Things I want to say about initiation

Ryan R. Wixom, Sandia National Laboratories

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Tadasana

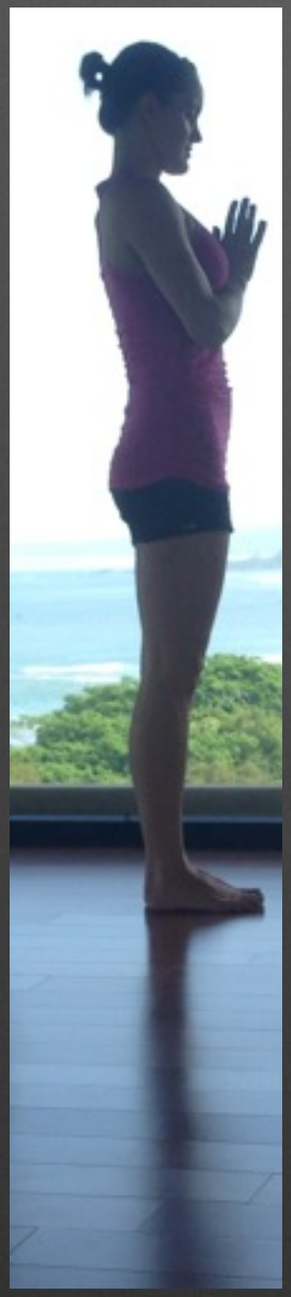
Salamba sirsasana

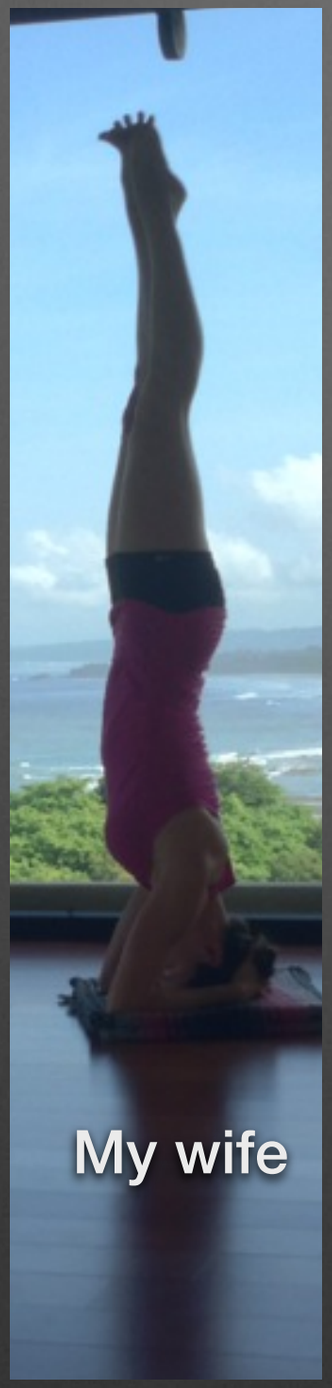
Ado Mukha Vrksasana

Shazaaaaaam

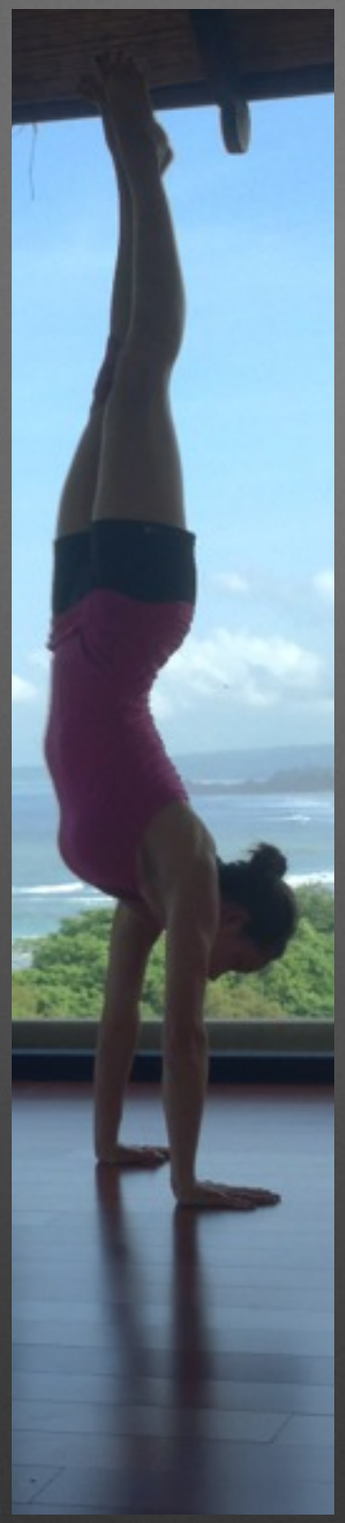
B.K.S. Iyengar

Savasana





My wife



One of these things is…
<u>very much</u> like the others.

B.K.S. Iyengar: Now 95yo

The fundamental principles are the same

What the hell does this have to do with initiation?

Impact, mostly magic, DETONATION.

Exploding Foil Initiator-chip slapper

SDT

Homogeneous v. Heterogeneous

Entirely different physics and chemistry

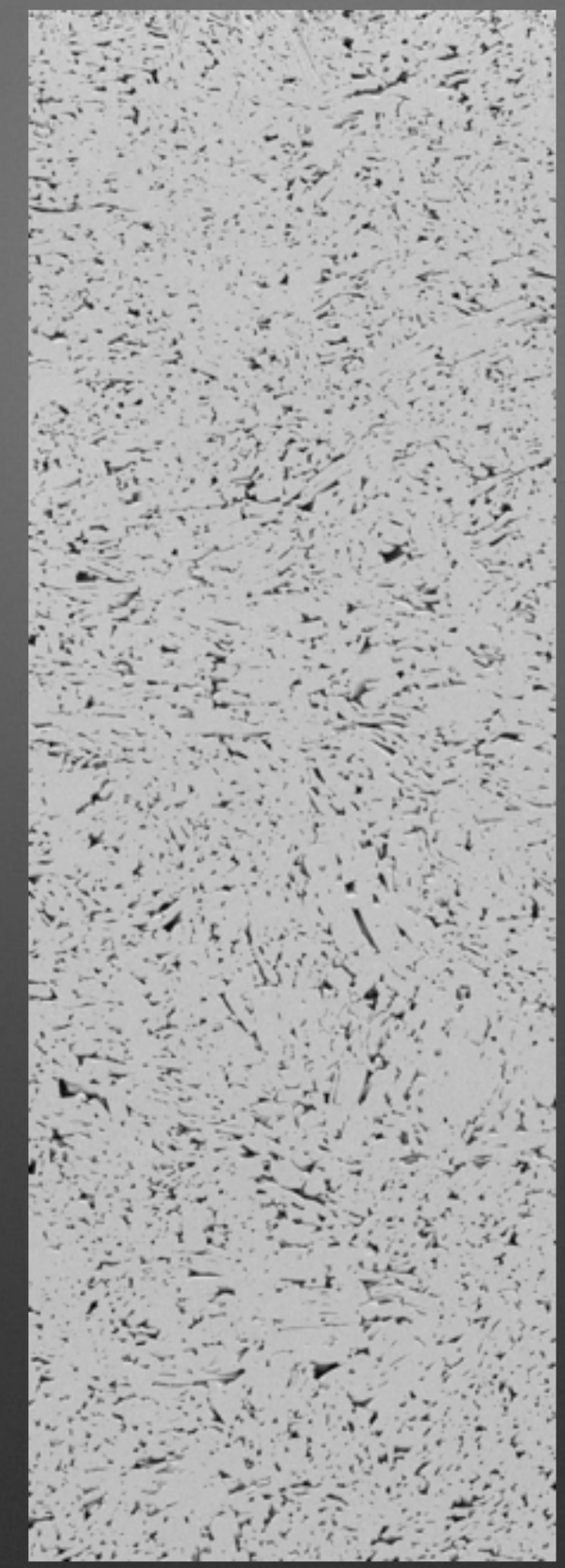
HUH?

DDT

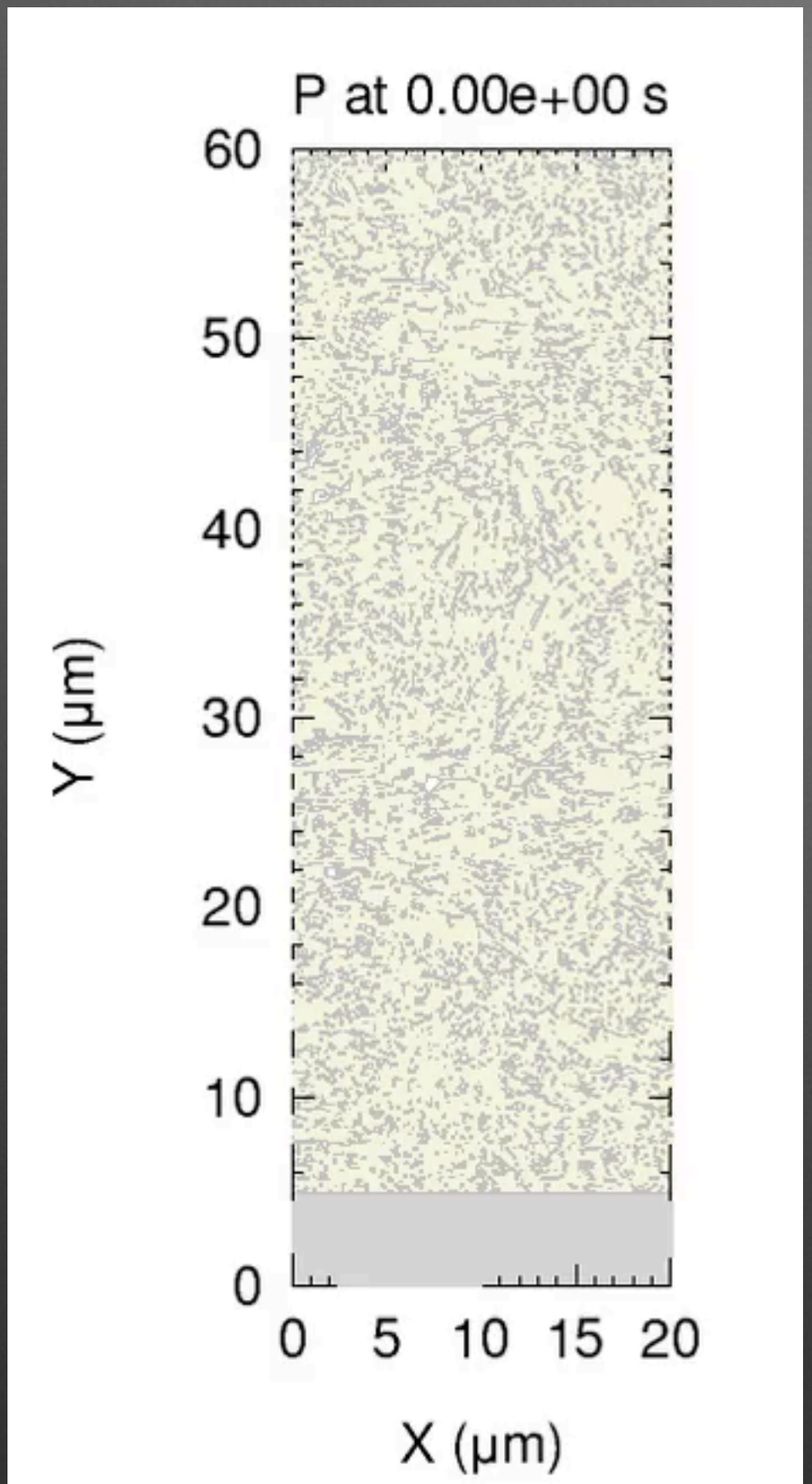
Thermal, burning, faster burning, magic, Detonation

