

Catastrophic Interface Debonding in Energetic Materials

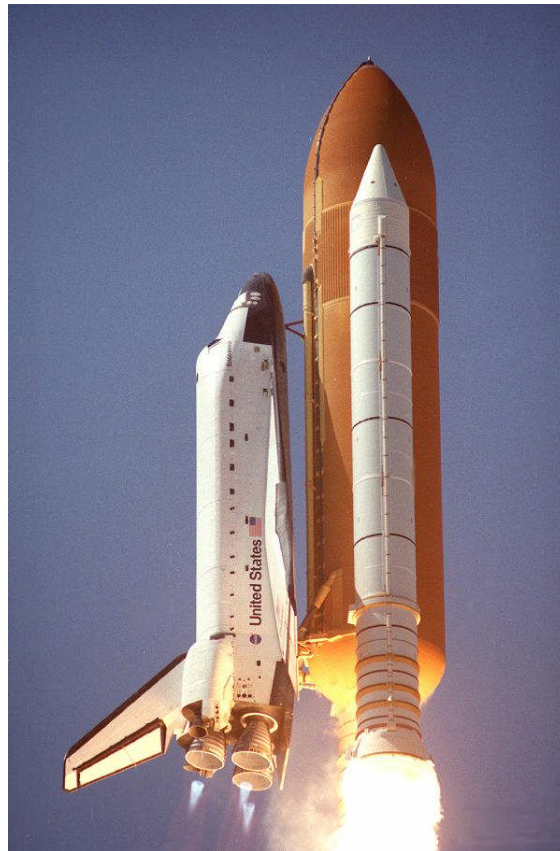
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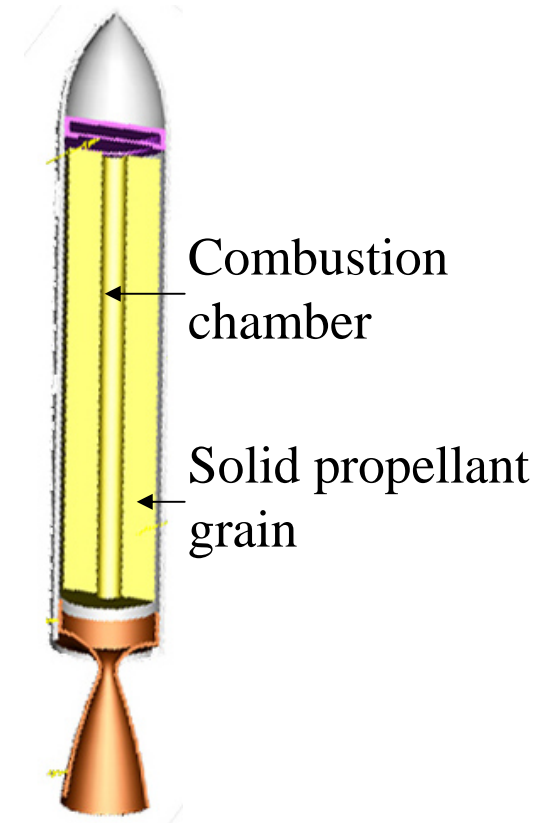
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University of Manchester

Solid Propellant Rocket Burning Rate – Chamber Pressure



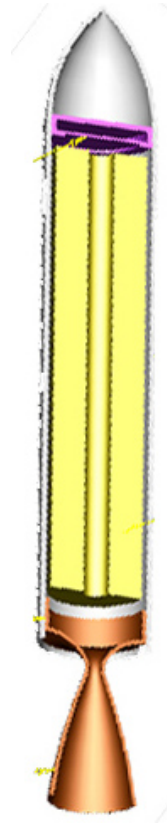
NASA space shuttle



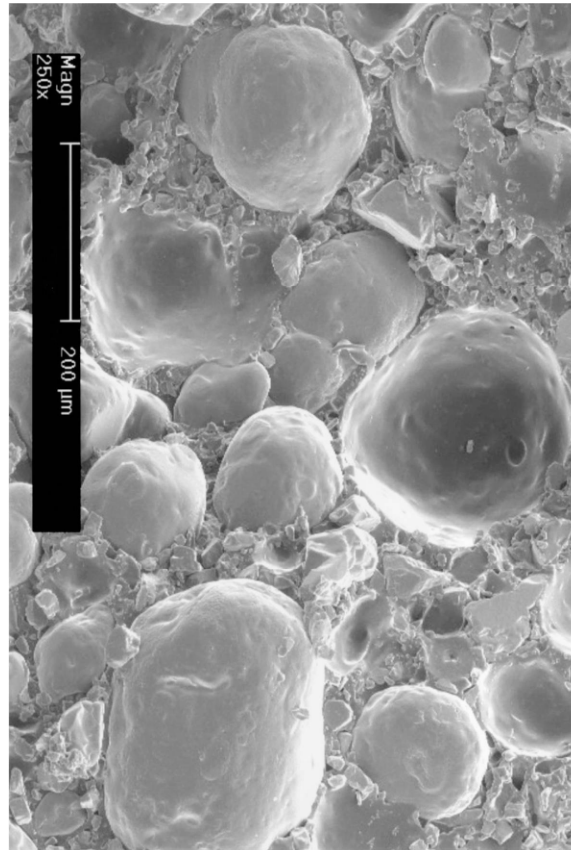
Solid propellant rocket

- The burning rate increases with the chamber pressure, and the chamber pressure increases with the burning rate.

