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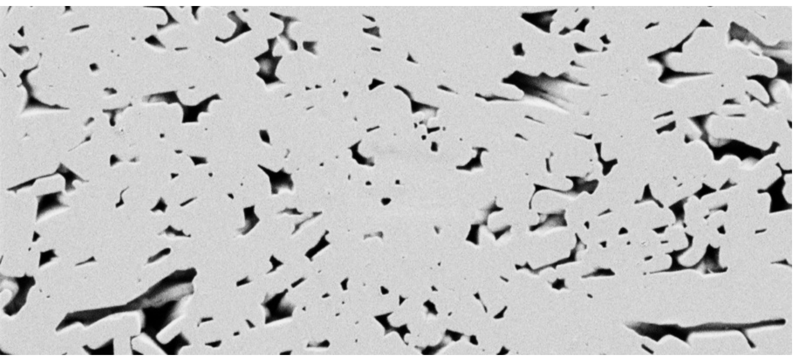

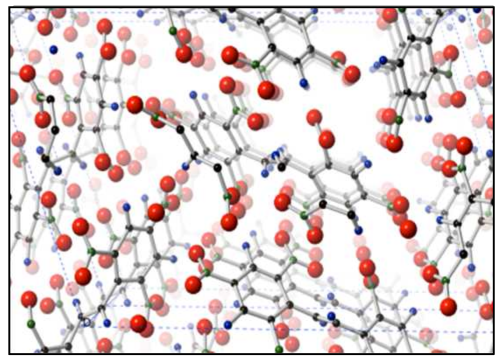

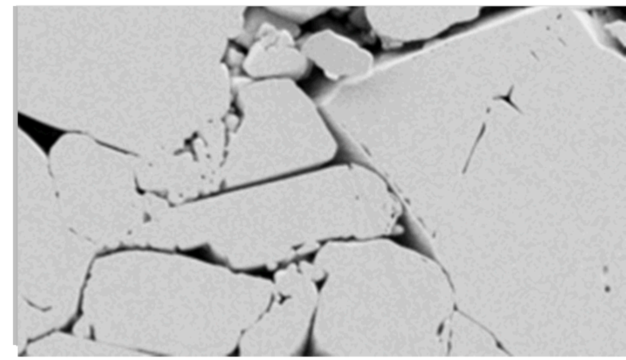

The Growing Impact of Grain-Scale Modeling

Cole Yarrington, Ryan Wixom

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Science-based understanding of shock initiation.

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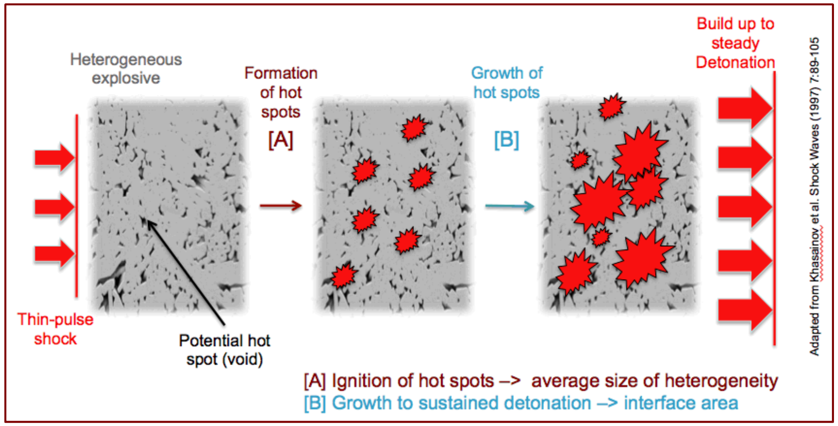


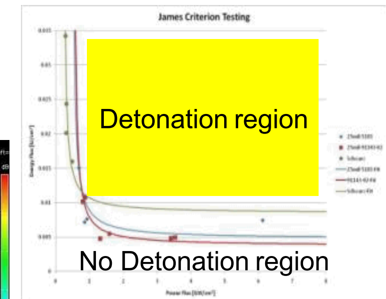
Technology

Science

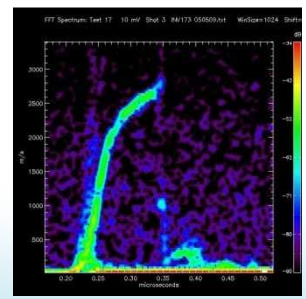
Performance Char.

Microstructure Characterization

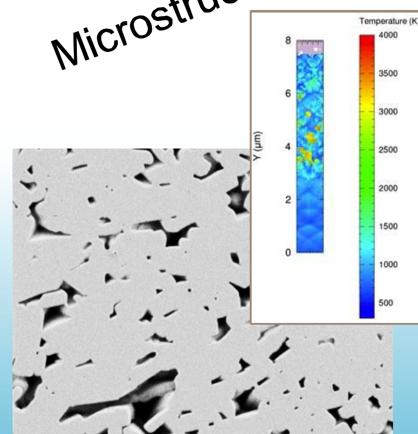
Equation of State / Chemistry



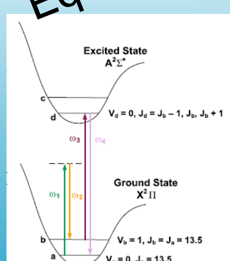
Energy flux vs. power flux of slapper for HNS-FP initiation

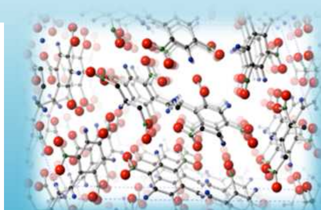


Velocimetry of flyer



X-section of HNS pellet, and grain-scale hydrocode simulation



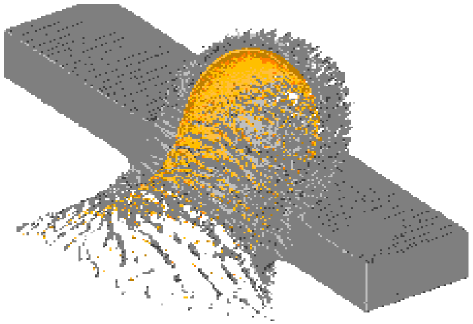


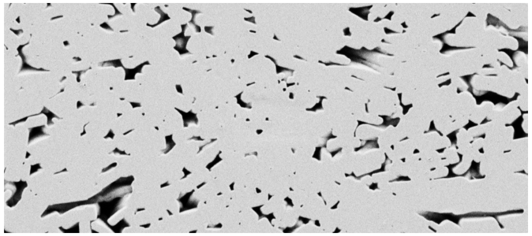
HNS crystal structure

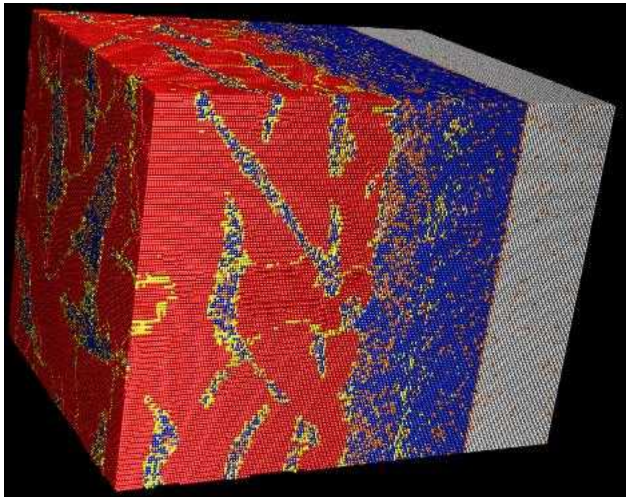
Time scale: $10^{-12} – 10^{-9}$ s

Atomic Molecular Microscale Mesoscale Continuum

Mesoscale Approaches







Continuum

~Avagadro's number

Resolution

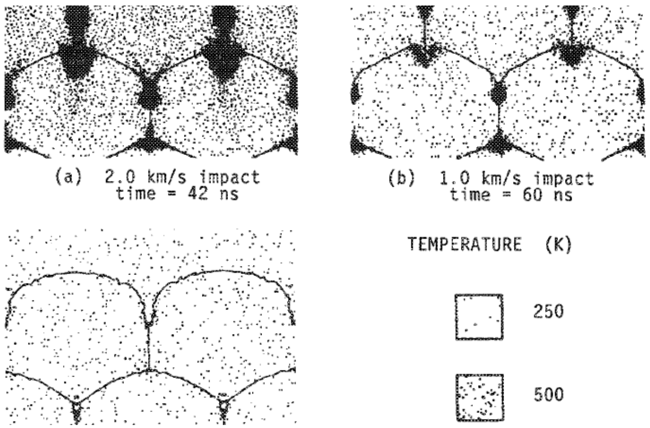
Mesoscale

~1x10^3 to 1x10^9 atoms

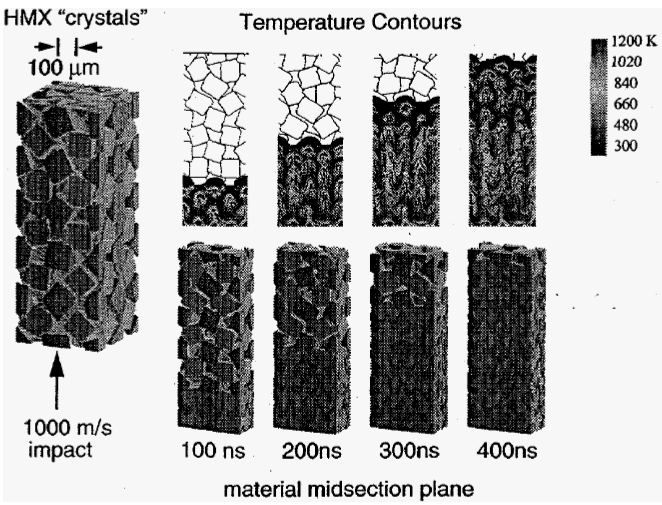
Scaling

Atomistic - Molecular

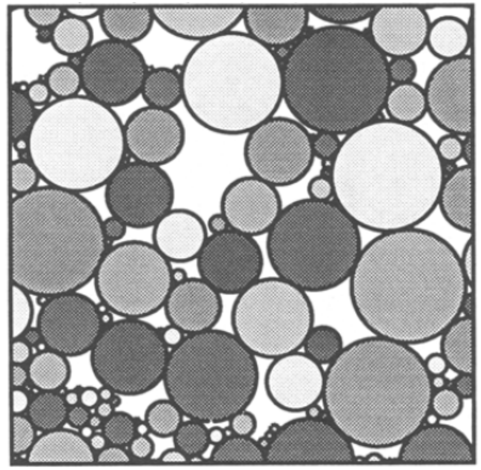
Where did it start?



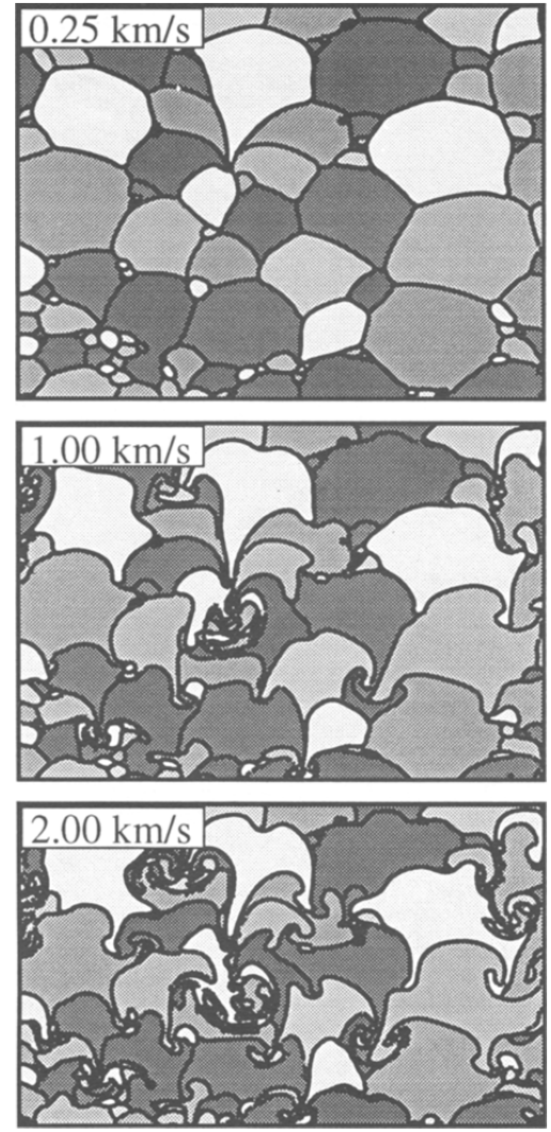
Williamson, R.L., *Parametric studies of dynamic powder consolidation using a particle-level numerical model.* Journal of Applied Physics, 1990. 68: p. 1288-1296.