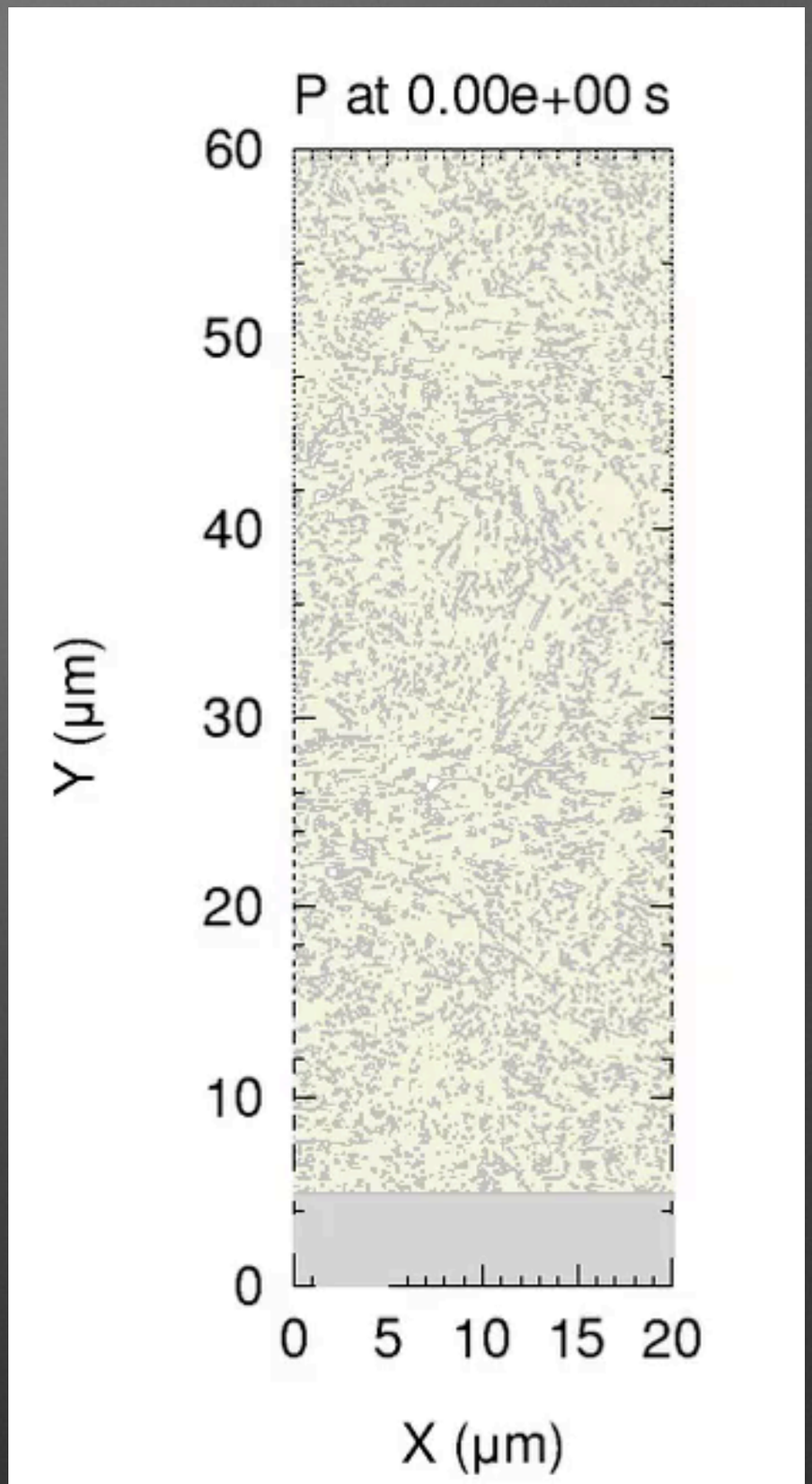
Exploding Bridge Wire

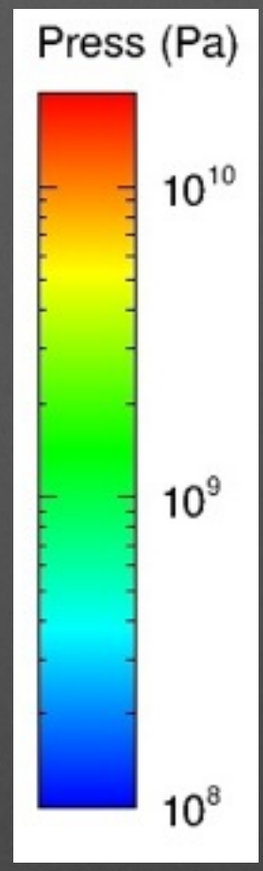
HNS-FP
90% TMD



Al flyer
1.5 km/s

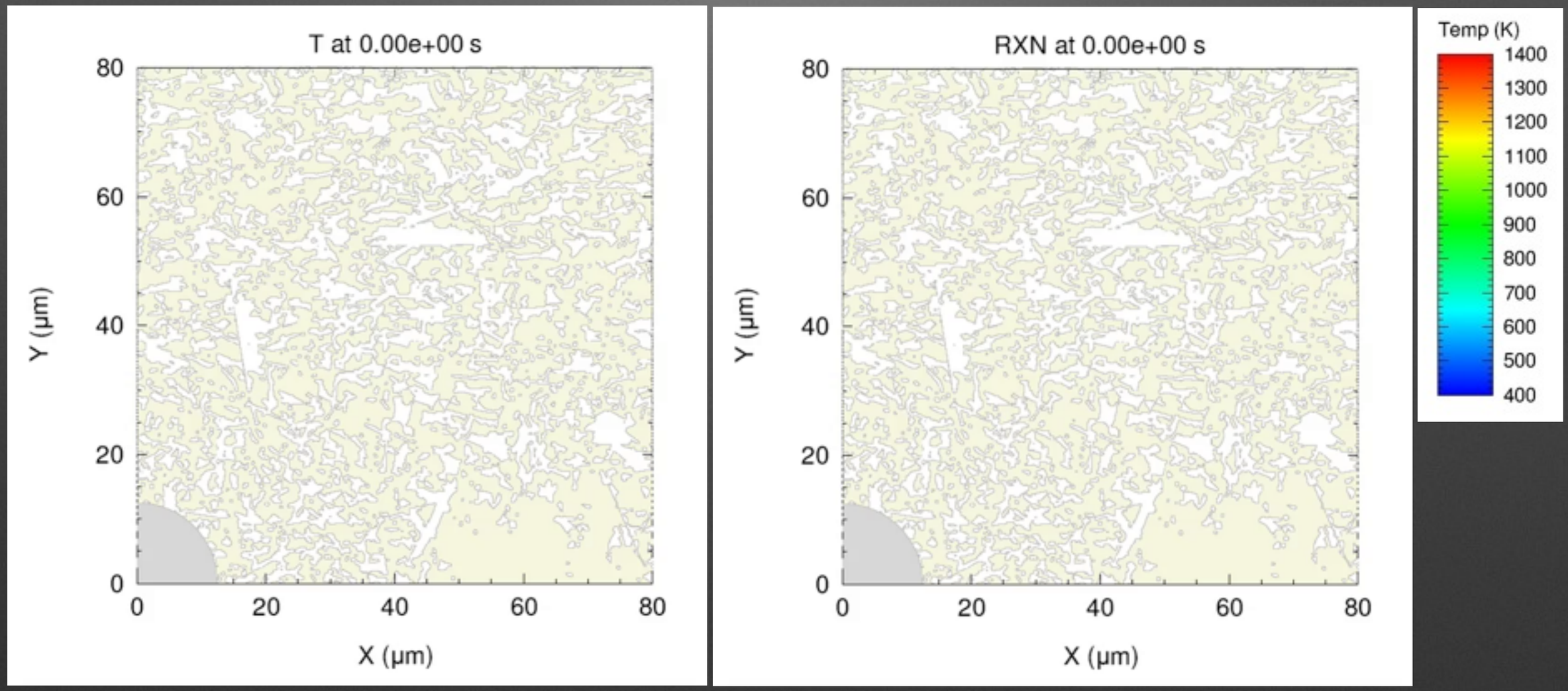






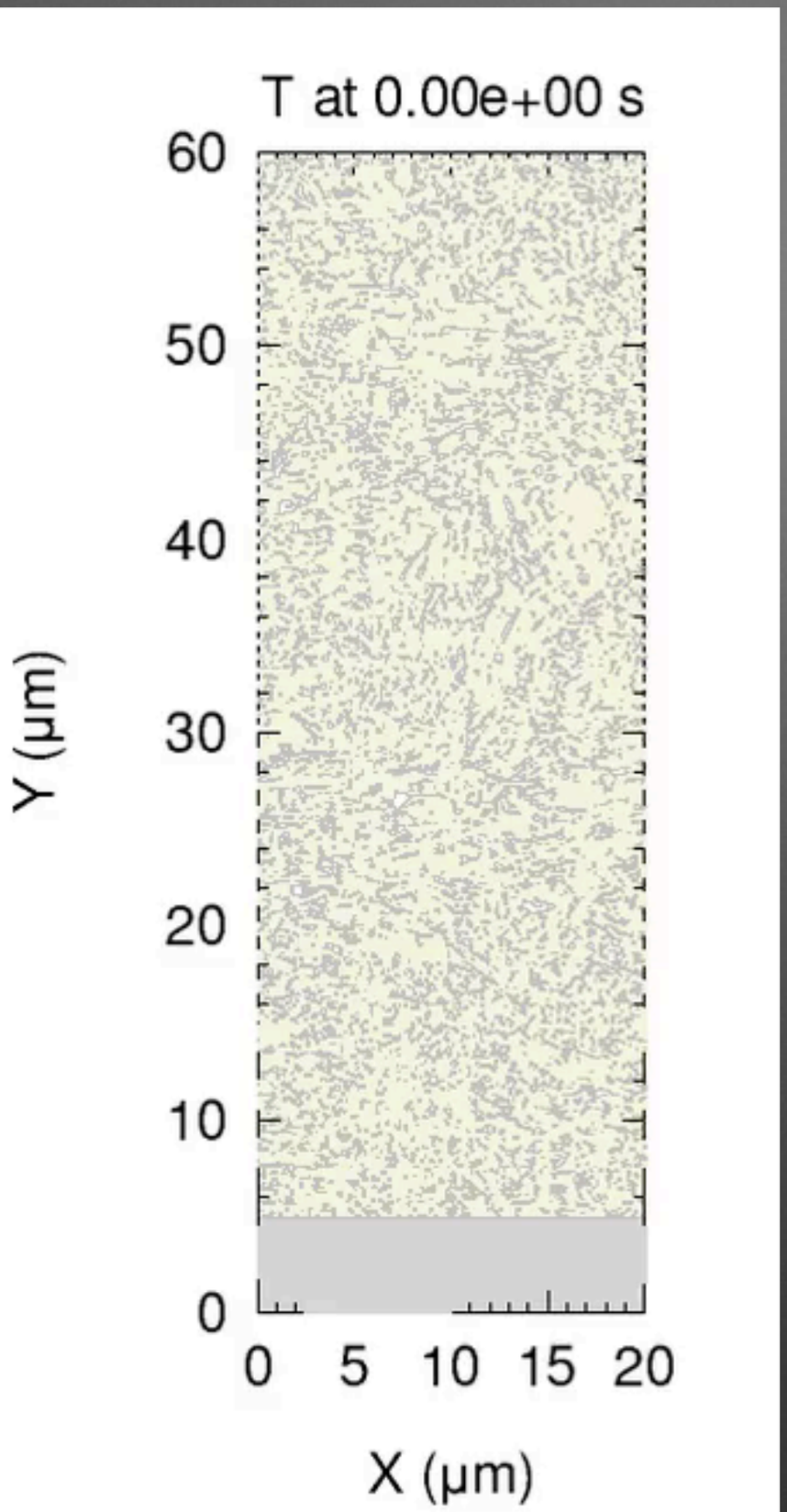
Al flyer
2.5 km/s

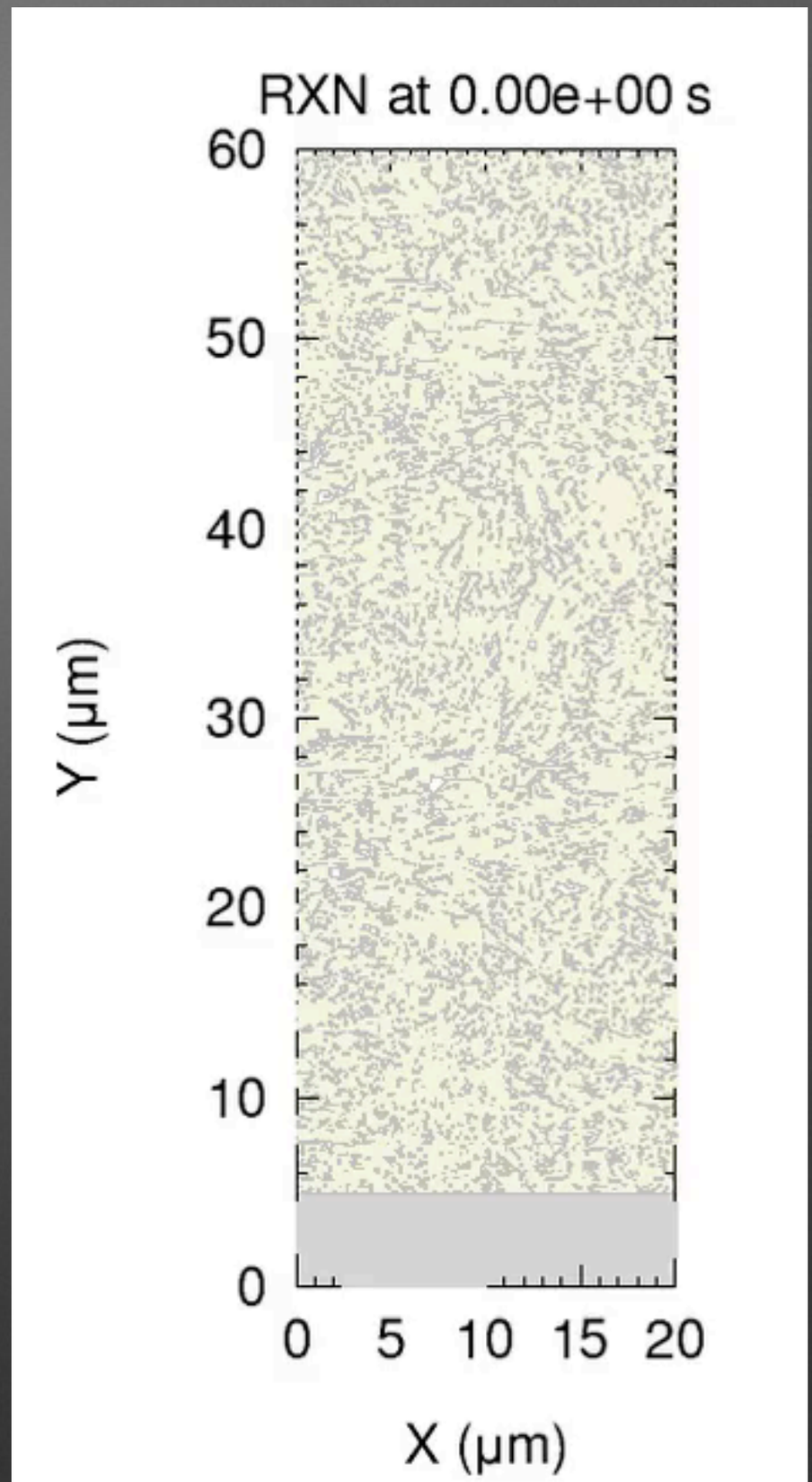
Grain-scale simulation of EBW



Temp HE (K)