Microstructure of Solid Propellant



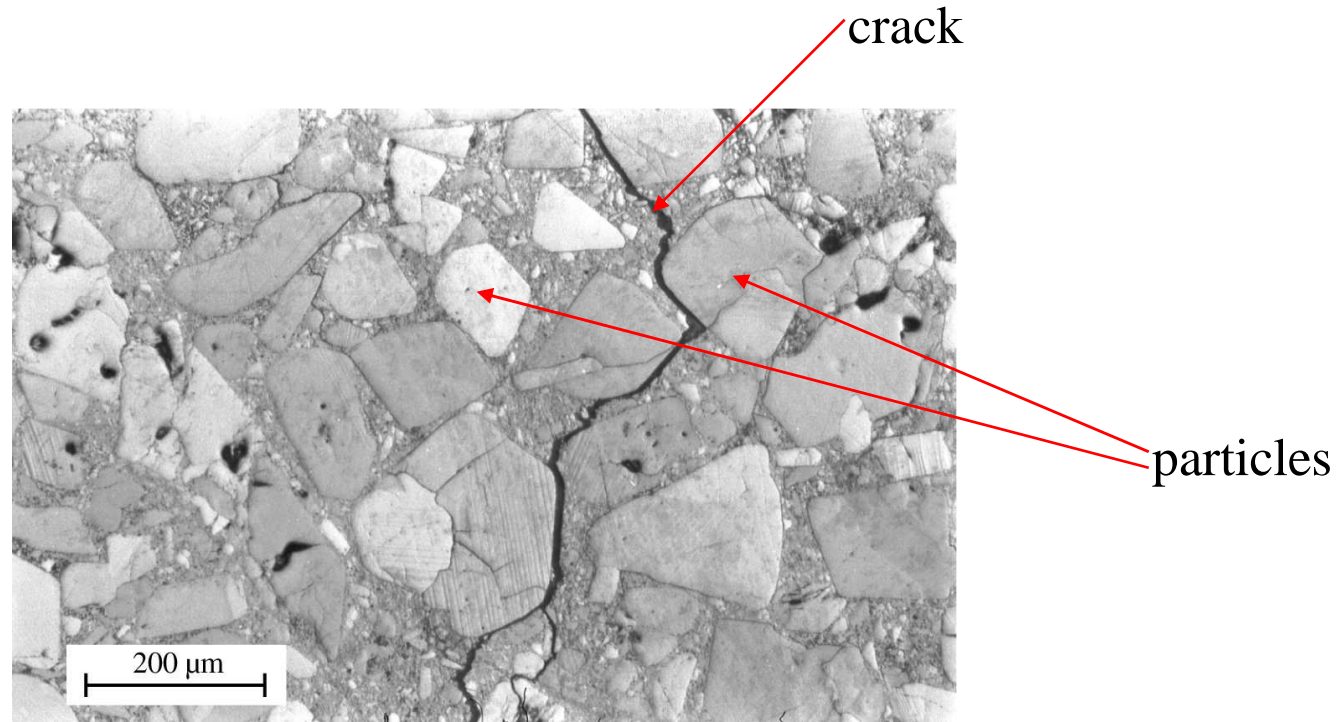
Solid rocket



Microstructure of solid propellant material
Ide et al., 1999

- Particle/binder with interfaces
- Bimodal particle size distribution
- Large particle volume fraction
- Fracture mainly along interfaces

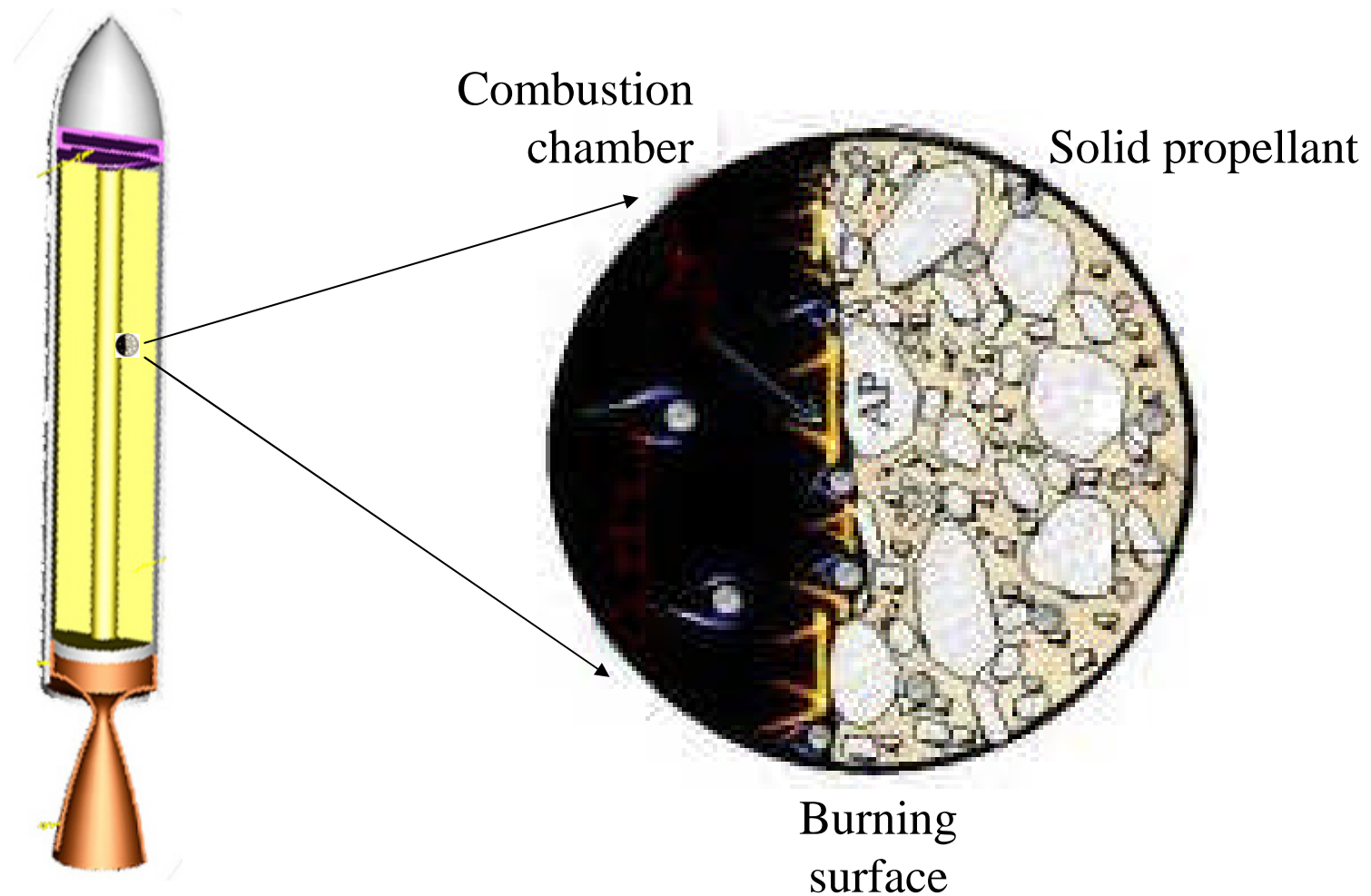
Crack Propagation along Particle/Binder Interfaces



Rae *et al.* 2002. Cavendish Laboratory, Cambridge

- Cracks propagate mainly through interface debonding.

