# Computational Modeling of Brittle Materials Under Dynamic Conditions

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## Outline

- **Experimental observations**

- **SCRAM and DCA (Dominant Crack Algorithm) Models:**
  - ***Continuum-level* models based on statistical consideration of defects.**

- **Calculations and data for explosives & ceramics**

- **Summary/discussions**

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**Dienes, Addessio, Lewis (LANL)**

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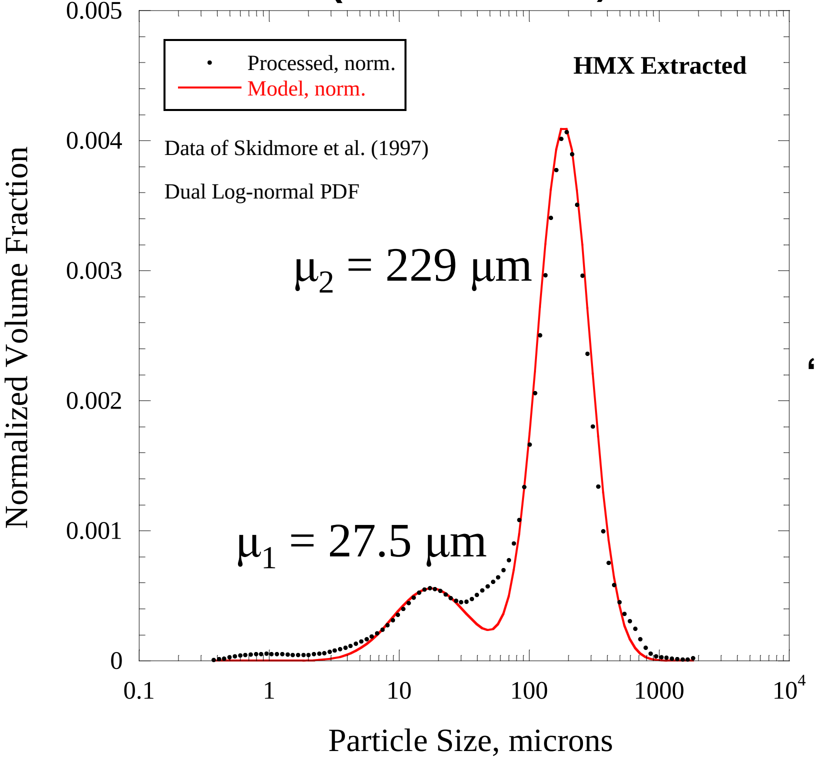
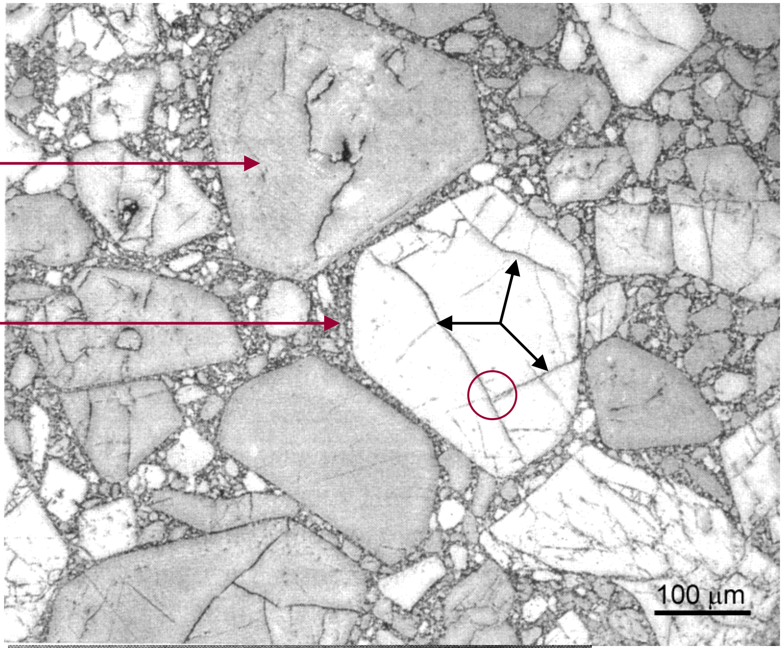
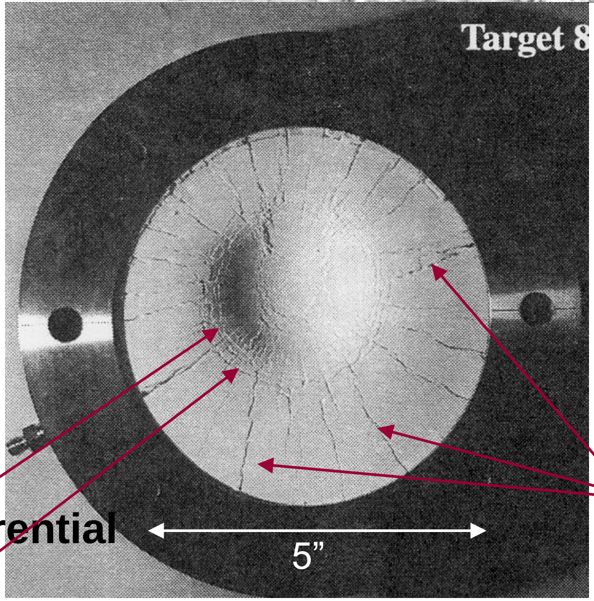
# Damage and Failure in Brittle Materials
# (explosives, ceramics, propellants, concrete, *sea ice*, etc.)

