reduction in the activation energy and increase in the pre-exponential factor. Connections to continuum-level models for shock initiation are described. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. It is approved for unlimited release with document number LLNL-ABS-768121.

Matthew Kroonblawd
Lawrence Livermore Natl Lab

Date submitted: 22 Feb 2019

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