Baer, M.R., Graham, R.A., Anderson, M.U., Sheffield, S.A., and R.L. Gustavsen, *Experimental and Theoretical Investigations of Shock-Induced Flow of Reactive Porous Media.* In *1996 JANNAF Combustion Subcommittee and Propulsion Systems Hazards Subcommittee Joint Meeting.* 1996. Monterey, CA.

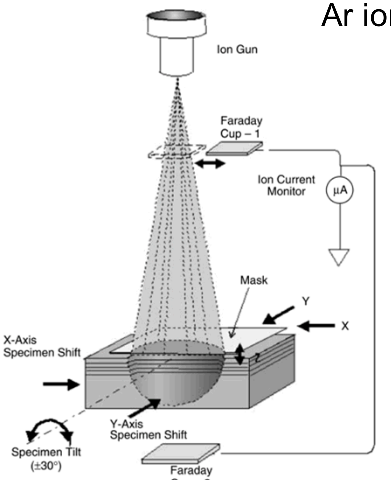


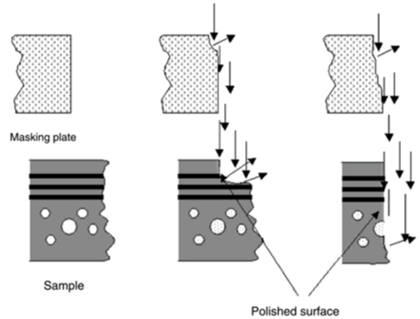
Benson, D.J., and Nellis, W.J., *Numerical simulation of the shock compaction of copper powder.* AIP Conference Proceedings, 1994. **309**: p. 1243-1246.



Characterizing pellet microstructure

Ar ion cross-section polishing: 2D





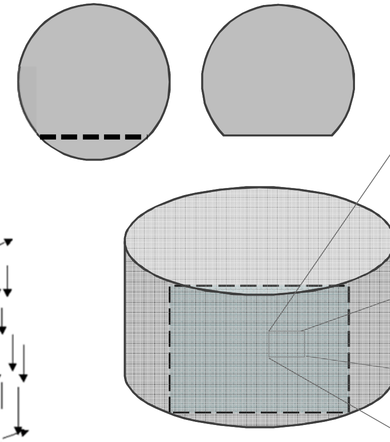
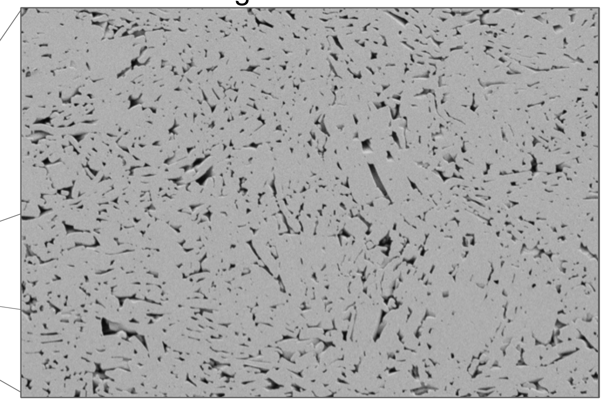
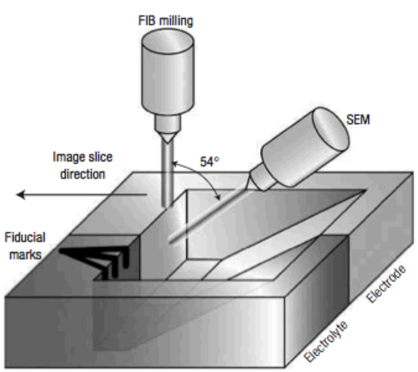


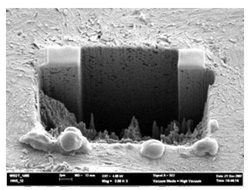
Image width: 25 um

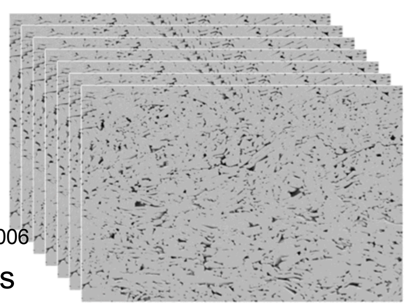


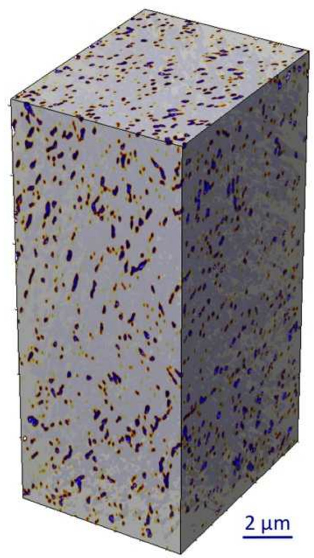
HNS-FP, 90% TMD

Focused ion beam nanotomography: 3D data

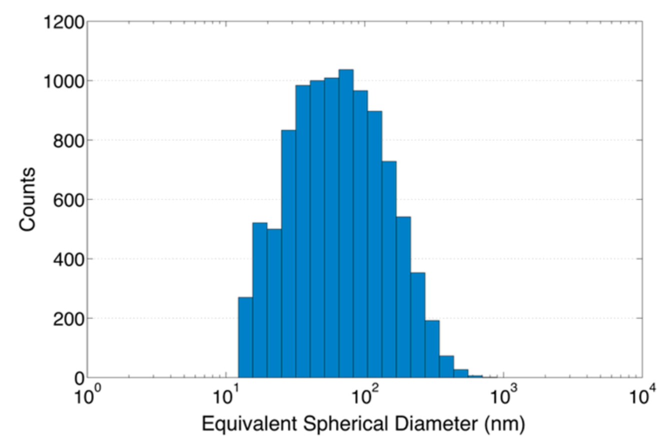








80,000 pores, mean diameter 86.3 nm

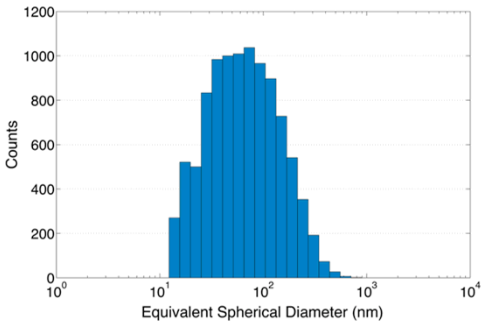


Wilson et al. Nature Materials, VOL 5, JULY 2006

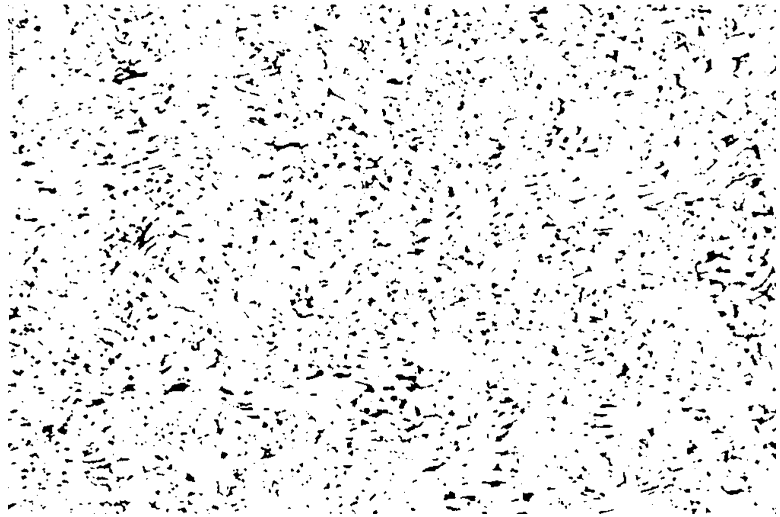
Nanotomography: 25 nm slices

Wixom et al. J. Mater. Res. 25 1362 (2010).

