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The Effects of Microstructure on the Propagation of Shock Waves in Porous Energetic Materials

Ryan R. Wixom
Manager - Nanostructure Physics
Center for Integrated Nanotechnologies (CINT)
Sandia National Laboratories

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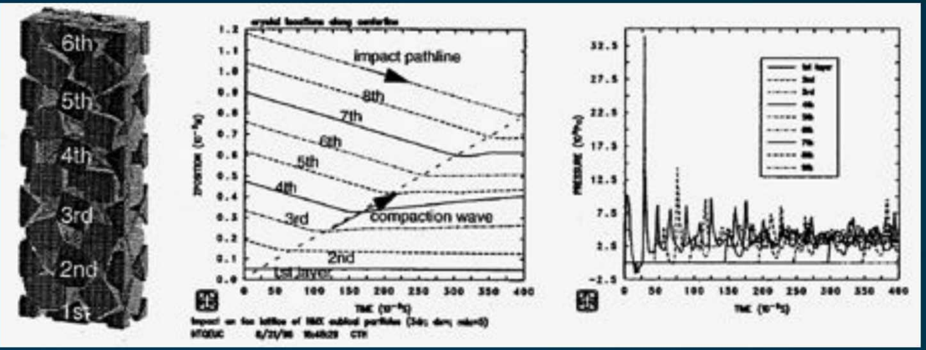
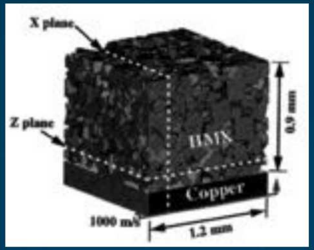
Mel Baer

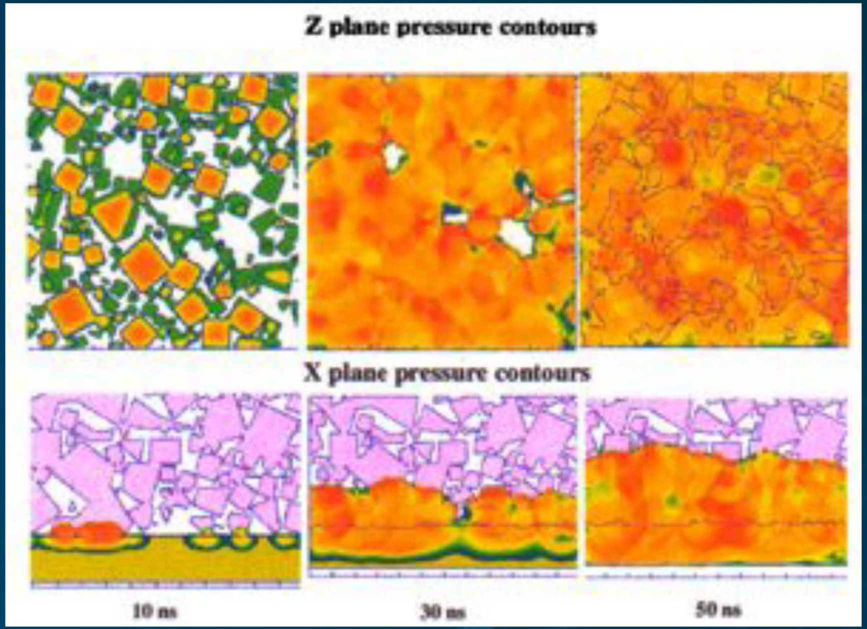
- §Baer, 1996 [1]
- §Mie-Gruneisen
- §Elastic perfectly plastic yield – 1kbar
- §Hot spots scale with particle size



Baer, 2000 [2]

History Variable Reactive Burn (HVRB)
HMX distribution 68% TMD
Reaction concentrated at large particle centers





[1] Baer, M. R., Graham, R. A., Anderson, M. U., Sheffield, S. A. and Gustavsen, R. L., "Experimental and Theoretical Investigations of Shock-Induced Flow of Reactive Porous Media" *1996 JANNAF Combustion Subcommittee and Propulsion Systems Hazards Subcommittee Joint Meeting*, Monterey, CA, November 1996.
[2] Baer, M. R., "Computational Modeling of Heterogeneous Reactive Materials at the mesoscale" *AIP Conference Proceedings*, Vol. 505, pp. 27-33, 2000.

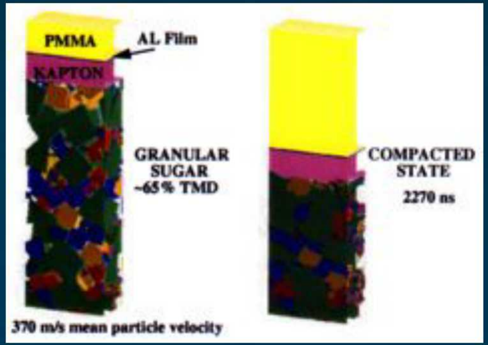
§Baer, 2002 [3,4]

