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Measuring and modeling the electronic structure of explosives at the explosive/air interface.

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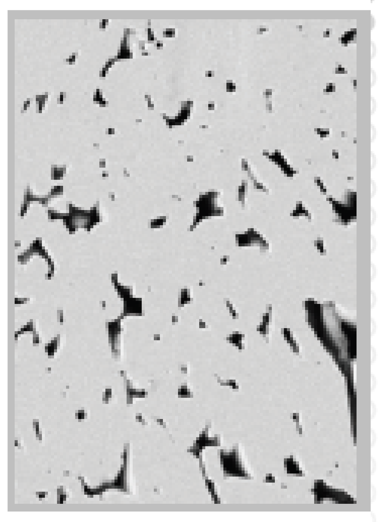

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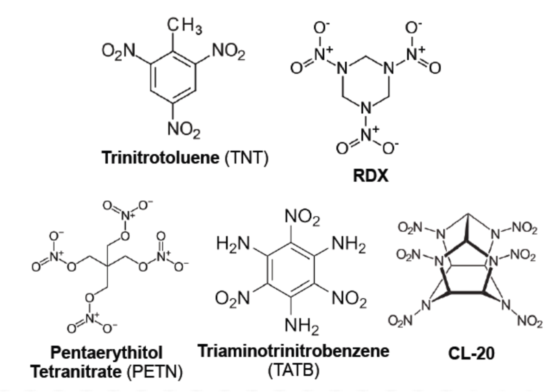
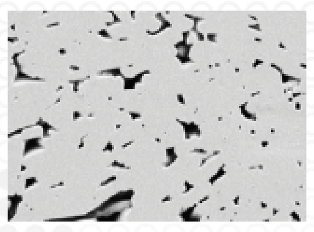
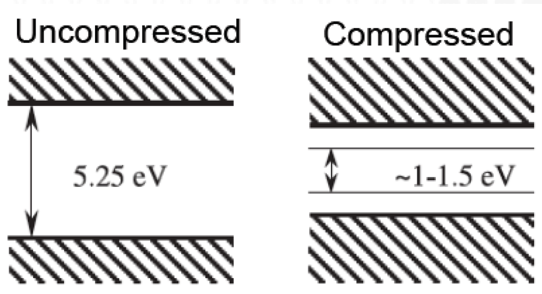
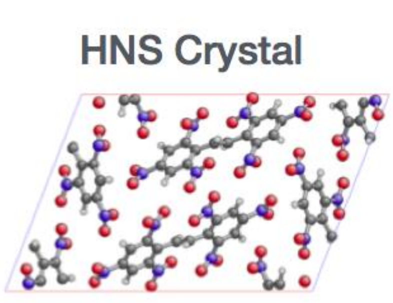
Motivation





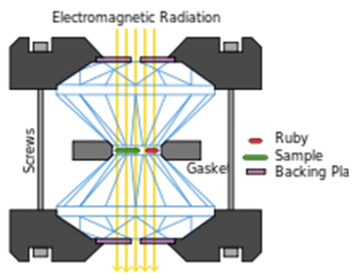


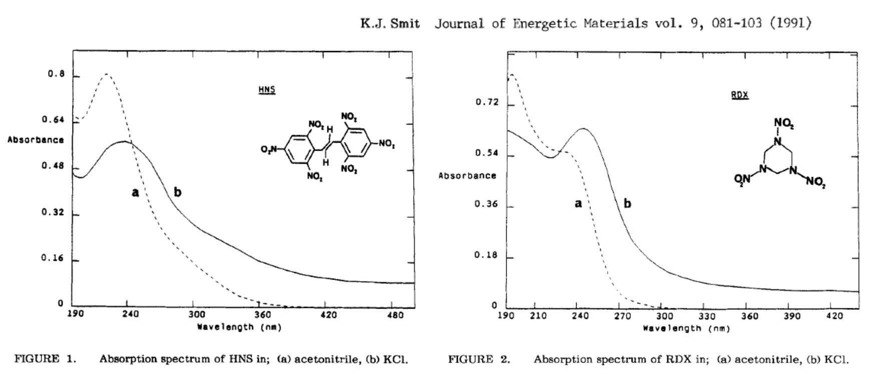
Kuklja *Appl. Phys. A* **76**, 359 (2003)



- Secondary explosives are ***stable molecules*** that react rapidly under shock compression.
- Voids and grain boundaries significantly increase the sensitivity and rate of initiation.
- Theorists predict pressure induced band gap reduction occurs and may drive rapid reactivity.
- Pressure induced gap compression has never been observed on the timescale of shock-rise.
- Explosive at void or grain boundary surface may experience increased band gap compression.

