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Effects of Microstructure and Binder on the Shock-to-Detonation Behavior of Hexanitrostilbene (HNS)

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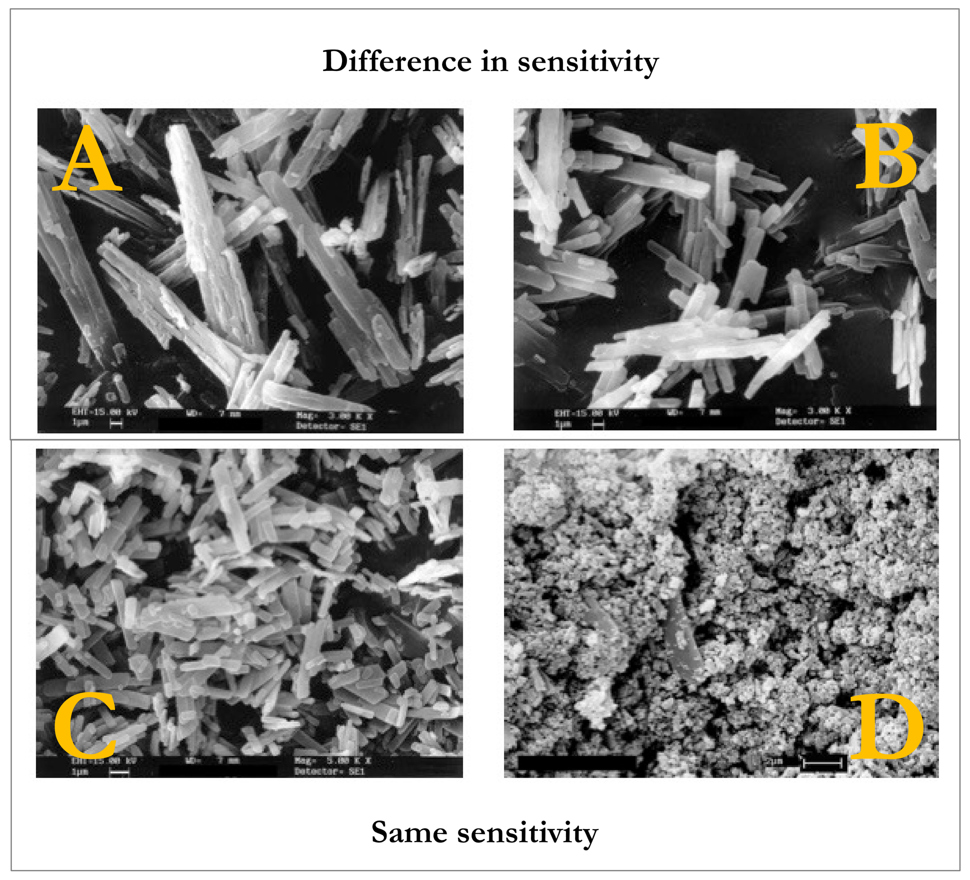
EXPLOSIVE TECHNOLOGIES GROUP 7550

Motivation

Specification and acceptance criteria for explosive powders represent a technical challenge:

- How do physical properties of powders relate to detonation performance of pressed pellets?
- Which physical properties should be specified and what are the acceptable limits?
- What do we really mean by "performance"?

Example: Initiation sensitivity of pressed pellets made from fine-grained HNS powder



Several batches of fine-grained HNS powder were produced according to the same specification:

- Top: Two **physically similar** batches of powder exhibited **different initiation sensitivity**
- Bottom: Two **physically different** batches of powder exhibited **similar initiation sensitivity**

