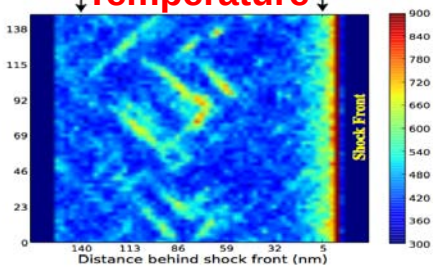
General, Unified, Multiscale Modeling to Predict the Sensitivity of Energetic Materials (MURI), PI: Donald L. Thompson, University of Missouri - Columbia

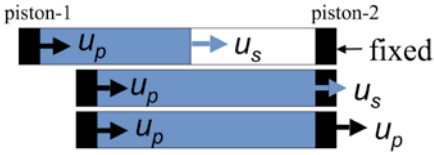
Objective: Develop methods spanning all scales for predicting the properties of energetic materials relevant to understanding detonation sensitivity.

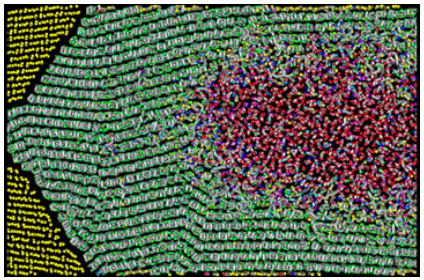
Scientific Challenges.
- Accurate reactive potential
- Extension of MD methods to sufficient temporal and spatial scales to simulate energy localization and initiation of chemistry under practical conditions of thermo-mechanical load
- Sequential and concurrent multiscale methods

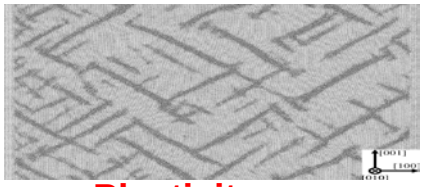
Temperature



Shocks







Plasticity

Hotspot formation

Major Accomplishments:
•Improved shock front absorbing boundary condition method & performed MD studies of shocked RDX. • Develop automated analysis of post-shocked materials. • Parameterized of bond-charge electrostatic model for H, F, C systems. • Implemented bond-charge model in simulation software. • Discovered two mechanisms relating interface faceting to sensitivity of PBXs. • Simulated "nano-jetting" and characterized its role in initiation at voids, including a new analytic model • Developing new temporal and spatial scaling from molecular detonation to hot spot initiation. • Calculated the elastic constants and studied the basis set effects on the results

Personnel: 7 graduate students, 0 undergraduates, 3 postdoctoral, 3 faculty members

Army Relevance: The successful completion of this project will provide the Army with improved computational tools on atomic & mesoscopic scales and physical insights that collectively will enhance efforts to develop new insensitive munitions

Funding profile: FY05 $85.7k FY06 $401.8k FY07 $472.5k FY08 $419.7 FY09 $527.6

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