Pressure – Burn – Microstructure

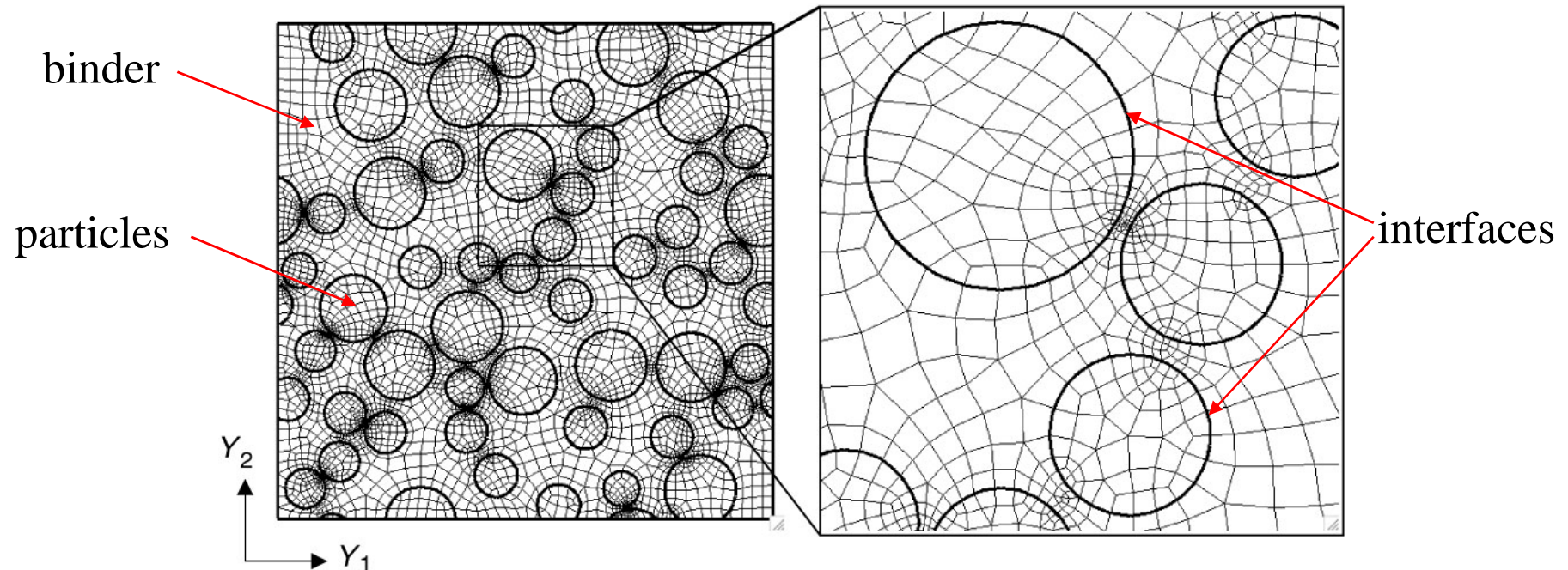


- Relatively small defects, like debonded interfaces and cracks, can lead to catastrophic failure.

Objective

To establish a **stability criterion**
for interface debonding in plastic bonded energetic materials

What Do Simulations Tell Us?

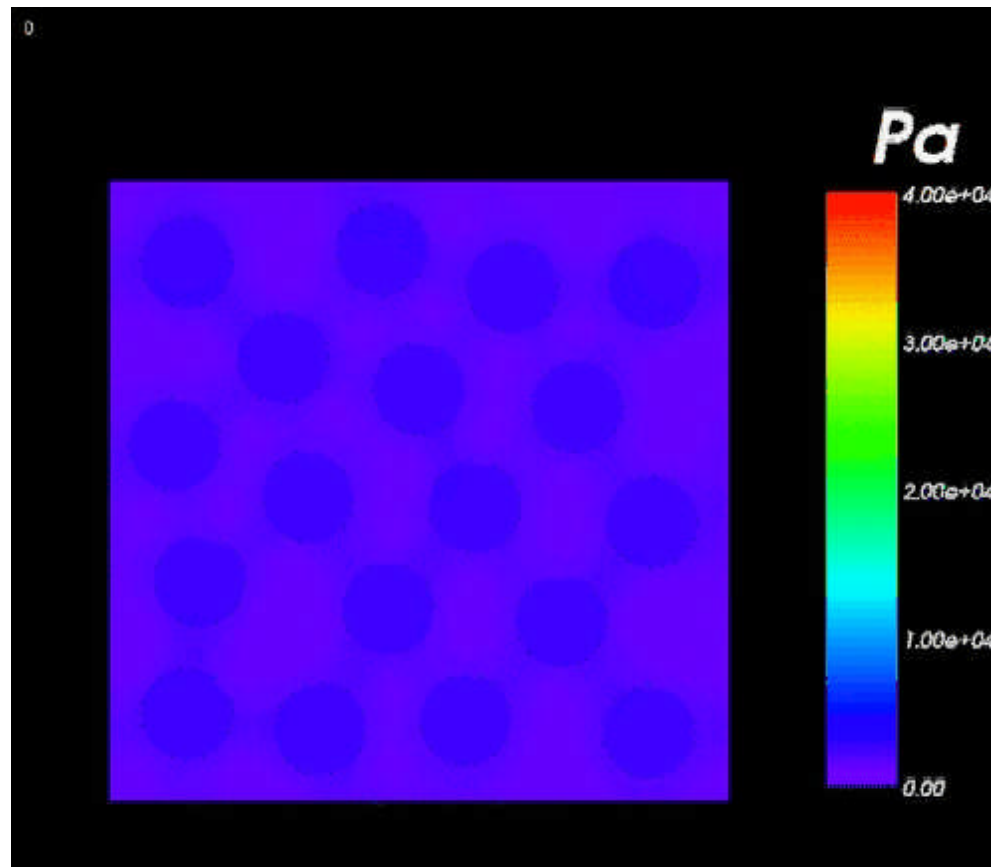


Inglis, Geubelle, Matous, Tan and Huang, 2007, Mech. Mater.

- Macroscopic strain imposed as a body force applied at microscale
- 4-noded cohesive element at interfaces
- Periodic boundary conditions

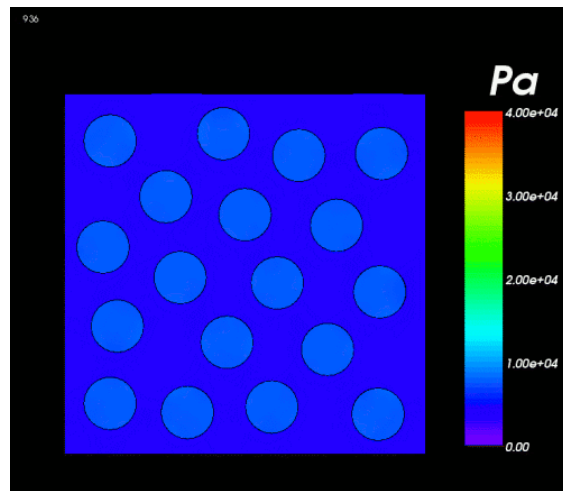
Material Subject to Increased Loading

- Material subjects to equibiaxial strain
- Color-scale represents von Mises stress