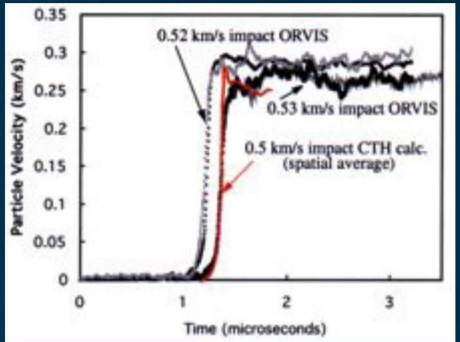
§Shock wave transmission through sugar

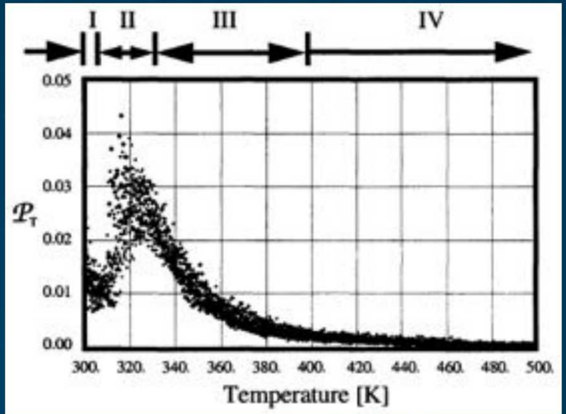
§ORVIS comparison

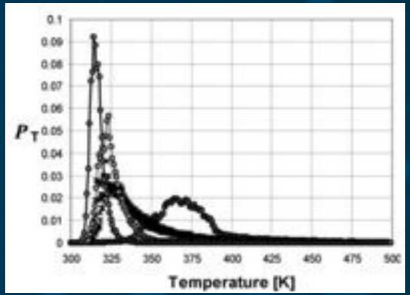
§Identified temperature distribution regimes

§Suggested link to stochastic differential equations







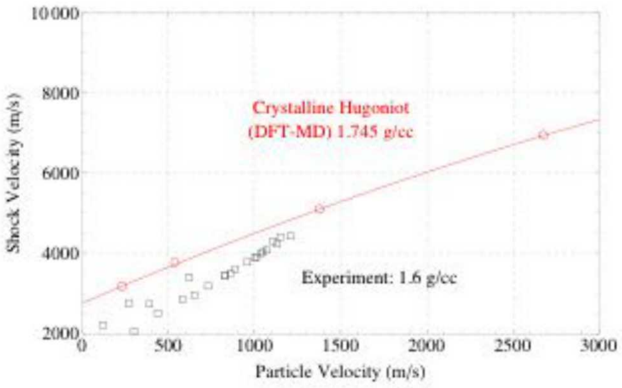


[3] Baer, M. R. and Trott, W. M., “Theoretical and Experimental Mesoscale Studies of Impact-Loaded Granular Explosive and Simulant Materials” *Proceedings of the 12th Detonation Symposium*, pp. 939-950, San Diego, CA, August 2002.

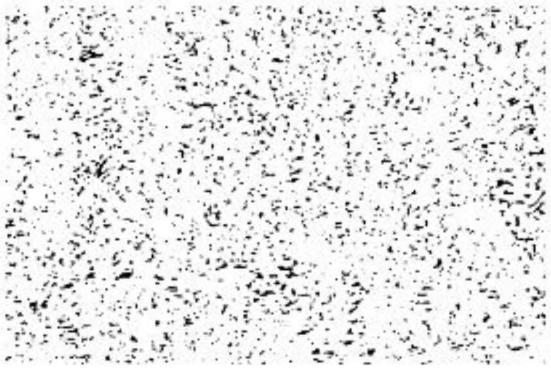
[4] Baer, M. R. and Trott, W. M., “Mesoscale Descriptions of Shock Loaded Heterogeneous Porous Materials” *AIP Conference Proceedings*, Vol. 620, pp. 713-716, 2002.