1400
1300
1200
1100
1000
900
800
700
600
500
400





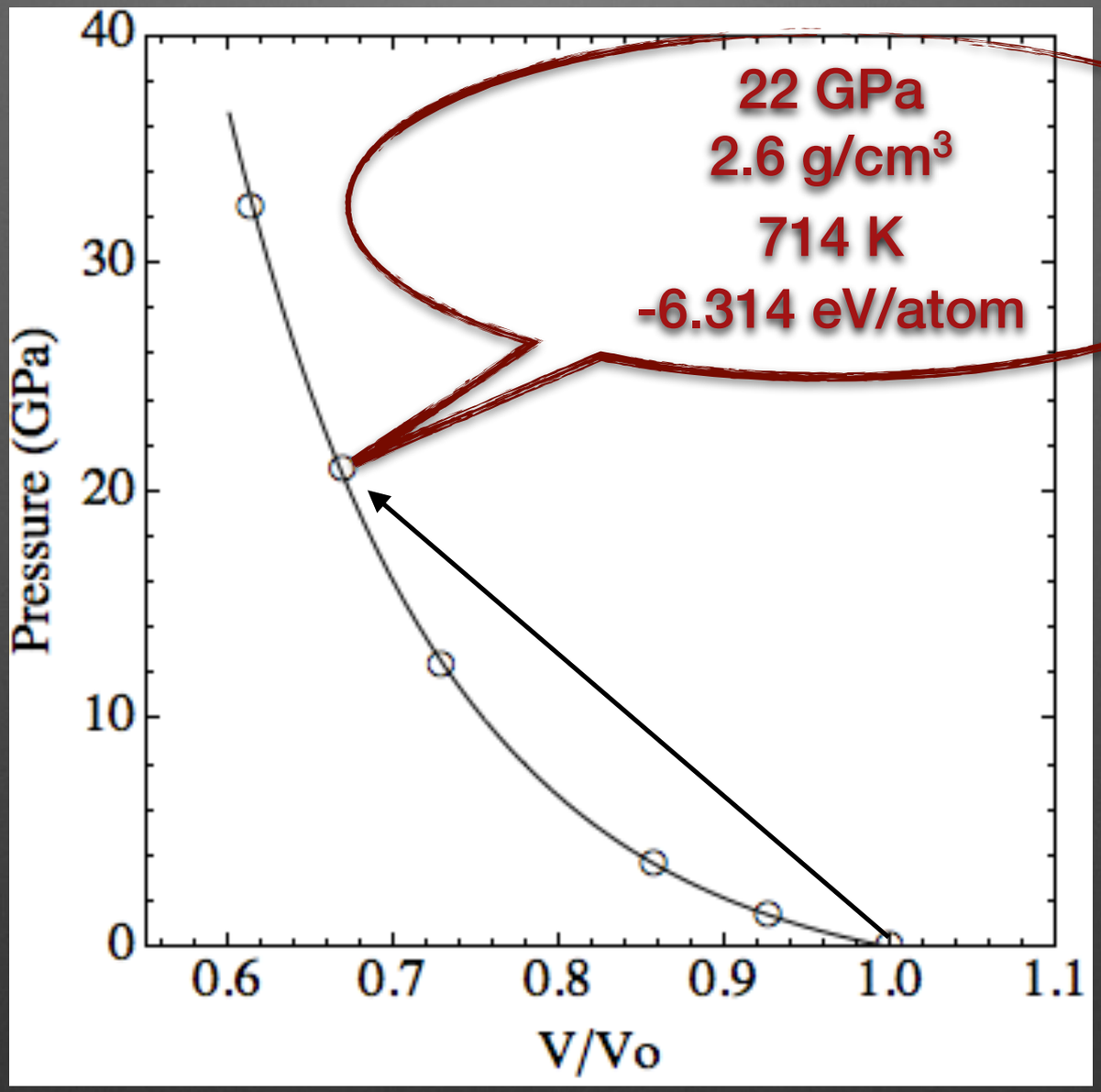
XRN

10^{0}
10^{-1}
10^{-2}

Al flyer
1.5 km/s

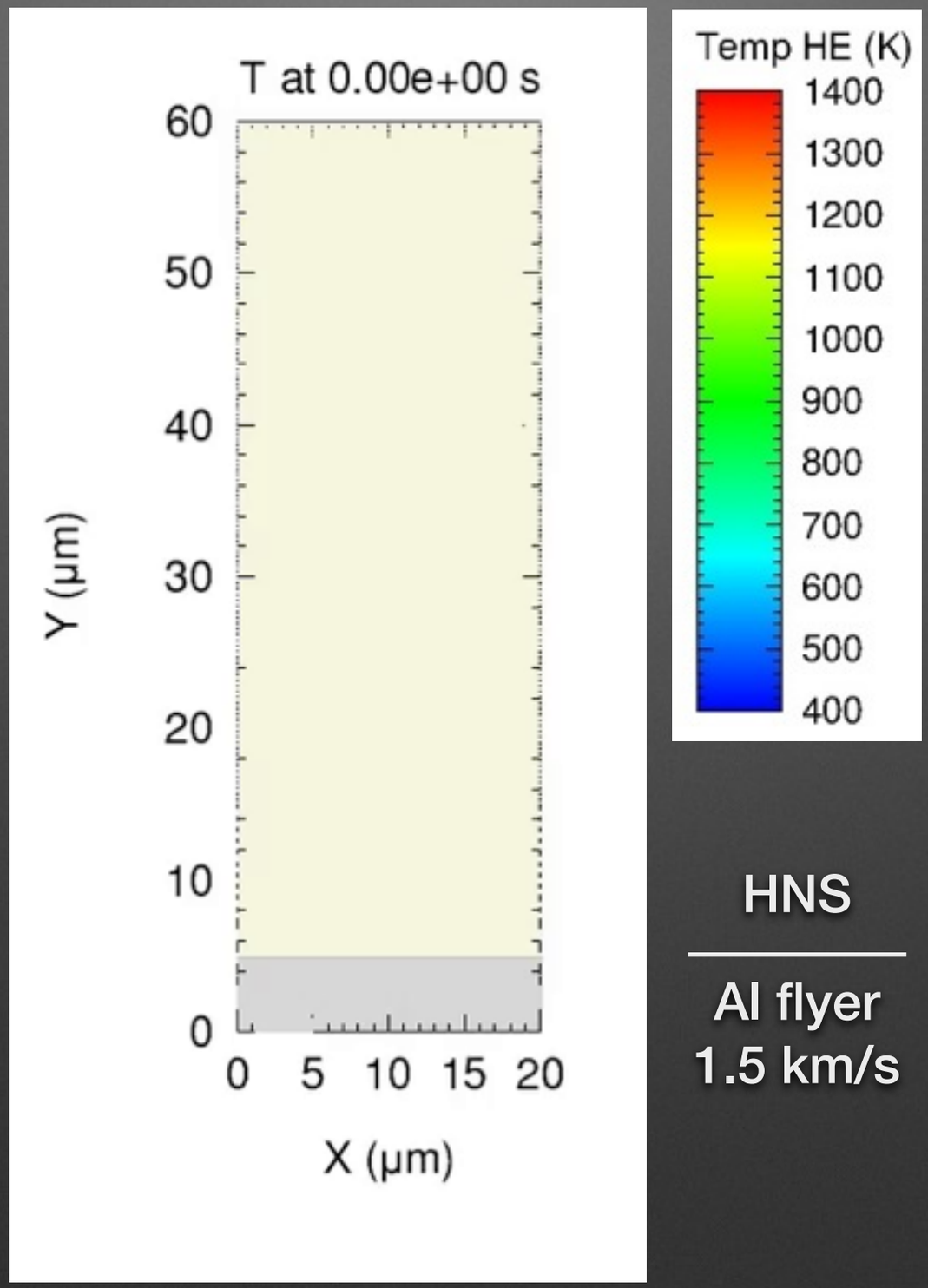
That's right… a shock wave isn't a pressure wave.

A shock is a propagating change of thermodynamic state.



Rayleigh line connects two thermodynamic states
Volume, Pressure, Temperature, Internal Energy

A shock is also a thermal pulse

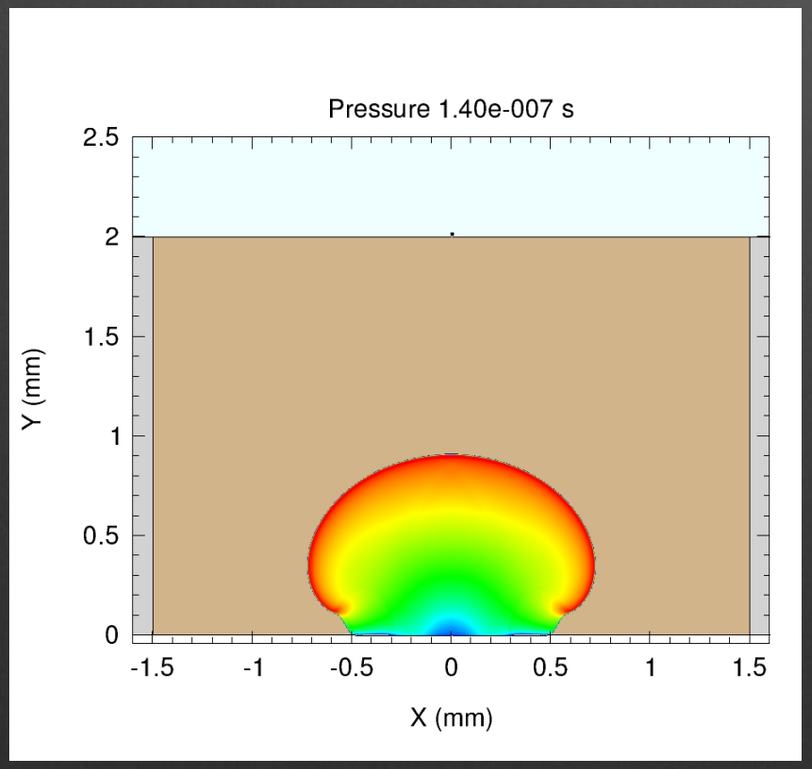


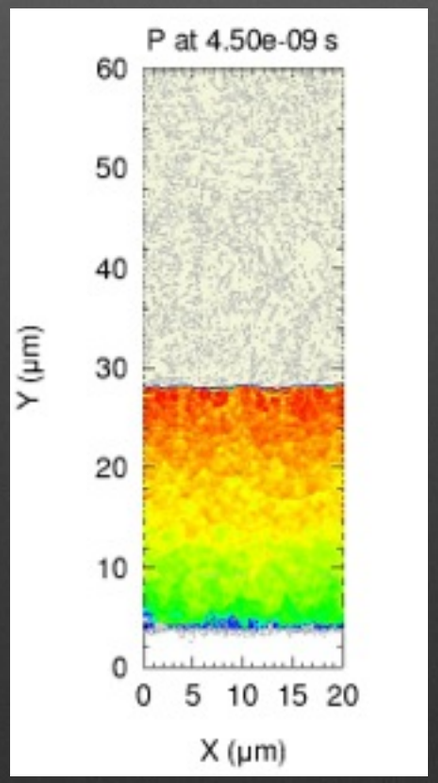
HNS

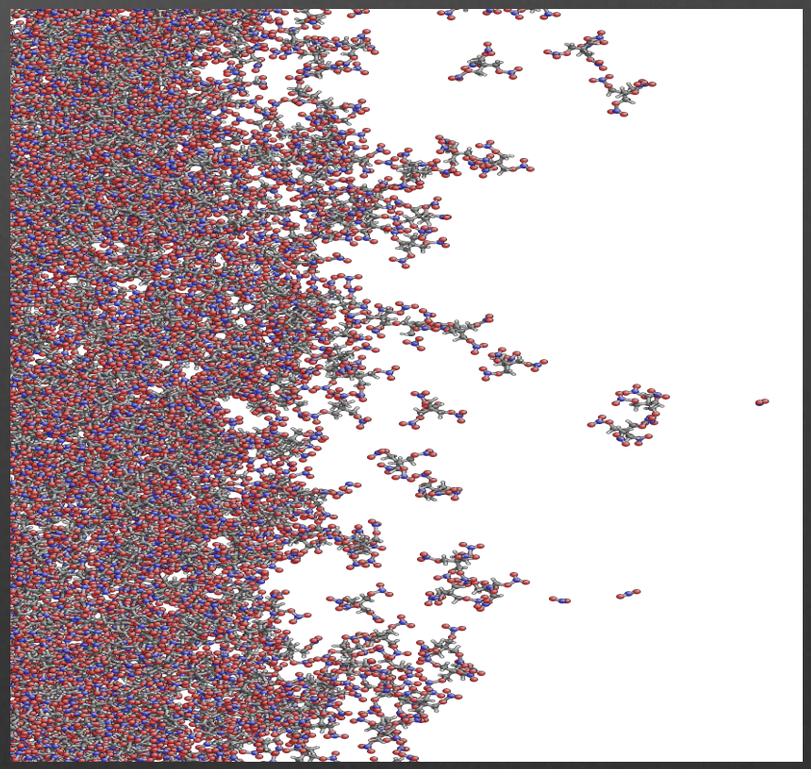
Al flyer
1.5 km/s

Question: Do EBWs function by SDT or DDT?

Answer: Frankly, … I don’t really care.