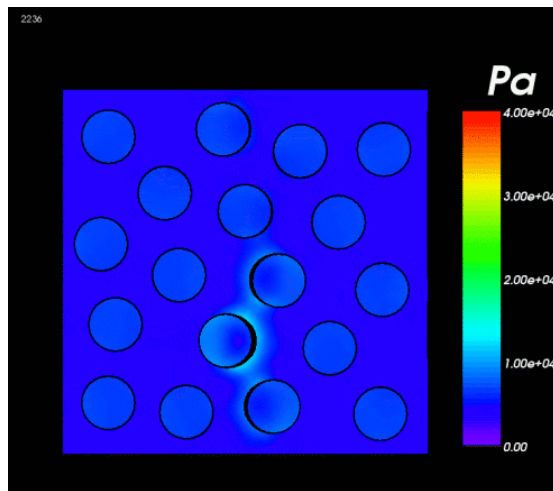


Catastrophic Interface Debonding

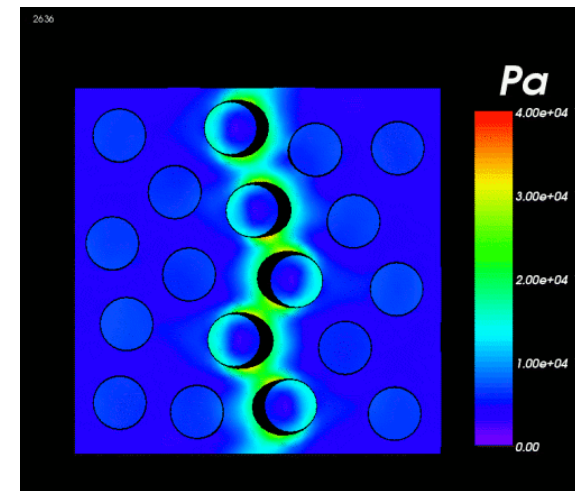
Increasing equibiaxial load



Uniform debonding



Sudden non-uniform
debonding

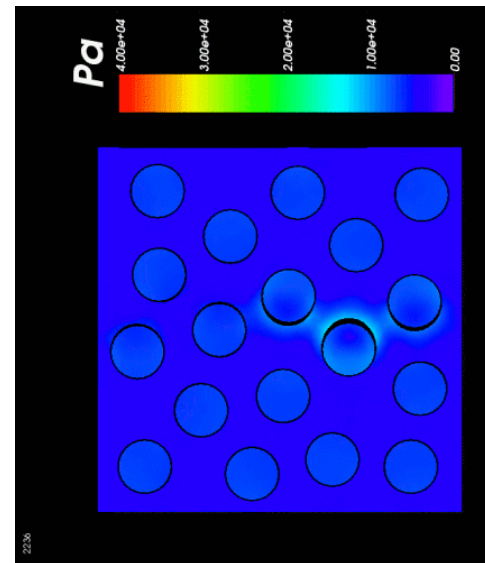
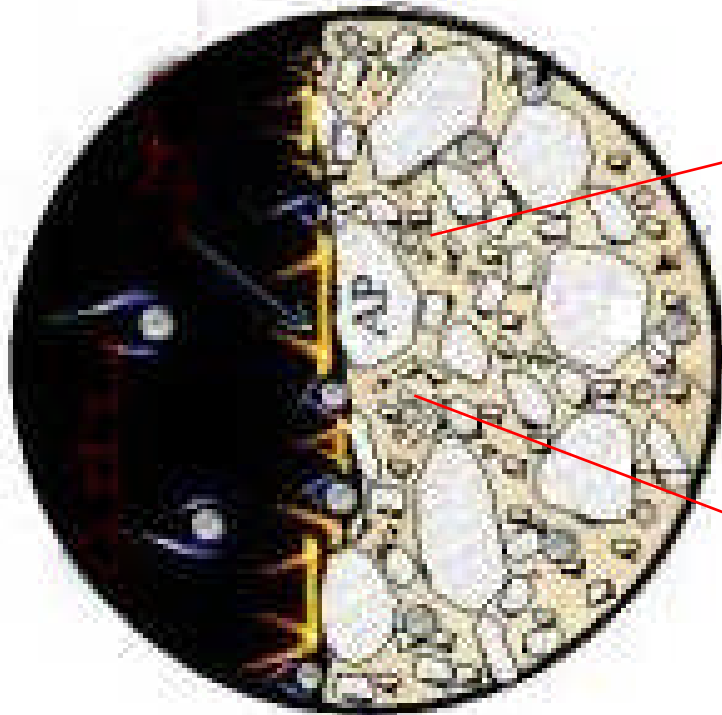


Collapse of interface
debonding
→ Crack formation

- Sudden interface debonding under quasi-static loading

Deflagration to Detonation Transition

Increasing chamber pressure



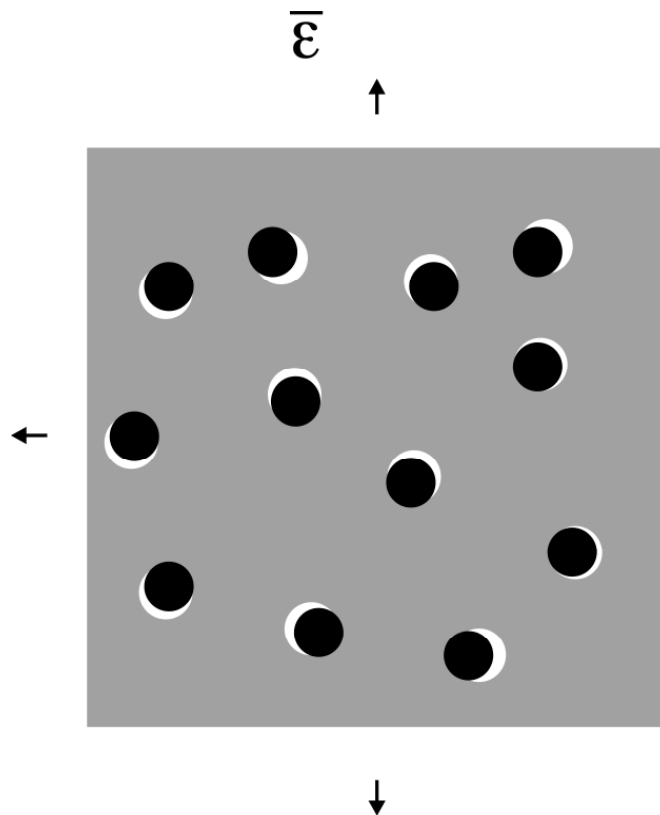
- Sudden interface debonding -> hot spots
- Pressurised cracks

Strain Energy Density in Hydrostatic Tension

$$\Pi([\mathbf{u}]) = \frac{1}{\Omega} \left\{ \frac{1}{2} \int_{\Omega} \sigma_{ij}([\mathbf{u}]) \varepsilon_{ij}([\mathbf{u}]) dV + \int_{S_{\text{int}}} \phi([\mathbf{u}]) dA \right\}$$

interface cohesive energy

strain energy in the matrix and particles



Π is a functional of displacement jump $[\mathbf{u}]$ at interfaces.