# Cracking in an Explosive (PBX 9501)

**size distribution of HMX Grains (Bronkhorst et al.)**







Disk of explosive after impact

Idar et al, 1998

**Heterogeneous**:
HMX crystals & Polymer Binder

**Distribution of HMX grains is random:**
**Bi-modal distribution (229/27.5 μms)**

**Microcracks in the "pristine" sample:**
**different sizes & orientations**

# Ceramic Armor under Ballistic Impact

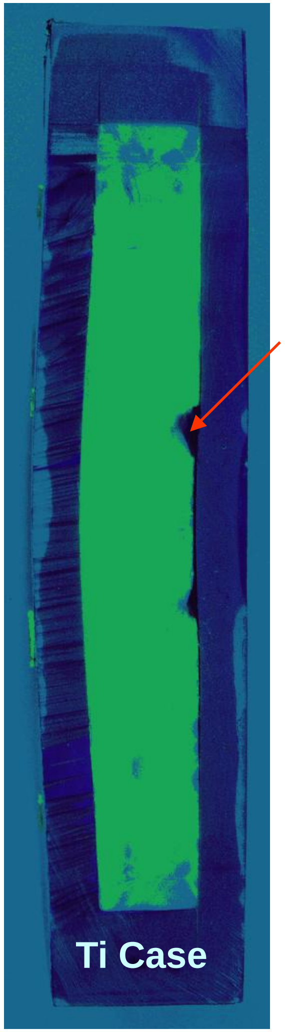
- Ceramic disk: Coors AD 995 (1/2" thick, 4 in diameter)

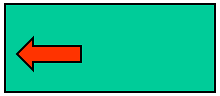
- Casing (3 pieces): Ti-6Al-4V
2 cover plates (1/4 " thick each)
Ring (5" diameter, ½ " thick)

- Impactor: Lexan rod
1.5" long , ¾ " diameter

- Impact velocity: 1.56 km/s

Can we predict the *location and size* of the failed ceramic?





Bingert et al

Sectioned Post-Mortem sample

# Computational Modeling

# Challenges

- **Events taking place at length scales below the *grid resolution* can have significant effects on the damage and failure**

- **Challenges:**
  - **how far do we need to go down in *scales* (meso/micro scales?)**