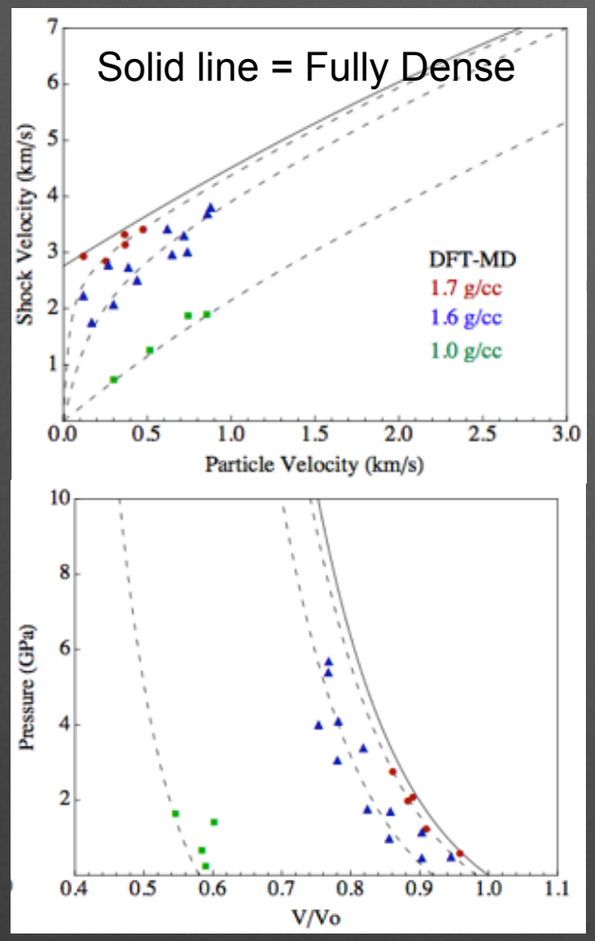




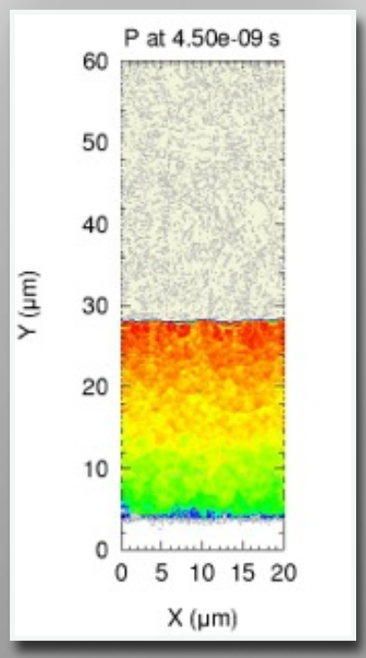


Continuum → Microscale → Atomic Scale

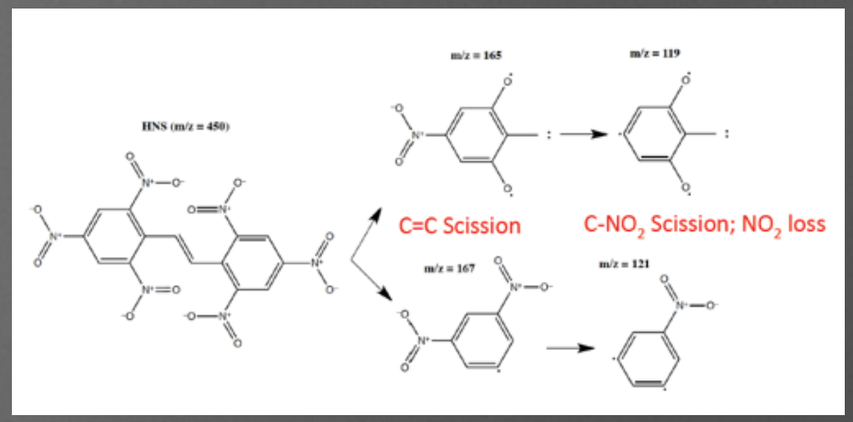
Predictive Simulation of Initiation



Equation of State

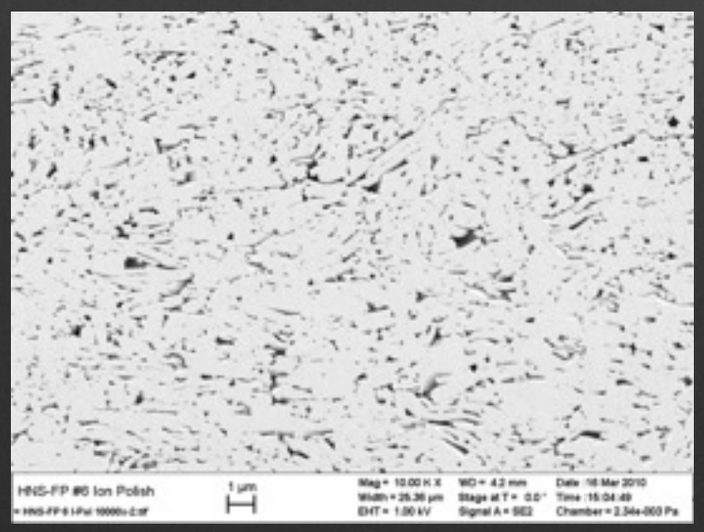


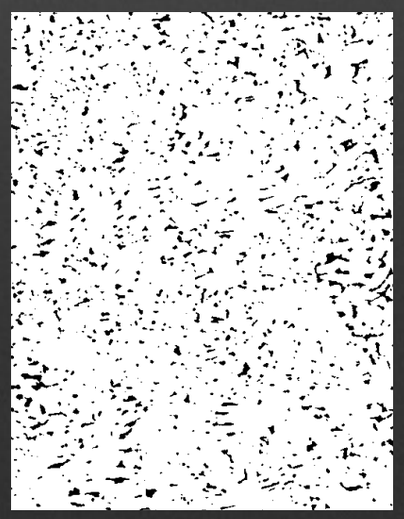
Chemical Reactions

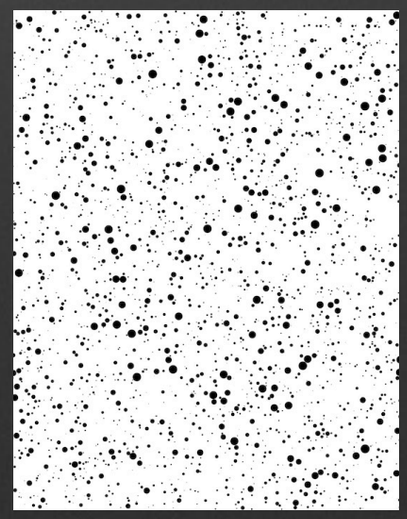


$$d\lambda/dt = (1-\lambda)F\exp(-\Theta/T)$$

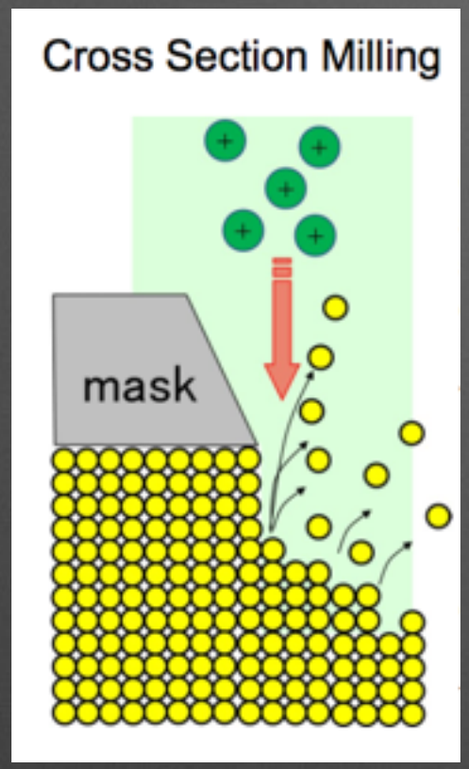
Physical Representation / Microstructure

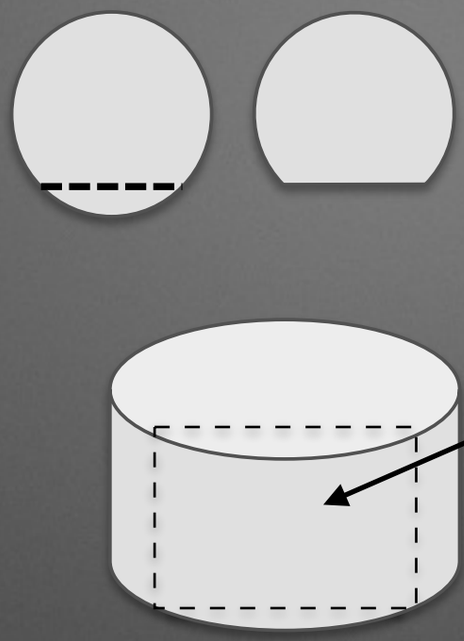


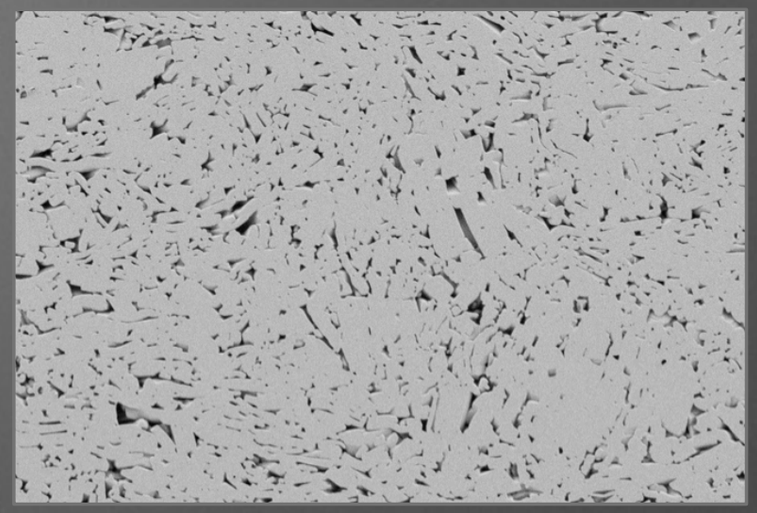




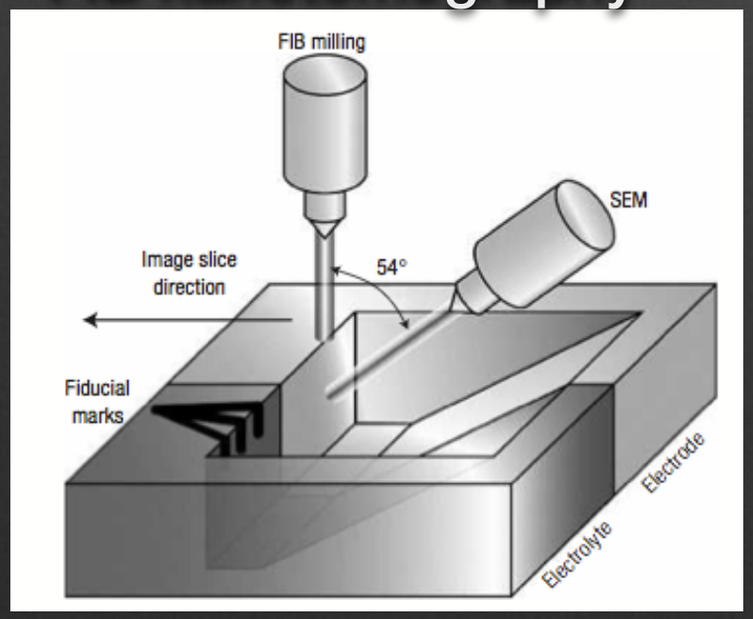
Ion Beam Techniques for X-Sectioning Explosives

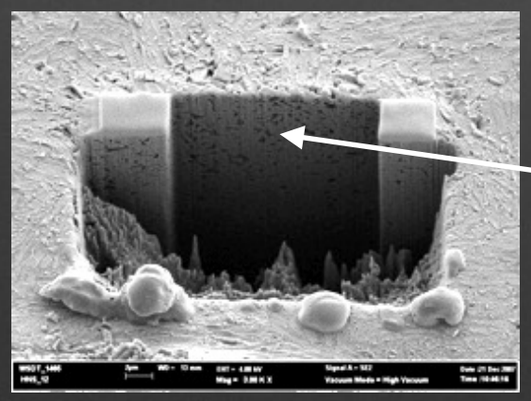




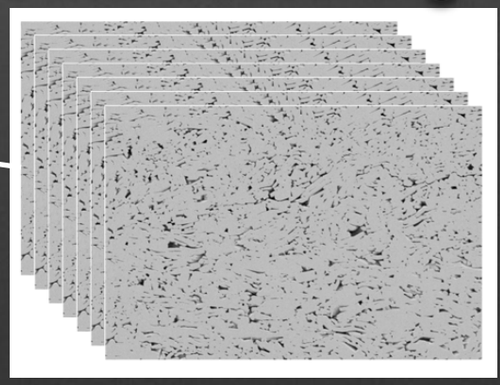


FIB nanotomography

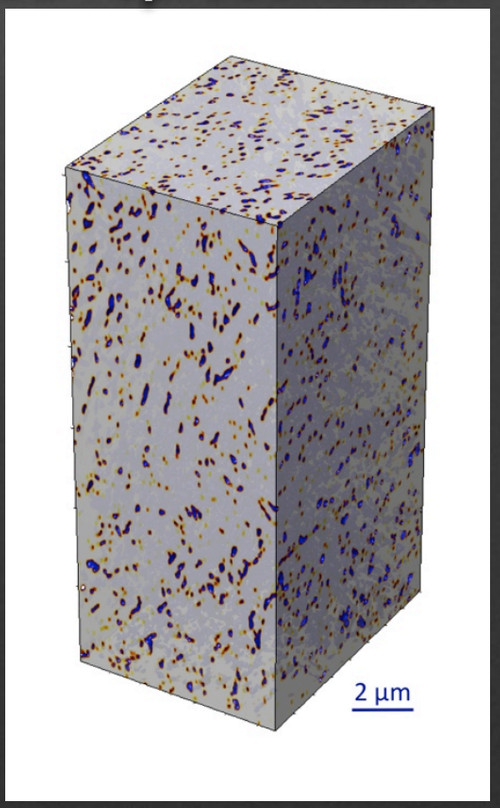




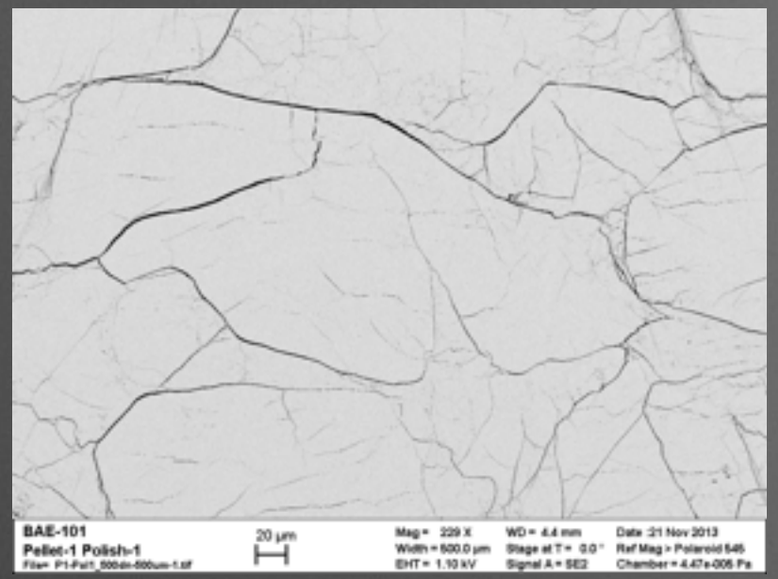
Serial sectioning

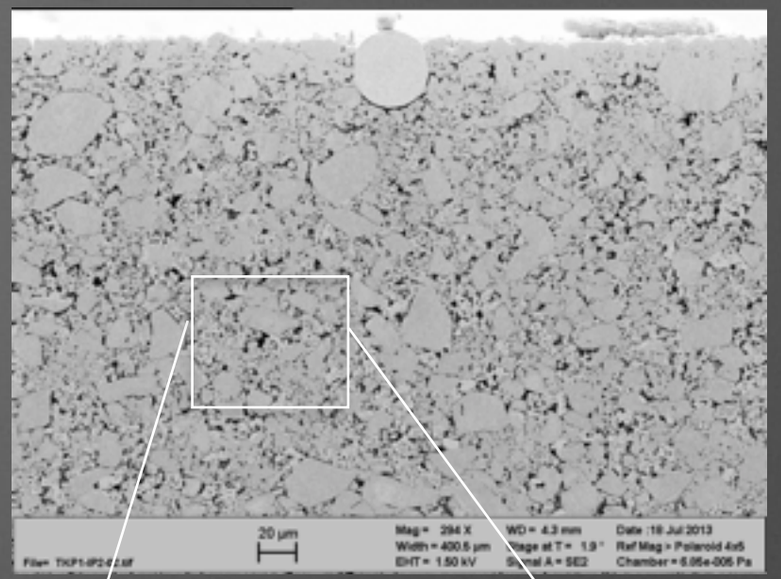


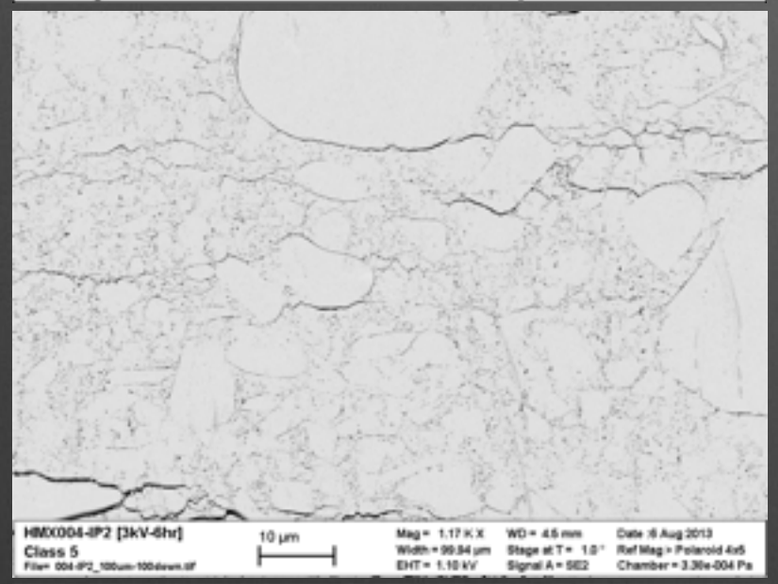
3D representation

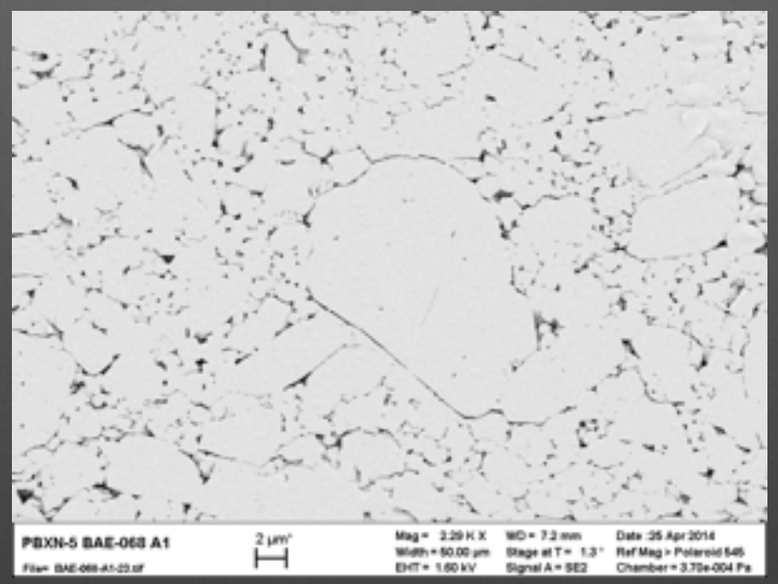


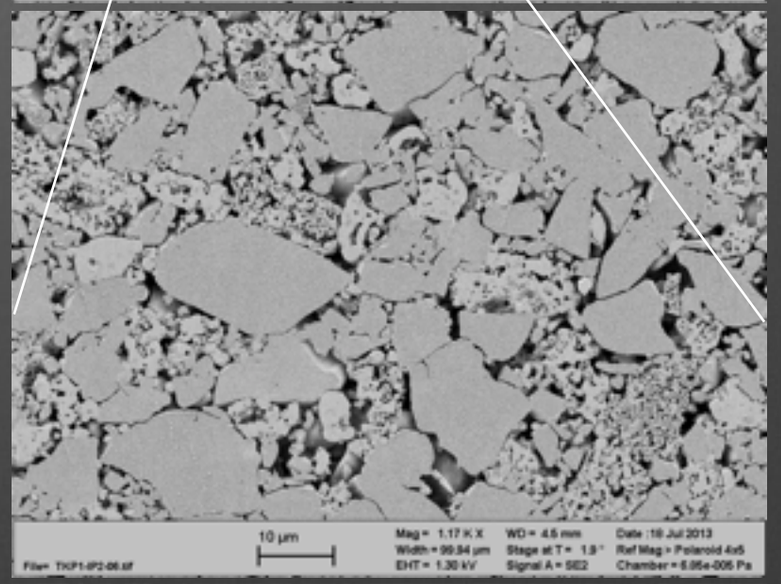
HNS, PETN, HMX, PBX, TATB, CL-20, Pyro, Propellant…