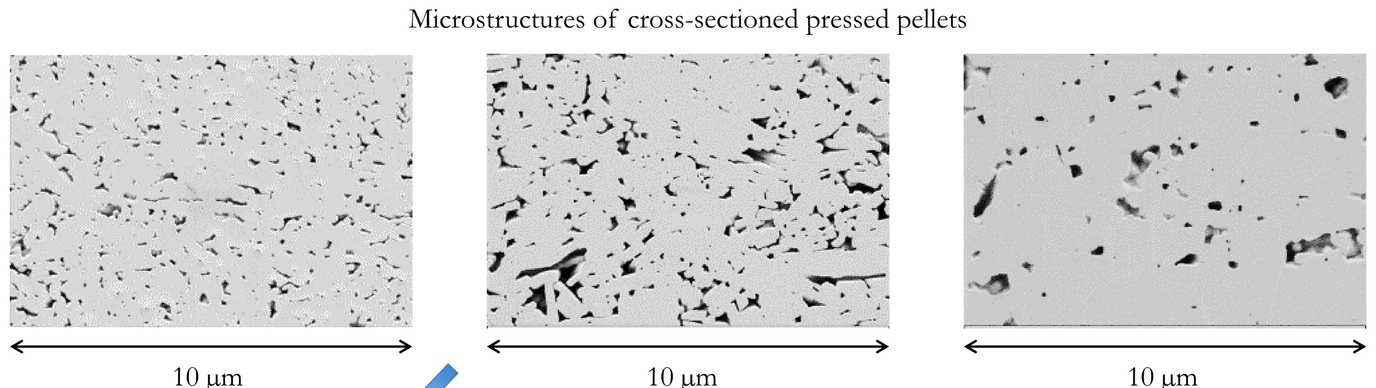
Characteristics of loose powder do not always correlate with performance of **pressed pellets.**

- Pressing powder to a high density (e.g. 90% TMD) can break or deform the particles and create new features such as voids or cracks
- During shock initiation, the shock wave energy is localized at these defects, creating "hot spots" which govern the detonation process

Modeling and Simulation Methods

Mesoscale simulations of shock initiation may provide insight into the relationship between microstructure and performance of high explosives

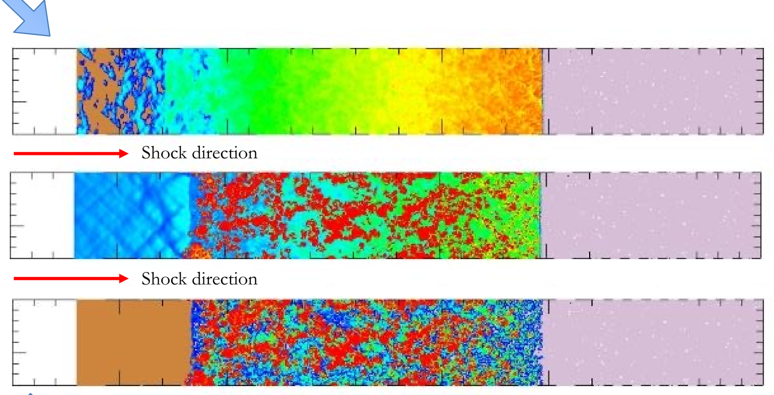
Microstructures of cross-sectioned pressed pellets



Import experimental SEM images into CTH as initial microstructures

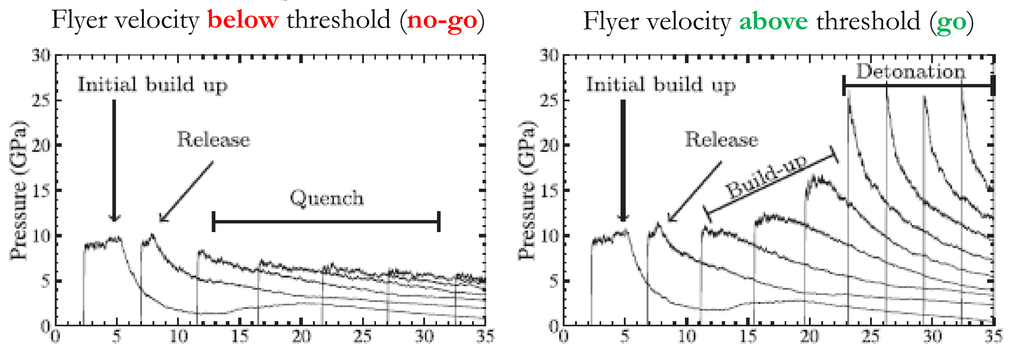
Shock-to-detonation simulations:

- Use CTH shock hydrocode
- Vary flyer thickness
- Vary flyer impact velocity
- Different initial microstructures



Track pressure with gauges placed at various depths below impact surface

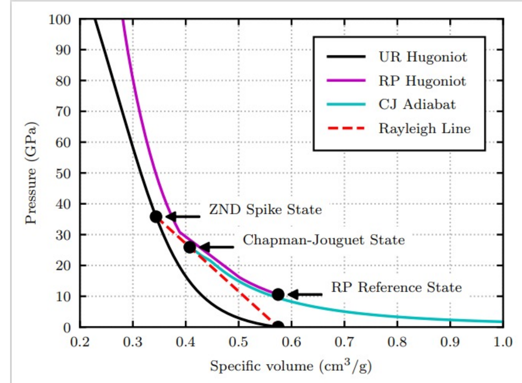
Flyer velocity **below** threshold (**no-go**) Flyer velocity **above** threshold (**go**)



Model Calibration for HNS

- **Leverage prior experimental data** for thin-flyer initiation of fine-grained HNS where we have threshold flyer velocities for various flyer thicknesses.
- In this work, we **calibrate a mesoscale HNS model** with respect to the 11 μm flyer results and test the model validity against the other data for different flyer thicknesses.

Flyer Material	Flyer thickness (μm)	Threshold velocity (km/s)
Parylene	29	2.678
Parylene	21	2.635
Parylene	11	3.236
Parylene	6	4.483



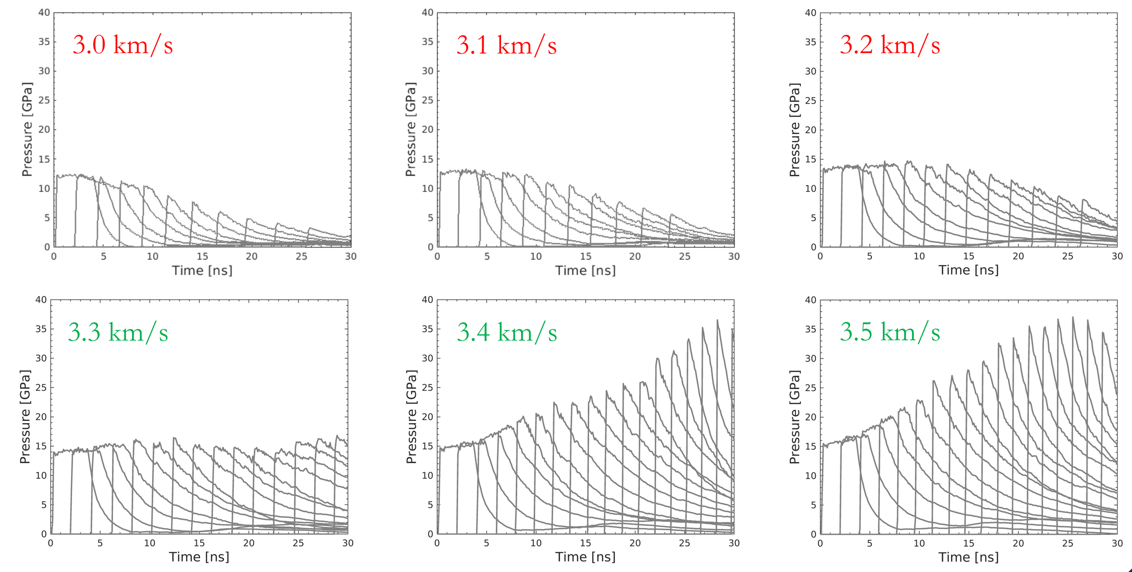
Unreacted (UR) and reaction products (RP) Hugoniots for fully dense (solid) HNS. The initial state is at zero pressure. A detonation wave shocks the material along the Rayleigh Line to the ZND spike pressure. Products expand to the CJ state and down the CJ adiabat.

