



Micro-structural Effects on the Ignition Behavior of Various HMX Materials

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Minding the Gap between the Continuum and Mesoscale



Air Force Research Laboratory
Integrity ★ Service ★ Excellence

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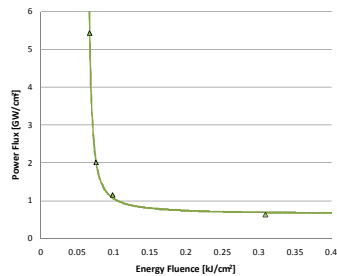


Objective & Background



- **Objectives:** Assess the utility of using an ignition model based upon James' work as a tool to quantify effects of bed microstructure on ignition behavior. Quantify bed microstructures and ignition behavior to assist in the future validation of modeling and simulation efforts focused on understanding mesoscale effects on reactive systems

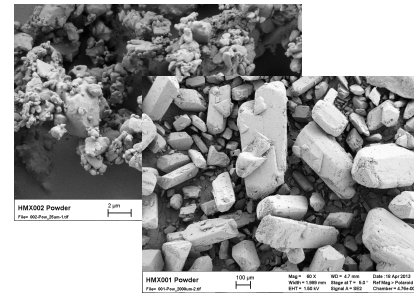
Measured Ignition Behavior



James Phenomenological Ignition Model

$$\frac{E_c}{E} + \frac{\Sigma_c}{\Sigma} = 1$$

Do Ignition Parameters Strongly Correlate to Measurable Bed Structures?



$$E_c \stackrel{?}{=} E_c(d, L, \dots)$$

$$\Sigma_c \stackrel{?}{=} \Sigma_c(d, L, \dots)$$

L & S = bed microstructure parameters

Can we incorporate this information into future AND conventional models?

$$\frac{d\lambda}{dt} = I(1 - \lambda)^b \left(\frac{\rho}{\rho_0} - 1 - a \right)^x + G_1(1 - \lambda)^{c_1} P^y + G_2(1 - \lambda)^{c_2} P^z$$

$$\frac{\rho}{\rho_0} - a = 1 = \frac{E_c(d, L)}{E} + \frac{\Sigma_c(d, L)}{\Sigma}$$

"a" correlates to Σ_c

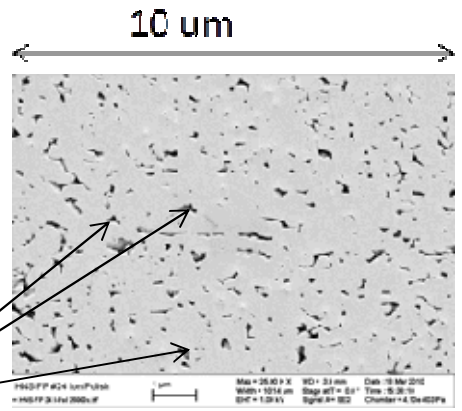
- We have studied the *ignition* behavior of HMX materials ranging from smaller size particle class 5 material to a coarser class 3 material as a means to answer these questions
 - Subsequent studies will assess effects on growth to completion



Shock to Detonation Phenomena: Ignition followed by Growth to Completion

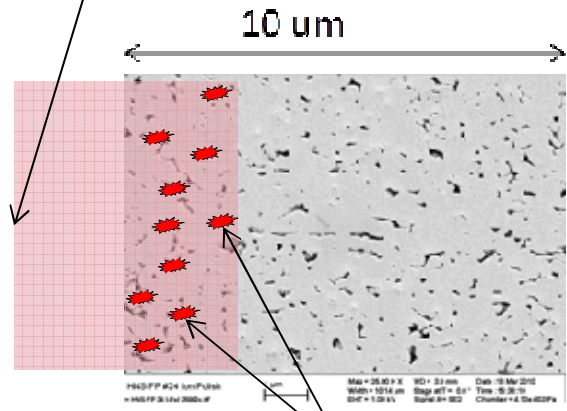


Packed Granular Bed



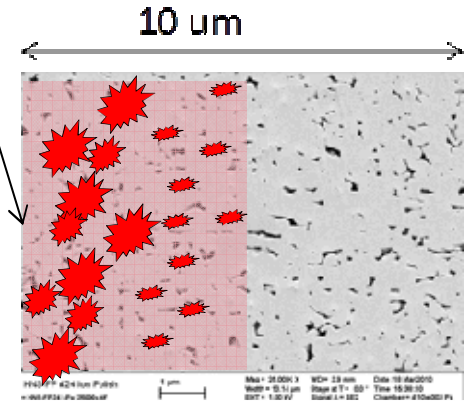
Bulk Powder

Rear of Shock Wave
Relieves pressure and
temperature which can
quench reactions



- Energy localizations raise temperatures resulting in reaction
- Pore sites are primary bed structure we initially seek to correlate to “hot spots”

Simple picture but underlying question is how to properly describe ignition and then quantify effects of microstructure



- Shock supports the growth of reaction site such that they coalesce constructively for the case of a successful ignition event
- For a failed ignition the shock relief drops the temperatures locally and quenches reactions