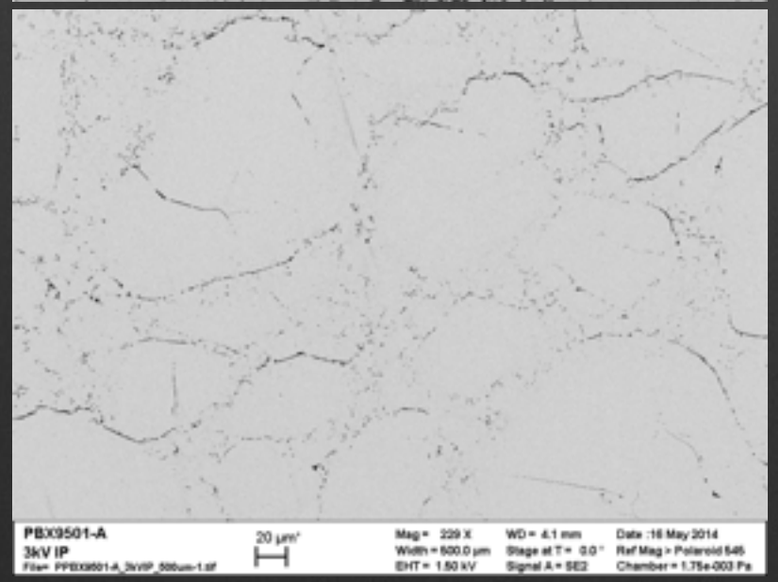


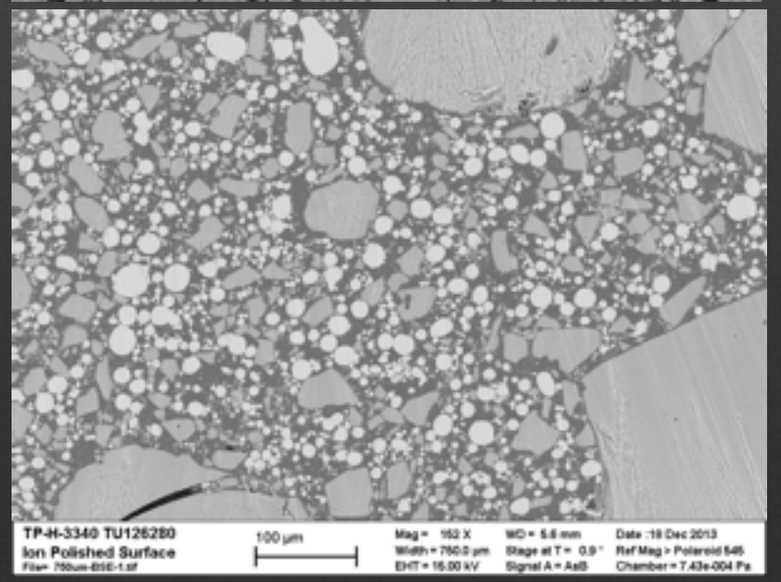




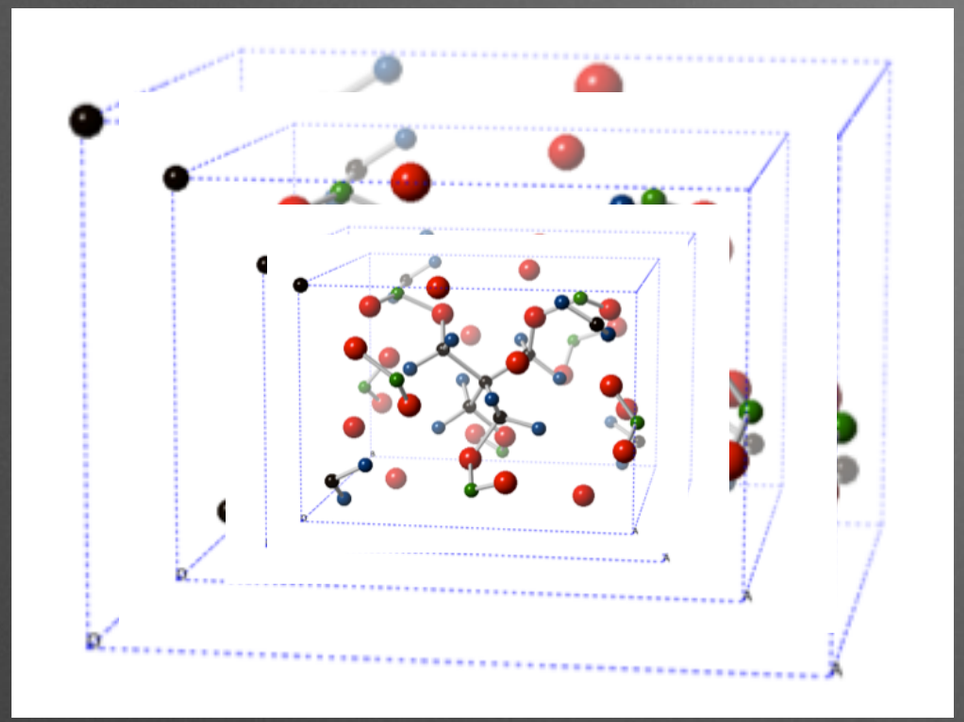








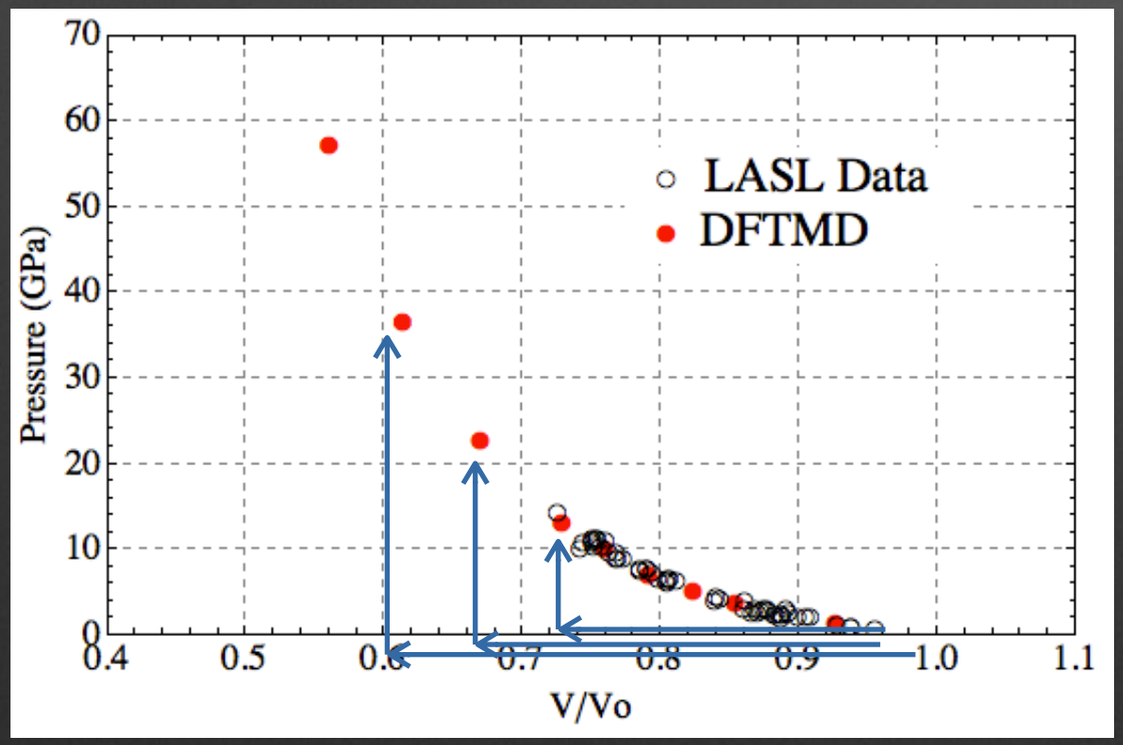
Frist Principles Predicted Equation of State

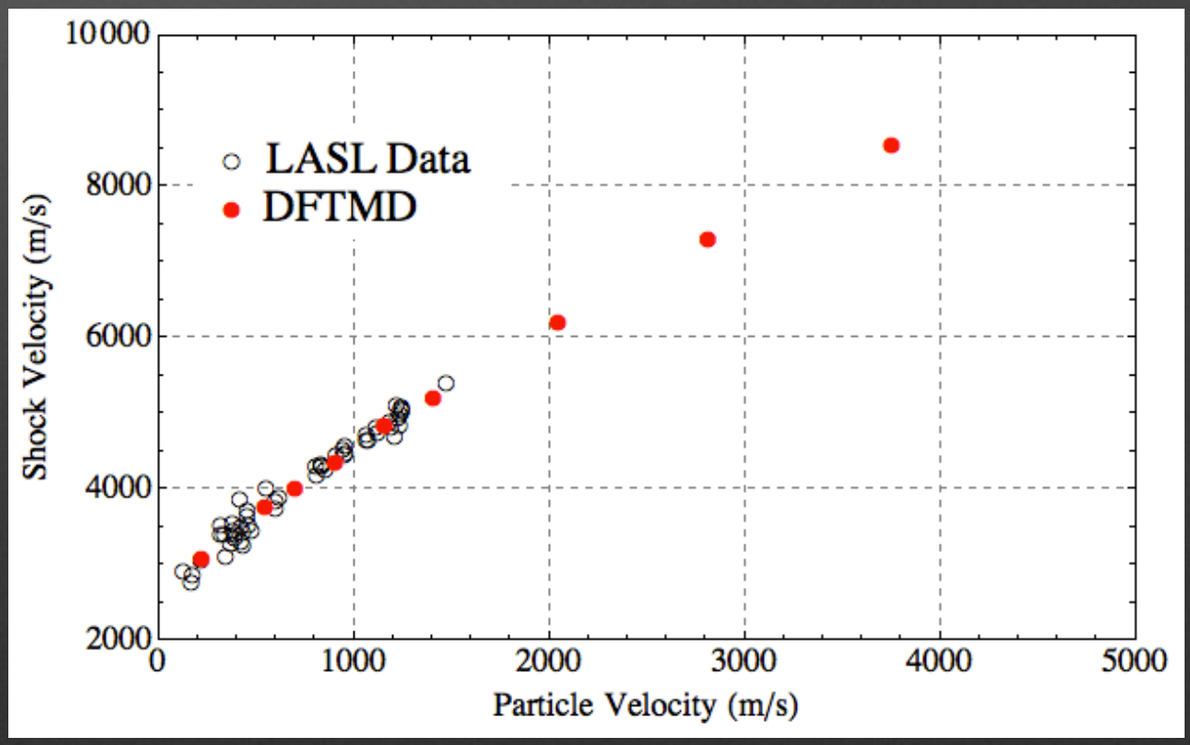


$$\rho_o D = \rho_1 (D - u_1)$$

$$P_1 = \rho_o D u_1$$

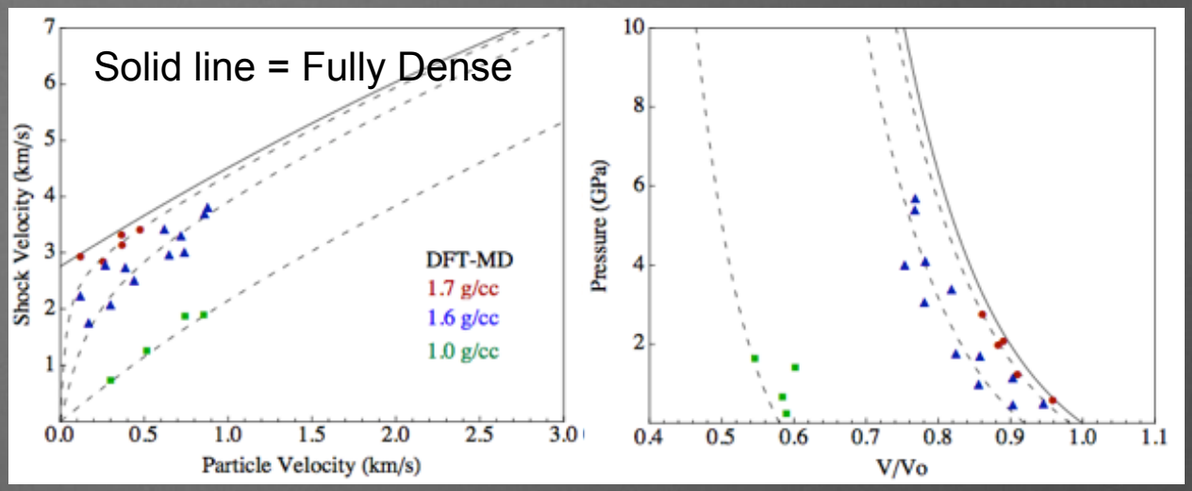
$$E - E_o = \tfrac{1}{2}(P + P_o)(V_o - V)$$