  - **What about the history of *defects*?**

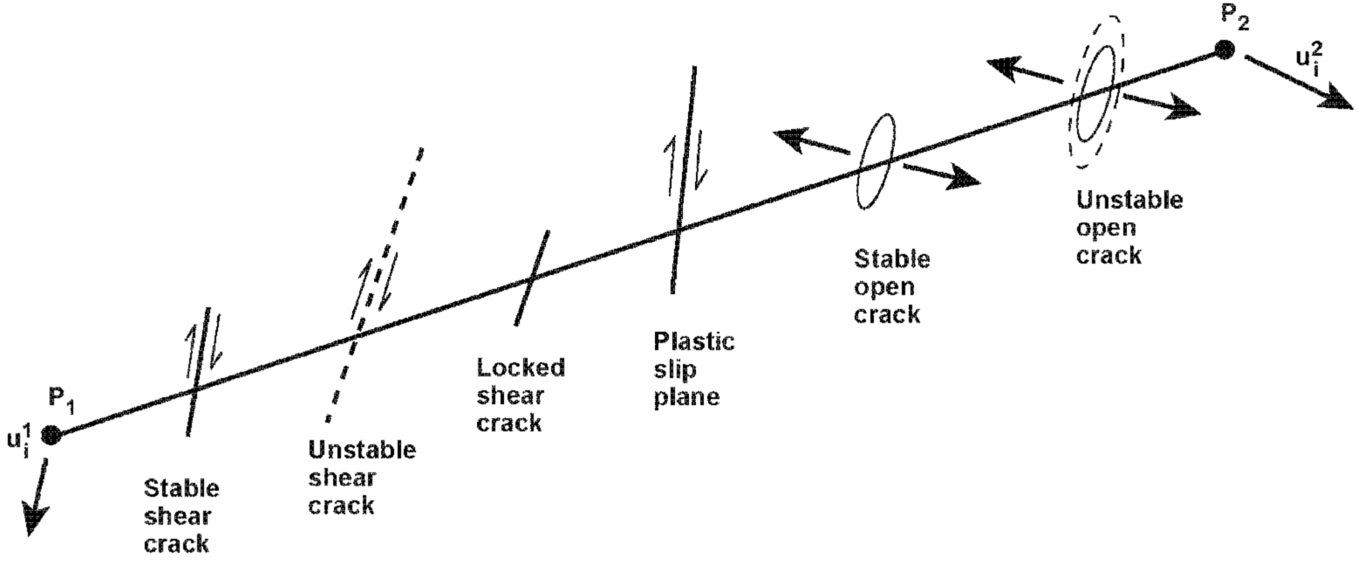
  - **How do we connect the mechanics/physics of different scales? (e.g., grain-level mechanics)**

  - **What about convergence and stability of the *numerical solution* (i.e., *ill-posedness*/Hadamard instability)?**

# Models based on statistical consideration of defects (cracks)

- SCRAM
- DCA

# Superposition of Strain Rates



## Defects idealized in the model

**Difference in velocity**

$$\Delta \mathbf{u} \equiv \mathbf{u}^2 - \mathbf{u}^1 = \sum \Delta \mathbf{u}^c + \sum \Delta \mathbf{u}^d$$

**Discont.**

**Continuous Deformation**

## Statistical averaging

**(probability density function)**

$$\mathbf{d} = \mathbf{d}_m + \mathbf{d}_c + \mathbf{d}_g + \mathbf{d}_p$$

**Total Stretch**

**(rate of deformation)**

$$\mathbf{d} \equiv (\nabla \mathbf{u})_{sym}$$

**Matrix**

**Crack**

**Crack growth**

**Plastic**

# **SCRAM**: Model for damage, failure and initiation of brittle materials

# Impact Initiation Scenario

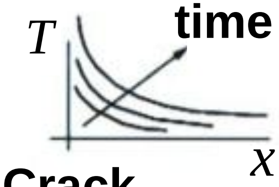
Shock wave activates shear cracks.

**Shock Compression**

Shear cracks grow easily in HMX, inhibited by binder.

Shear cracks grind and produce heat.

$x$ **Normal to Shear crack**



Heat conducted away from sliding interface; temperature rise causes cooking of HMX. $\dot{T} = DT_{xx} + qZe^{-E/kT}$

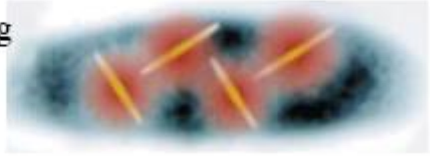
**Sub-grid model**

HMX reaches ignition point (Linan & Williams or IGNC) $T > T_c$

Burned gases open cracks, create initial high-pressure zone. Opening inhibited by inertia, stiffness, and damping.

$$m\ddot{w} + c\dot{w} + kw = pA \qquad p = f(M,T)$$

Burning increases general pressure, accelerating burn in adjoining hot spots.