A **reactive burn model** tracks the evolution of the material from an unreacted state to a fully reacted state. We use a temperature-dependent form for these Arrhenius kinetics:

$$k = A\exp(-E/RT)$$

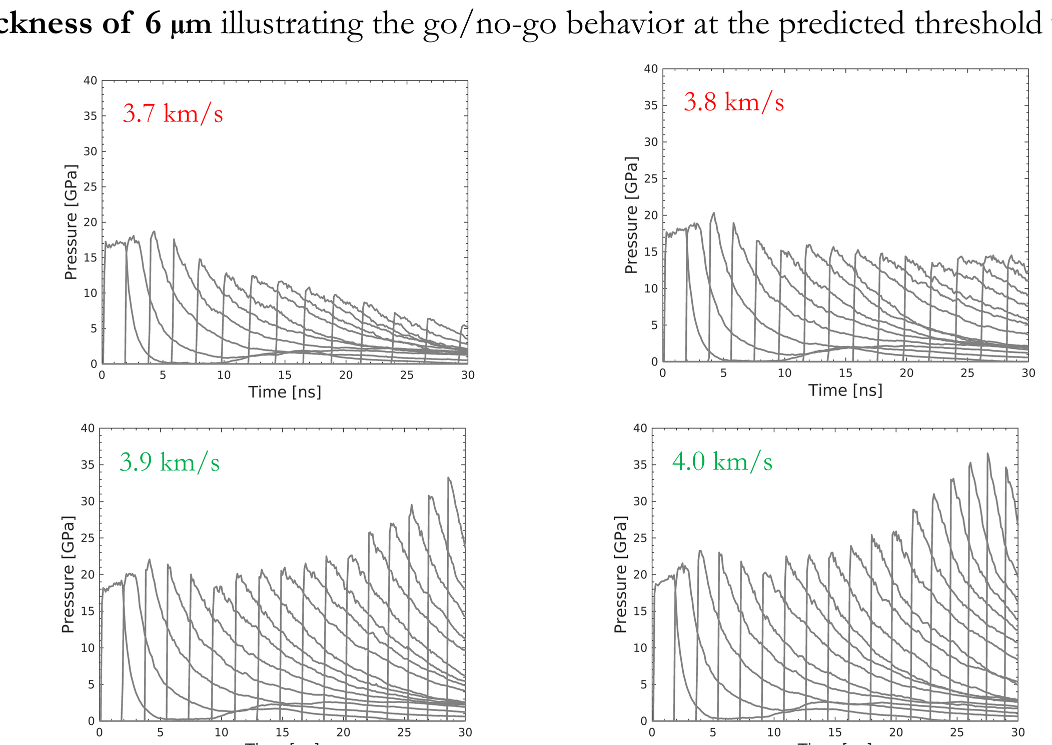
There are two parameters: activation energy (E), and the pre-exponential factor (A). The activation energy is fixed from values in the literature, which is based on thermal time-to-explosion data, while the **frequency factor is adjusted to match the experimental threshold velocity data.**

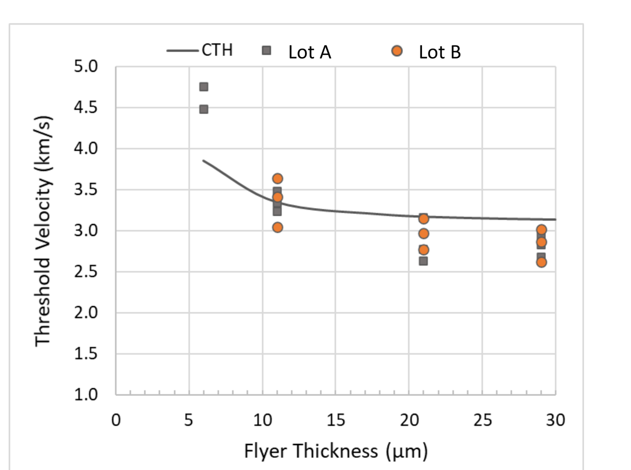
Pressure profiles as a function of flyer velocity for the calibrated HNS model with A = 3.51e11 illustrating the **go/no-go behavior at the threshold velocity.**



