

Abstract Submitted
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Measuring HOMO/LUMO gap of explosive film at air interface using ESFG: model for explosive at void surface DARCIE FARROW, IAN KOHL, SEAN KEARNEY, STEPHEN RUPPER, LAURA MARTIN, KATHY ALAM, ROBERT KNEPPER, JEFFERY KAY, Sandia Natl Labs — Vibrational broadband sum frequency generation has enabled measurements of heat transfer/disorder under shock compression on monolayer length scales (Carter, JPCA, 2008). At Sandia, we are extending this approach to examine shock-induced changes in the electronic structure of secondary explosives at surfaces using electronic sum frequency generation (ESFG)(Yamaguchi, JCP, 2008). Theoretical studies suggest explosives at voids and grain boundaries may have different reactivity than bulk material based on shifts in the bandgap at defects (Kuklja, Appl. Phys. A 2003). We seek to measure these electronic shifts for the first time using a thin film explosive samples as a model for the void surface. We will report electronic sum frequency data from vapour deposited thin film explosive compared to UV/Vis data of the bulk film at ambient pressures and discuss application of ESFG technique to samples under shock compression.

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