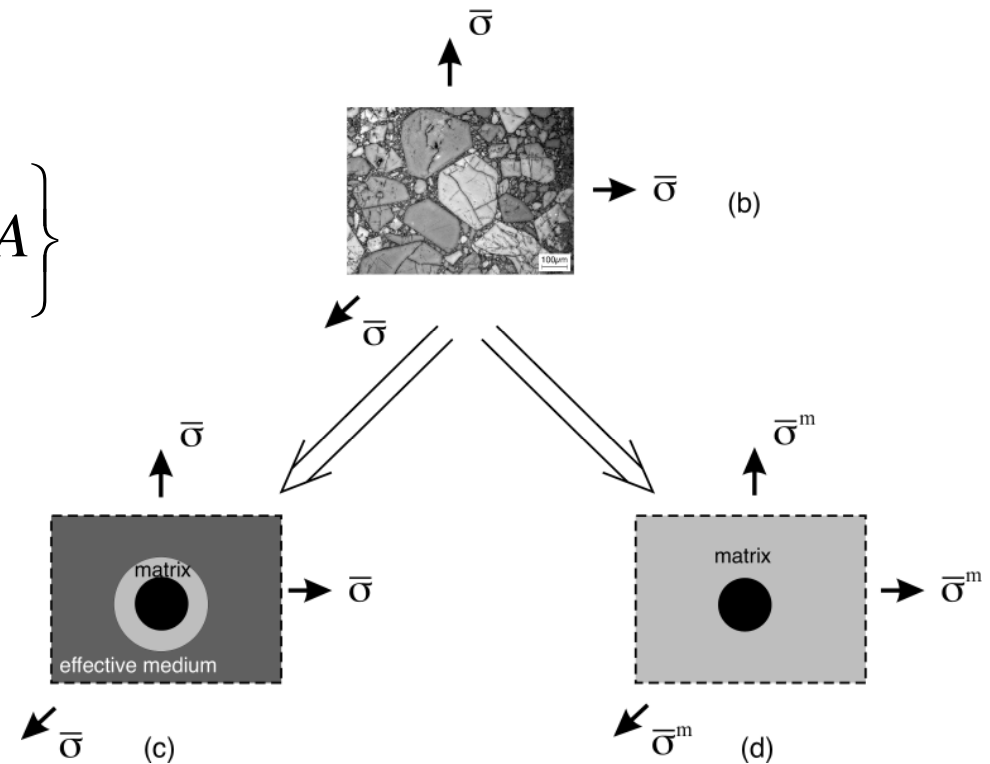
- Determine $[\mathbf{u}]$ by minimizing $\Pi([\mathbf{u}])$

Tan *et al.*, 2005. *AIAA*

Tan *et al.*, 2006. *Int. J. Multiscale Comput. Eng.*

Homogenization Methods in Micromechanics

$$\Pi = \frac{1}{\Omega} \left\{ \frac{1}{2} \int_{\Omega} \sigma_{ij} \varepsilon_{ij} dV + \int_{S_{\text{int}}} \phi dA \right\}$$



Generalized Self
Consistent Method

Mori-Tanaka Method

- Mori-Tanaka method is extended to account for nonlinear interface debonding.

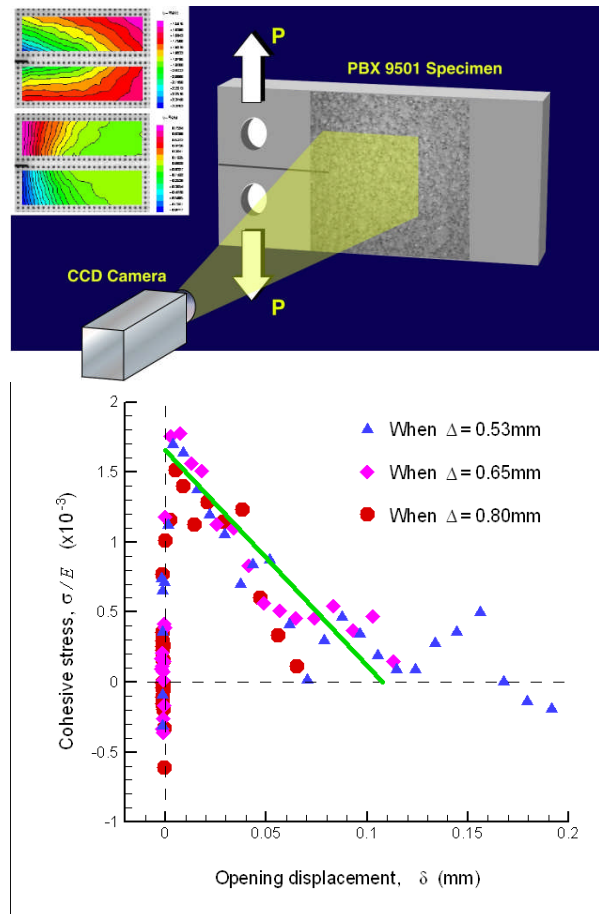
Tan *et al.*, 2005. *Int. J. Plasticity*

Tan *et al.*, 2007. *Int. J. Fract.*

Determine Interface Cohesive Law for High Explosives

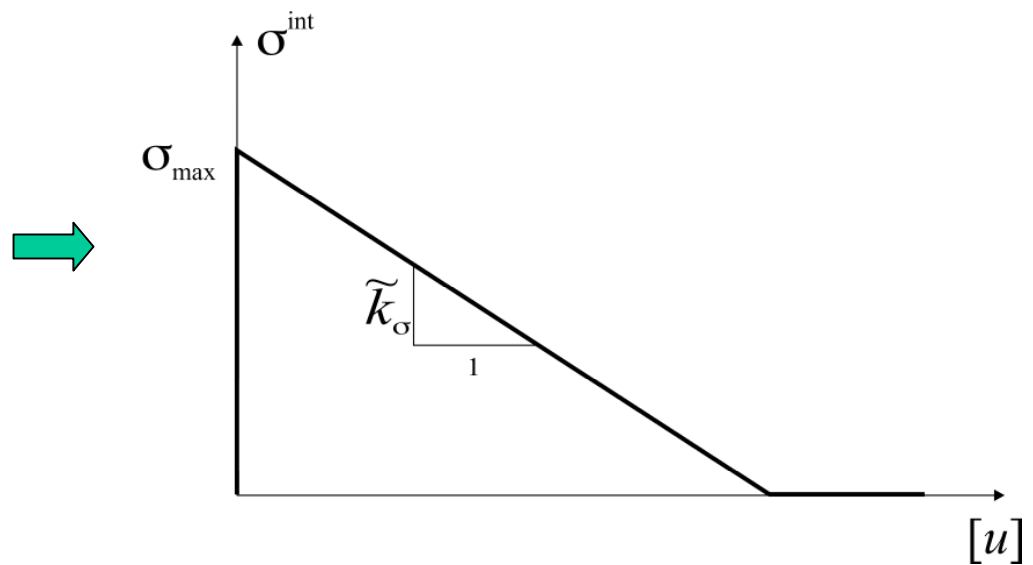
$$\Pi = \frac{1}{\Omega} \left\{ \frac{1}{2} \int_{\Omega} \sigma_{ij} \varepsilon_{ij} dV + \int_{S_{\text{int}}} \phi dA \right\}$$