Approaching Shock of finite width & amplitude

Voids & Interfaces are potential energy localization sites



Phenomenological Ignition Model



- Cooper¹ described ignition processes as hyperbolic functions
 - Described ignition process for stab and hotwire igniters
 - Those efforts utilized Power vs. Energy relationships
- James² defined a criterion that correlates ignition to Energy Flux and Specific Kinetic Energy as a hyperbolic function for shock phenomena
 - Captured ignition data previously inconsistent with the Walker-Wasley
- Welle³ defined a modified ignition relationship
 - Exponential form
 - Utilizes shock power flux versus energy fluence
 - Incorporates a third constant that affects the rate at which the hyperbolic functions transitions from an power to energy flux limited condition

Modified Ignition Relationship

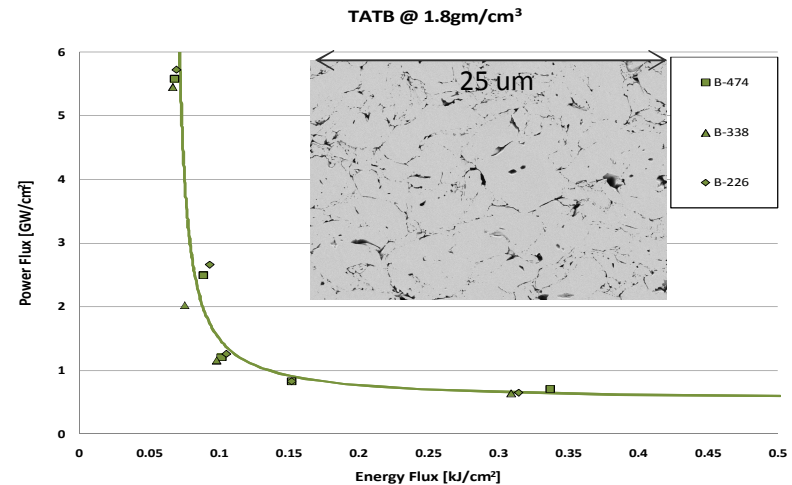
Ignition Relationship

$$E_f = E_c \cdot \exp\left(\frac{-\Pi_a}{\Pi_c - \Pi}\right)$$

Supporting Relationship

$$\Pi = P U_p$$

$$E = P U_p \tau$$



1. Cooper, P.W., *Explosives Engineering*, Wiley-VCH, Inc., pp. 325-345 (1996)
2. James, H.R., *An Extension to the Critical Energy Criterion Used to Predict Shock Initiation Thresholds*, Propellants, Explosives, Pyrotechnics. 21: 8-13 (1996).
3. Welle, E.J., Breaux, B.A., Thorn, C.S., Wixom, R.R and Dudley, E.C., *Ignition Studies and Understanding the Large Scale Gap Test*, Hugh James Initiation Workshop, (October, 2011)

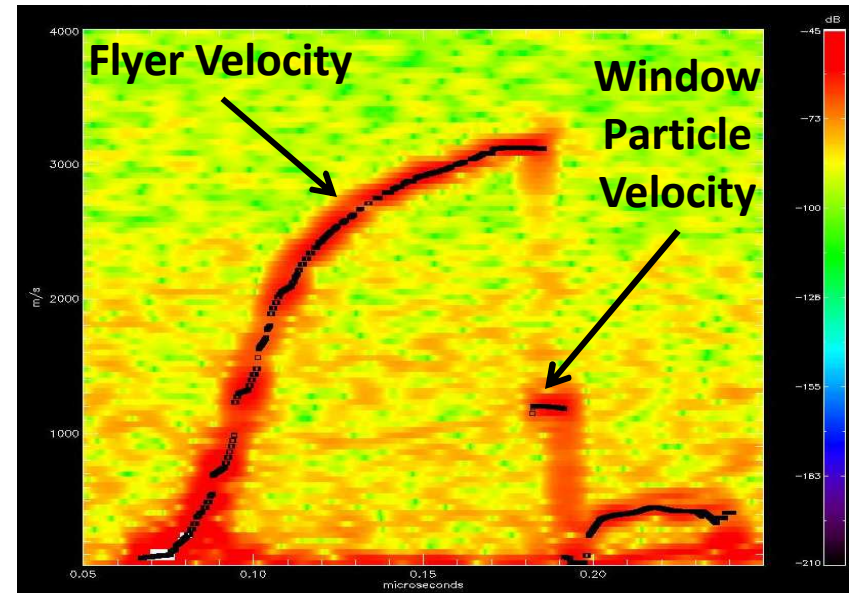


Ignition Model Data Sets



- Data sets that allow for the parameterization of the Hugh James Ignition model
 - Threshold testing to determine mean firing conditions using E-gun
- 10kV E-Gun
 - Equivalent series $R=75\text{m}\Omega$, $L=65\text{nH}$ and $0.9\ \mu\text{F}$
- Bridge & Flyers
 - 3.8 mm Square
 - 30 and 53 μm thick Parylene-C flyers
 - 127 and 203 μm thick polyimide flyers
- Velocity measurements of the flyers at those conditions
 - Photonic Doppler Velocimetry