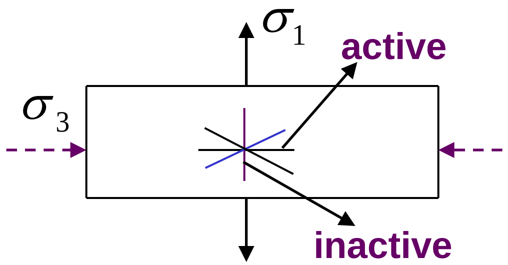


Cracks coalesce when percolation threshold is exceeded, causing general explosion.

# Dominant Crack Algorithm (DCA) Model (Zuo et al., 2006- )

- Damage surface is derived from the instability condition for the critical crack orientation;
- New damage surface has similar features to that in ISOSCM, but removes a discontinuity existed in ISOSCM;
- Crack opening strain is more consistent with physics-- only the tensile principal stresses contribute to the crack opening strain. Material response can be anisotropic.
- Damage evolution (growth rate of the mean crack radius) is given by the energy release rate for the crack along the *critical* (most unstable) orientation.
- Including a nonlinear EOS and porosity growth.

**Zuo, et al., (2006, 2008, 2010, 2011, 2012)**



# Crack strain (damage)

**Total strain is the sum of matrix strain and crack strain:**

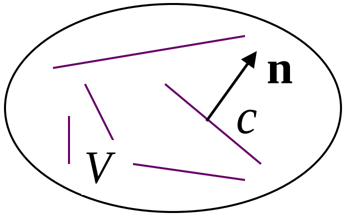
$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_m(\boldsymbol{\sigma}) + \boldsymbol{\varepsilon}_c(\boldsymbol{\sigma}, \bar{c})$$

**Matrix strain:**

$$\boldsymbol{\varepsilon}_m(\boldsymbol{\sigma}) = \mathbf{C}^m \boldsymbol{\sigma} \qquad \mathbf{C}^m = \text{Matrix Compliance}$$

**Crack strain:**

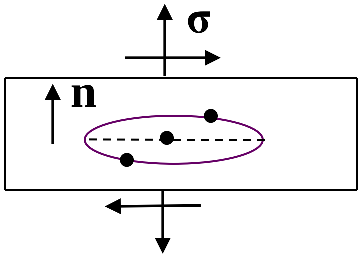
$$\boxed{\boldsymbol{\varepsilon}_c(\boldsymbol{\sigma}, \bar{c}) = \sum_{\Omega, c} \Delta\boldsymbol{\varepsilon}_c(\boldsymbol{\sigma}, c, \mathbf{n})}$$



**For a crack set:**

$$\Delta\boldsymbol{\varepsilon}_c(\boldsymbol{\sigma}, c, \mathbf{n}) = \beta c^3 \left( \mathbf{c}^o + \mathbf{c}^s \right) \boldsymbol{\sigma} n(c, \mathbf{n}, t) \Delta c \Delta\Omega$$

$$\boxed{n(c, \mathbf{n}, t) : \text{crack number density dist.}}$$



**Fabric tensors :**

$$\mathbf{c}^o = \mathbf{b} - \nu \mathbf{a} \qquad \mathbf{c}^s = \mathbf{b} - 2\mathbf{a}$$

$$\mathbf{a} = \mathbf{n} \otimes \mathbf{n} \otimes \mathbf{n} \otimes \mathbf{n} \qquad \mathbf{b} = \mathbf{i} \wedge \mathbf{n} \otimes \mathbf{n} + \mathbf{n} \otimes \mathbf{n} \wedge \mathbf{i}$$

**Material damage:**

$$\boxed{\boldsymbol{\varepsilon}_c(\boldsymbol{\sigma}, \bar{c}) = \mathbf{D}\boldsymbol{\sigma} = \left( \mathbf{C}^o + \mathbf{C}^s \right) \boldsymbol{\sigma}} \quad \text{added compliance}$$