Macroscopic cohesive law



Interface cohesive law

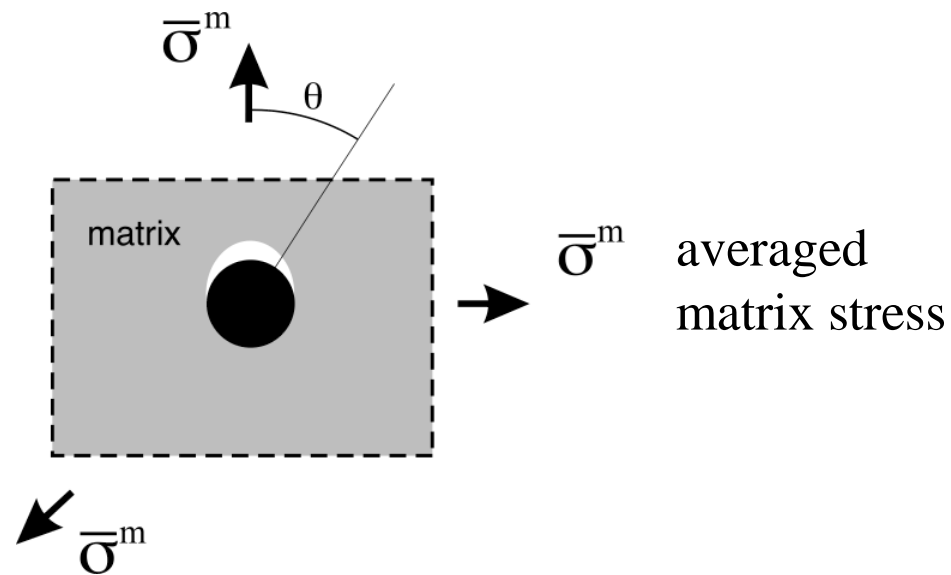
softening modulus: $\tilde{k}_{\sigma} = 17\text{MPa/mm}$
 interface strength: $\sigma_{\text{max}} = 1.66\text{MPa}$



Tan *et al.*, 2005. *J. Mech. Phys. Solids*

Interface Displacement Jumps

Goal:
$$\Pi([\mathbf{u}]) = \frac{1}{\Omega} \left\{ \frac{1}{2} \int_{\Omega} \sigma_{ij}([\mathbf{u}]) \varepsilon_{ij}([\mathbf{u}]) dV + \int_{S_{\text{int}}} \phi([\mathbf{u}]) dA \right\}$$



Interface opening $[u]$

$$\frac{[u]}{a} = A_0 + \begin{cases} A_u \cos \theta & \theta \in [0, \pi/2] \\ 0 & \theta \in [\pi/2, \pi] \end{cases}$$

Quadratic Form of Total Potential Energy

- Total potential energy density can be expressed in a **quadratic** form of A_u when subject to hydrostatic loading

$$\Pi(A_u) = c_0 + c_u A_u + c_{uu} A_u^2$$

For rigid particle embedded in incompressible matrix under hydrostatic tension:

$$c_{uu} = \frac{3}{2} \mu_m \left(1.0225 - f - \frac{\tilde{k}_\sigma a}{6\mu_m} \right)$$