Flyer Velocity at Mean Fire



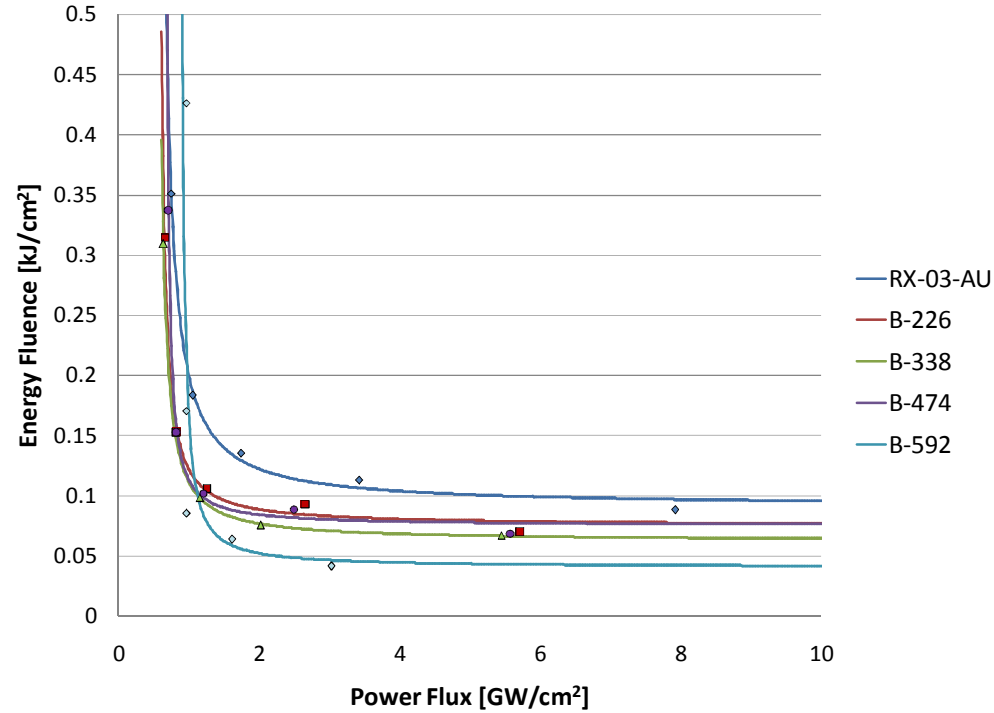


Historical Data: TATB Thin Pulse Ignition Studies



- TATB materials evaluated at 1.8gm/cm^3
 - Data harvested from 7th Intl. Det. Symp.¹
- Variations in Π more significant than E

Material	Surface Area m^2/gm	Particle Size Arithmetic Mean μm
B-592	4.323	9
RX-03-AU	0.539	58
B-474	0.513	17
B-338	0.43	21
B-226	0.539	58



¹Honodel, C.A., Humphrey, J.R., Weingart, R.C., Lee, R.S. and Kramer, P., Shock Initiation of TATB Formulations, Proceedings of the 7th Symposium (International) on Detonation, pp. 425-434, Annapolis, MD, (June 1981).

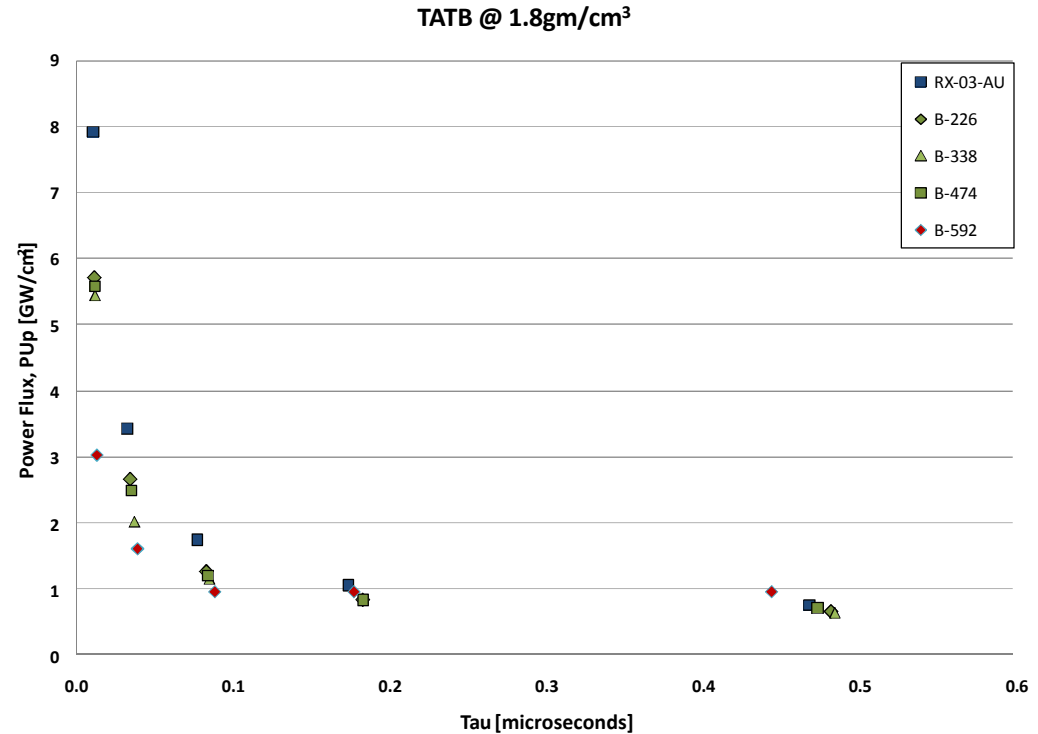
Material	Π @ $E=0.4\text{kJ/cm}^2$ GW/cm^2	E @ $\Pi=7.0\text{GW/cm}^2$ kJ/cm^2	Π % Diff	E % Diff
RX-03-AU	0.71700	0.0979	18	130
B-226	0.62580	0.0780	3	84
B-338	0.60899	0.0655	0	54
B-474	0.69860	0.0769	15	81
B-592	0.91425	0.0425	50	0