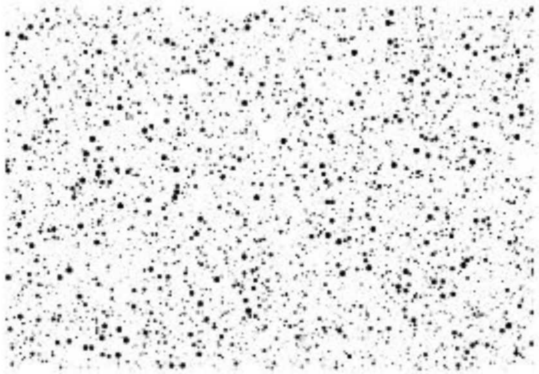
Mesoscale Model Elements

EOS



Microstructure



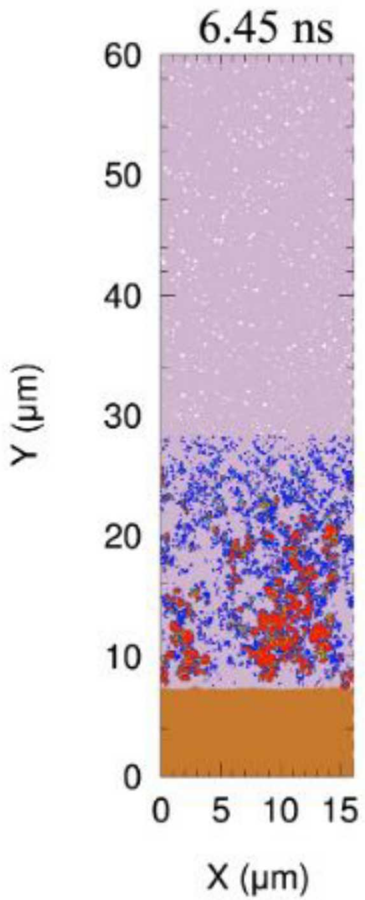


Constitutive

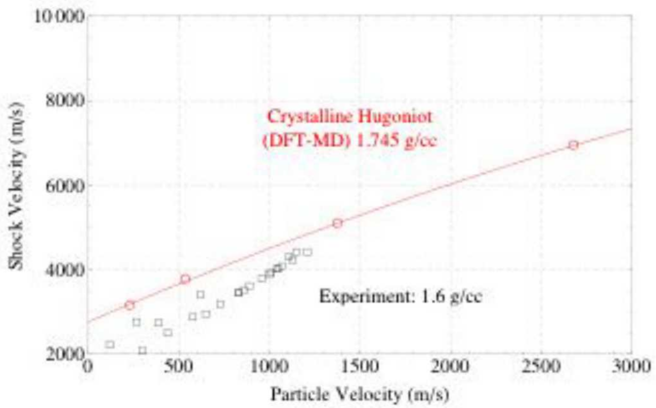
$$\sigma_{ij} = \bar{P}\delta_{ij} + S_{ij}$$

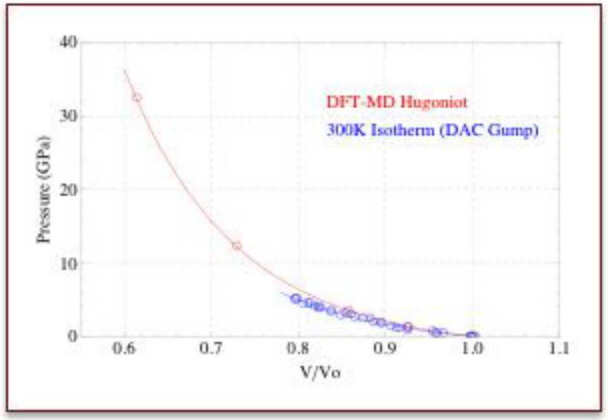
Reactive Burn

$$\frac{d\lambda}{dt} = (1-\lambda)F\exp(-\Theta/T)$$



EOS for Crystalline HNS





1. Predicted with DFT-MD, no empirical parameters
2. VASP software, AM05 functional, NVT dynamics.
3. Using temperature to build complete EoS. [7]

It ends with a table

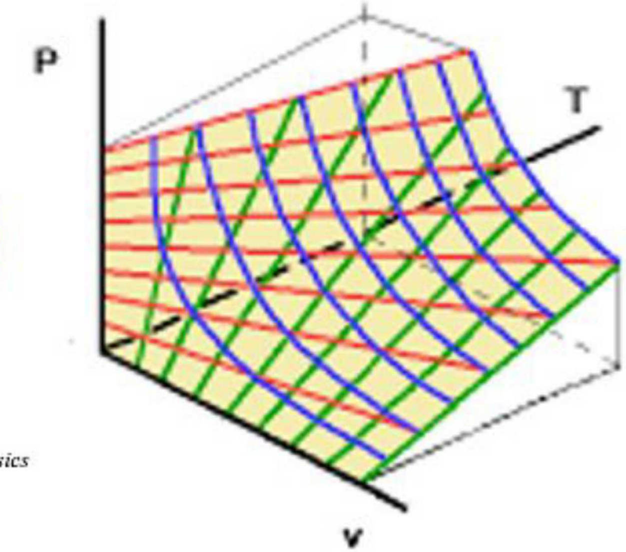
$$\left(\frac{\partial p}{\partial e}\right)_v = \frac{\Gamma(v)}{v}$$