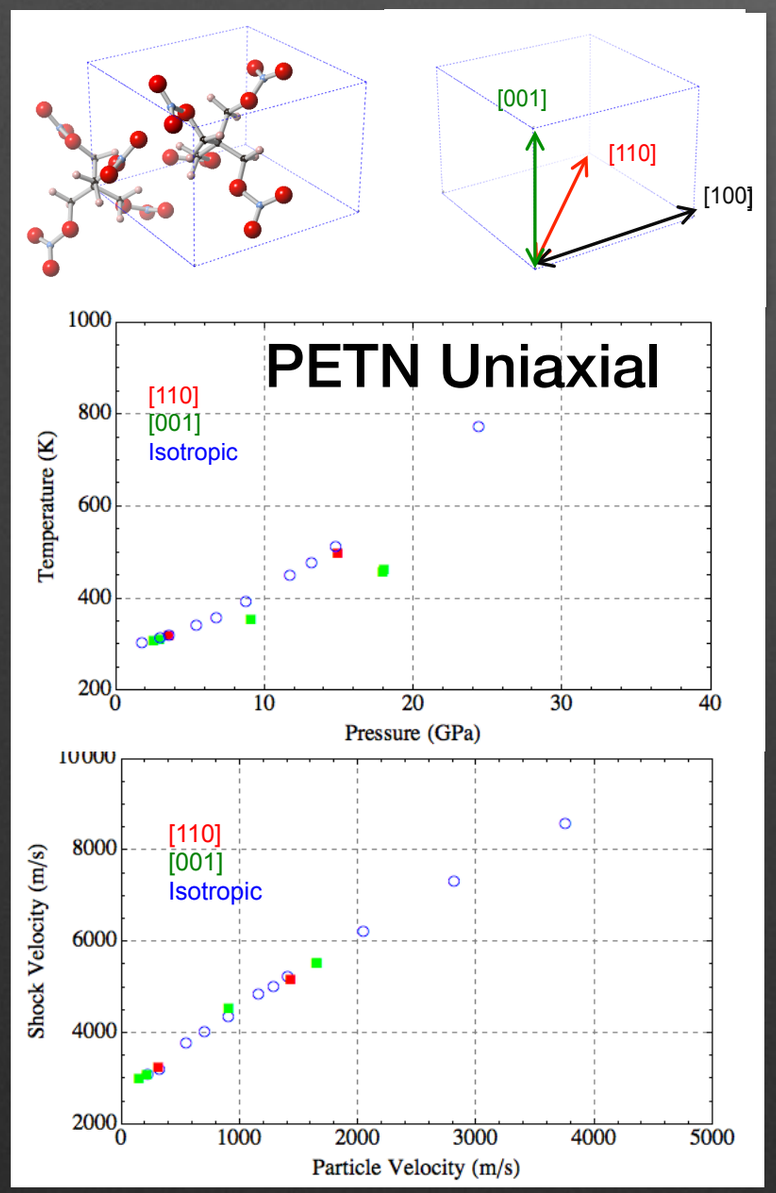


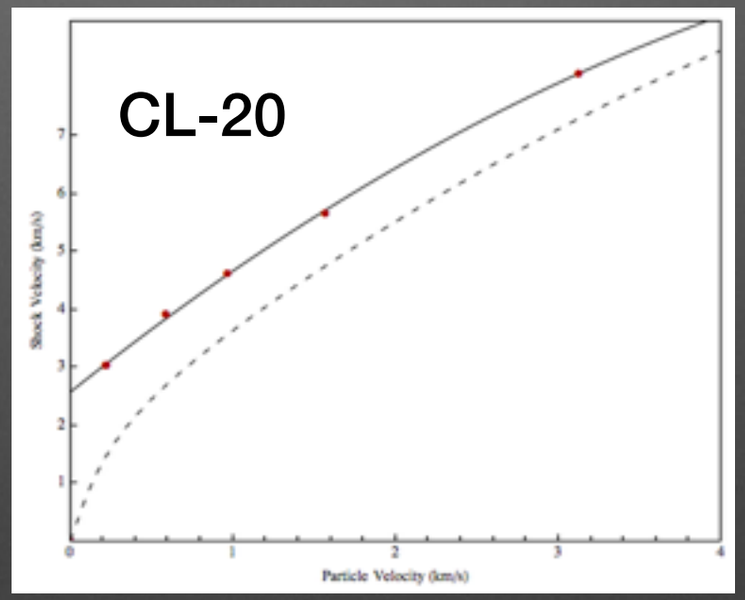


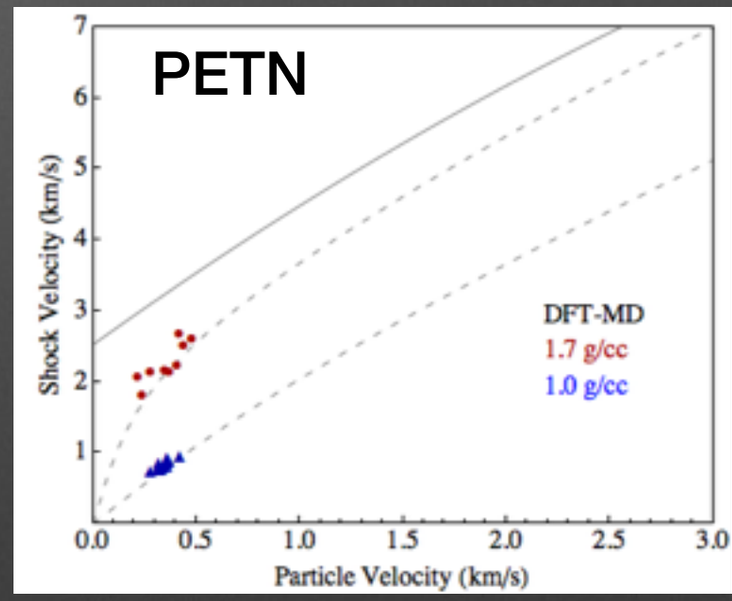
Gobs of Un/partially Published EOS

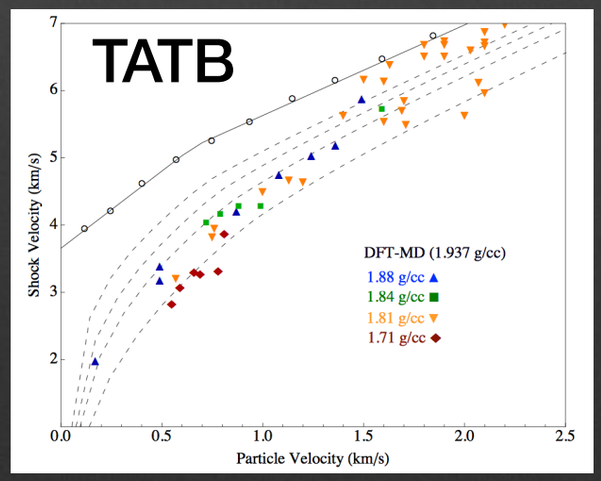
Orientation	Expt.[29]	This work		
	Stress (GPa)	Stress (GPa)	U_s (km/s)	U_p (km/s)
[110]	8.40	12.7	5.0	1.621
[001]	13.3	19.9	6.0	2.118
[100]	31.3	21.1	6.0	2.231

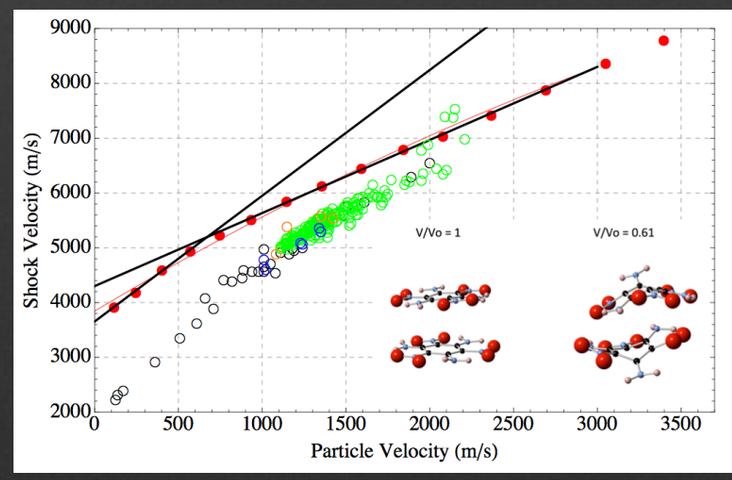












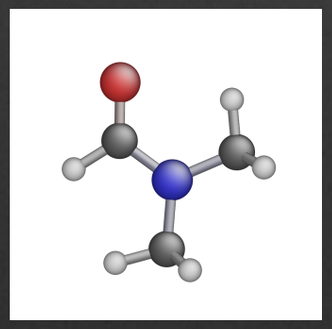
Validation of the DFT-MD Isotherm (HNS)

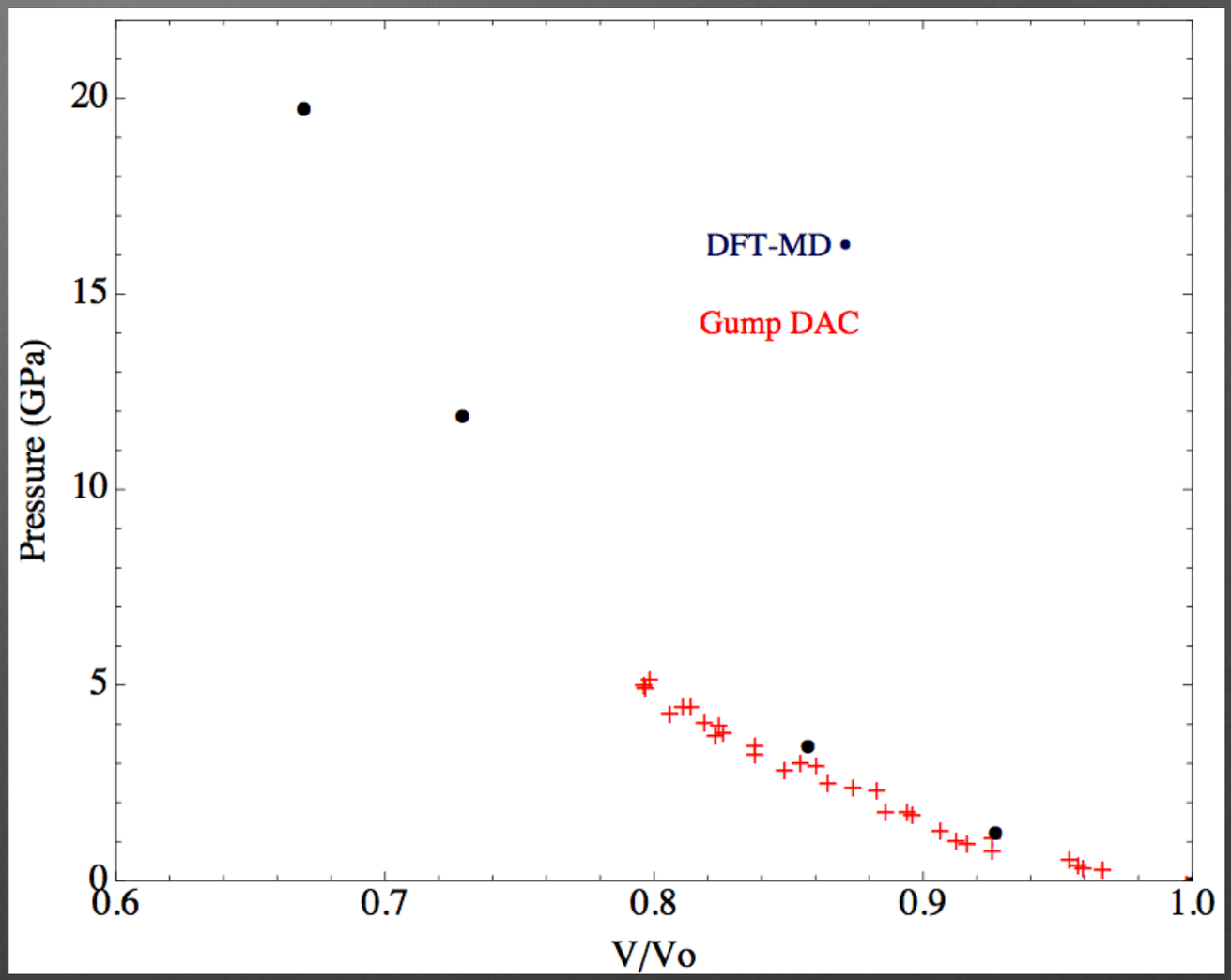
Why am I not right?

It must be the experiment!

- degradation of the sample
- not hydrostatic
- polycrystalline
- defects
- …

Solvent! DMF
Samples are 99.6% HNS





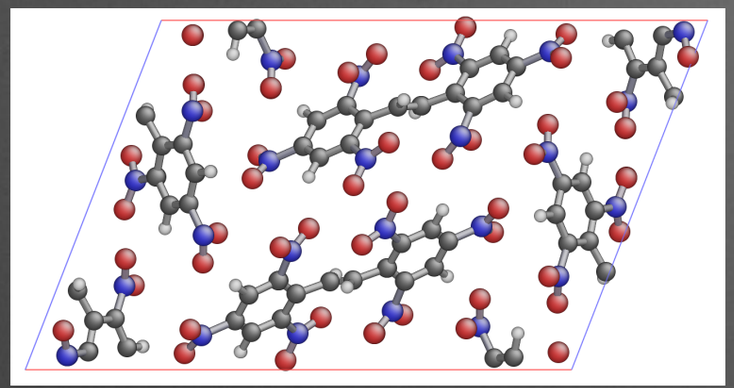
EQUATIONS OF STATE OF HEXANITROSTILBENE (HNS)

Jared C. Gump, Chad A. Stoltz, Brian P. Mason and Emily M. Heim[1]

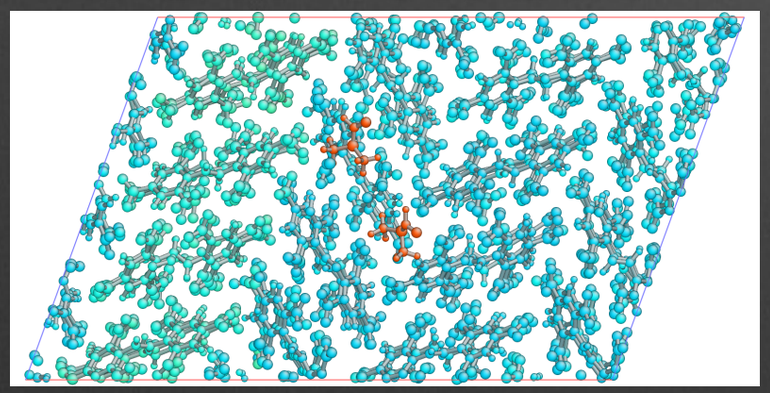
Naval Surface Warfare Center, Indian Head Division, Indian Head, MD 20640
[1]Naval Research Enterprise Intern Program

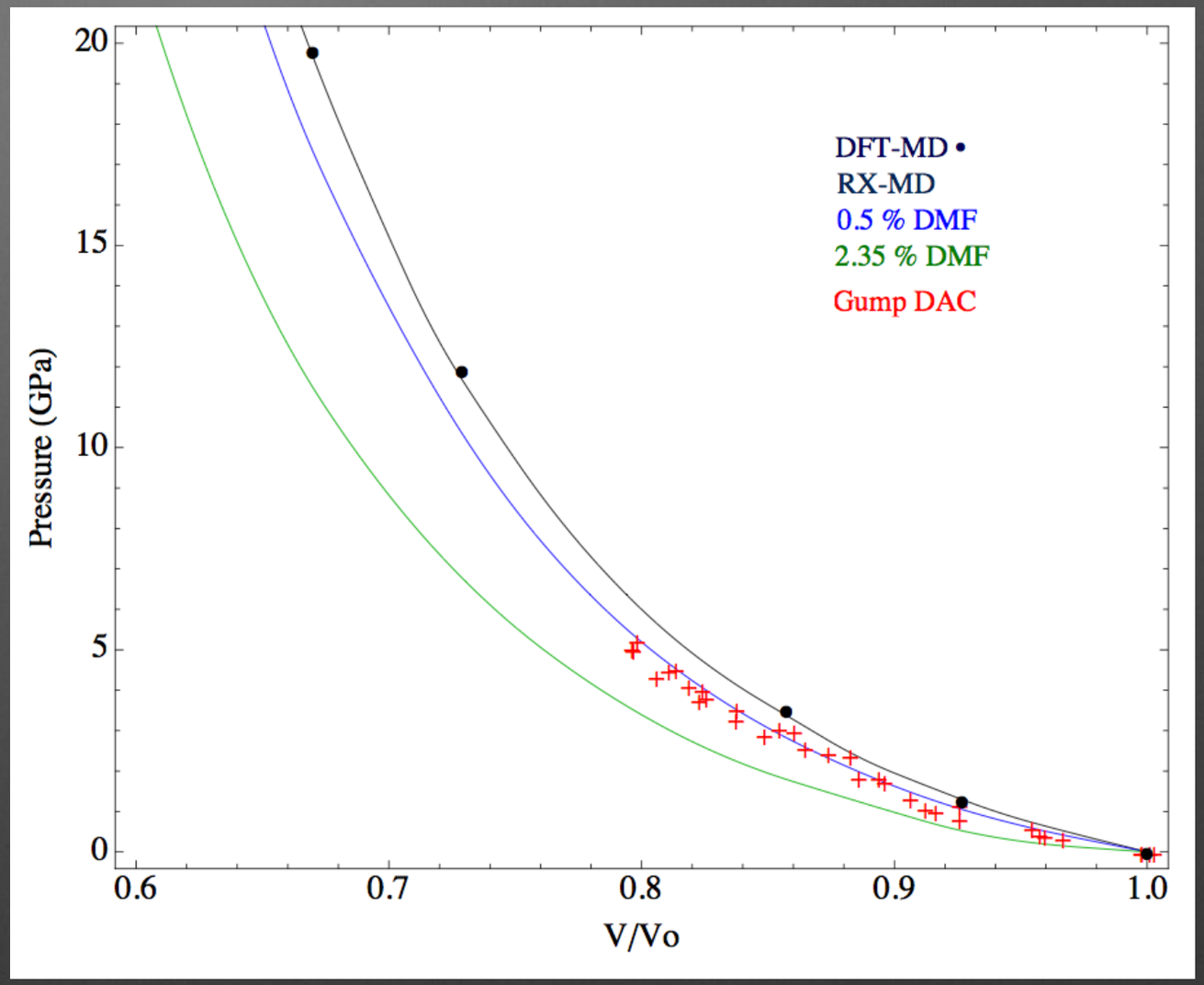
When we account for the solvent, we the calculation matches very well with experiment.