Trigger Condition



- Analyzed trigger term, Π_c , for constant spot sizes as a function of material lot
 - Π_c does not seem to be strongly affected by lot but instead by material
 - Chemical/reaction behavior (activation energy/critical temperatures) of material dominate behavior for a fixed spot size



Material	Π @ E=0.4kJ/cm ² GW/cm ²	E @ Π =7.0GW/cm ² kJ/cm ²	Π % Diff	E % Diff
RX-03-AU	0.71700	0.0979	18	130
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Ignition Phenomena Hypothesis

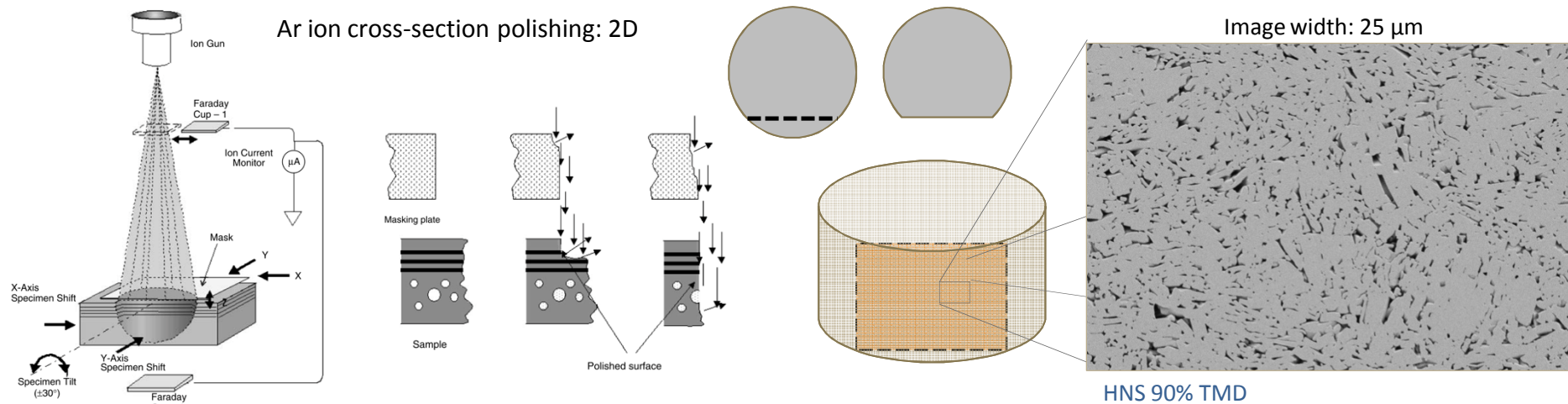
Effect of Microstructure



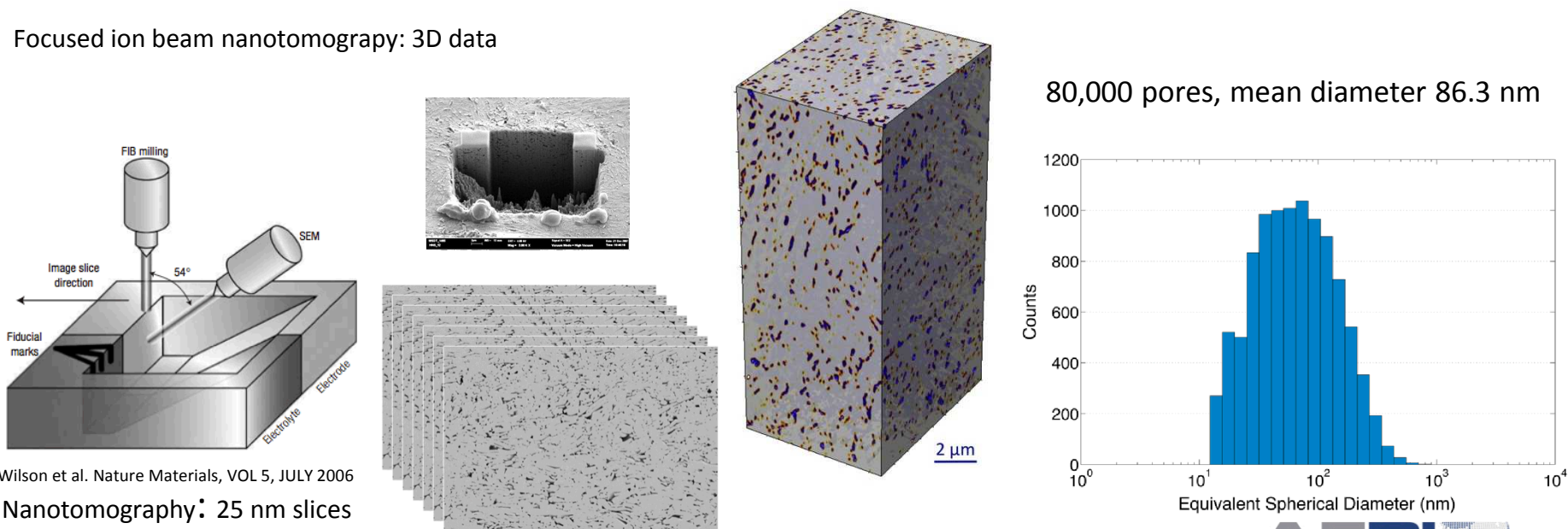
- What is controlling the ignition process?
 - Trigger condition, Π_c
 - Primarily controlled by material
 - Growth to successful ignition, $E_c = PU_p\tau$
 - Controlled by material and microstructure
 - Microstructure leads to critical hot spots
 - Temperature (Π_c) & Time ($E_c = PU_p\tau$): Critical temperatures must be established to trigger reaction and those reactions must be sustained long enough for ignition wavelets to effectively coalesce into a successful ignition wave