$$e(v,T) = e_c(v) + \int_0^T c_v(v,\hat{T})\,\mathrm{d}\hat{T}\,.$$

$$p(v,e) = \frac{\Gamma(v)}{v}e + \phi(v)$$

$$c_v(v_0,T) = \sum_{i=1}^{M} c_{v_i} E_i\left(\frac{\theta_i}{T}\right)$$

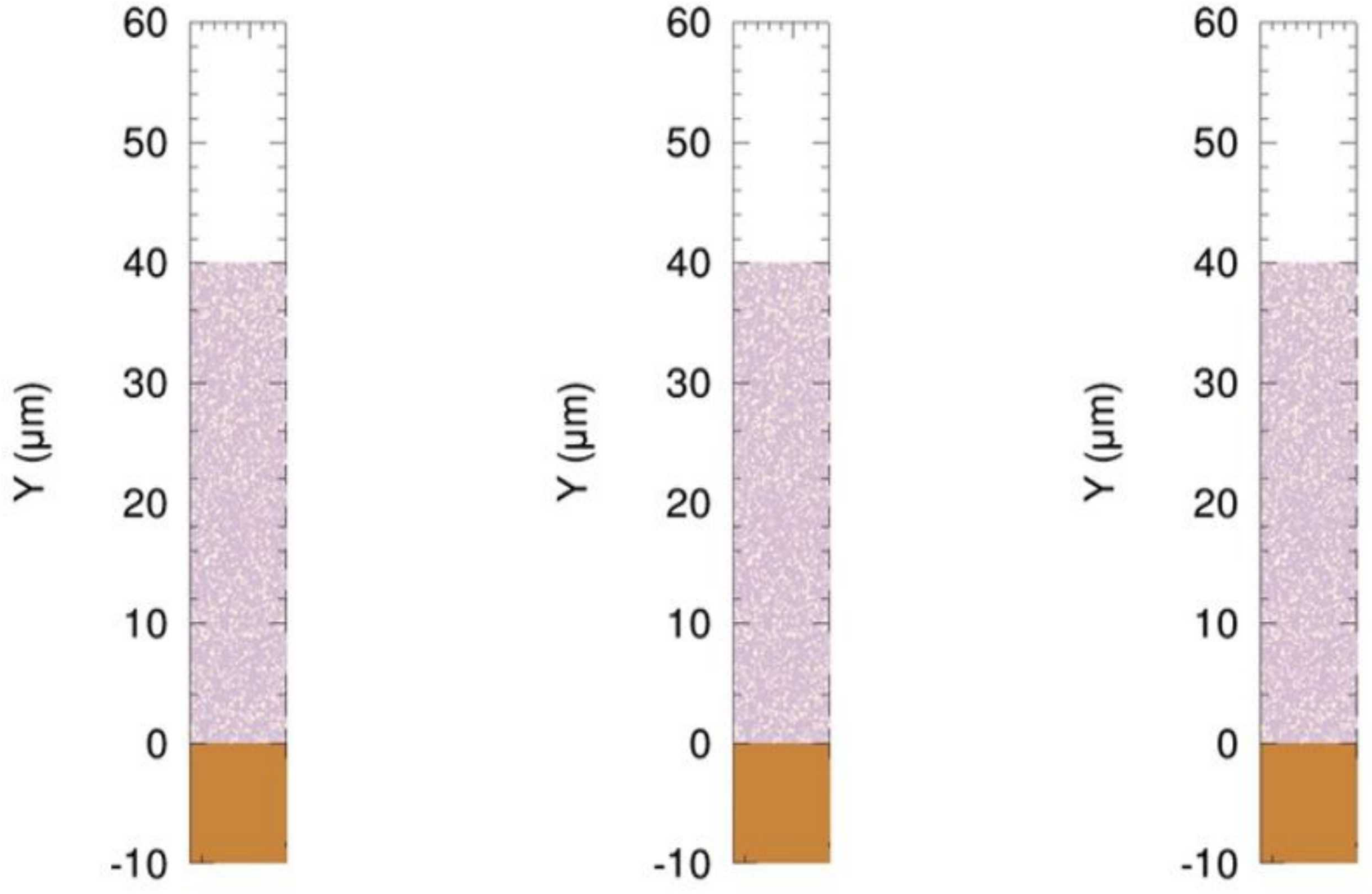
$$e_c(v) = -\tau(v)\int_{v_0}^{v} \frac{\phi_H(\hat{v})}{\tau(\hat{v})}\,\mathrm{d}\hat{v},$$



[6] Yarrington, C. D., Kittell, D. E., Wixom, R. R. and Damm, D. L., "A Mie-Grüneisen EOS with Non-Constant Specific Heat" *Journal of Physics Conference Series*, Vol. 500, p. 052053, 2014.

[7] Kittell, D. E. and Yarrington, C. D., "A Physically-Vased Mie-Gruneisen equation of state to determine hot spot temperature distributions" *Combust. Theor. Model.*, Vol. 20, pp.941-957, 2016.

Failed shock to detonation transition



P, T, & Rxn at 0.000000e+00

Constitutive Models (Strength)

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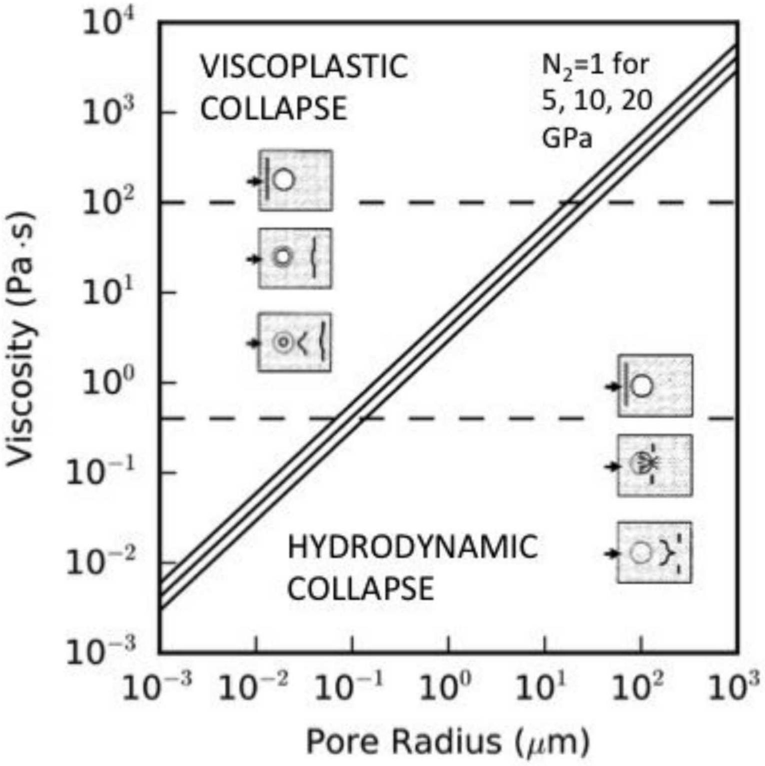
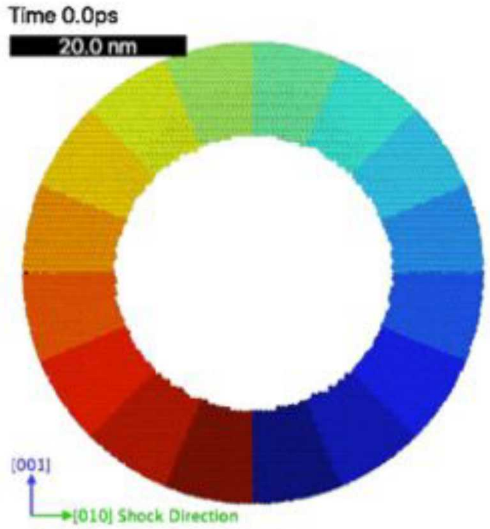
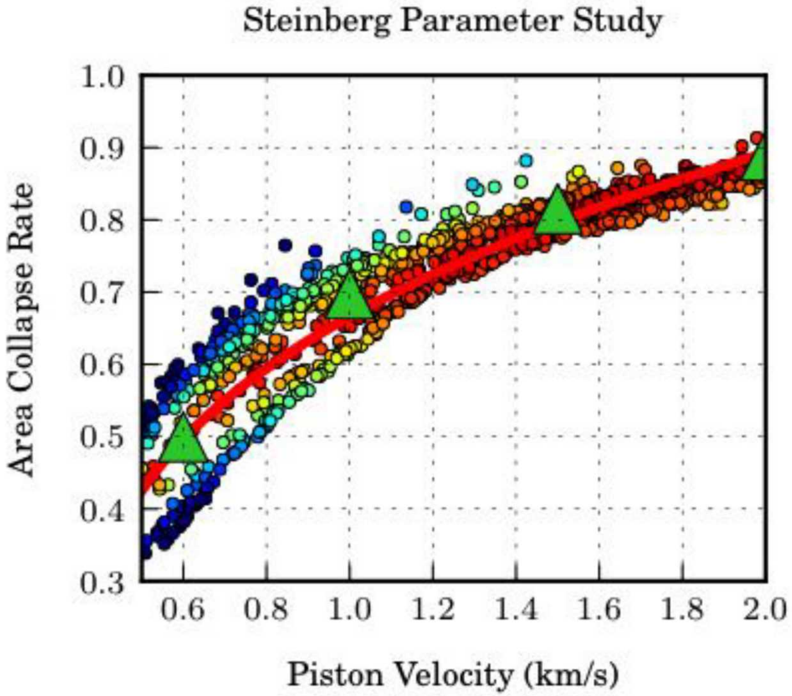