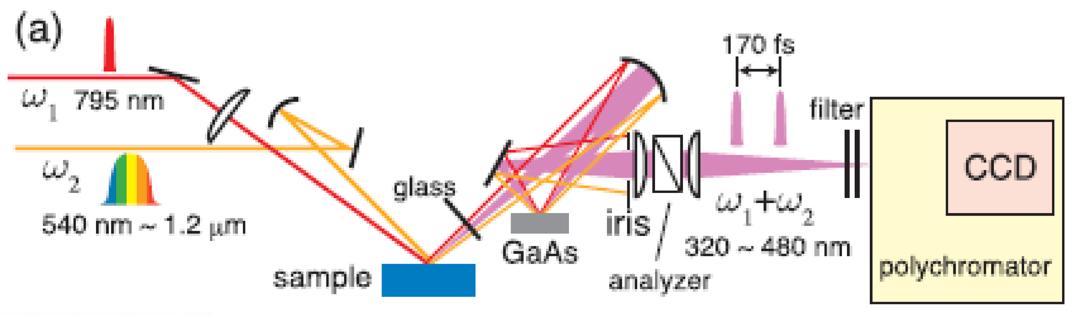
UV/Vis Spectra films/ crystal





- Spectra will be taken of films and powder at ambient and static pressure s < 25 GPa.
- Quantify band gap compression in bulk material and compare to predictions in previous work.

ESFG at Explosive Film/Air



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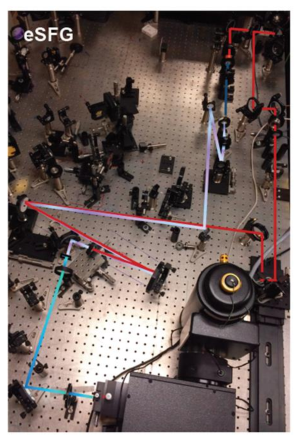
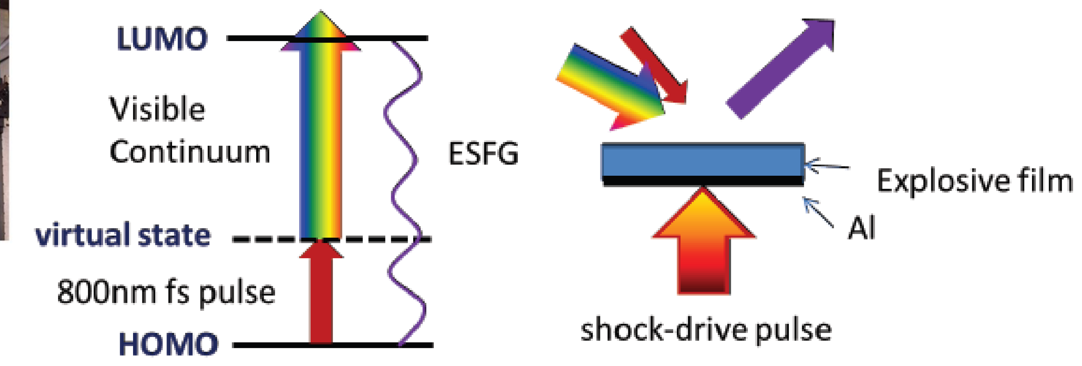
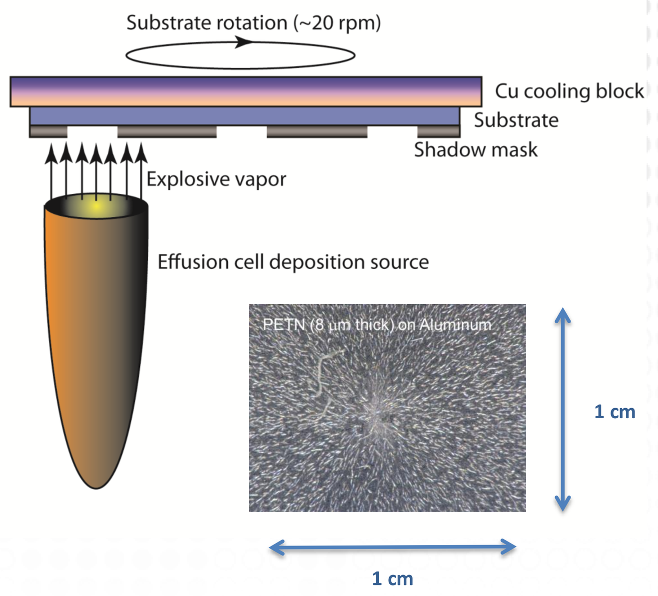
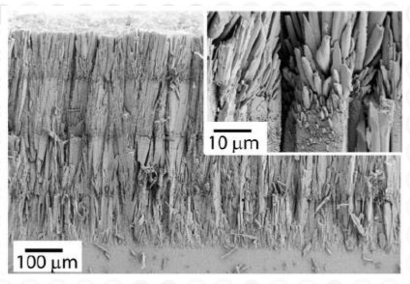