- Several lots of HMX were chose due to their wildly different bulk powder particle sizes in an attempt to generate significantly different microstructures



Characterizing Microstructure via Ion Cross-sectioning Techniques



Focused ion beam nanotomography: 3D data



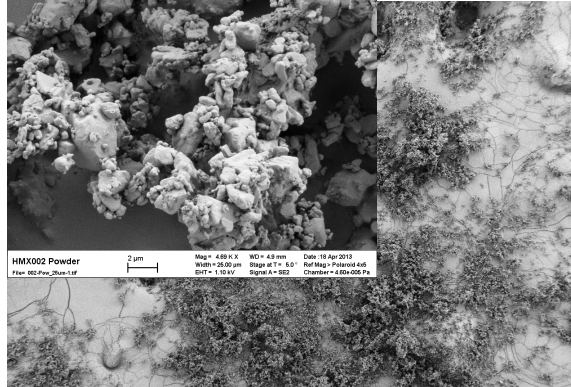
Wilson et al. Nature Materials, VOL 5, JULY 2006
Nanotomography: 25 nm slices



HMX Powders



HMX001 Powder
 File= 001-Pow_2000um-2.tif
 100 µm
 Mag = 60 X WD = 4.7 mm Date :18 Apr 2013
 Width = 1.989 mm Stage at T = 5.0 ° Ref Mag > Polaroid 4x5
 EHT = 1.50 kV Signal A = SE2 Chamber = 4.76e-005 Pa



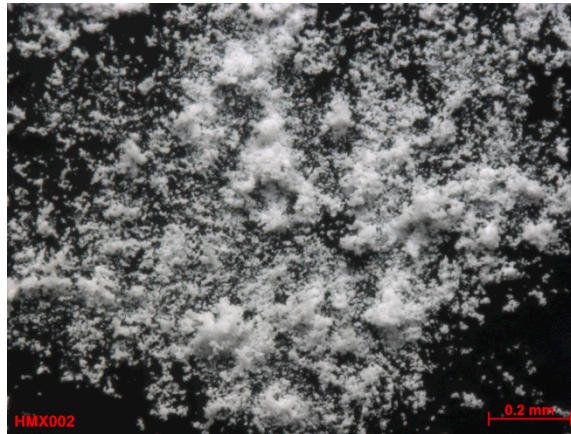
HMX002 Powder
 File= 002-Pow_2000um-1.tif
 2 µm
 Mag = 488 X WD = 4.8 mm Date :18 Apr 2013
 Width = 25.00 µm Stage at T = 5.0 ° Ref Mag > Polaroid 4x5
 EHT = 1.50 kV Signal A = SE2 Chamber = 4.68e-005 Pa



HMX003 Powder
 File= 003-Pow_2000um-2.tif
 100 µm
 Mag = 69 X WD = 4.5 mm Date :18 Apr 2013
 Width = 2.023 mm Stage at T = 5.0 ° Ref Mag > Polaroid 4x5
 EHT = 1.50 kV Signal A = SE2 Chamber = 4.68e-005 Pa