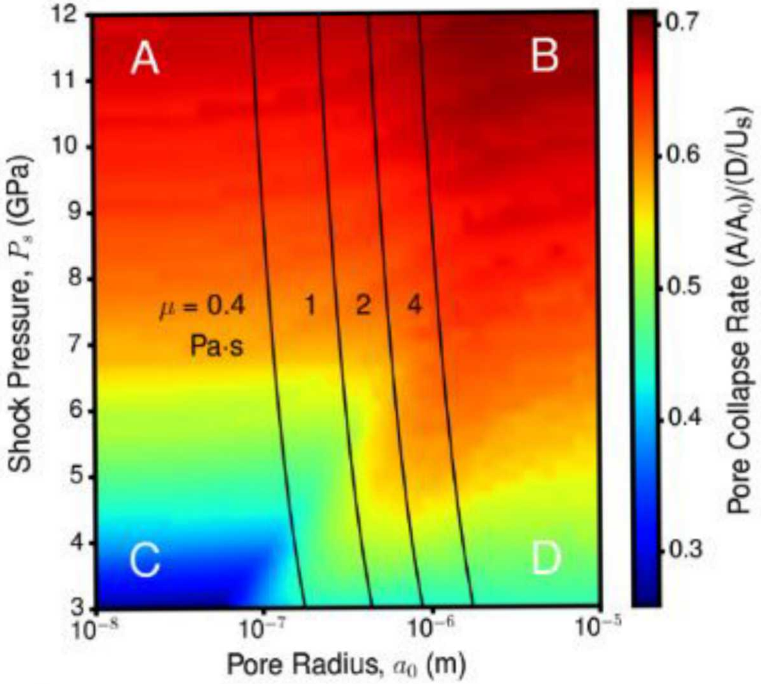


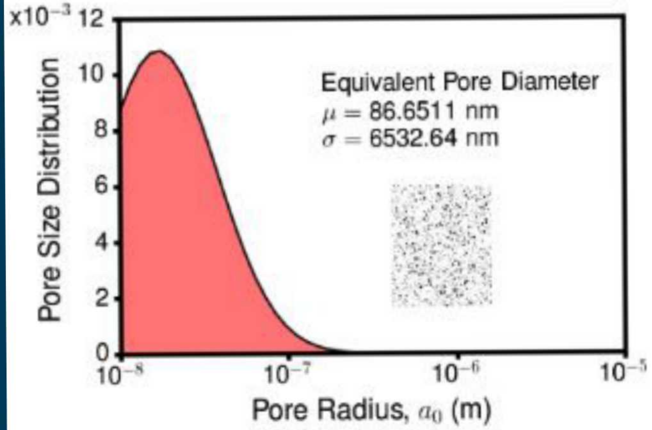
$$Y = \left\{ Y_T\left(\dot{\varepsilon}_p, T\right) + Y_A f\left(\varepsilon_p\right) \right\}$$

$$\dot{\varepsilon}_p = \left\{ \frac{1}{C_1} exp\left[\frac{2U_K}{kT} \left(1 - \frac{Y_T}{Y_P}\right)^2 \right] + \frac{C_2}{Y_T} \right\}^{-1}$$

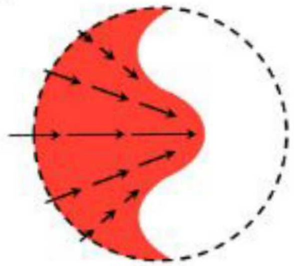
[9] Wood, M. A., Kittell, D. E., Yarrington, C. D. and Thompson, A. P., "Multiscale Modeling of Shock Wave Localization in Porous Energetic Material" *Phys. Rev. B*, Vol. 97, p. 014109, 2018.

