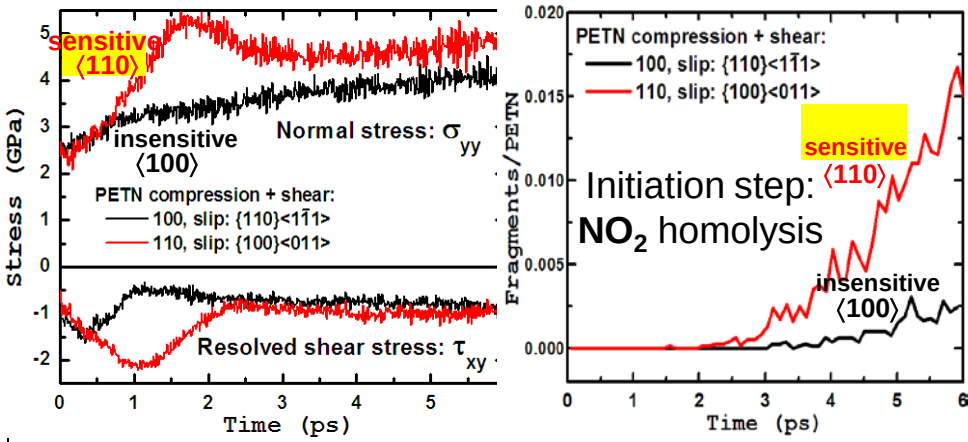
Fundamental chemistry and physics of munitions under extreme conditions (MURI): William A. Goddard, Micael Ortiz, Caltech

Objective: 1. Develop simulation methodology validated by experiment to elucidate the chemical and physical processes governing the initiation and sensitivity of energetic materials (EM) under shock, shear, and thermal impact. 2. Develop a physically based multiscale methodology for the prediction of shock driven ignition of heterogeneous polycrystalline high energetic materials.

Scientific Challenges.

- Development of a multiscale methodology which can be linked to reactive molecular dynamic simulations of HE materials.
- Develop transferable reactive force field ReaxFF for modeling of shock, flame, and detonation in EM
- Develop techniques for modeling mechanical and thermal effects on initiation and sensitivity of EM



ReaxFF prediction of experimentally-observed anisotropy of shock sensitivity in single-crystal PETN

Major Accomplishments:

- Extension of the crystal plasticity model by making use of the information coming from Gamma surface computations to include more general molecular crystalline classes
- Dynamic Shear Compression methodology to predict anisotropy of sensitivity of single crystal EM under shock and shear impact
- Empirical correction of DFT to predict equilibrium density of EM and equation of state at high strain
- Large-scale parallel ReaxFF simulations of shock initiation of EM crystals with and without defects

Personnel: 2 Faculty, 2 Research Scientists, 3 Doctoral Students, 1 Graduate Student

Army Relevance: Provide new computational tools for predictive modeling to test new HE compositions and packing strategies to:

- reduce HE sensitivity, and
- retain or improve HE performance
- in new generations of insensitive munitions

Total funding FY05 $300k, FY06 $600k, FY07 $600k, FY08 $482k, FY09 $659k, FY10 $350k

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