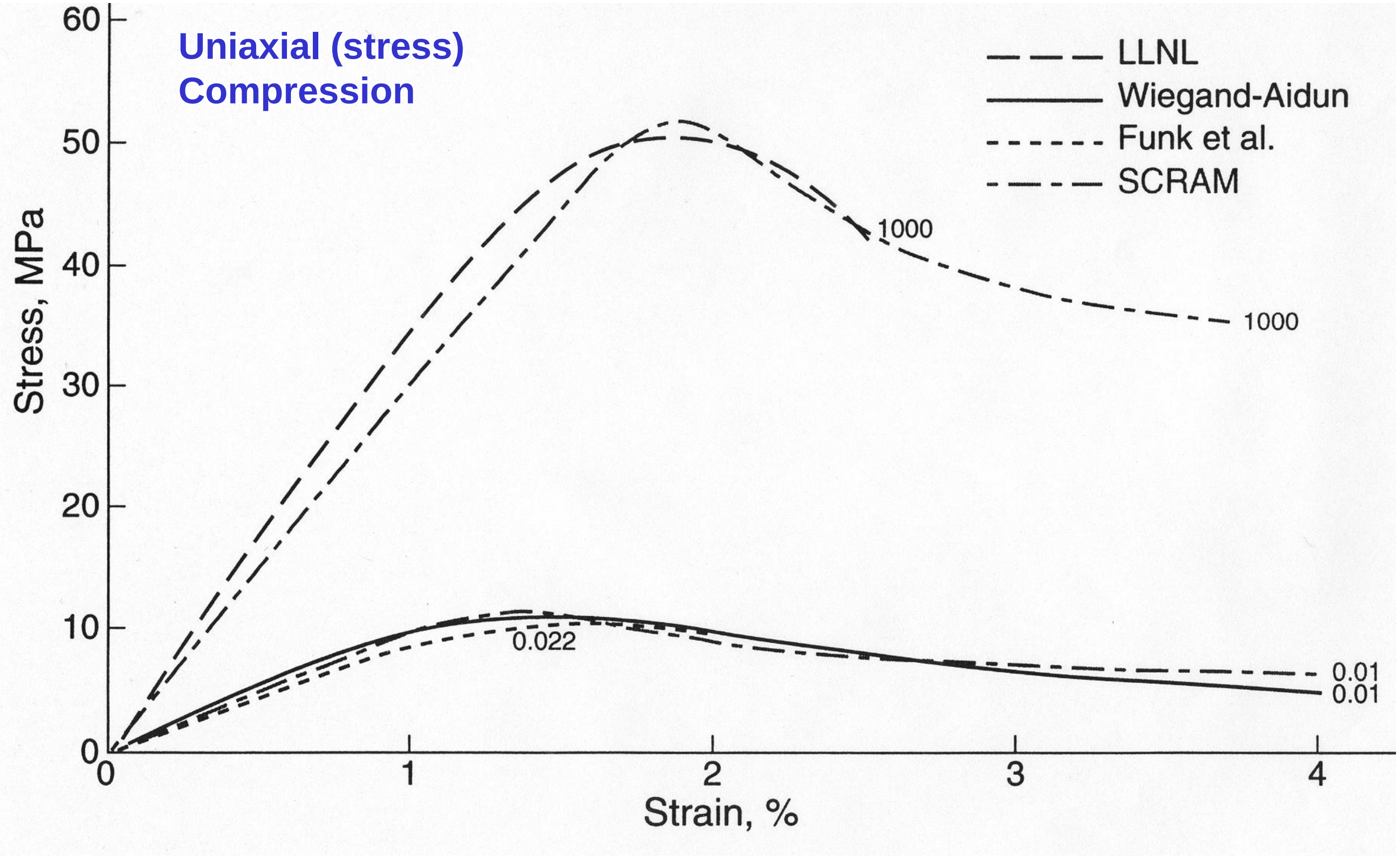
$$\mathbf{C}^o = (2 - \nu) \beta \int_\Omega \int_c n(c, \mathbf{n}, t) \mathbf{c}^o c^3 dc d\Omega \qquad \text{open cracks}$$

$$\mathbf{C}^s = \beta \int_\Omega \int_c n(c, \mathbf{n}, t) \mathbf{c}^s c^3 dc d\Omega \qquad \text{shear cracks}$$