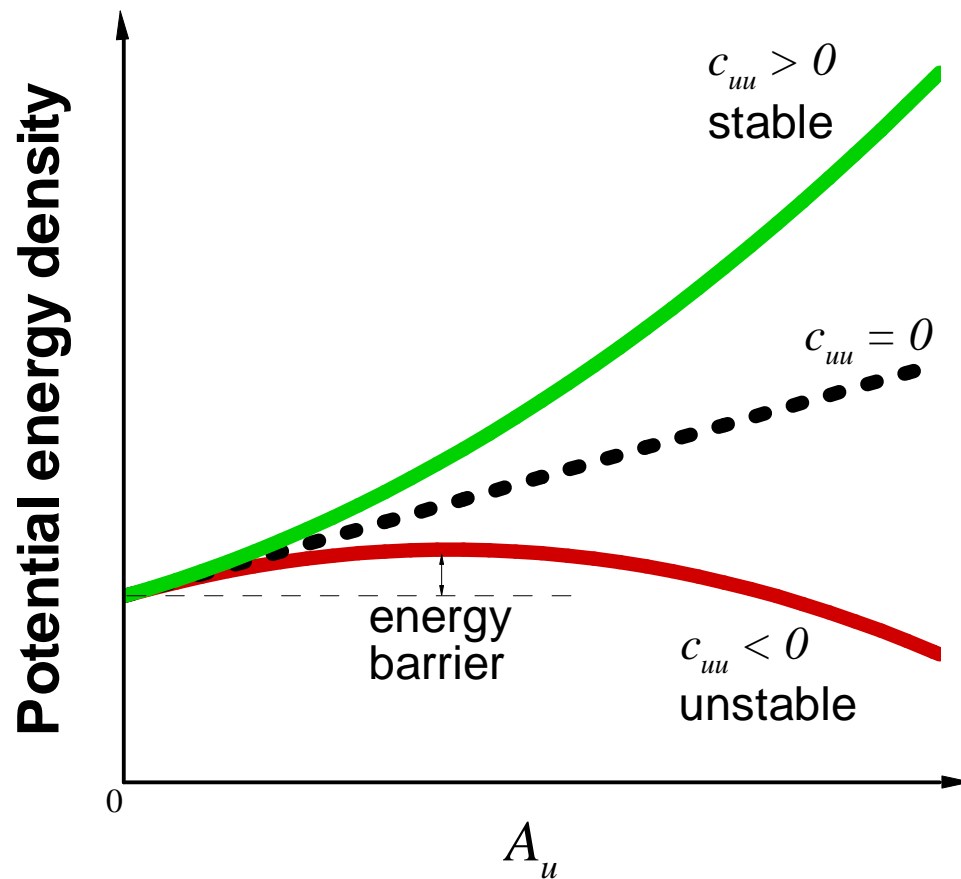
f : particle volume fraction

\tilde{k}_σ : interface softening modulus

a : particle radius

μ_m : shear modulus of matrix

Stability Criterion for Interface Debonding

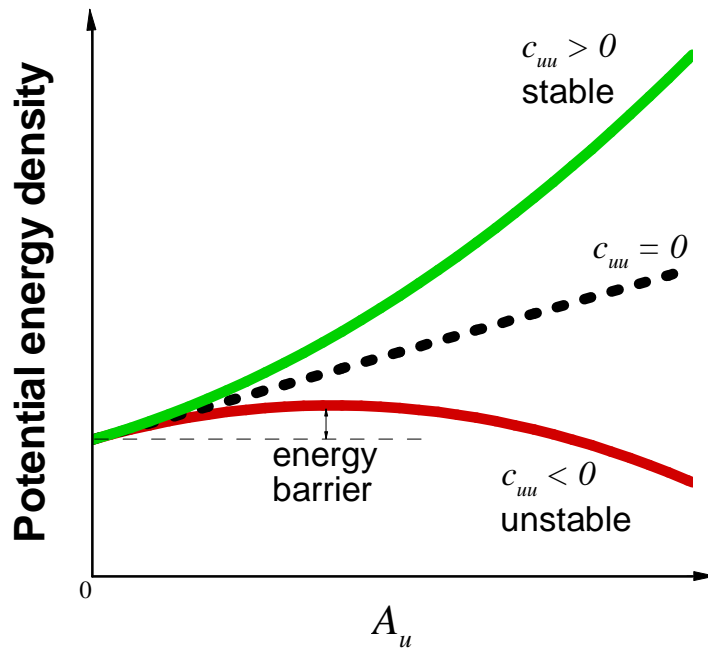


$$c_{uu} = \frac{3}{2} \mu_m \left(1.023 - f - \frac{\tilde{k}_\sigma a}{6\mu_m} \right)$$

$c_{uu} > 0$: stable debonding
 $c_{uu} < 0$: unstable debonding

A_u : Magnitude of non-uniform interface opening

Case Study I: Particle Size Effect



critical particle radius

$$a_{cr}^{stability} = 6(1.023 - f) \frac{\mu_m}{\tilde{k}_\sigma}$$

Plastic Bonded Explosives

interface softening modulus: $\tilde{k}_\sigma = 0.017 \text{ MPa} / \mu\text{m}$ Tan *et al.*, 2005

large particle volume fraction: $f = 69.5\%$ Skidmore *et al.*, 1997

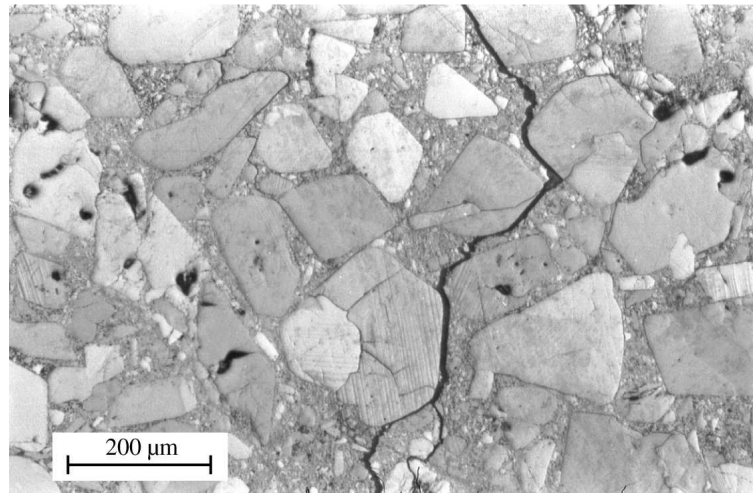
matrix modulus: $\mu_m = 0.334 \text{ MPa}$ Cady *et al.*, 2000



$$a_{cr}^{stability} \approx 39 \mu\text{m}$$

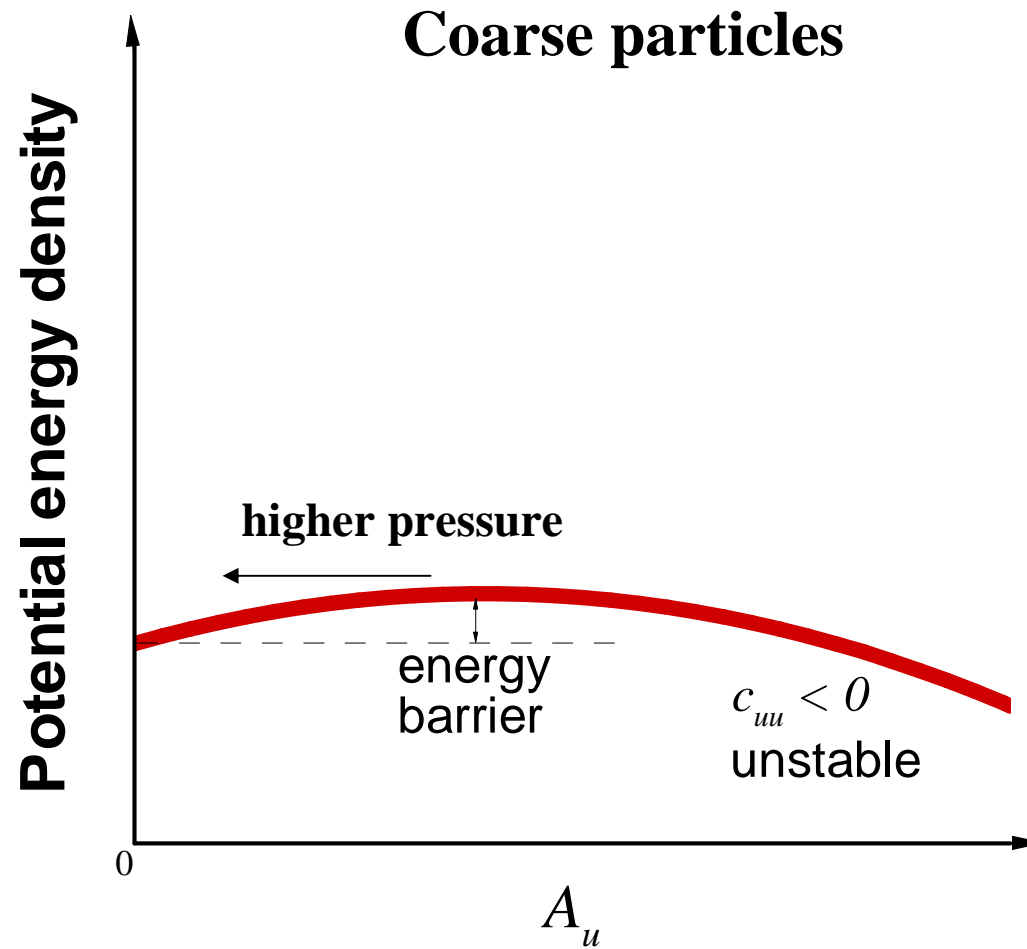
Performance versus Sensibility

$$a_{cr}^{stability} \approx 39 \mu m$$



Balancing the performance and sensibility through changing the particle size distribution

Size Effect on DDT



→ Deflagration to Detonation Transition (DDT)