Grain-scale hydrocode simulation w/ statistically equivalent microstructure

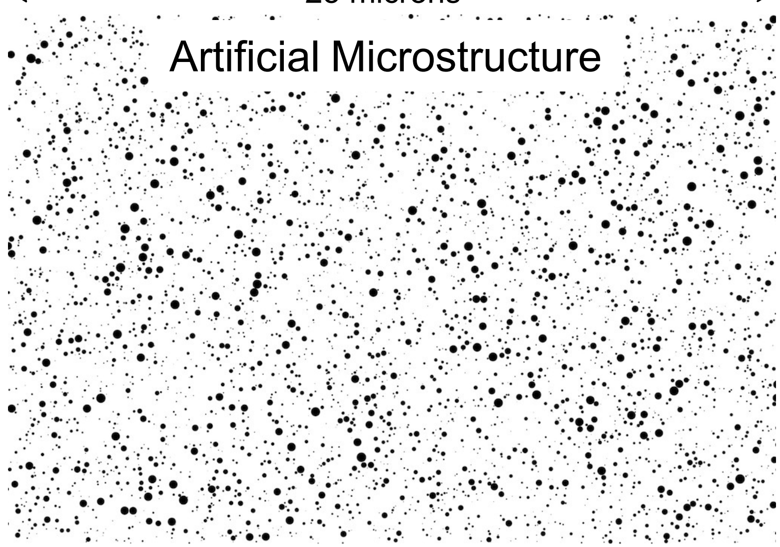


Real Microstructure

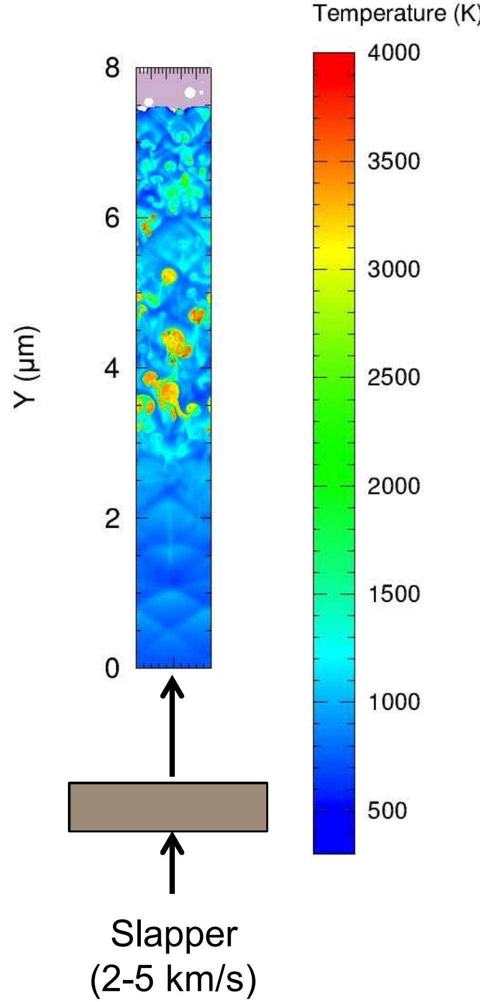


25 microns

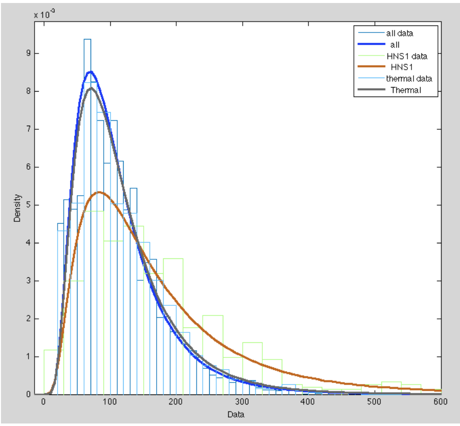
Artificial Microstructure



Snapshot from hydrocode simulation

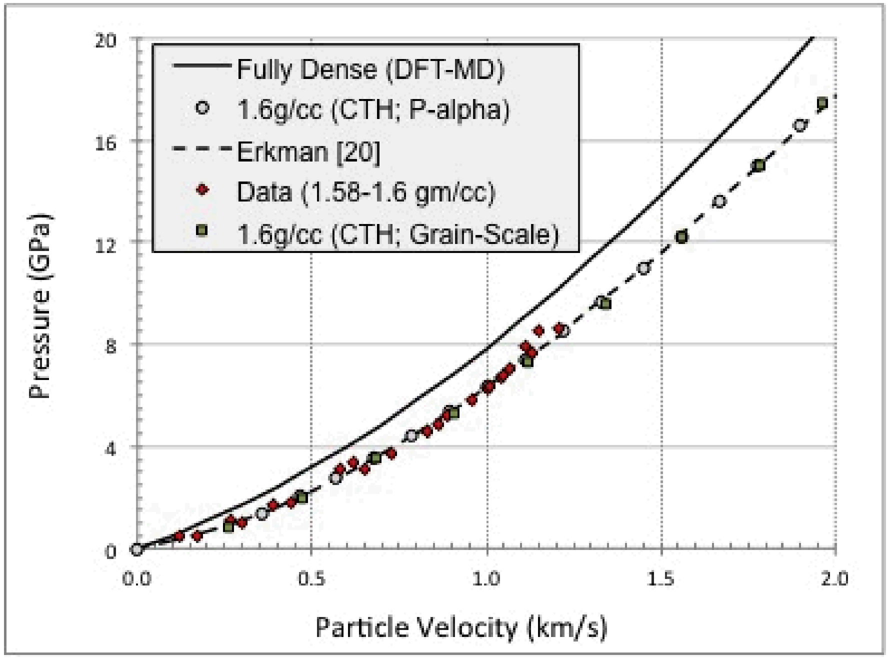


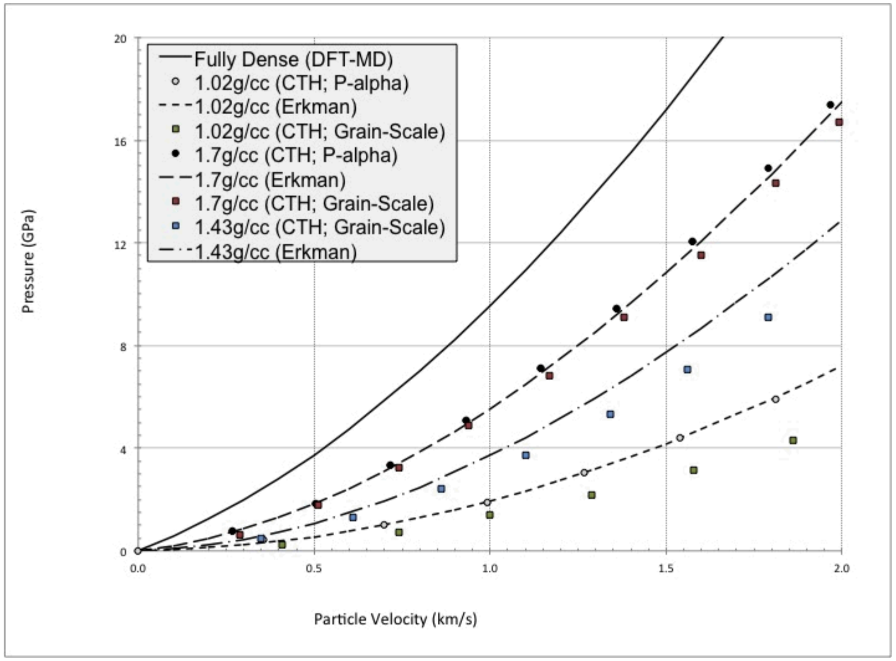
What features are important to initiation?



Bulk Hugoniot predictions

- HNS grain scale simulations were validated at 92% TMD with historical Hugoniot data
- CL-20 was simulated at 50, 70, and 84% TMD
- Strength not a factor at these conditions



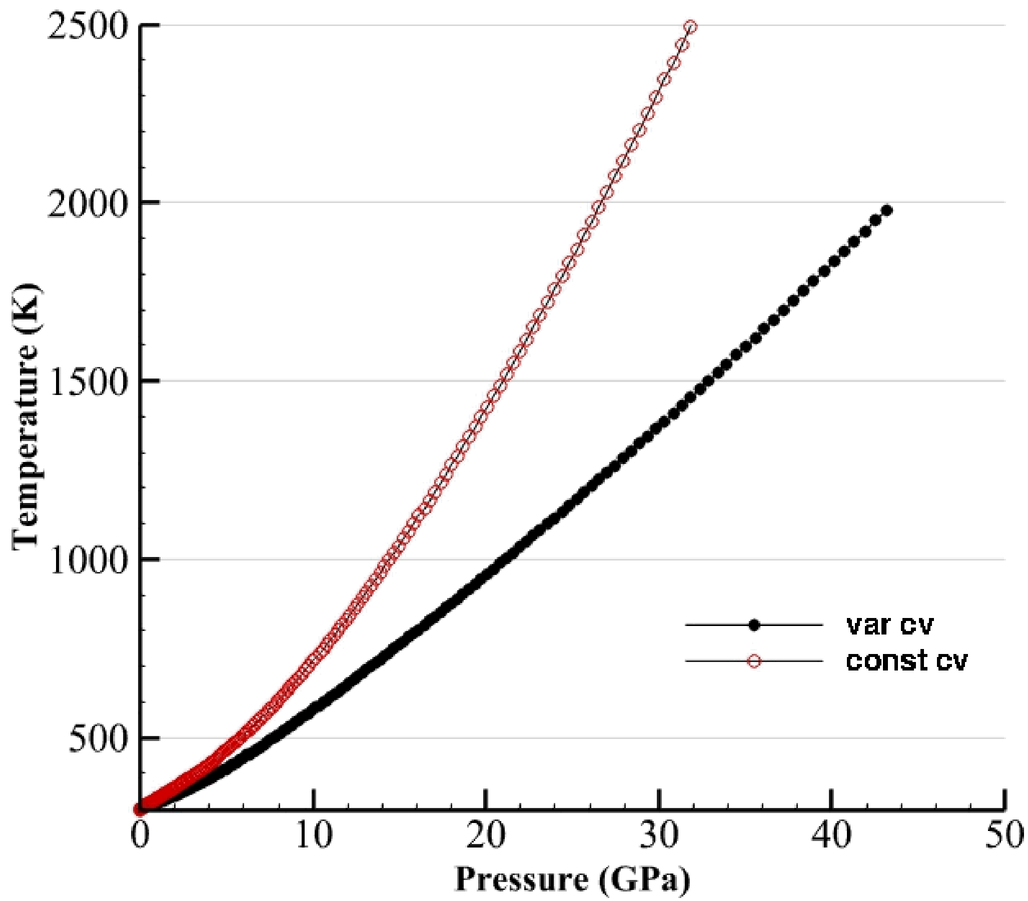


Temperature dependent reactive burn

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

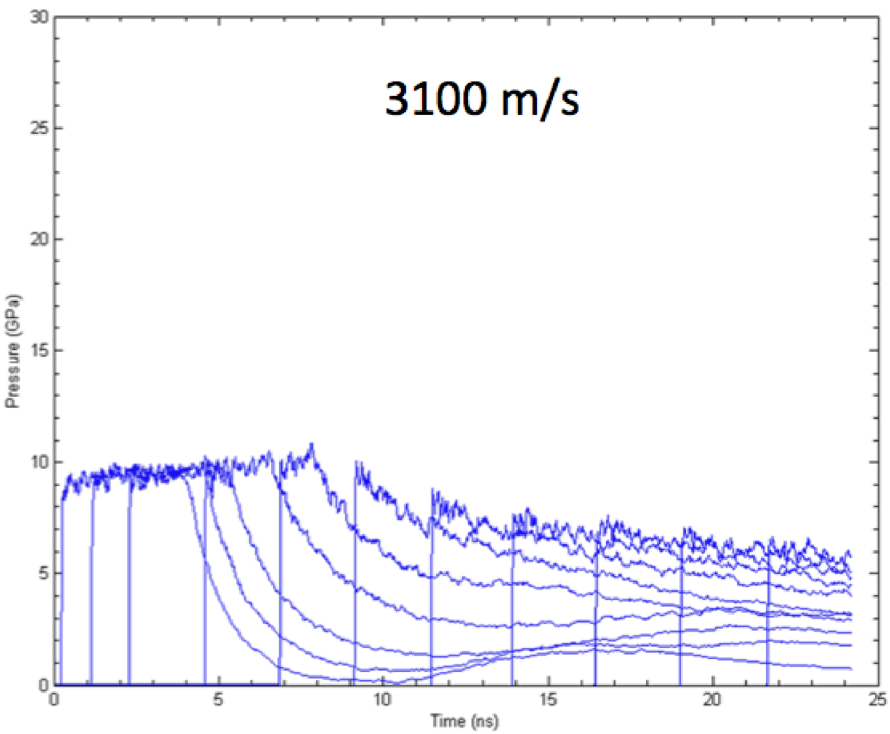
$$\Theta = \Theta_0(1 + A_P P)$$

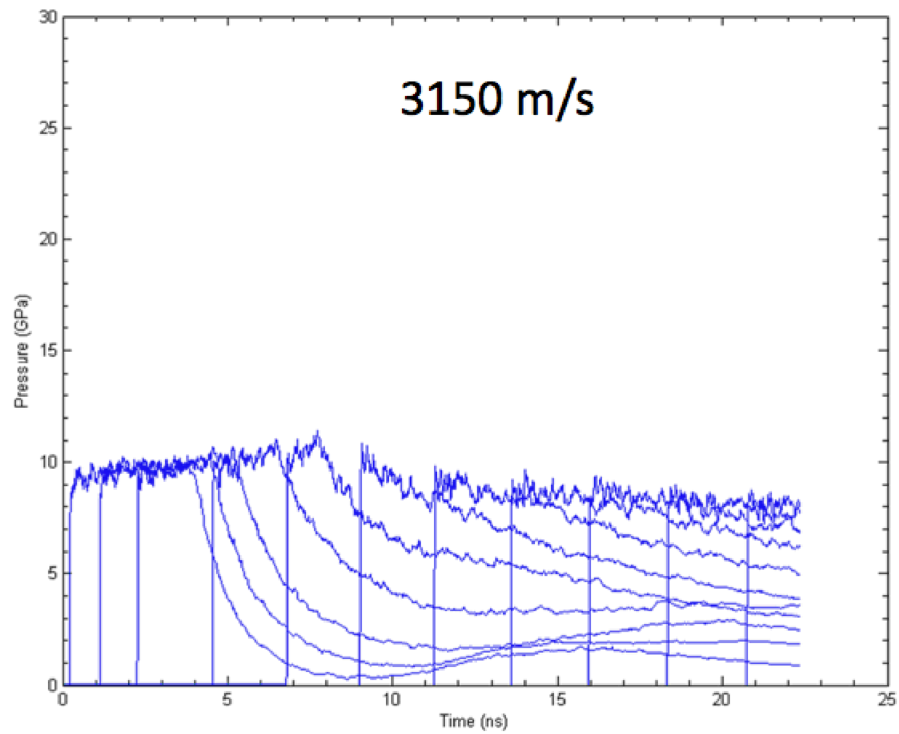
- Consistent temperatures obtained through variable specific heat Mie-gruneisen EOS
- Activation energy based on thermal decomposition data (127 kJ/mol [Cooper]
- Pre-exponential parameter was fit to shock initiation threshold data



Shock-to-detonation transition near threshold:

Bulk-average pressure history at various distance from the impact surface (1, 5, 10, 20, 30, 40, ... μm)