HMX001 0.2 mm



HMX002 0.2 mm



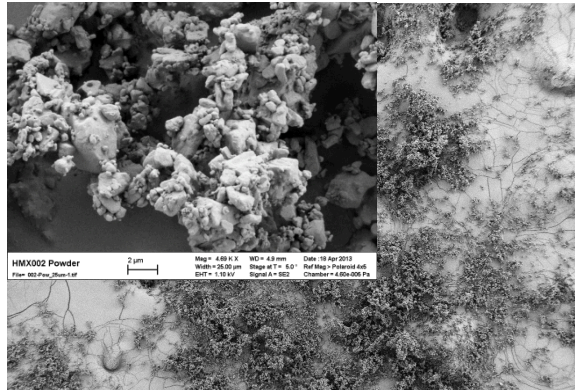
HMX003 0.2 mm



HMX Microstructures



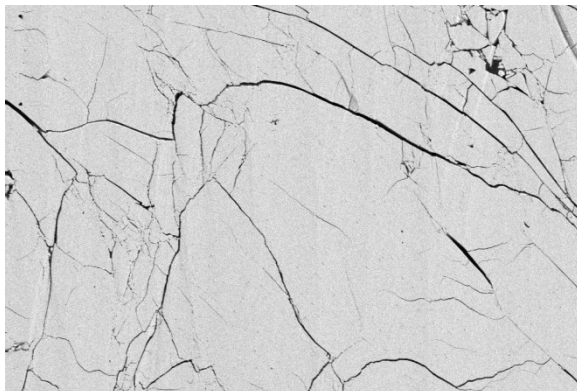
HMX001 Powder
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 100 µm
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 Width = 1.989 mm Stage at T = 5.0 ° Ref Mag > Polaroid 4x5
 EHT = 1.50 kV Signal A = SE2 Chamber = 4.76e-005 Pa



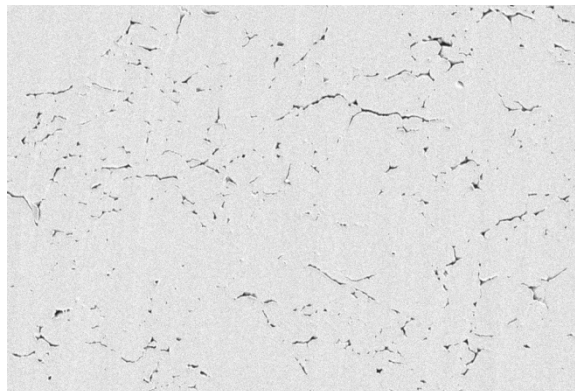
HMX002 Powder
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 2 µm
 Mag = 458 X X WD = 4.8 mm Date :18 Apr 2013
 Width = 25.00 µm Stage at T = 5.0 ° Ref Mag > Polaroid 4x5
 EHT = 1.50 kV Signal A = SE2 Chamber = 4.68e-005 Pa



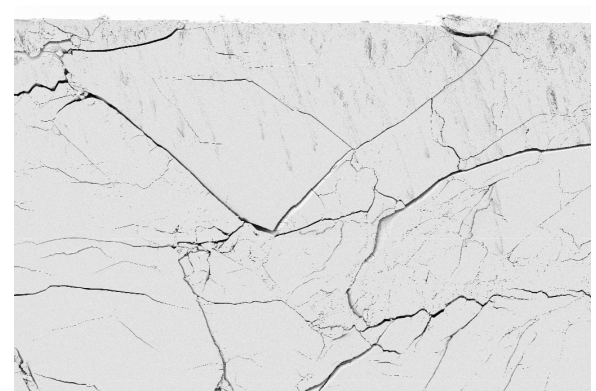
HMX003 Powder
 File= 003-Pow_2000um-2.tif
 100 µm
 Mag = 69 X WD = 4.5 mm Date :18 Apr 2013
 Width = 2.023 mm Stage at T = 5.0 ° Ref Mag > Polaroid 4x5
 EHT = 1.50 kV Signal A = SE2 Chamber = 4.68e-005 Pa



HMX01-IP5
 File= HMX01-IP2_03.tif
 10 µm
 Mag = 1.17 K X WD = 3.9 mm Date :14 Jun 2013
 Width = 59.94 µm Stage at T = 0.0 ° Ref Mag > Polaroid 4x5
 EHT = 1.50 kV Signal A = SE2 Chamber = 7.17e-005 Pa



HMX02-IP6
 File= HMX02-IP6_22.tif
 1 µm
 Mag = 7.82 K X WD = 3.9 mm Date :14 Jun 2013
 Width = 16.00 µm Stage at T = 0.0 ° Ref Mag > Polaroid 4x5
 EHT = 1.50 kV Signal A = SE2 Chamber = 7.84e-005 Pa



HMX003-3 IP 3kV-9hrs
 File= 003-IP2_100um-1.tif
 10 µm
 Mag = 1.17 K X WD = 2.9 mm Date :17 May 2013
 Width = 100.0 µm Stage at T = 0.3 ° Ref Mag > Polaroid 4x5
 EHT = 1.10 kV Signal A = SE2 Chamber = 3.49e-005 Pa