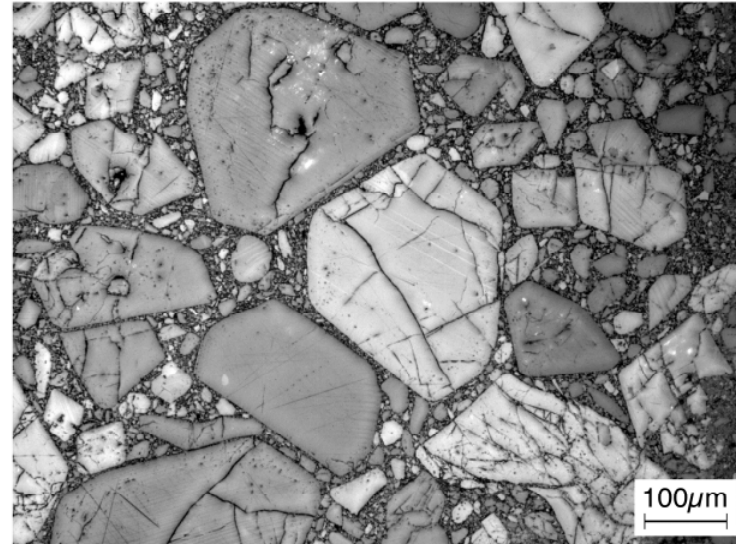
Case Study II: Macroscopic Deformation during Compression

8% volume increase
when HMX particles transfer
from β -phase to δ -phase.

$$a_{cr}^{stability} \approx 39 \mu m$$

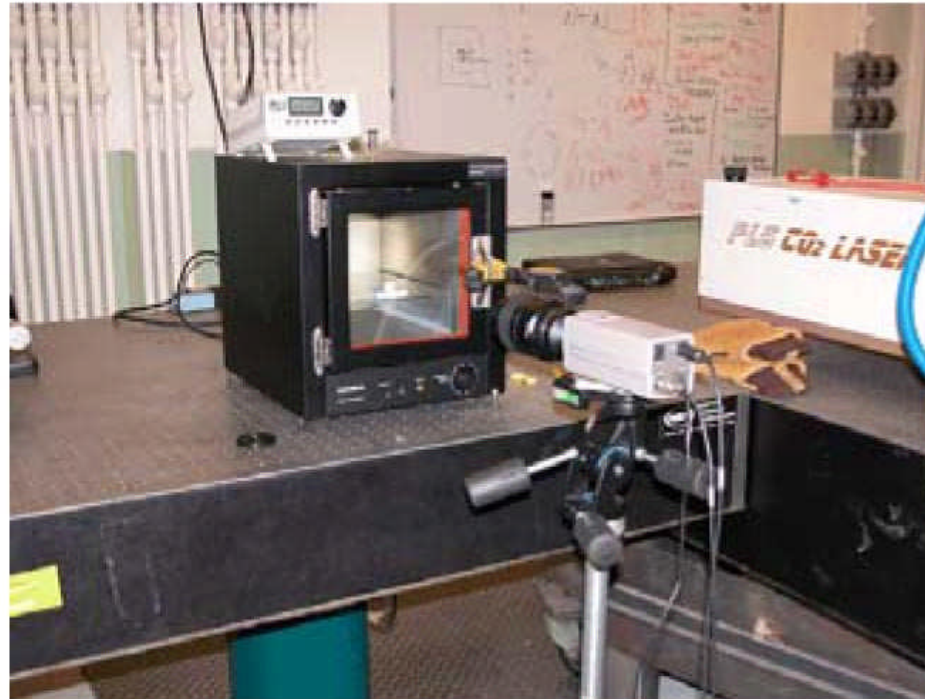
Average radius of coarse particles is $125 \mu m$.

PBX 9501 High Explosive



- Microscopically, each particle may debond suddenly in a random direction.
- Macroscopically, deformation field is **chaotic**.

Experimental Setup for Slow Heating of PBX 9501 Sample

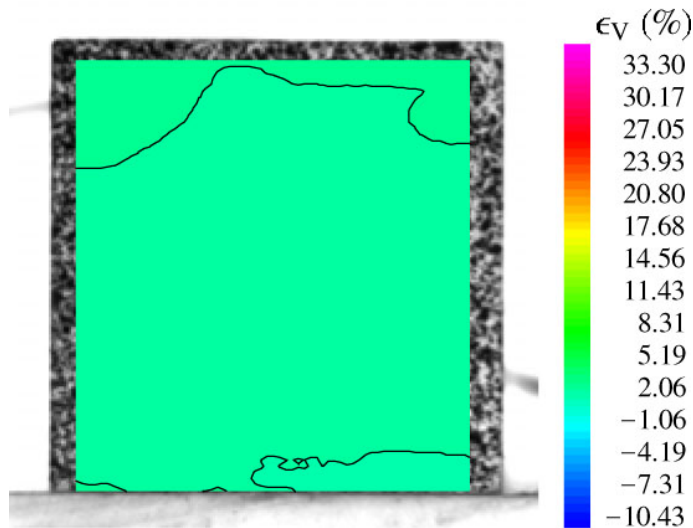


- Cubic sample of size 12.7mm
- Free standing sample
- Temperature ramps from 33°C to 195°C in one hour

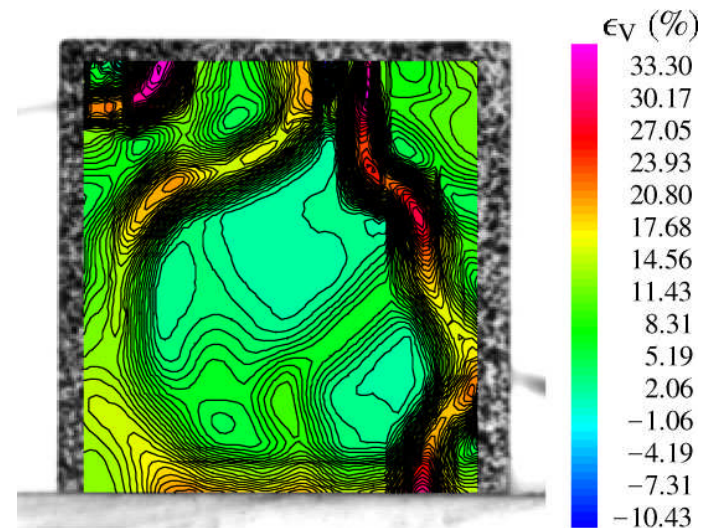
Evolution of the Deformation Field



Strain Field



below transformation temperature



around transformation temperature

- low strain -> chaotic deformation field

Summary

- A stability criterion for interface debonding is established for energetic composite materials.
- Catastrophic interface debonding is observed in numeric simulations.
- Catastrophic interface debonding contributes to the chaotic deformation during the phase transformation of HMX particles.
- Application: safety of solid rocket propellant.