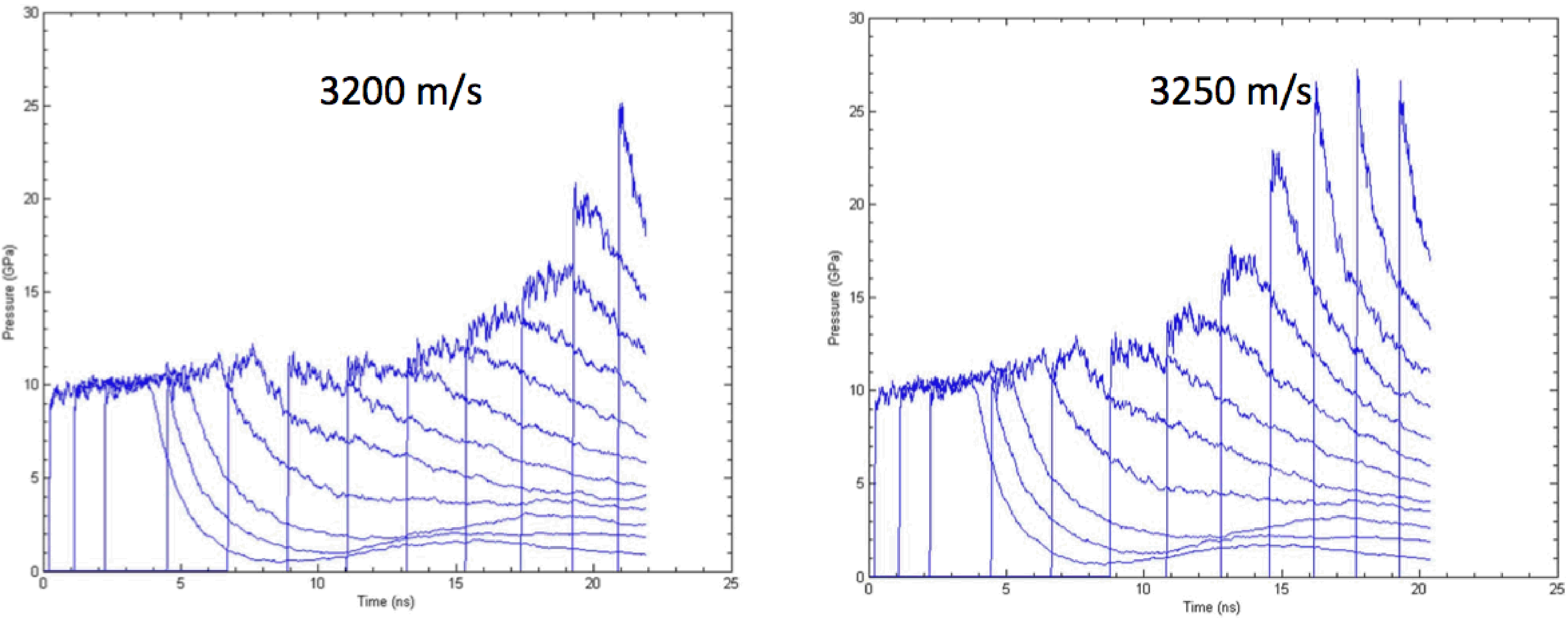




(*Experimental threshold is ~ 3200 m/s)

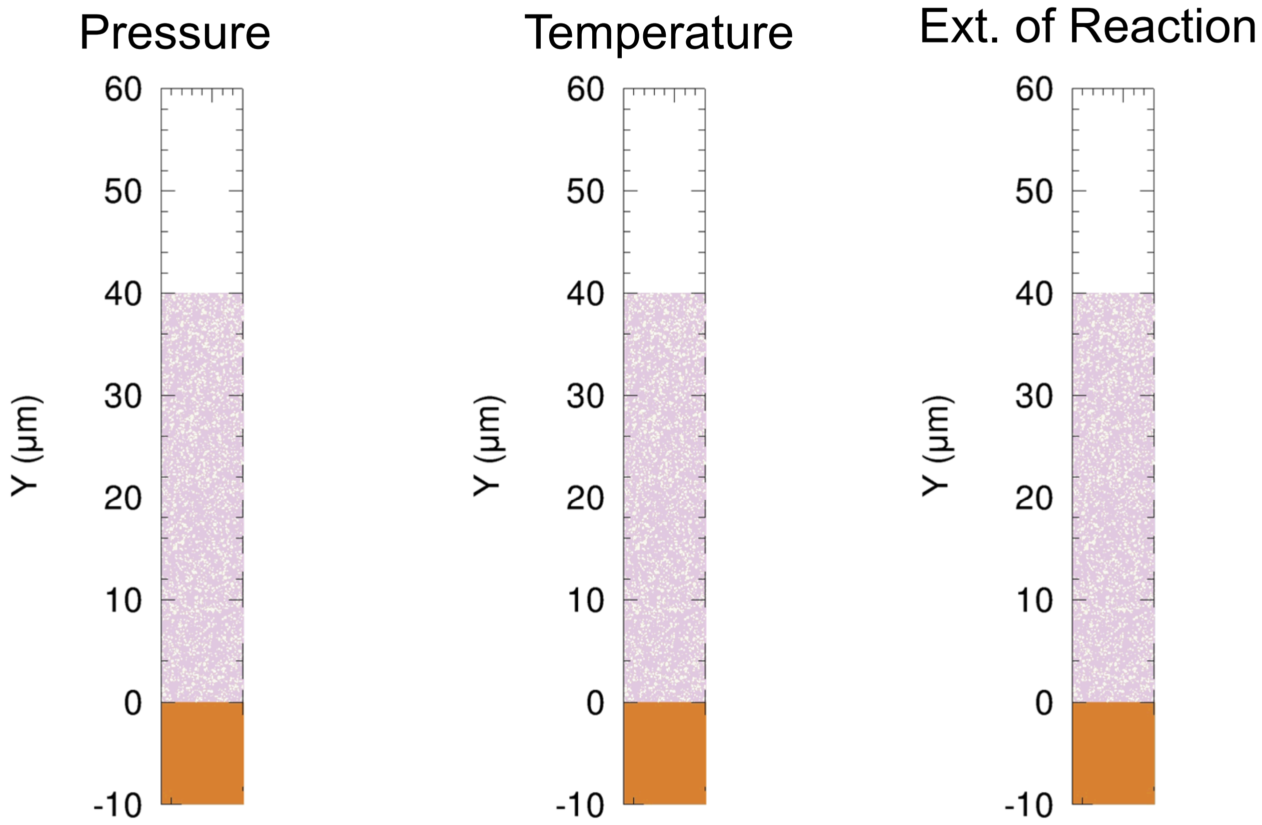
Shock-to-detonation transition near threshold:

Bulk-average pressure history at various distance from the impact surface (1, 5, 10, 20, 30, 40, ... μm)



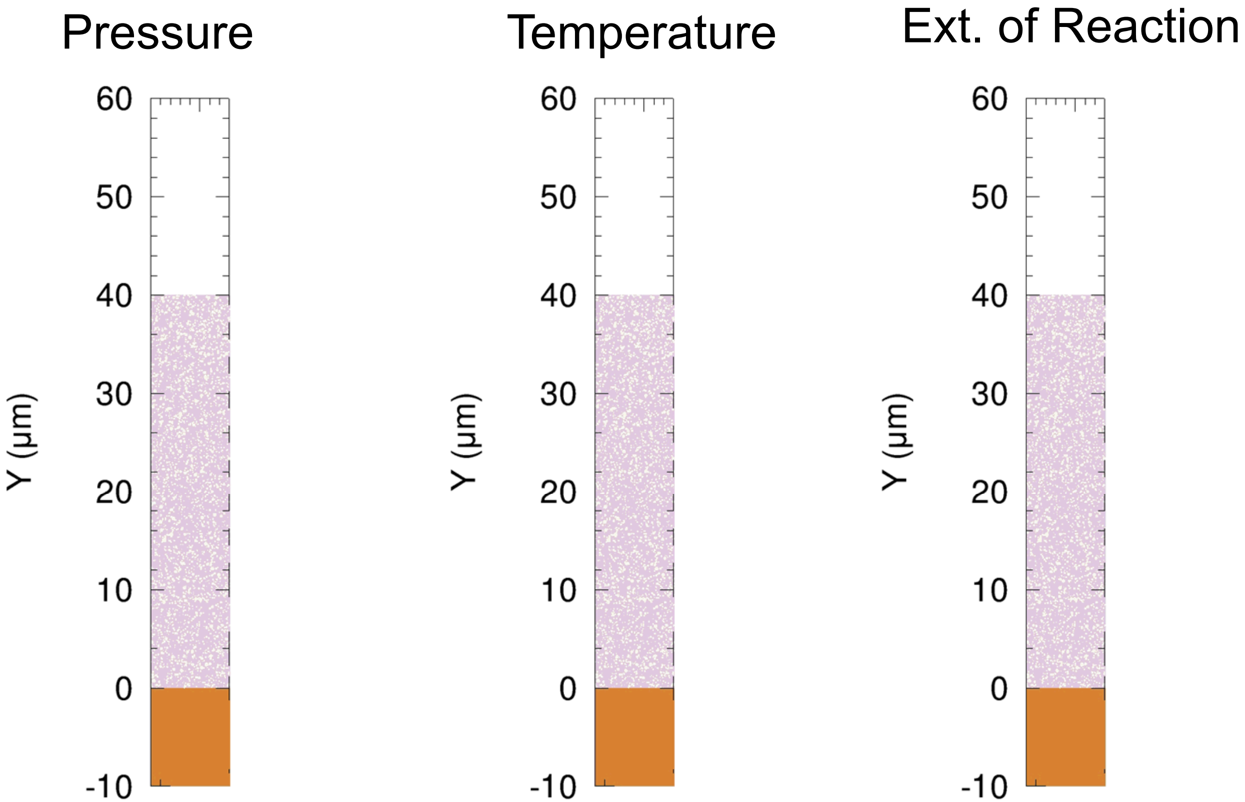
(*Experimental threshold is ~ 3200 m/s)

Shock-to-detonation transition below threshold:



P, T, & Rxn at 0.000000e+00

Shock-to-detonation transition above threshold:



P, T, & Rxn at 0.000000e+00

Where are we going

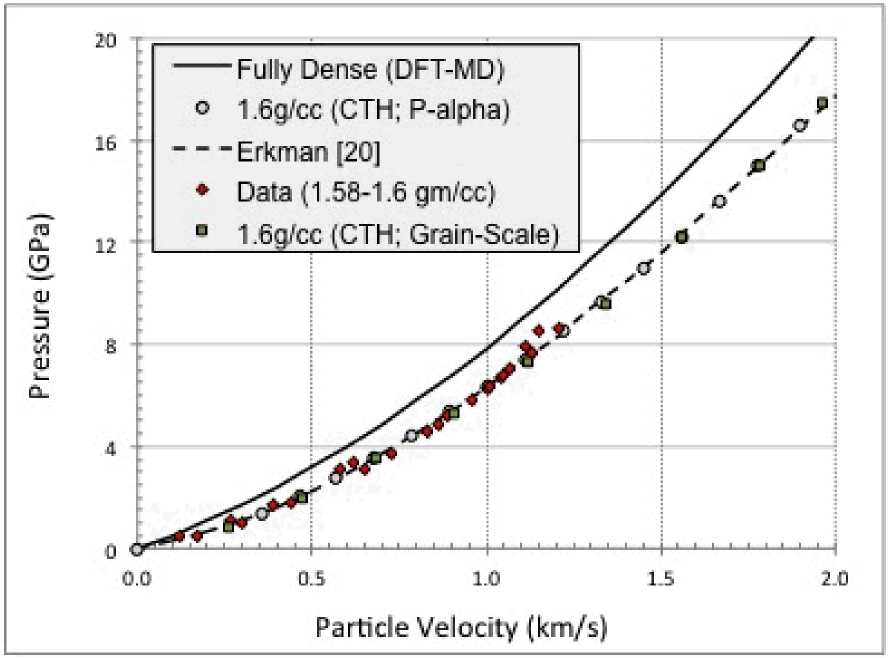
- Grain scale modeling has been used to investigate pore collapse, coallescence, prediction of bulk properties, run up to detonation and failure
- Computational cost can still be expensive
- Large impact to be gained by mining the data
- Determine statistical correlations relevant to the microstructure → response
  - What are the key metrics
- Suggest model forms for next generation continuum models

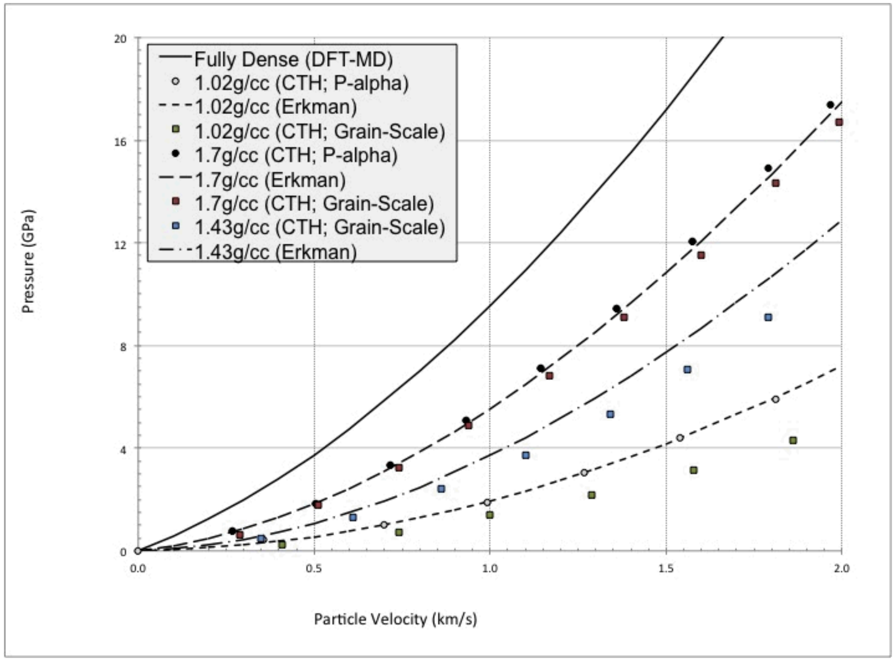
Questions?