Threshold Flyer Velocity Predictions: I

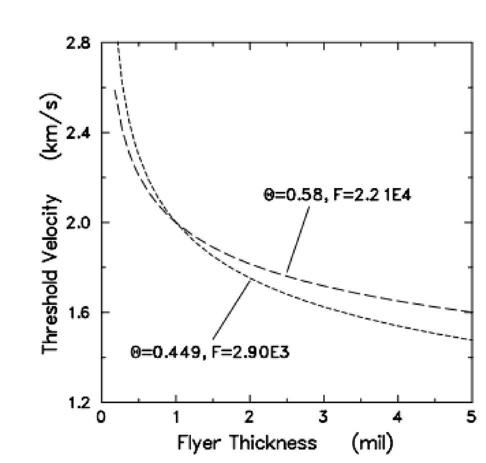
Pressure profiles as a function of flyer velocity using the **calibrated HNS model with a thinner flyer thickness of 6 μm** illustrating the go/no-go behavior at the predicted threshold velocity.





Comparison of simulation predictions with experimental threshold data for two lots of fine-grained HNS.

- We under predict threshold velocities for thin flyers while over predicting threshold velocities for thicker flyers.
- Model kinetics can be fine-tuned for a better match with experiments.

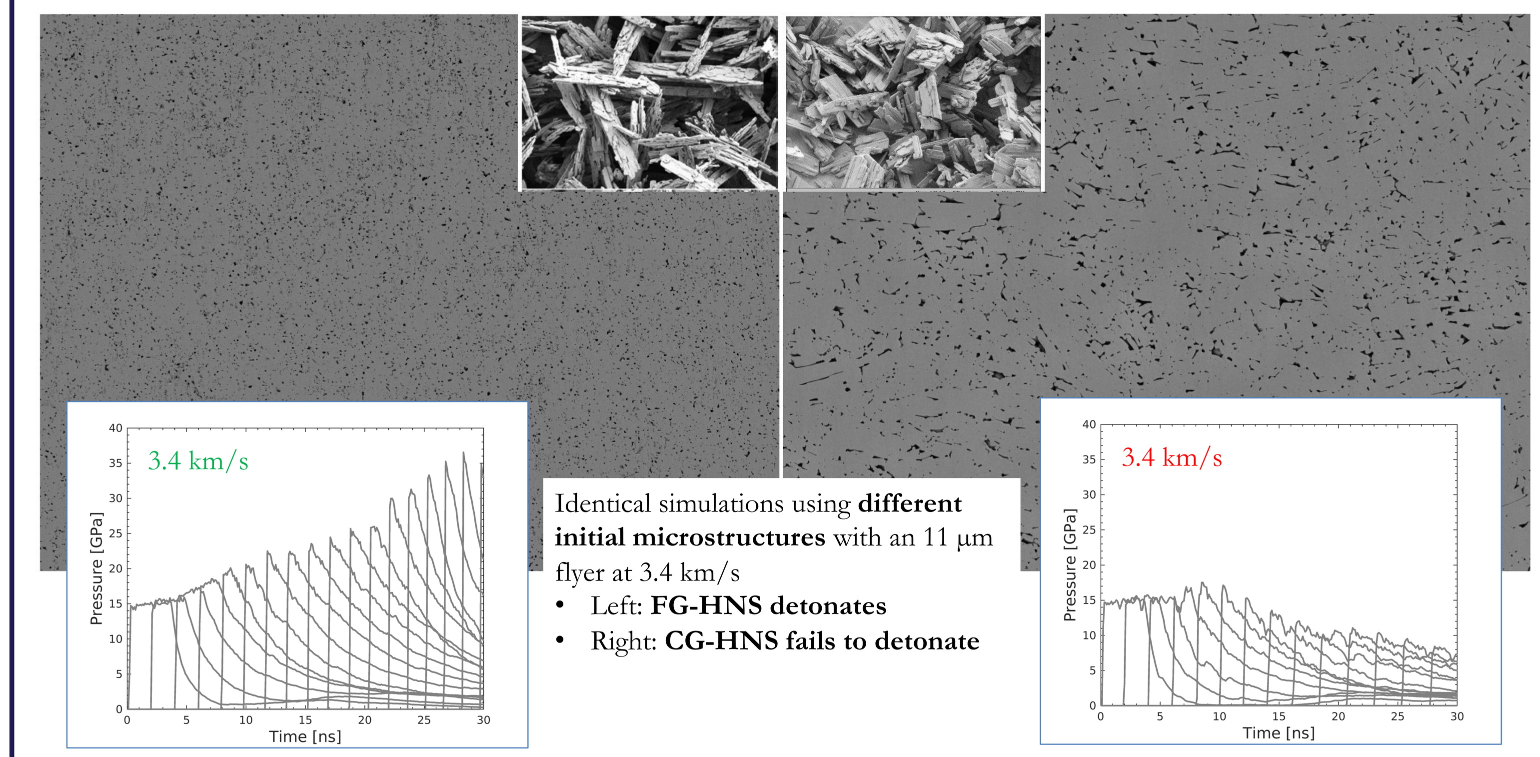


From Kerley: Threshold velocity vs. flyer thickness depends on **two parameters in Arrhenius models.**