Pore Collapse Rate – Frey Mapping [9]

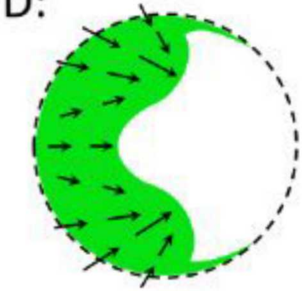




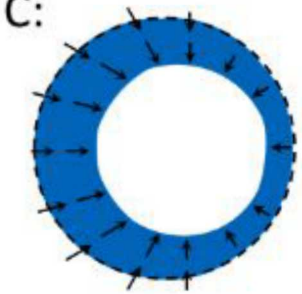
A, B:



D:

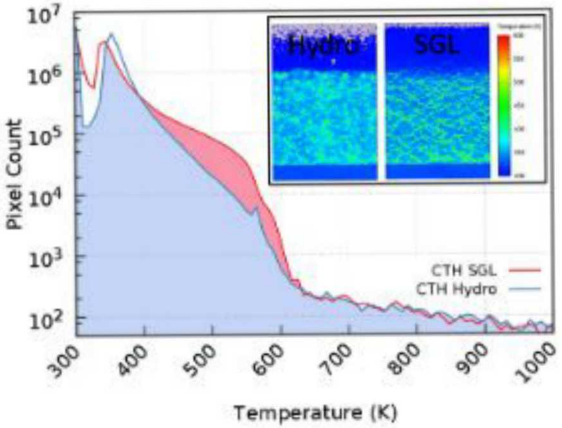


C:

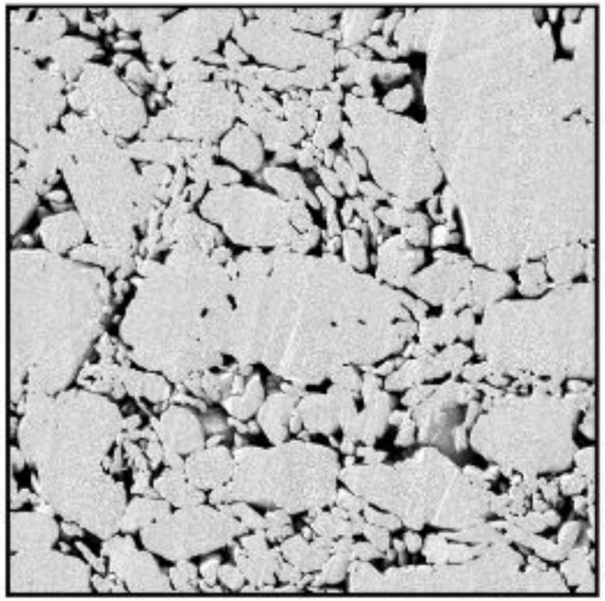


$$\sigma_{ij} = \bar{P}\delta_{ij}$$

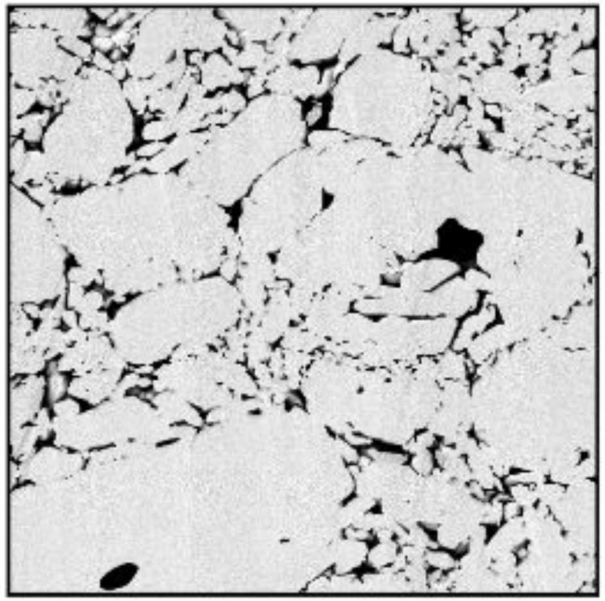
$$\sigma_{ij} = \bar{P}\delta_{ij} + S_{ij}$$