Extras

Bulk Hugoniot predictions

- HNS grain scale simulations were validated at 92% TMD with historical Hugoniot data
- CL-20 was simulated at 50, 70, and 84% TMD

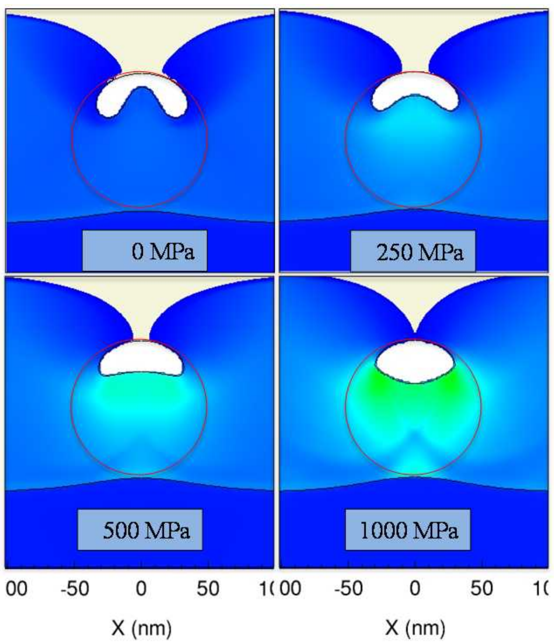


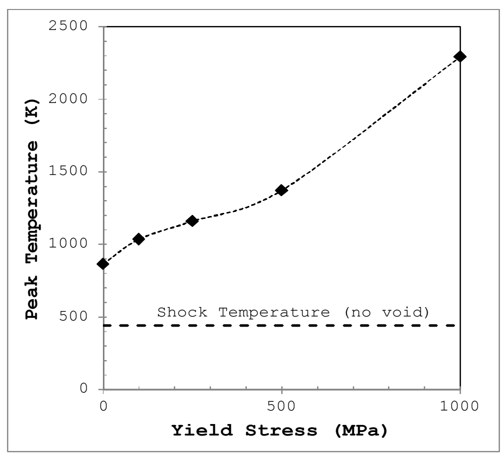


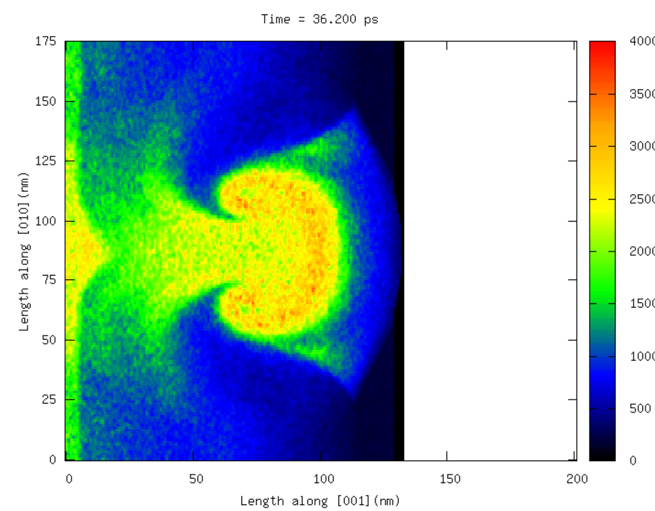
Material Strength

- Material strength has been shown to have a strong effect on pore collapse states
  - 6 Gpa shock (Us – 4.2 km/s)
  - 0 – 1000 Mpa
  - 443 K – 765 K (before jet impact)
  - 1030 K – 1200 K (after jet impact)

- MD simulations of pore collapse
- ReaxFF based on CHO combustion and CHNO nitramine force fields







Calibrating Strength Models

- Lack of experimental data on HNS
- MD pore collapse used as substitute
- Lagrangian tracers surrounding pore
- Average state time history used as objective function
- Convergence achieved for two strength models
- Future work will focus on irreversible work as an objective, calibration at multiple stress conditions

$$Y = Y\left(\varepsilon^{p}, \dot{\varepsilon}^{p}, T\right) = \left[A + B\left(\varepsilon^{p}\right)^{N}\right]\left[1 + C\ln\left(\dot{\varepsilon}^{p}\right)\right]\left[1 - \Theta_{h}^{m}\right]$$

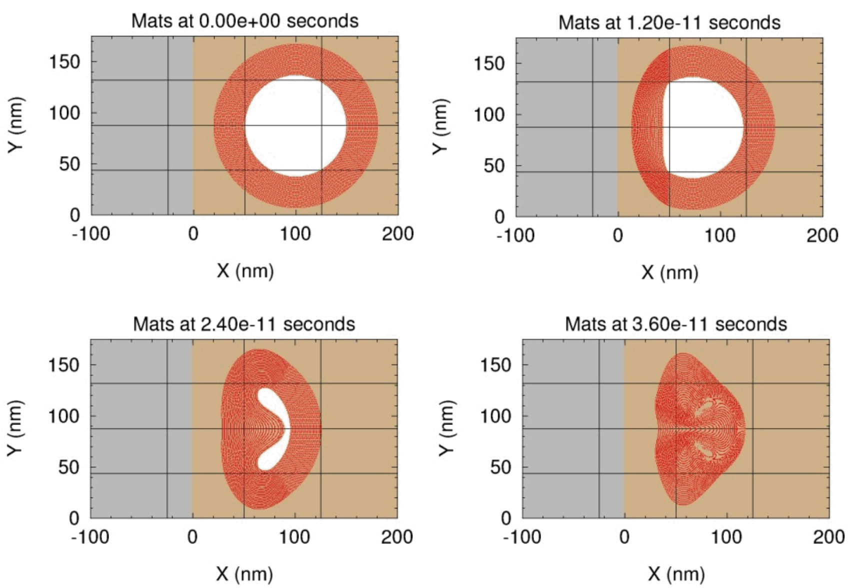
$$\Theta_{h} = \frac{T - T_{r}}{T_{M} - T_{r}}$$

EPPVM

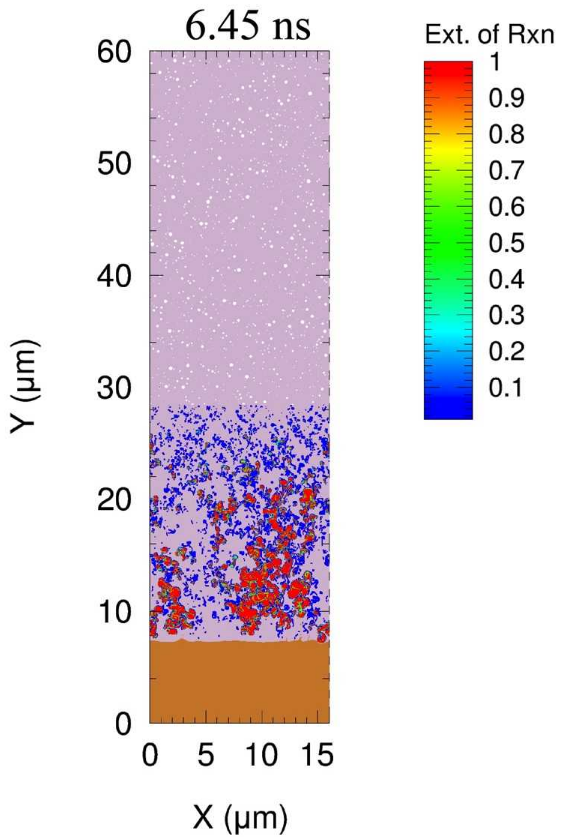
- Yield Strength –
- Poisson's Ratio –
- Melt Temp. – 316 ° C

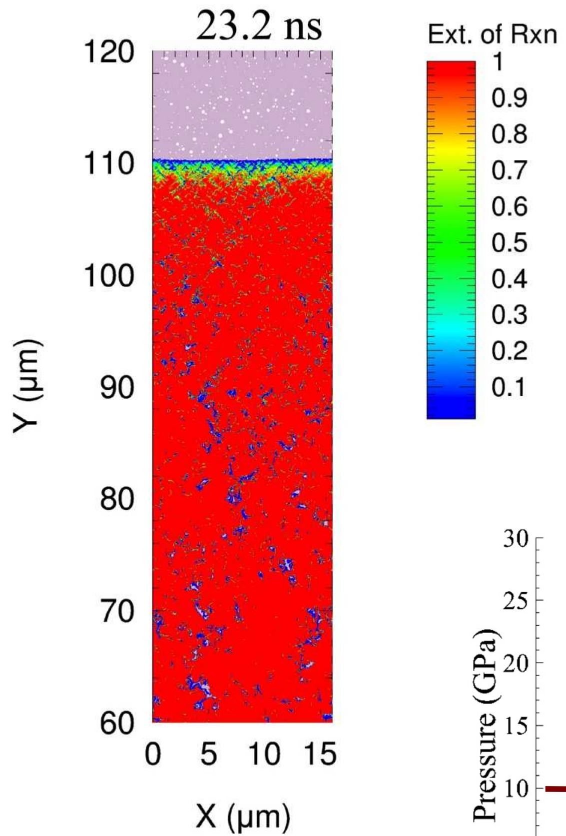
Johnson Cook

- A –
- B –
- C –
- N –
- M -



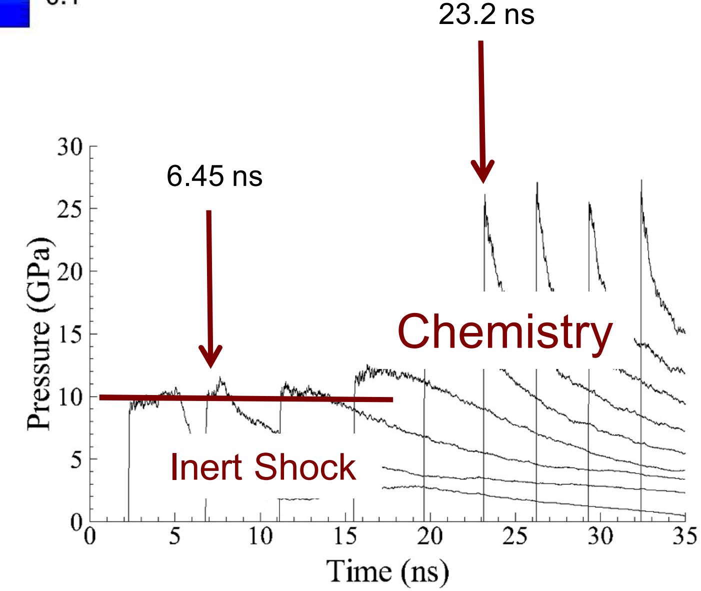
Grain-scale simulation of SDT in HNS





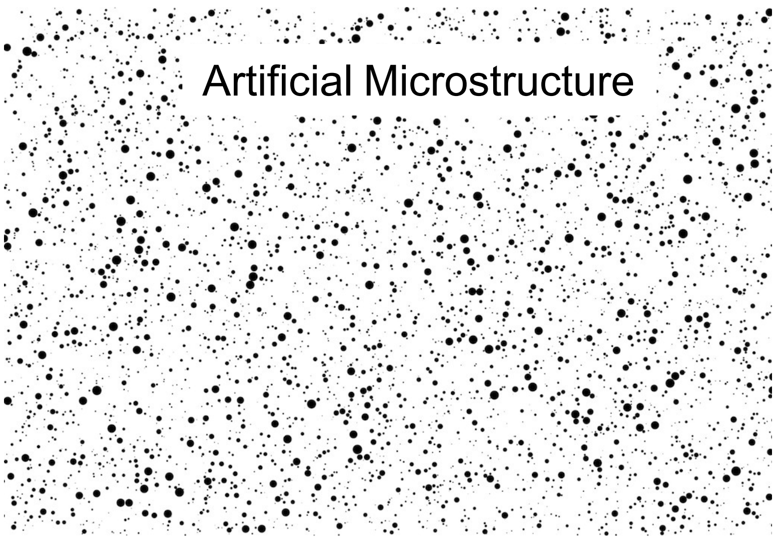
Reaction rate is based on Temperature
Example: Arrhenius burn model (ARB)