- We held activation energy constant and calibrated the pre-exponential factor.
- Activation energy may also be adjusted for high pressure shock compression state.

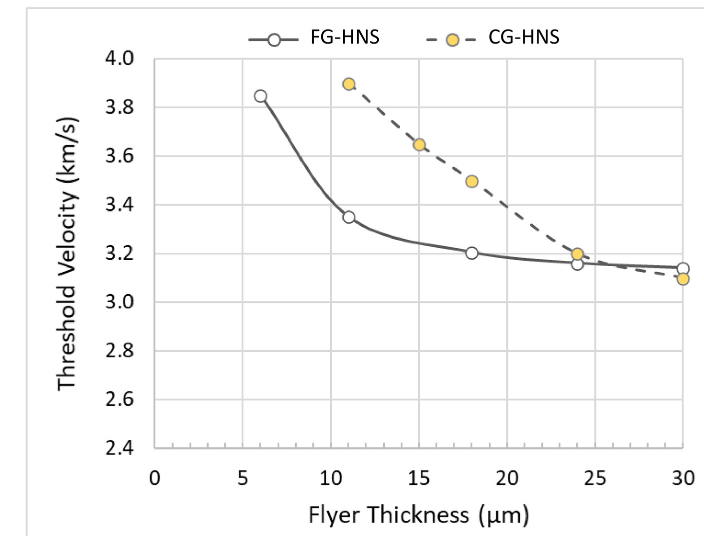
Threshold Flyer Velocity Predictions: II

Fine-Grained HNS vs. Coarse-Grained HNS



Identical simulations using **different initial microstructures** with an 11 μm flyer at 3.4 km/s

- Left: **FG-HNS detonates**
- Right: **CG-HNS fails to detonate**



Summarized threshold velocity vs. flyer thickness predictions for FG-HNS and CG-HNS

Predicted shift in performance between FG-HNS and CG-HNS due to the differences between the microstructures.

- CG-HNS is less sensitive for thin flyers
- Cross-over predicted for thicker flyers
- Experimental data for shock initiation of CG-HNS is needed