HNS Crystal



HNS w/ ~5% DMF





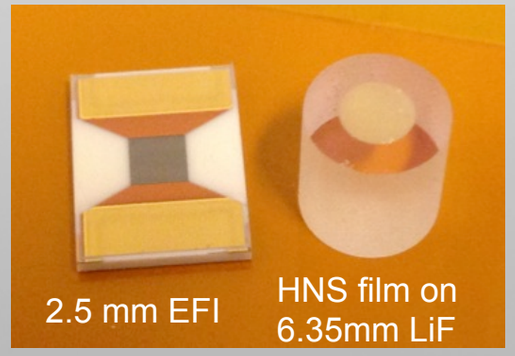
Microstructure: done

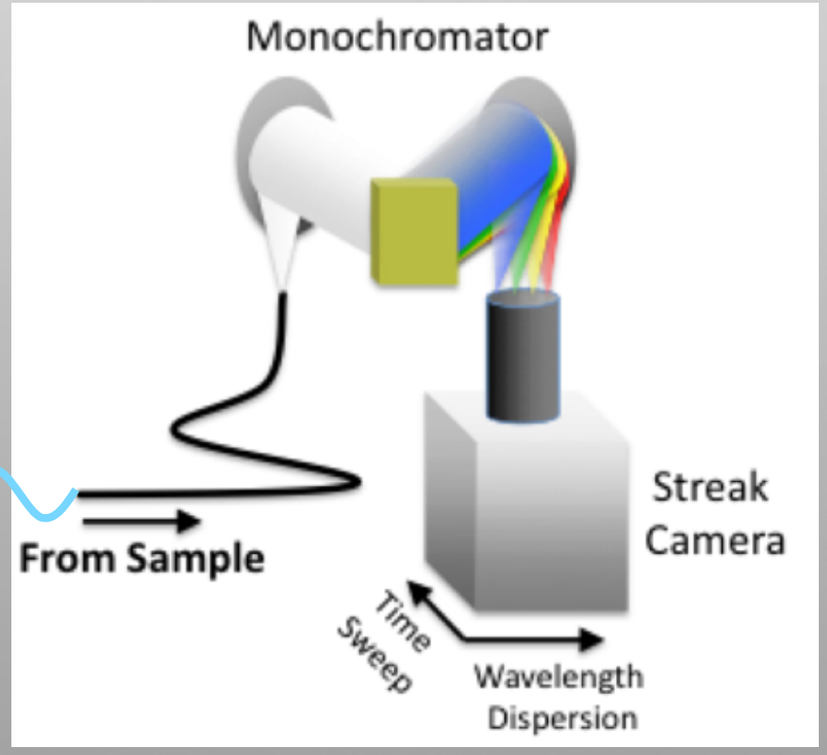
Equation of State: getting there

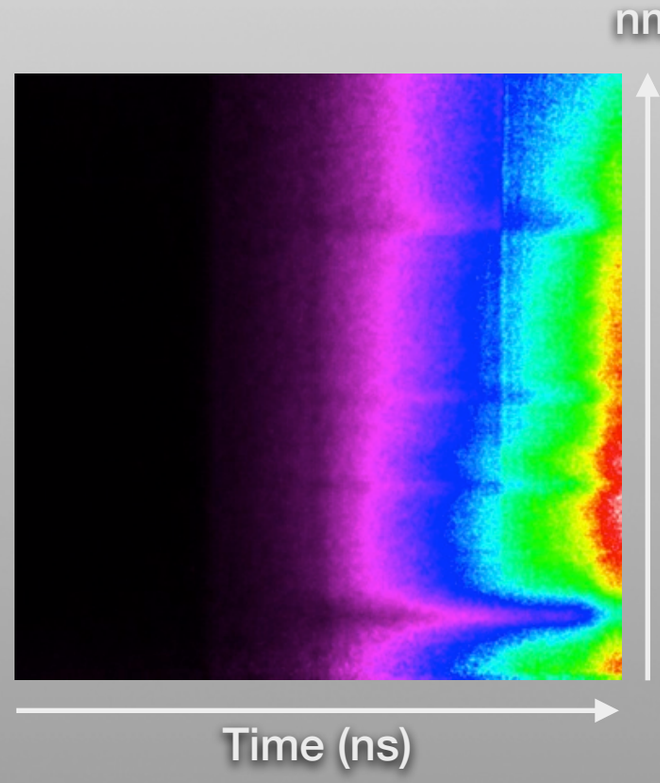
What about chemistry ?

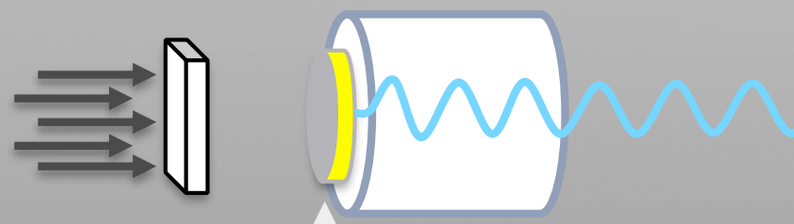
Can we capture emission from evolving intermediates/products?
Streak Spectroscopy: Experimental Configuration

Unique samples, dense explosive films onto optical windows









Flyer
20kV CDU

18-150um
HNS film

LiF Window

Streak Spectroscopy: Preliminary Results

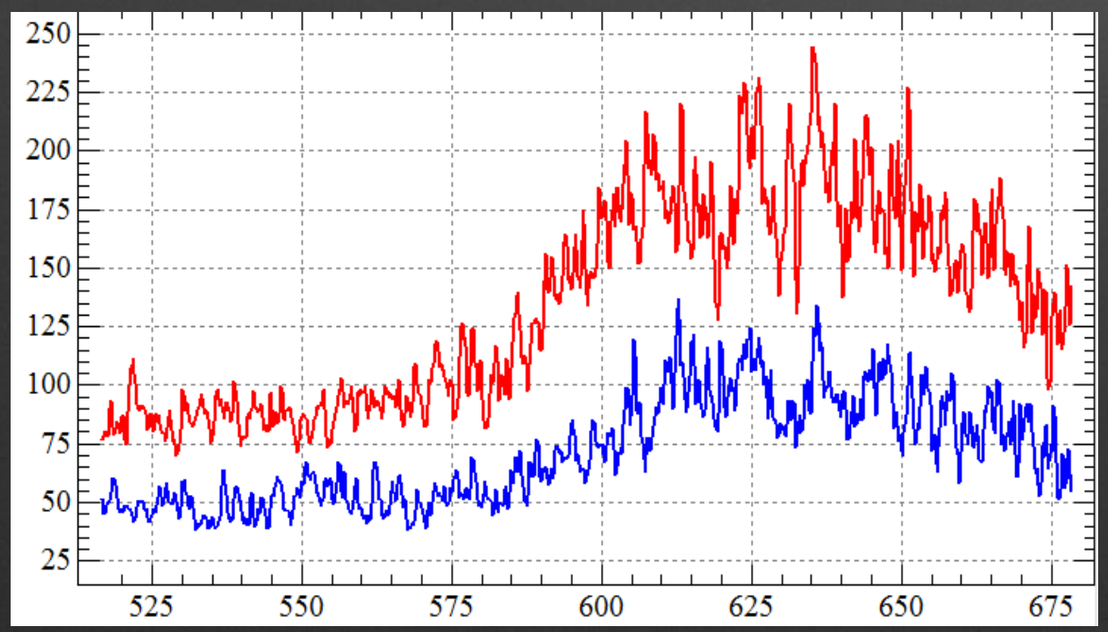
Actual Experiment lasts <60ns

Velocity Map

0 0.5 1 1.5 2 2.5 3

Raw PDV Data

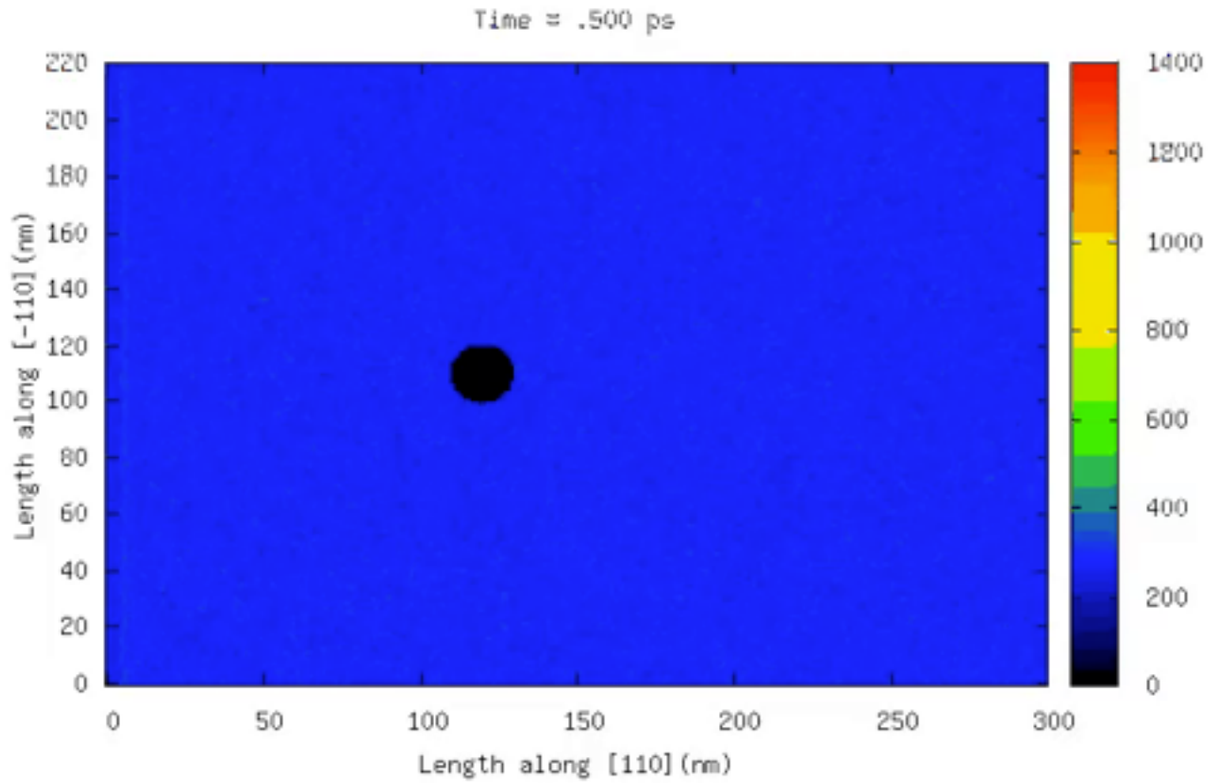
0 500 1000 1500 2000 2500 30



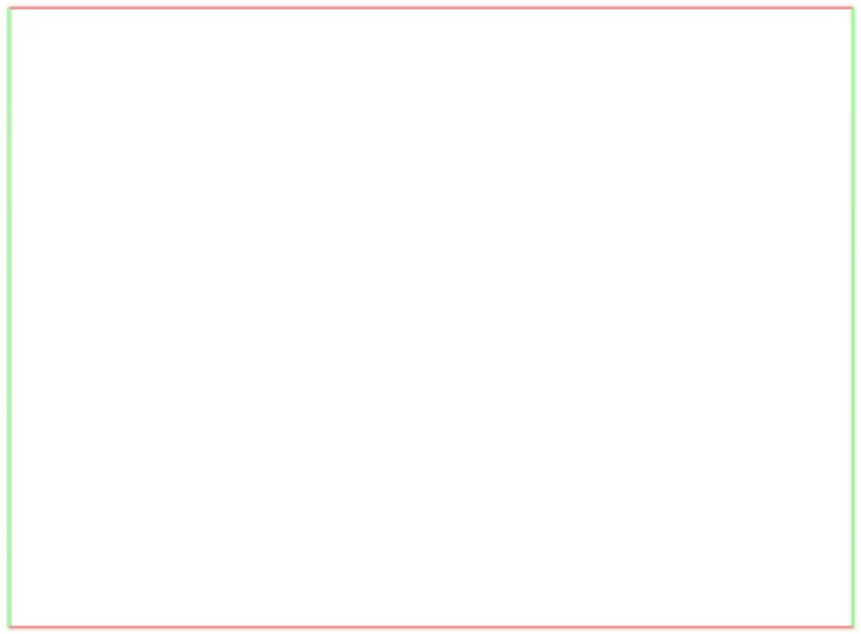
Large-scale Reactive NEMD Simulations

Can we use these to inform material models and chemical models?