Note scale: Image width 15um



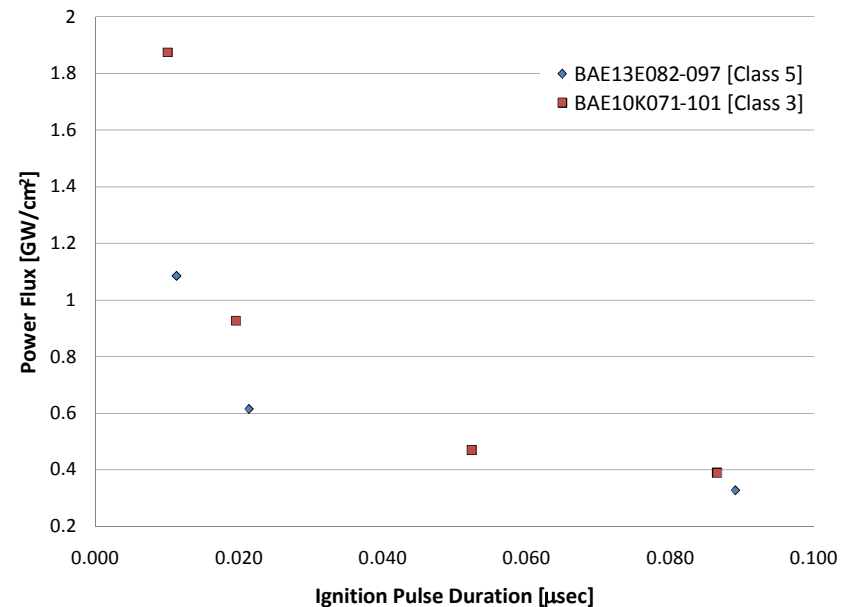
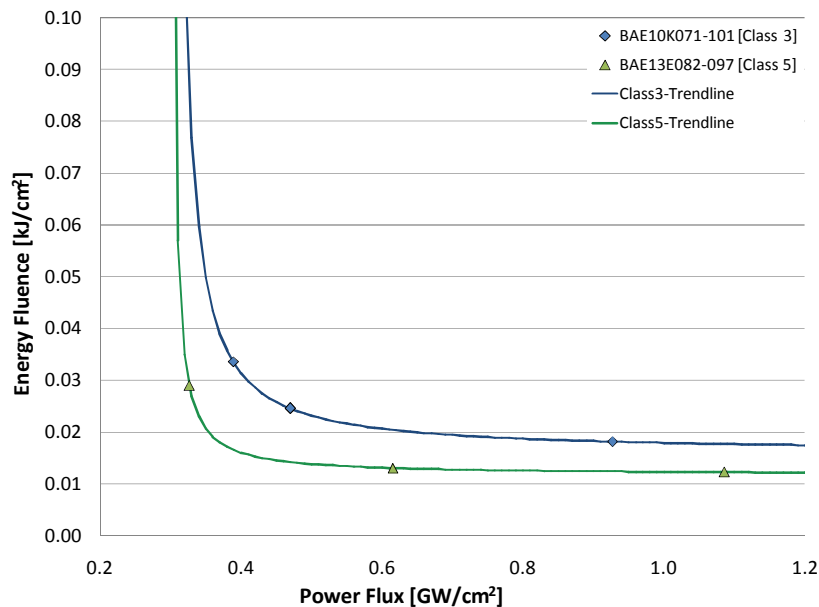


HMX Ignition Results



- Fit hyperbolic functions
- Ignition Pulse
 - $\delta T \approx 10 \rightarrow 90$ ns
 - $\delta x \approx 57 \rightarrow 410$ μm

- As with TATB data, Π_c does not seem to be strongly affected by lot but instead by material





Shock to Detonation Phenomena Revisited

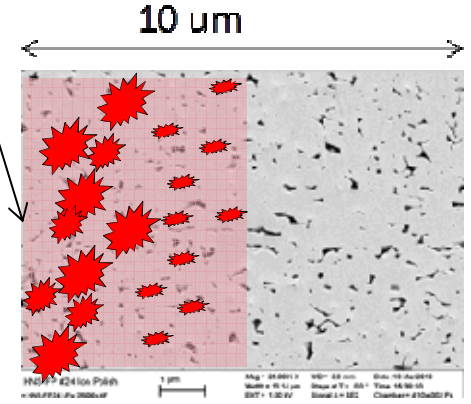
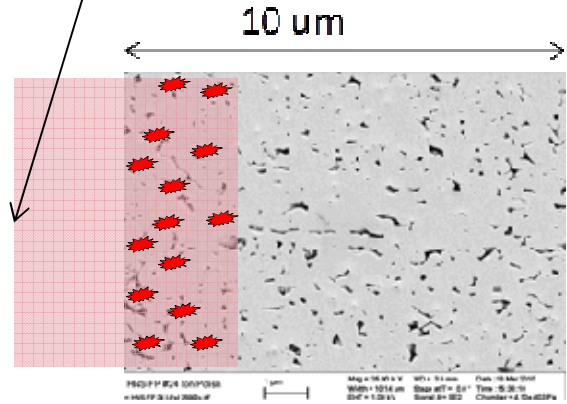
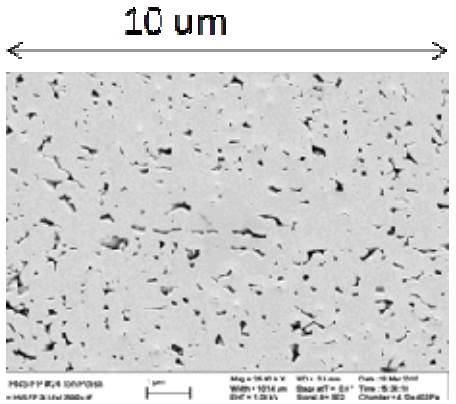


