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

SAND2016-5093C

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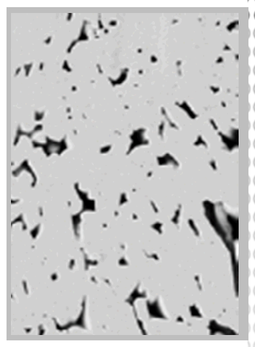

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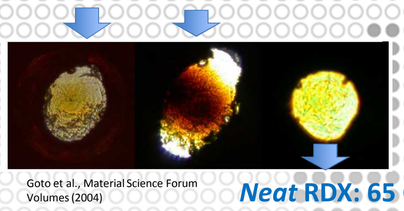
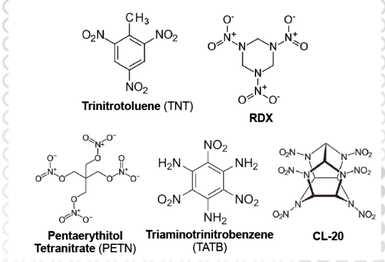
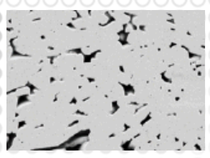
Motivation

RDX *in CsI*: 22GPa 48GPa

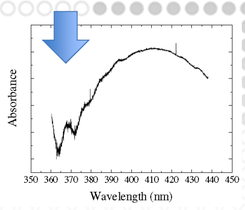


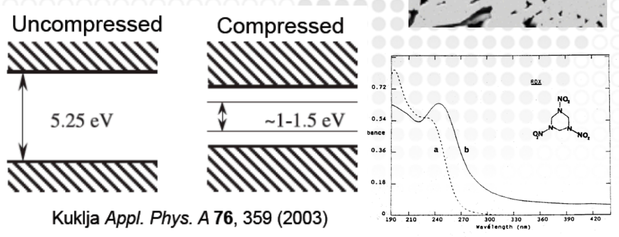
Goto et al., Material Science Forum Volumes (2004)





Neat RDX: 65 GPa

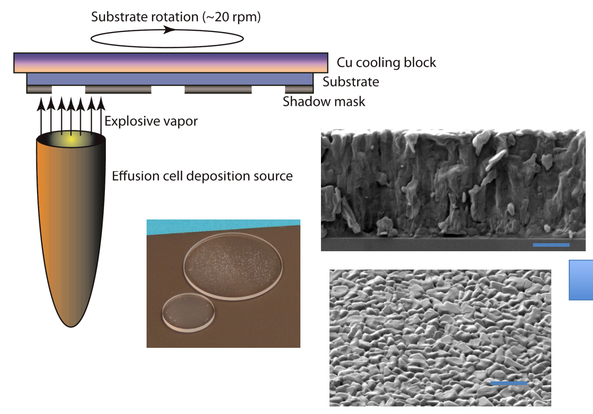




Kuklja *Appl. Phys. A* **76**, 359 (2003)

- 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 HOMO/LUMO gap reduction occurs and may drive rapid reactivity.
- Explosive at void or grain boundary surface may experience increased reduction in HOMO/LUMO gap.

Approach: Film/air interface faux void

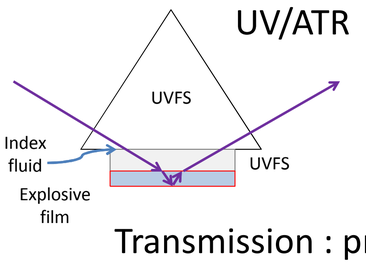


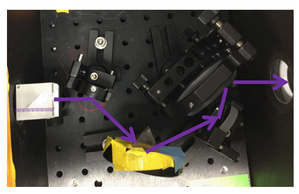
Surface specific UV/Vis Spectroscopy :

Electronic Sum Frequency Generation?

Measure UV/Vis spectra of a thin film explosive/air interface to observe *red shift in band edge*.

UV/ATR at film/air interface





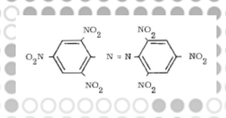
Transmission : prism + flat

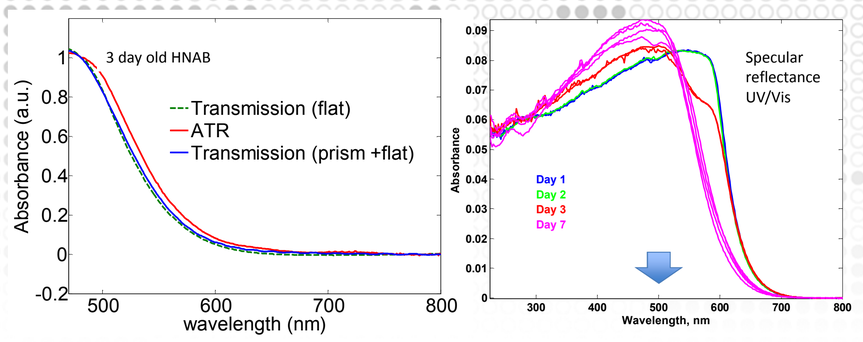
Transmission : flat only

- PerkinElmer Lambda 750 equipped with tungsten-halogen and deuterium sources, with PMT detection.
- Spectra taken of thin film in ***transmission*** mode through prism/index fluid and of flat/film sample to measure ***UV/Vis of bulk film.***
- ATR spectra for UVFS plate with and without thin film explosive. ***Red shift and/or change in shape indicate increased surface contribution to spectra.***