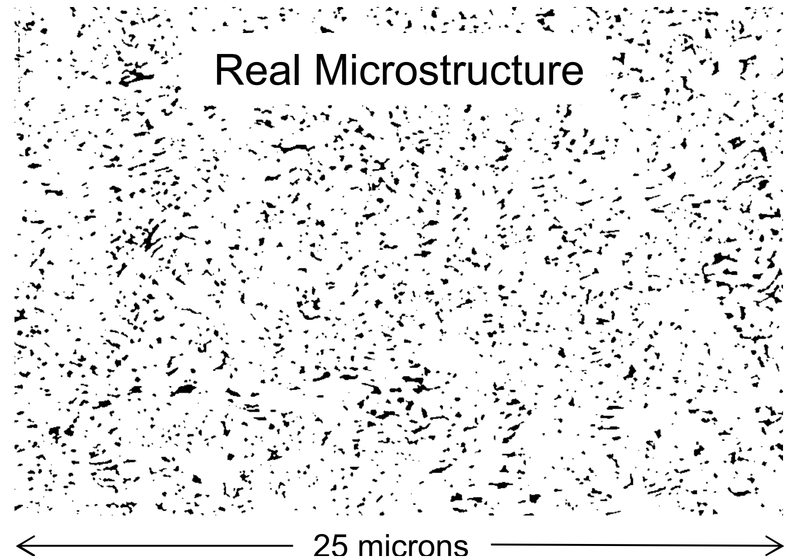
$$d\lambda / dt = (1 - \lambda) F \exp(-\Theta / T)$$

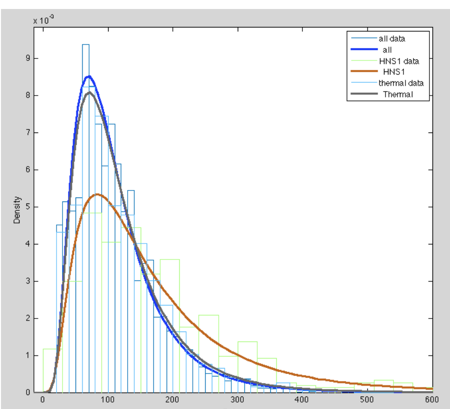


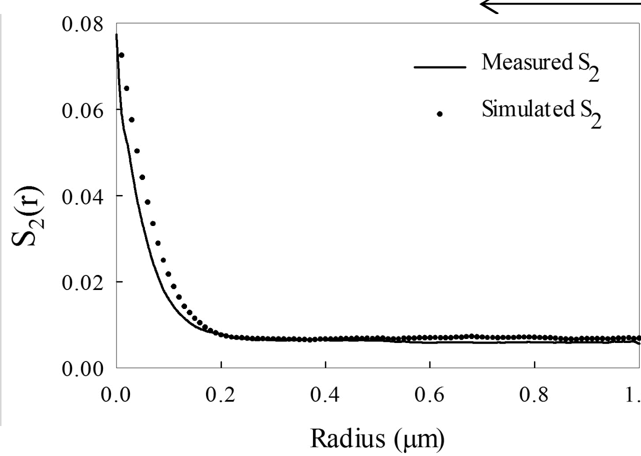
Simulations: 3.15 km/s, Mean pore size 86 um

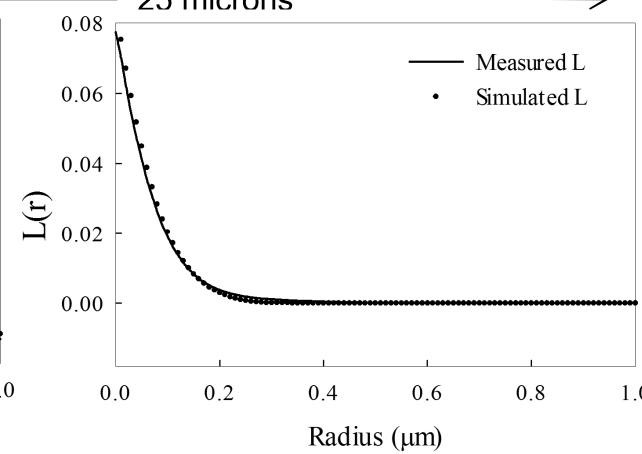
Reconstructed and measured microstructural statistics





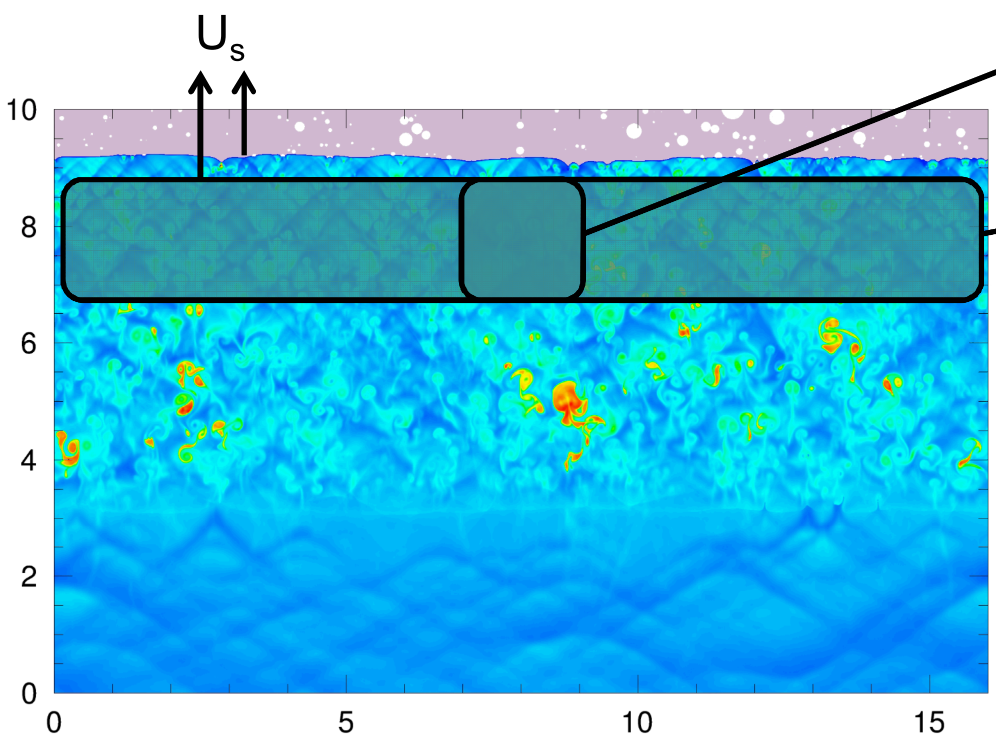


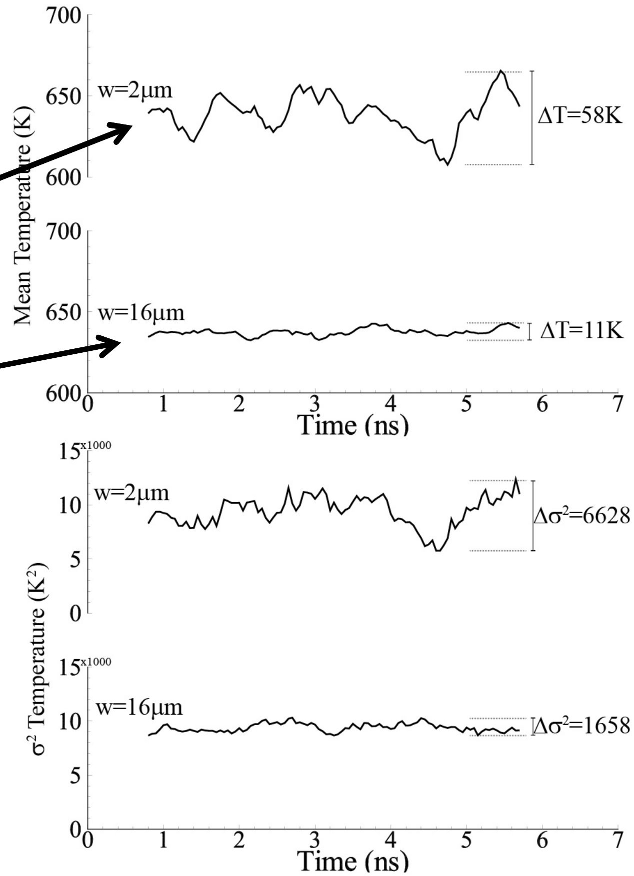




Determining the Representative Volume Element (RVE):

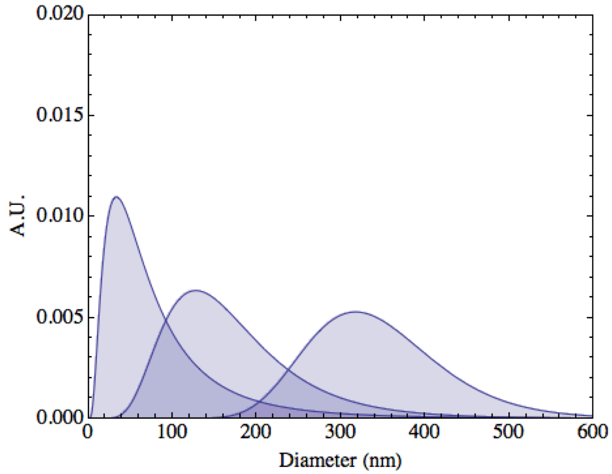
- Statistical relevance ensured by estimating the RVE
- RVE contains enough microstructure, but is smaller than the macroscopic length scale
- Temperature mean and variance

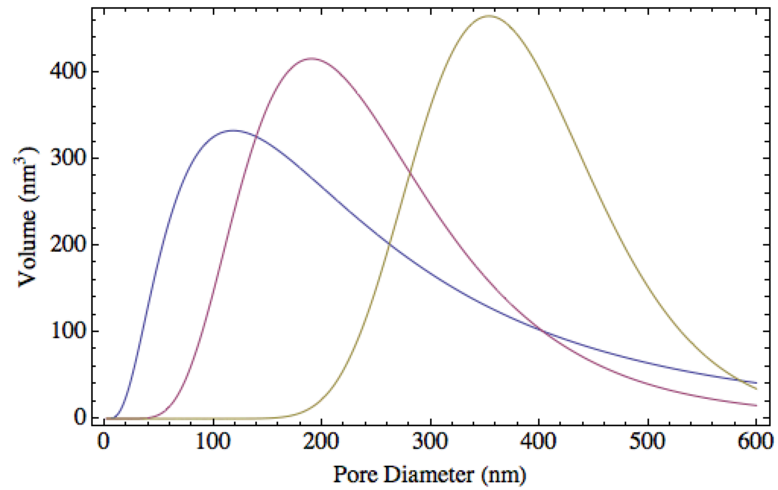




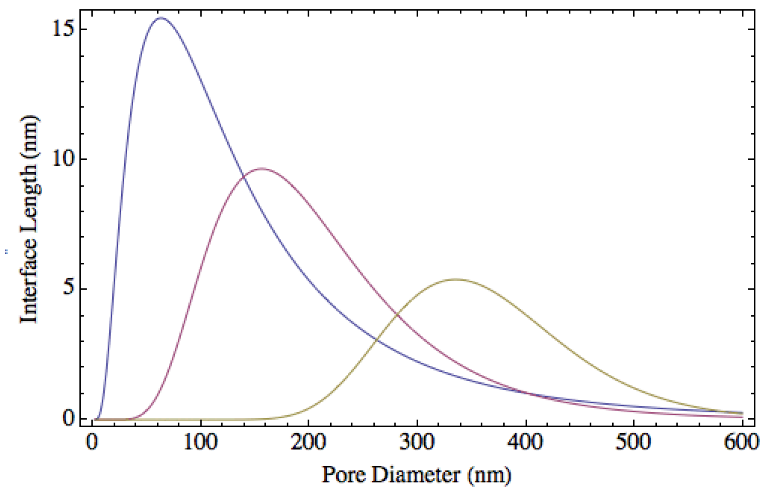
HNS initiation as a function of pore-size:

Simulations: 3.15 km/s, Mean pore size 86 um, 172 um , 344 um



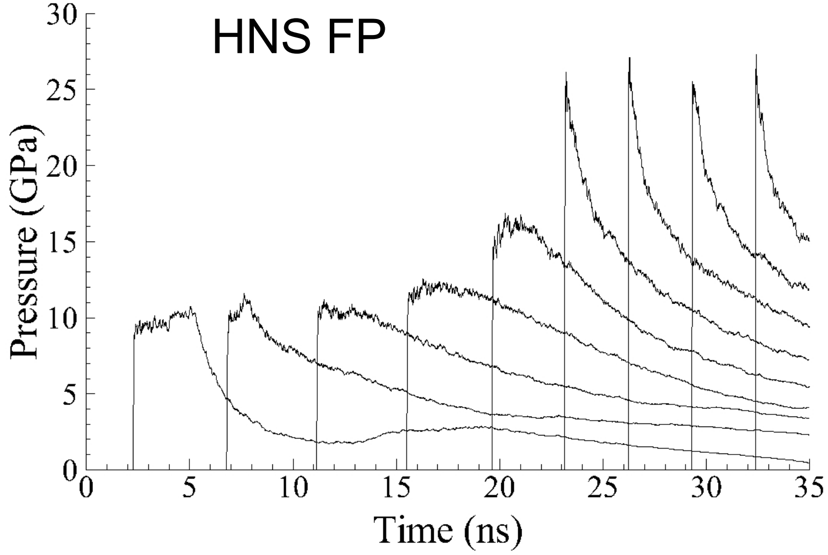


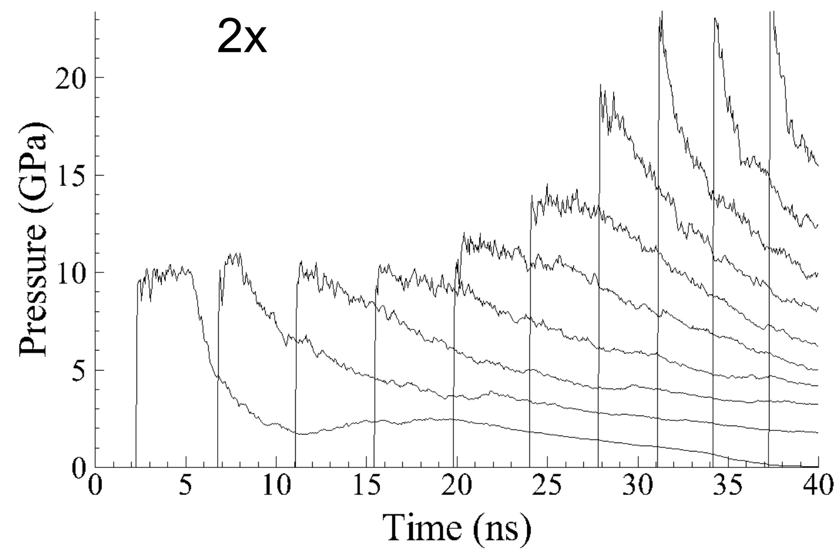
- Equal variance
- Mean increased by factor of 2 and 4
- Similar Volume, increased interface length

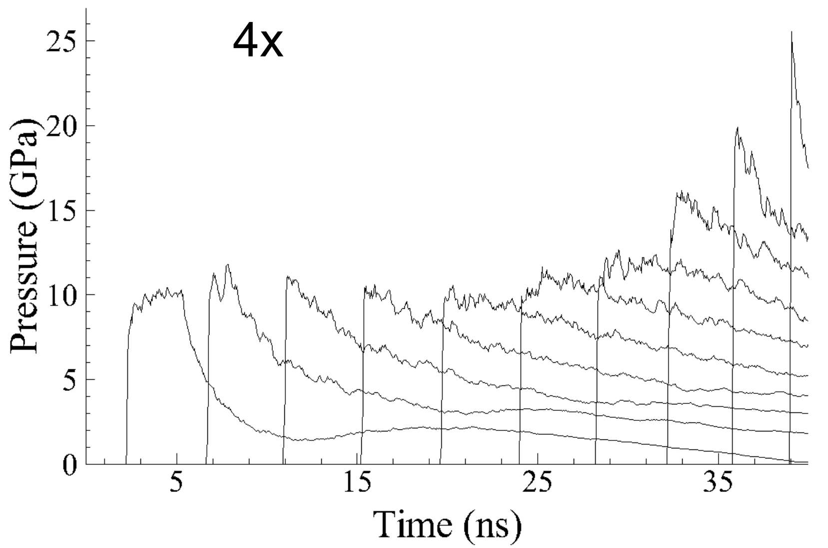


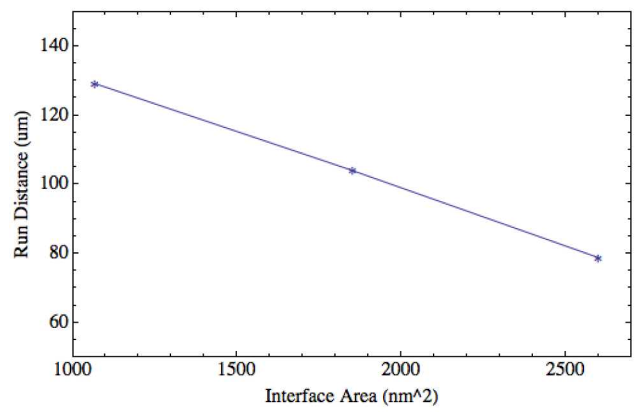
B.A. Khasainov, B.S. Ermolaev, H.N. Presles, P. Vidal, *On the effect of grain size on shock sensitivity of heterogeneous high explosives*, Shock Waves (1997) 7:89-105.

Run distance shifted with pore-size:

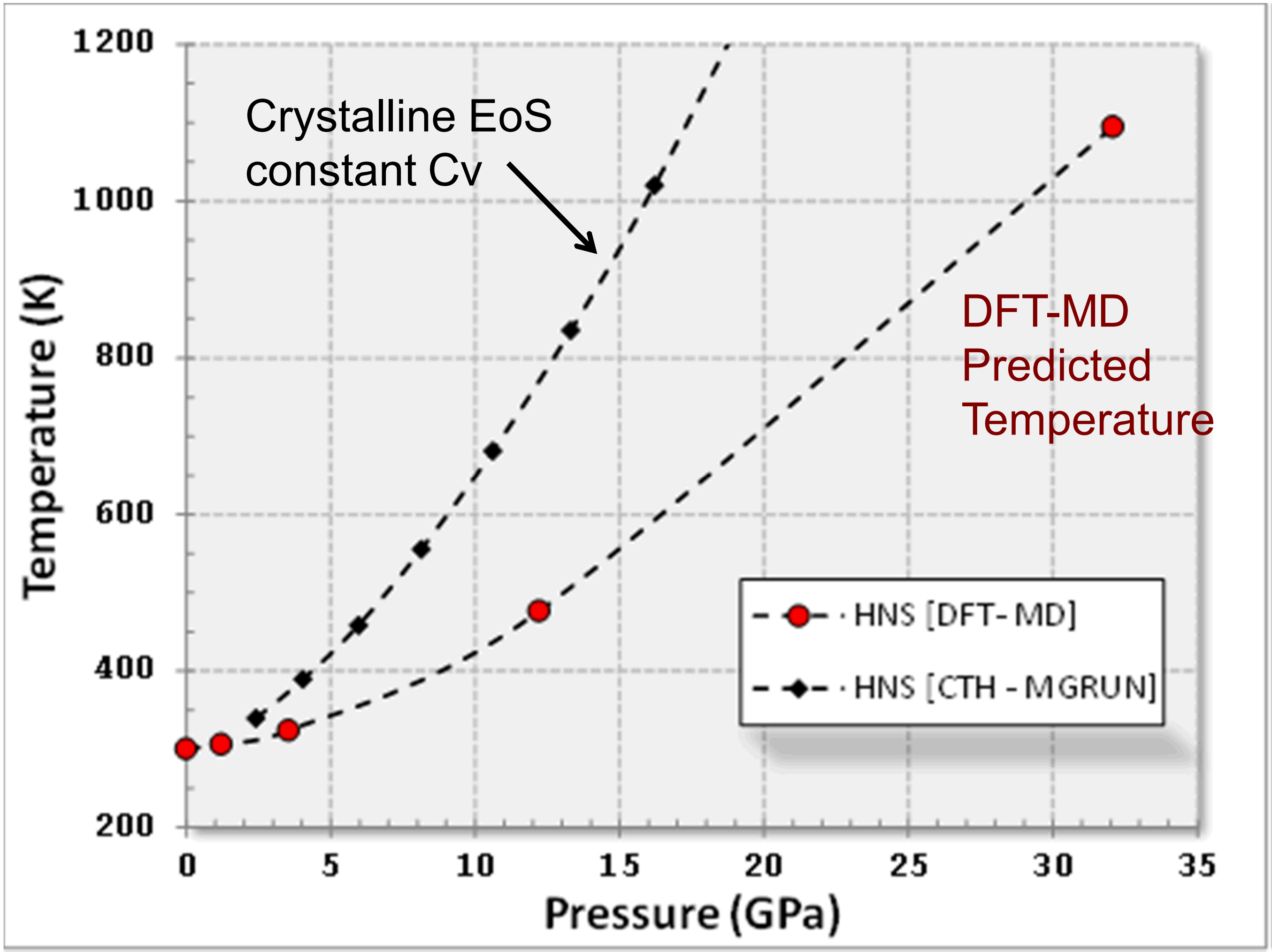






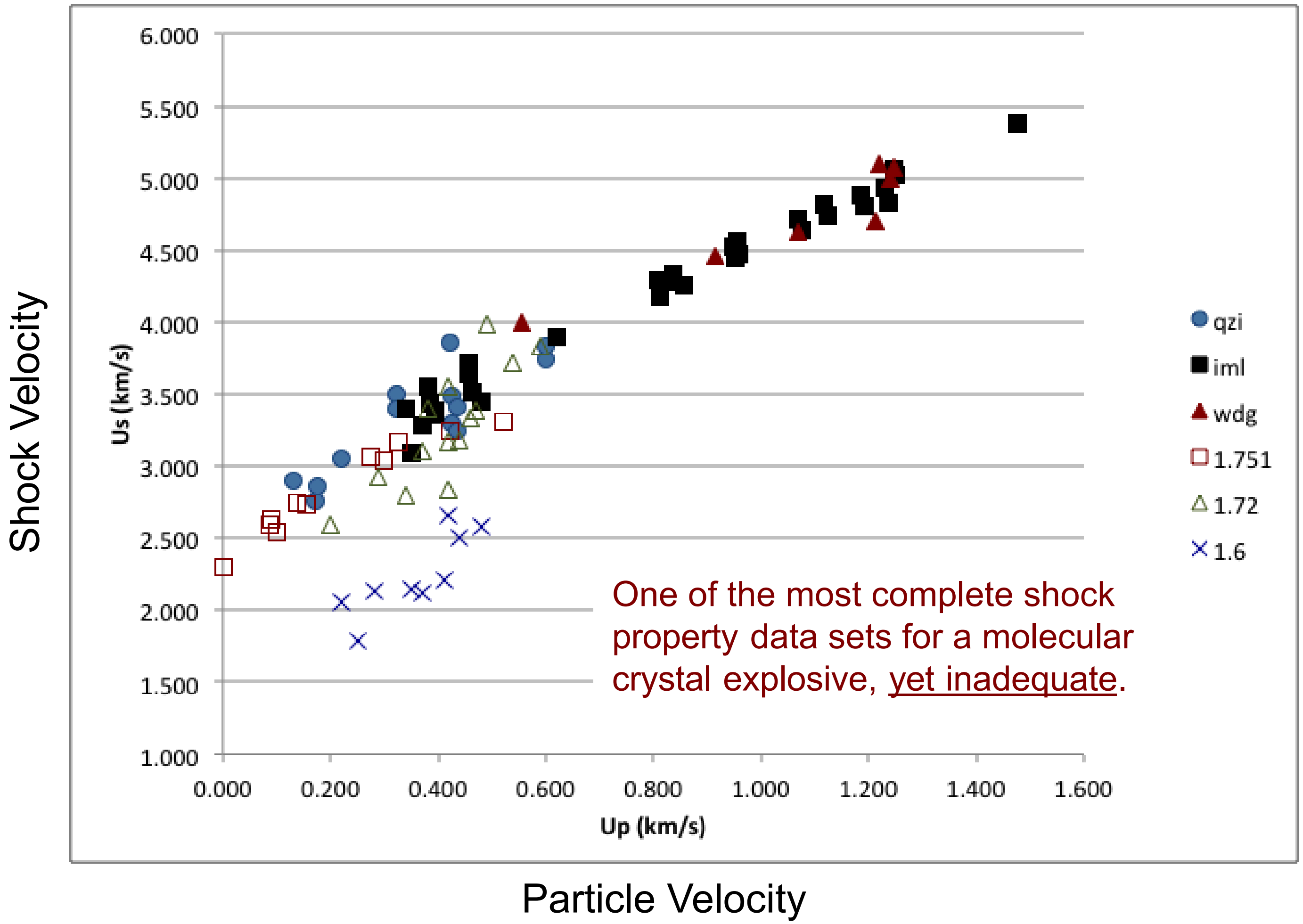


Demonstrating the EoS problem (Cv):



Experimental EoS for explosives

PETN Shock Hugoniot data from the LASL shock handbook (Marsh)



1) Not a straight line. 2) No information about temperature. 3) Data is usually low pressure.