Measurement combines broad-band continuum and narrow-band pulse to generate light at the sum of their frequencies within a few monolayers of the interface. Signal increases when sum matches the HOMO/LUMO gap.

Thin-film Explosive Samples

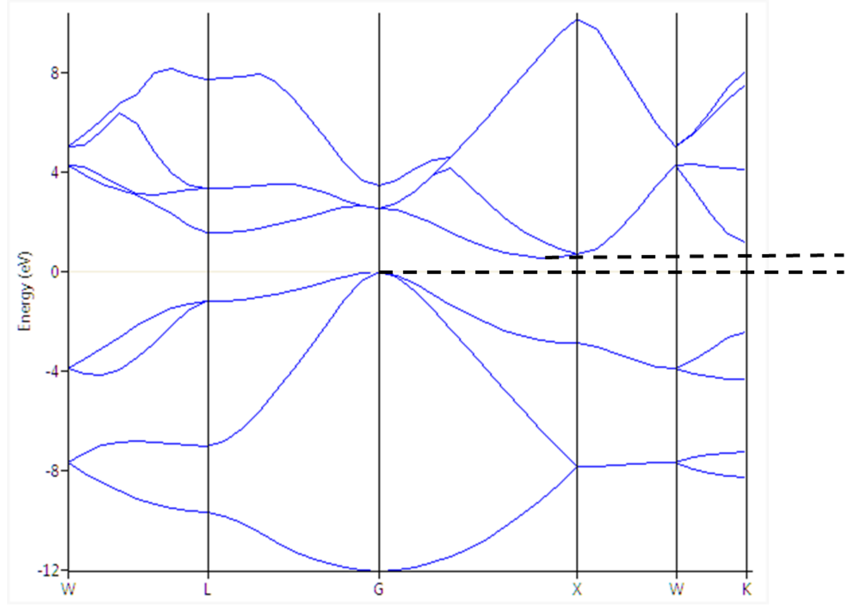




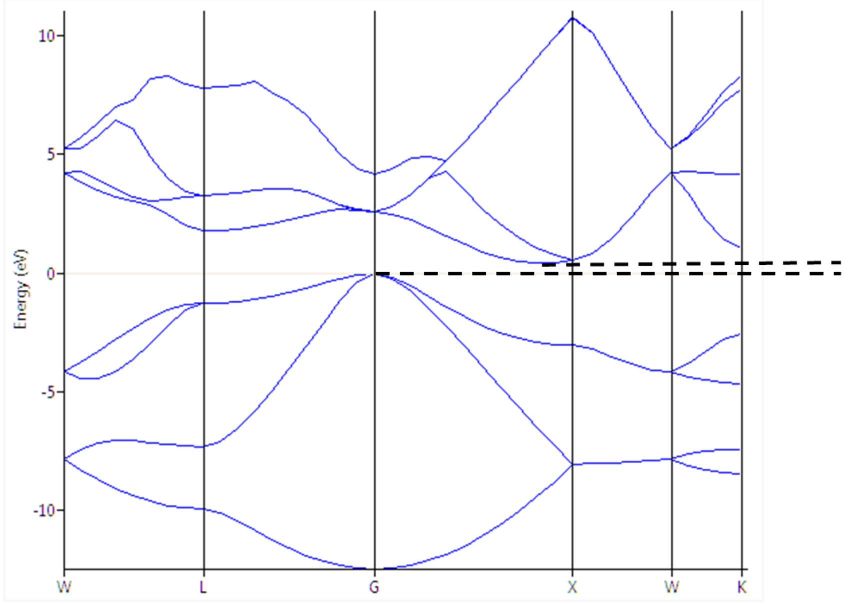
Knepper et al. *J.Mater.Res.* **26** (2011)

- 5- 8 um of PETN, HNS, CL20, HNAB or RDX will be vapor deposited over 1.5-2um Aluminum or UV fused silica.
- Samples are mounted in a reflection geometry.

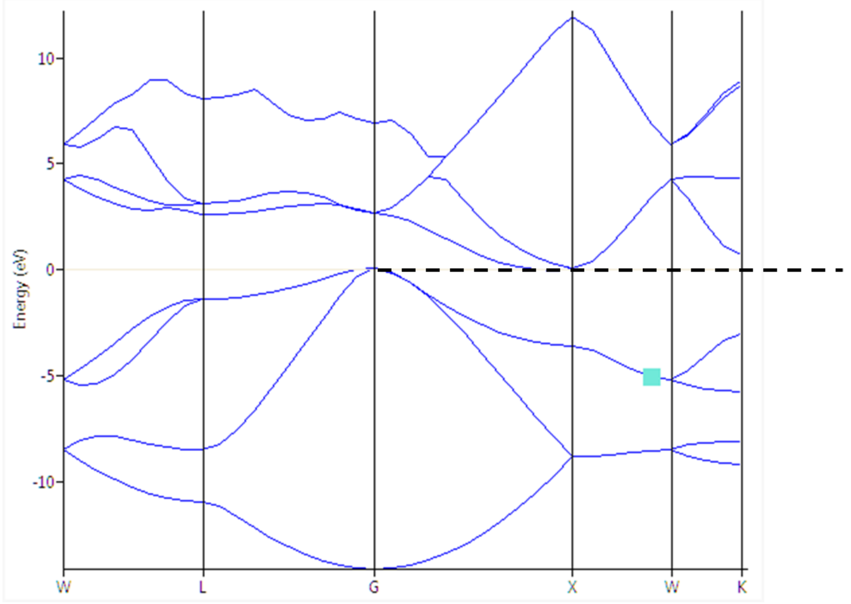
Modeling Band Gap Shift



Ambient Pressure

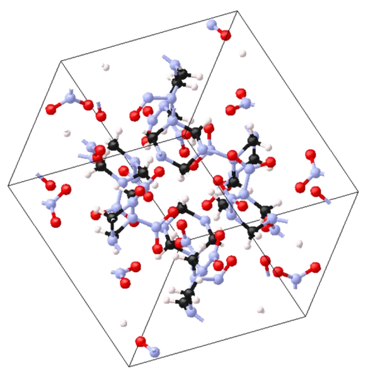


P= 10 GPa



P= 50 GPa

- Density functional theory used simulate shift in HOMO/LUMO gap of an extended lattice with pressure.
- Preliminary Calculations carried out on silicon as a function of pressure.
- Similar effects are expected to occur in explosive crystals. Calculations are currently being performed to assess pressure-induced band gap closure in RDX, HNS (hexanitrostilbene), PETN (pentaerythritol tetranitrate), and TATB (triaminotrinitrobenzene).



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