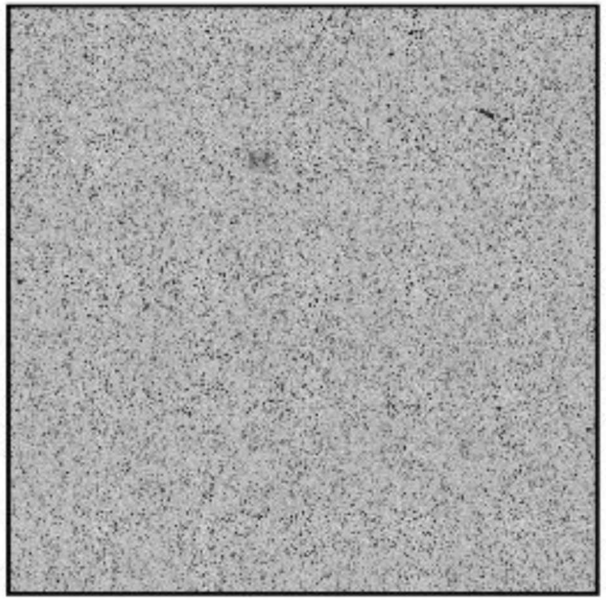
UF, 80% TMD



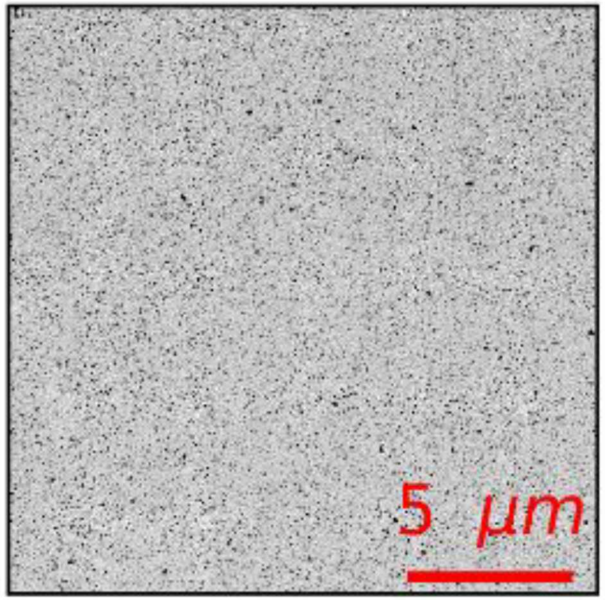
UF, 88% TMD

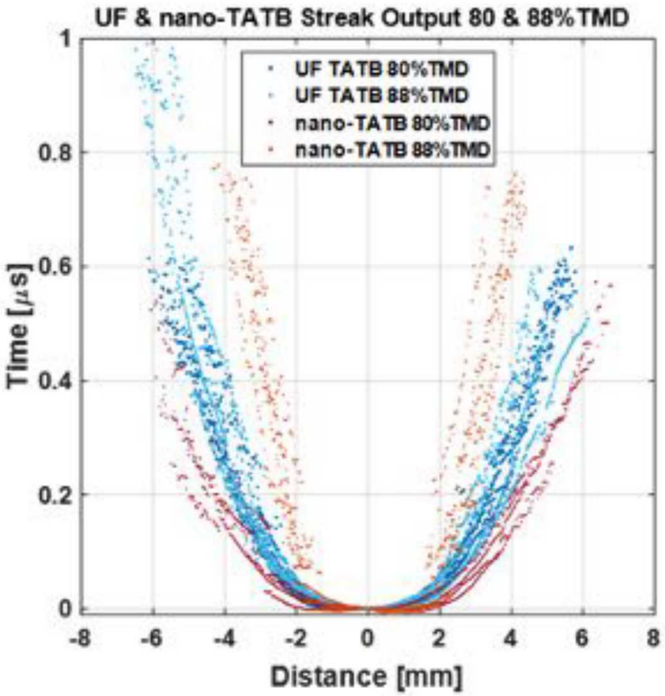


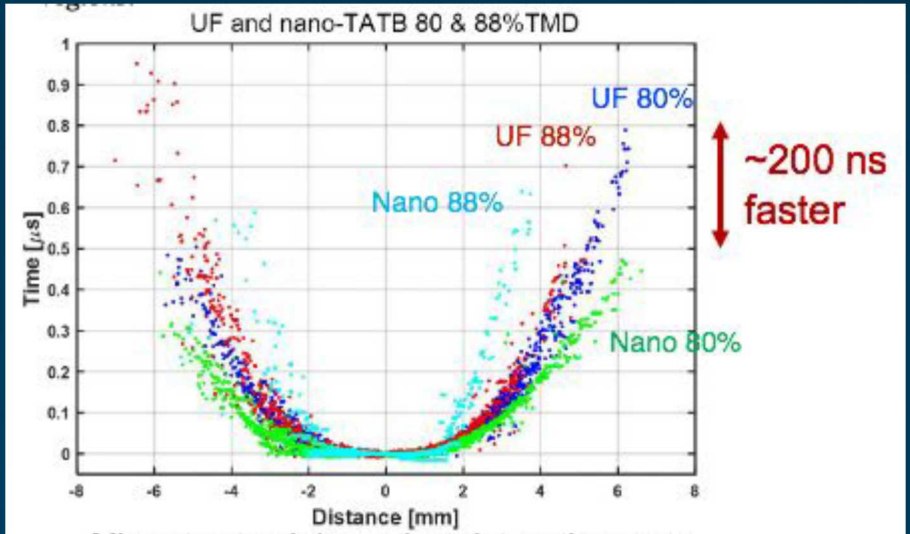
Nano, 80% TMD



Nano, 88% TMD







Microstructural dependent detonation wave
spreading in different grades of TATB

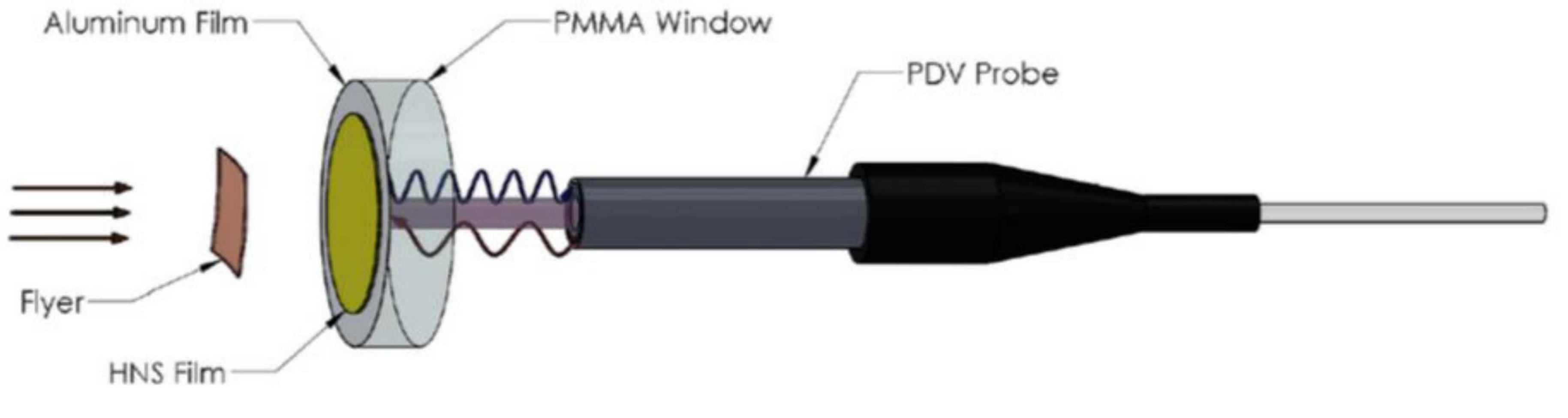
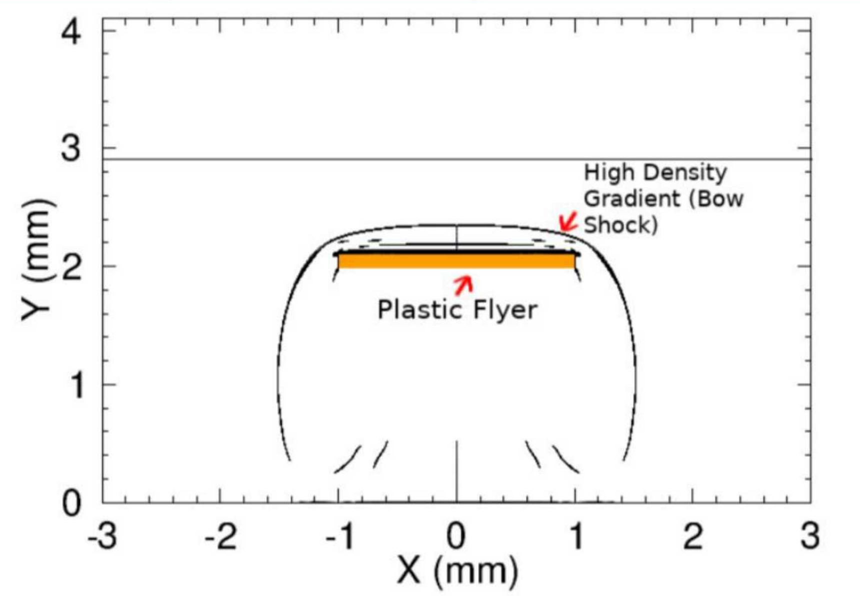