Density Functional Theory (DFT) and XC functionals:

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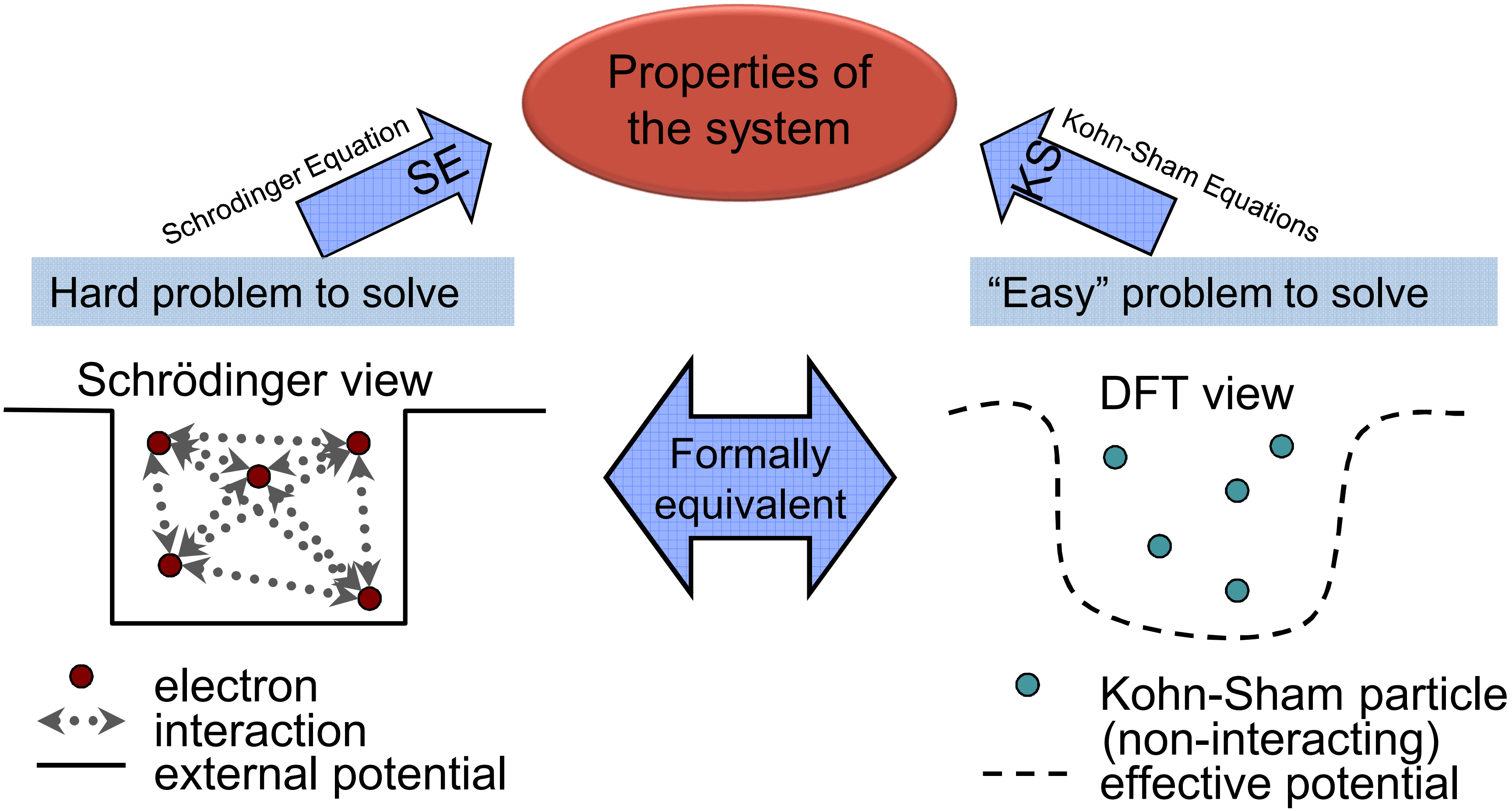
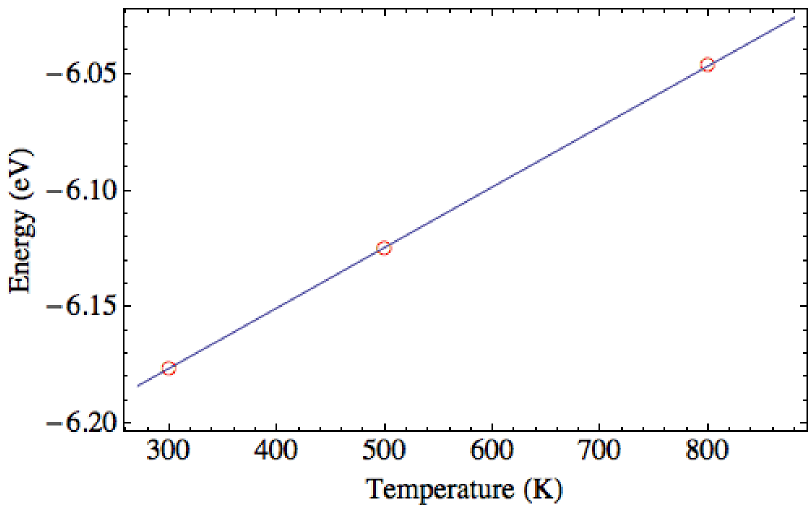
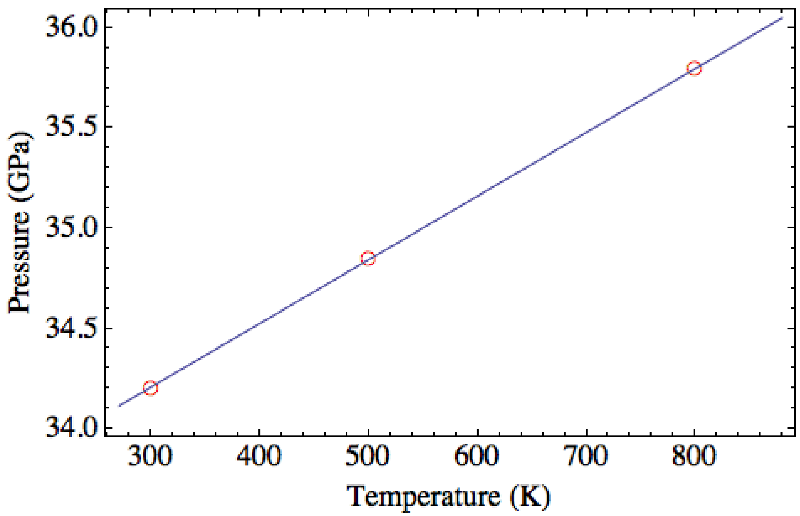


$$v_{eff}(\mathbf{r}) = v(\mathbf{r}) + \int \frac{n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\, d\mathbf{r}' + \frac{\delta E_{xc}[n(\mathbf{r})]}{\delta n(\mathbf{r})}$$

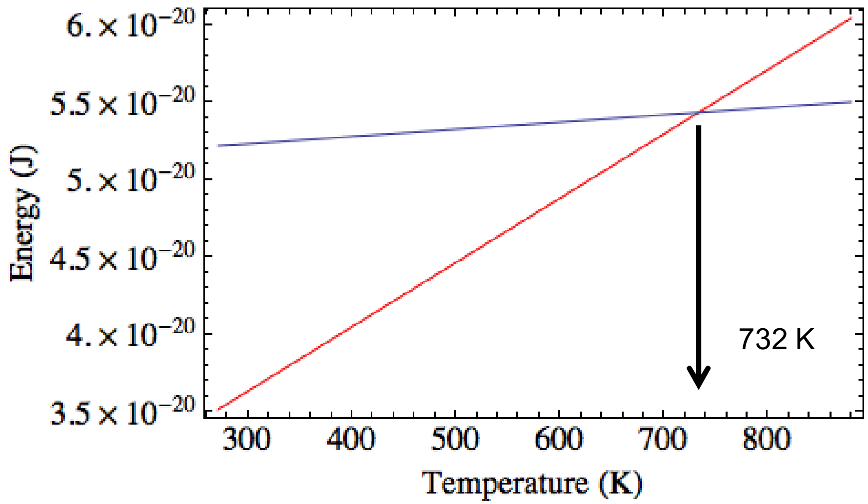
AM05, LDA, GGA, Meta-GGA, Hybrids

Finding the Hugoniot (TATB $V=0.85V_o$):





$$E(T) - E_o = \frac{1}{2}[P(T) + P_o][V_o - V]$$



Cataloging microstructures: X-sections of different types of HNS

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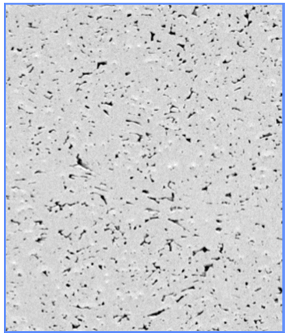
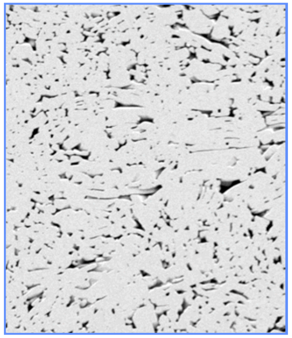
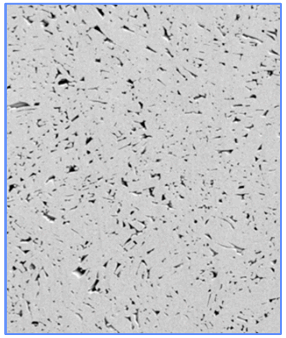
HNS FP (a)



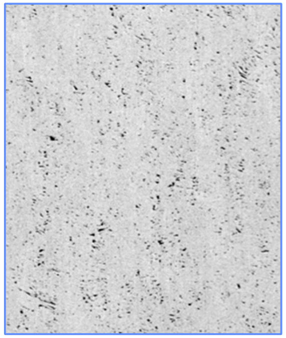
HNS FP (b)



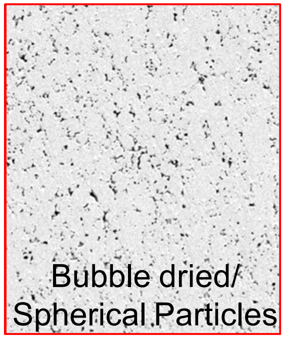
HNS FP (c)



HNS FP (d)

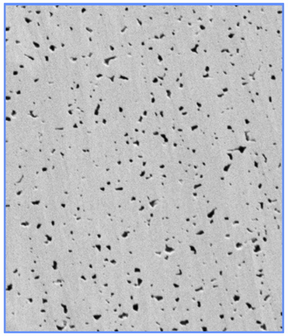


HNS BD

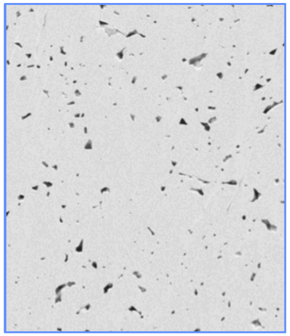


10 um

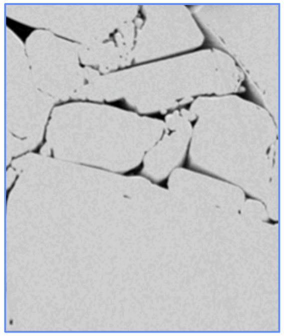
HNS/2% Kel-F



HNS-I



HNS-II



Type	Powder SSA (m2/g)	Interface Area (m2/g)	Avg. DIA (nm)	Avg dist to a pore (nm)	Density %TMD
		(0.15)	(10.0)	(10.0)	(.01)
HNS-FP (a)	6	1.77	136.6	136.0	0.925
HNS-FP (b)	5	2.10	254.5	130.7	0.875
HNS-FP (c)	10	1.98	152.6	131.2	0.914
HNS-FP (d)	16	3.61	74.2	78.3	0.921
HNS-BD	12	2.41	113.5	107.3	0.899
HNS+Binder	?	1.10	211.6	214.6	0.928
HNS-I	?	0.71	233.0	345.6	0.960
HNS-II	1	0.24	1363.8	1703.5	0.950

We have also have x-sections of thermally cycled HNS FP (a)