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Pressure dependence of electronic states in secondary explosives: comparison between bulk and air/explosive interface. Darcie Farrow, Ian Kohl, Kathy Alam, Laura Martin, Stephen Rupper, Hongyou Fan, Kaifu Bian, Robert Knepper, Michael Marquez, Jeffery Kay; Sandia National Laboratories, Albuquerque, NM 87185

Although shock initiation of explosives has been studied for decades, it is still not clear how shock waves initiate chemical reactions that lead to detonation. The mechanism of "hot spot" initiation is unclear. It is empirically well-known that material porosity enhances shock sensitivity, and it is often assumed that localized heating initiates reactions at defect sites. However, a wealth of evidence indicates that the mechanism may not be thermal heating, but rather spontaneous pressure-induced decomposition. This alternate mechanism is postulated to involve shock-induced changes in the electronic structure of the material, in which instantaneous reactions occur at the shock front, assisted by local distortion of electronic structure at defect sites. At present, no definitive measurement or calculation has proven or disproven this mechanism.

We are applying electronic sum frequency spectroscopy to directly measure the electronic absorption spectra of explosive films at an explosive/air interface and compare to UV/Vis spectra of the bulk film. We will then repeat measurement under static pressure using a diamond anvil cell to determine if this pressure-induced band gap compression is a factor in hot spot initiation during shock compression. We will report efforts to set up an ESFG measurement on vapor deposited HNS films.