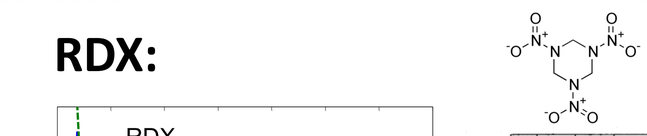
UV/ATR at ambient temperature/pressure

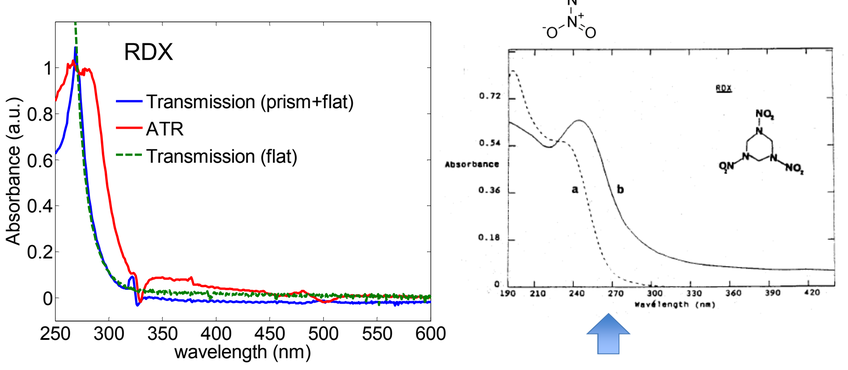
HNAB:





RDX:





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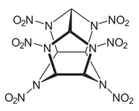
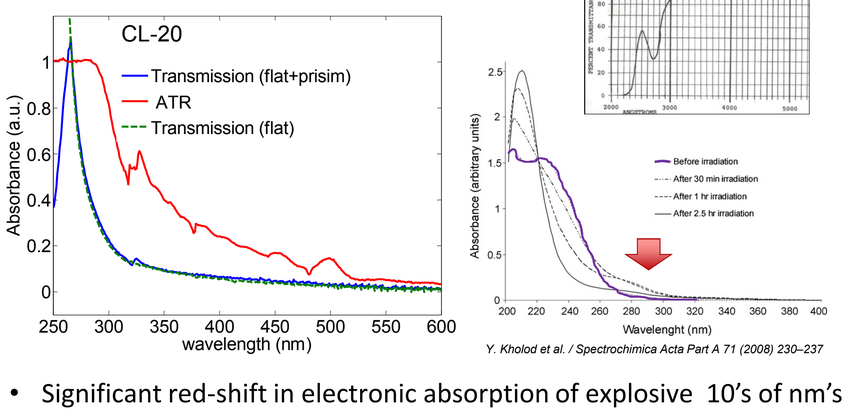
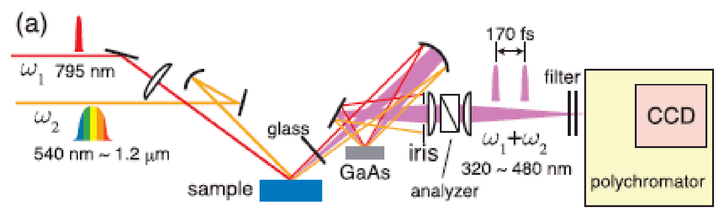




Y. Kholod et al. / Spectrochimica Acta Part A 71 (2008) 230–237

- Significant red-shift in electronic absorption of explosive 10's of nm's from the film surface compared to the bulk film .
- Red shift larger when bulk material band edge is in UV.

Next Step: Surface vs. film spectrum at elevated pressure



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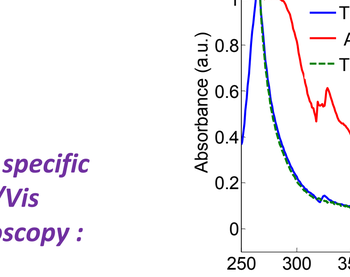
J. Chem. Phys. **129**, 101102 (2008)



- Performing a surface specific spectroscopy (UV/ATR or Electronic Sum Frequency Generation –ESFG) on sample under shock compression or static compression (DAC).
- Compare to TA or UV/Vis data of film under equivalent conditions.
- Use DFT models of material to understand changes in electronic structure in both systems.

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