Thermal Field



H_2O Formation

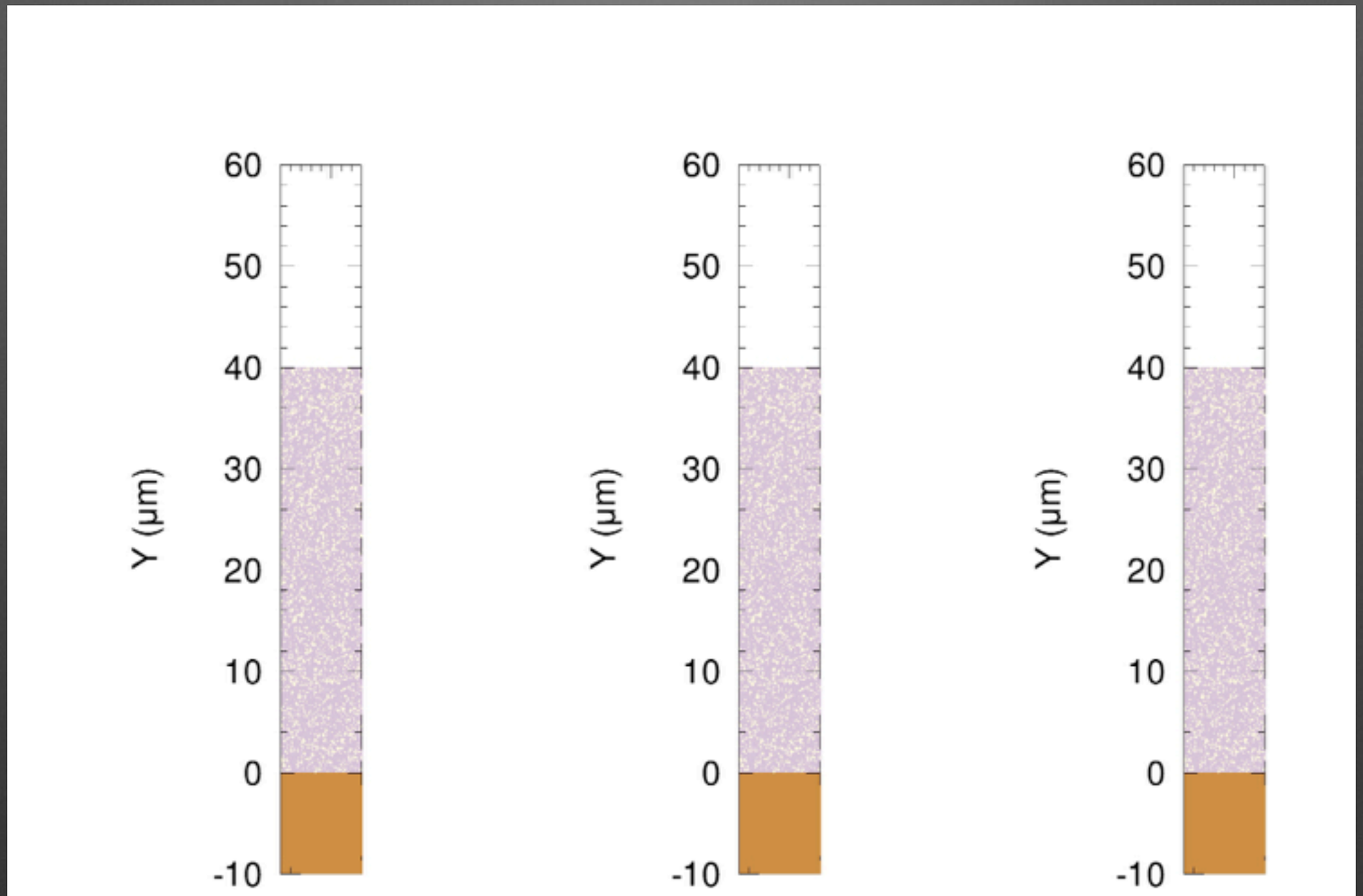


Shock wave in PETN localized at a void.

Up = 1.25 km/s

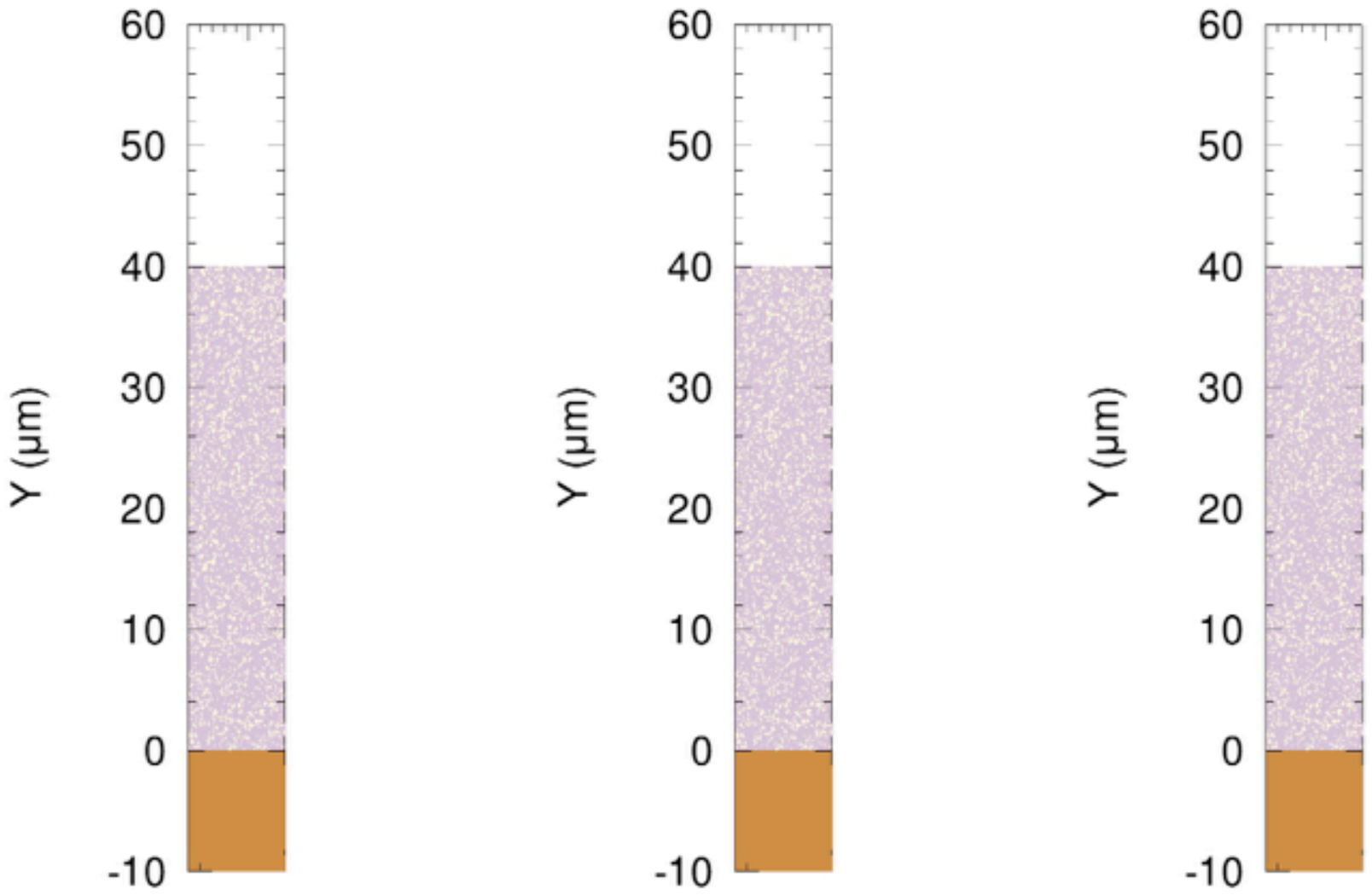
Simulation of successful initiation

HNS, 3100 m/s, Parylene-C flyer



Simulation of successful initiation

HNS, 3200 m/s, Parylene-C flyer

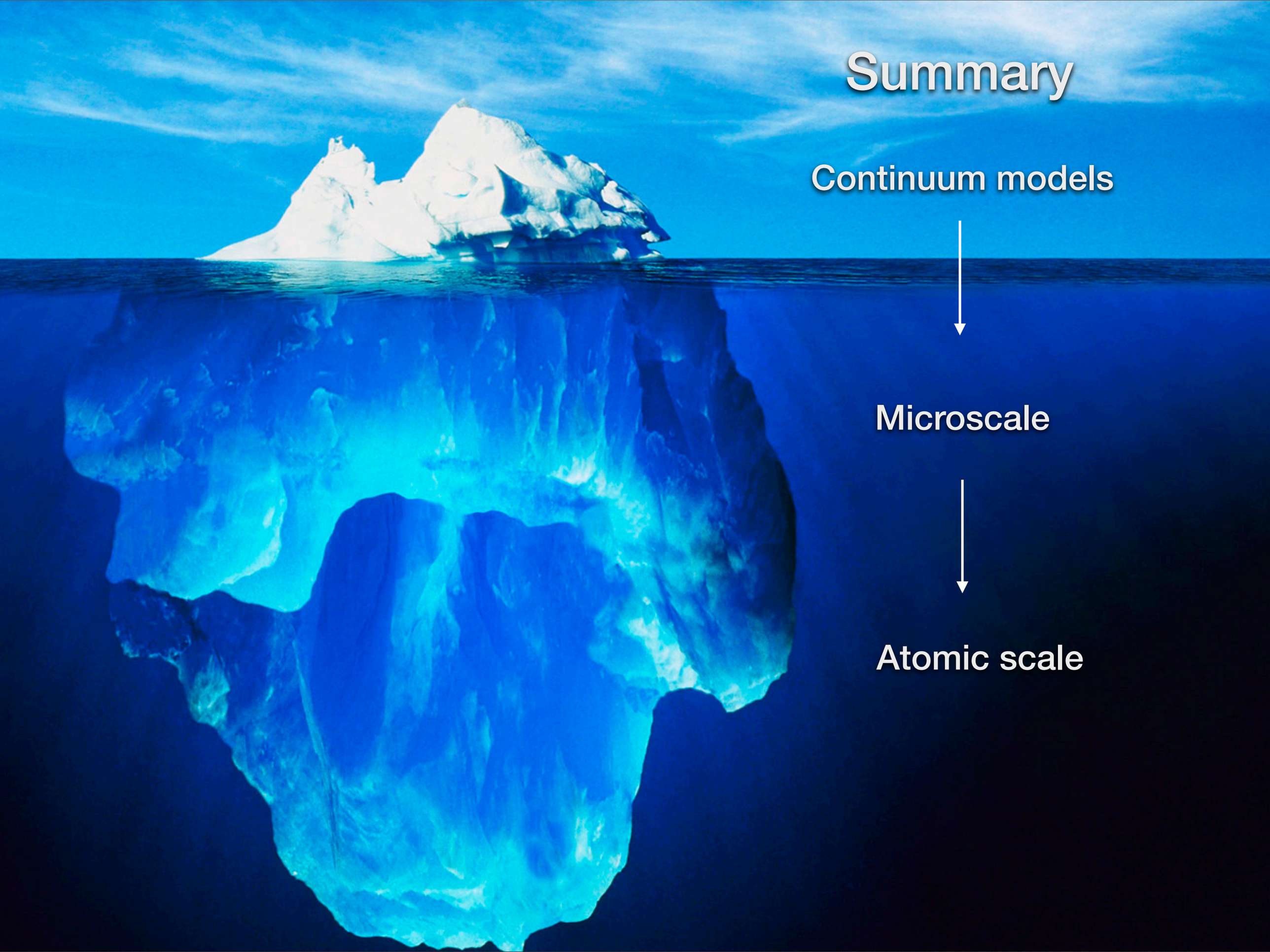


P, T, & Rxn at 0.000000e+00

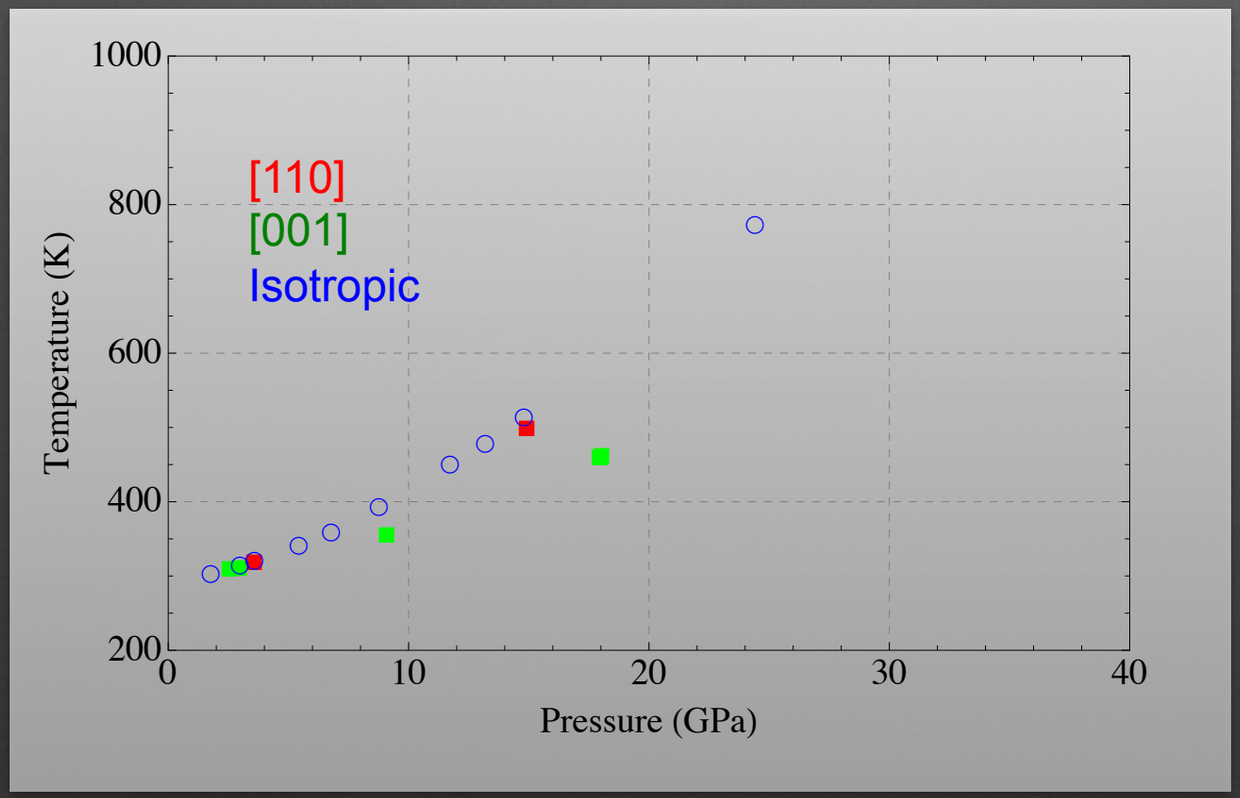
Mile 90 of the HardRock 100 Endurance Run

We've come pretty far. It's looking pretty good.

Sean Cunniff


Summary
Continuum models
Microscale
Atomic scale

Back-up Slides


1000
800
600
400
200
0
10
20
30
40
Temperature (K)
Pressure (GPa)
[110]
[001]
Isotropic

[1] $v U_S = v_0 (U_S - u_P)$ Rankine - Hugoniot Relations

[2] $P v_0 = u_P U_S$

[3] $e - e_0 = \frac{1}{2} P (v_0 - v)$

[4] $U_S = C_0 + S_1 u_P + S_2 u_P^2 \ldots$ Polynomial Fit

[5] $\Gamma = v \left(\frac{(P - P_0)}{(e - e_0)} \right)$ Gruneisan Parameter

Assume solid and porous material have the same refernce, $P_0 = P_0^* = 0$ and $e_0 = e_0^*$

[6] $P = \frac{\Gamma}{v} (e - e_0)$ (Solid) $P^* = \frac{\Gamma}{v} (e^* - e_0)$ (Porous*)

[7] $P - P^* = \frac{\Gamma}{v} (e - e^*)$ The two pressures can be related at any shock state, v

[8] $P - P^* = \frac{\Gamma}{v} \left(\frac{1}{2} P (v_0 - v) - \frac{1}{2} P^* (v_0^* - v) \right)$ by substituting [3] into [7]

[9] $P^* = P \frac{v_0 - v - \frac{2v}{\Gamma}}{v_0^* - v - \frac{2v}{\Gamma}}$ Where Gamma can be constant or dependent on density $\Gamma = \frac{\Gamma_0 \rho_0}{\rho}$

[10] $u_P^* = \frac{U_S^* (v_0^* - v)}{v_0^*}$ by solving [1] for particle velocity

[11] $U_S^* = v_0^* \sqrt{\frac{P^*}{(v_0^* - v)}}$ by substituting [10] into [2]

This does not depend on microstructure, only depends on initial density (... and purity)