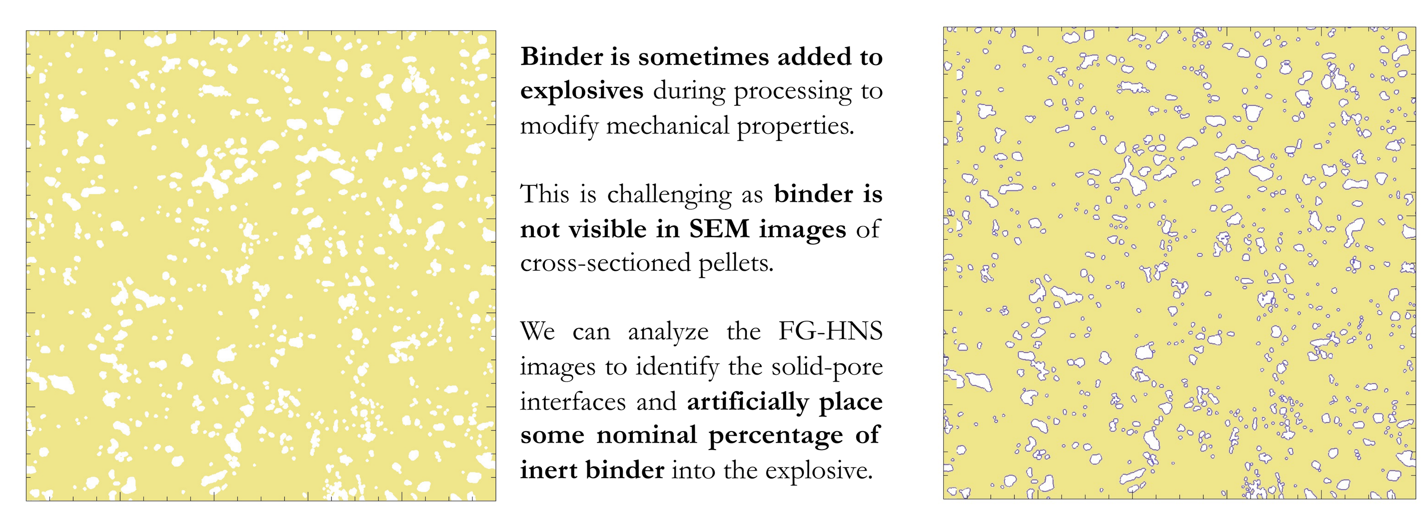
Predicted a cross-over in initiation sensitivity.

- Previously observed and discussed in the literature (e.g. Setchell, Khasainov, etc.)
- Includes both "low pressure" vs. "high pressure" shock regimes, and "short pulse" vs. "sustained shock" loading

Possible explanations:

- Duration of the shock pulse corresponds to a physical length-scale in the explosive
- Microstructure also has a characteristic length-scale(s)

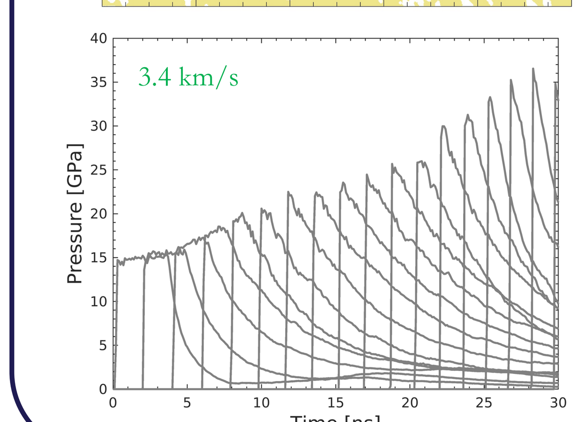
Fine-Grained HNS vs. Fine-Grained HNS with Binder



Binder is sometimes added to explosives during processing to modify mechanical properties.

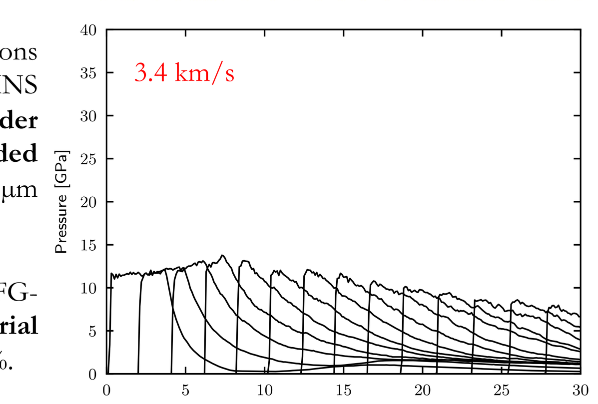
This is challenging as **binder is not visible in SEM images** of cross-sectioned pellets.

We can analyze the FG-HNS images to identify the solid-pore interfaces and **artificially place some nominal percentage of inert binder** into the explosive.



Pressure profiles for simulations of the exact same FG-HNS microstructure **without binder (left) and with 5% added binder (right)** for an 11 μm flyer at 3.4 km/s.

Simulations of binderized FG-HNS **predict that the material is less sensitive** by 15 – 20%.



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