Packed Granular Bed

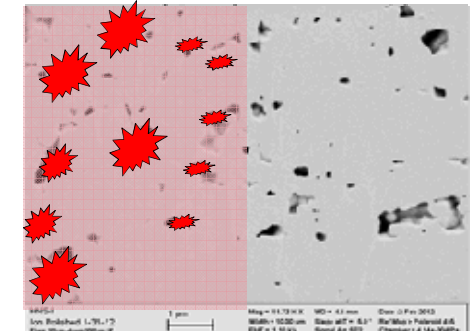
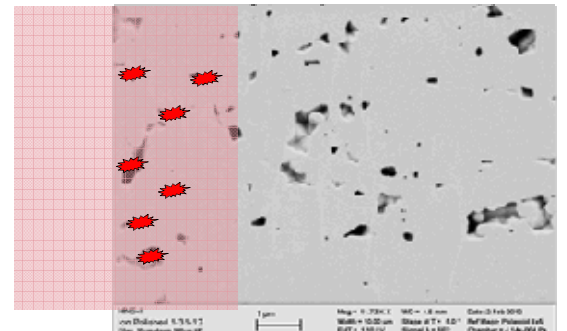
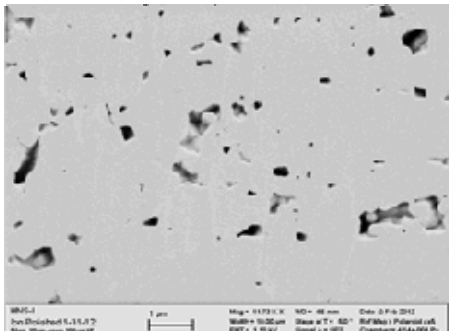
Rear of Shock Wave
Relieves pressure and
temperature which can
quench reactions

Due to bed structure, there are *few and farther apart localization sites* that require *shock pulse to be thicker in thin pulse regime* → $E_c \uparrow$

Approaching
Shock of finite
width &
amplitude



Approaching
Shock of finite
width &
amplitude





Summary



- Current data sets suggest Π_c is less sensitive to bed microstructures than E_c
- Initial micro-structural characterization results indicate that smallest E_c is present for material with smaller and more closely spaced pores
 - More thorough analysis of bed structures may produce better correlations between continuum ignition parameters and specific features of bed microstructure



Summary



- Current data sets suggest Π_c is less sensitive to bed microstructures than E_c
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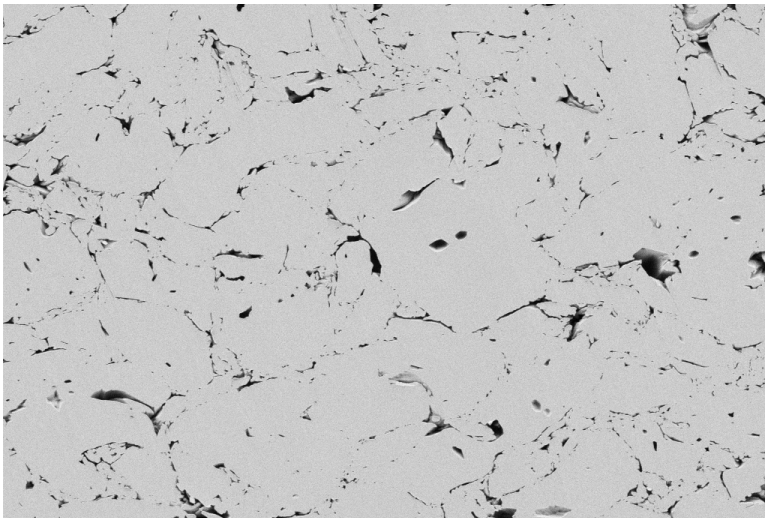


Questions?

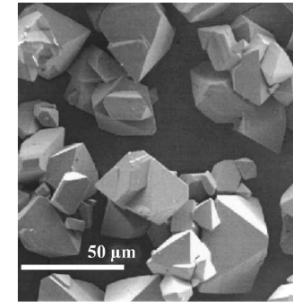




Extras



TATB den=1.8	1 μ m	Mag = 4.69 K X	WD = 3.4 mm	Date : 11 Oct 2012
File= 60down-25um-1.tif		Width = 25.00 μ m	Stage at T = 5.0 °	Ref Mag > Polaroid 4x5
		EHT = 1.20 kV	Signal A = SE2	Chamber = 1.93e-004 Pa



a) Detonator Grade HMX