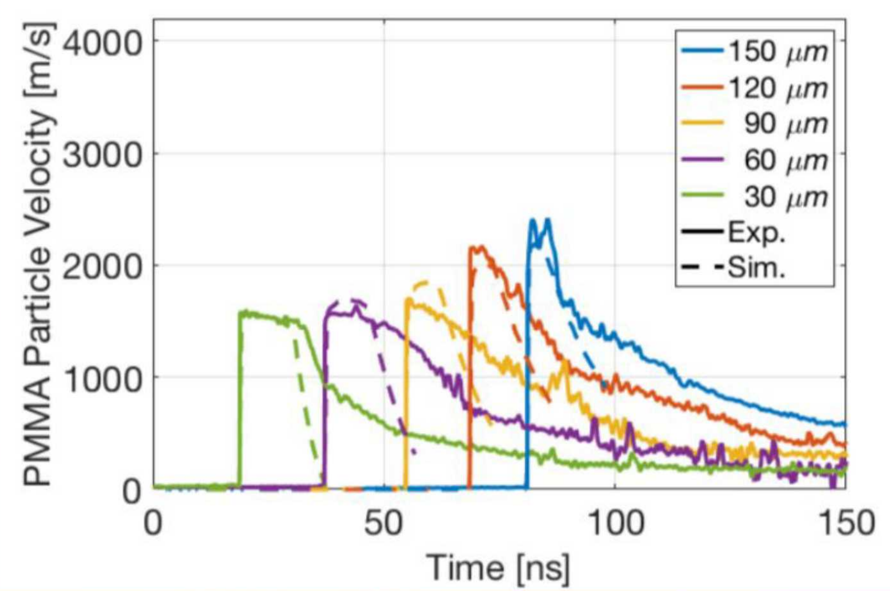


Figure: Schematic of experiment. Image from Olles et al.[2]





Conclusions:

- New way to observe initiation and run-to-detonation in energetic materials
- Calibration of chemistry models with full mesoscale representation
- Surprising effects of air on the results

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