# Model calculations and data
# (explosives & ceramics)

# Comparison of the Stress-Strain Responses with Data

**PBX (Plastic- Bonded eXplosive) 9501**
**at two strain rates (0.01/s and 1000/s)**



**Uniaxial (stress)**
**Compression**

**Model captures the data, including peak stress,**
**failure strain, and strain softening**

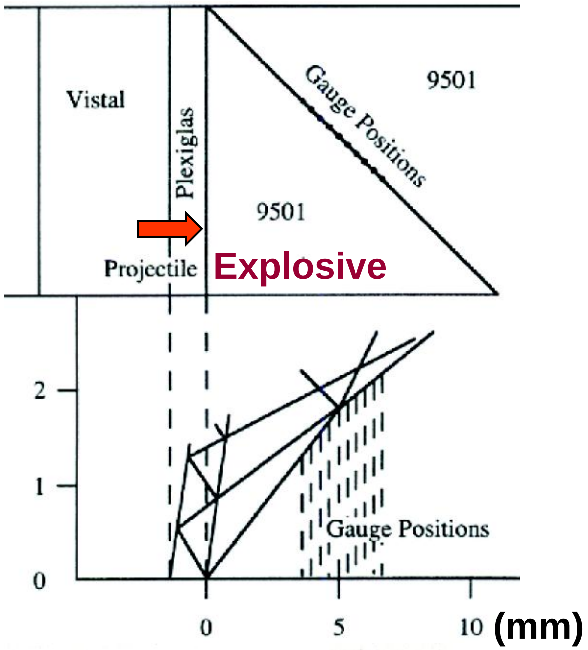
# Comparison with the Multiple-shock Experiment

- Experiment by Mulford et al. of LANL

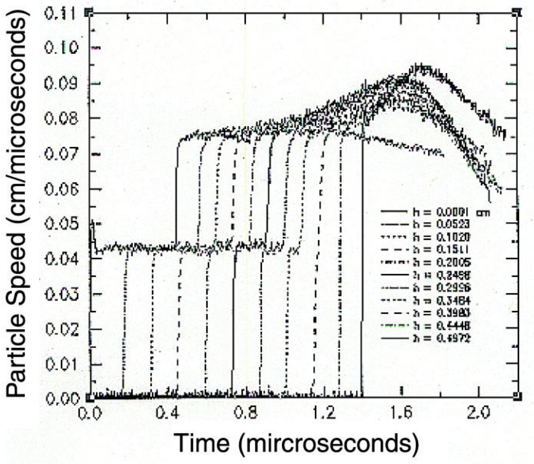
- Composite Impactor: Vistal ($Al_2O_3$) and Plexiglas (Kel-F);

- Plate thicknesses (mm):
  11 (Vistal) , 0.8 (Kel-F), 10 (HE);

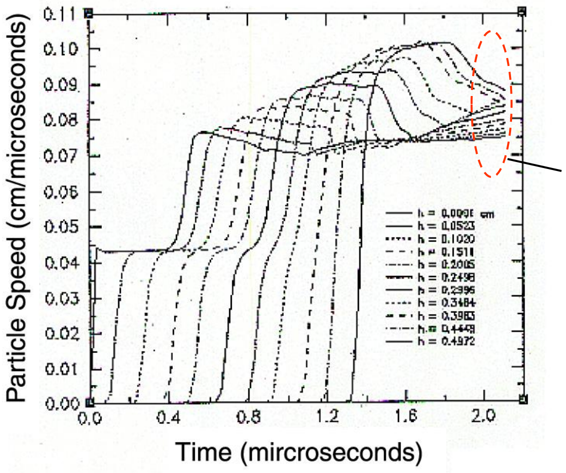
- Impact velocity: 911 m/s



Calculated particle velocity histories agree with data reasonably well.



**Measured**

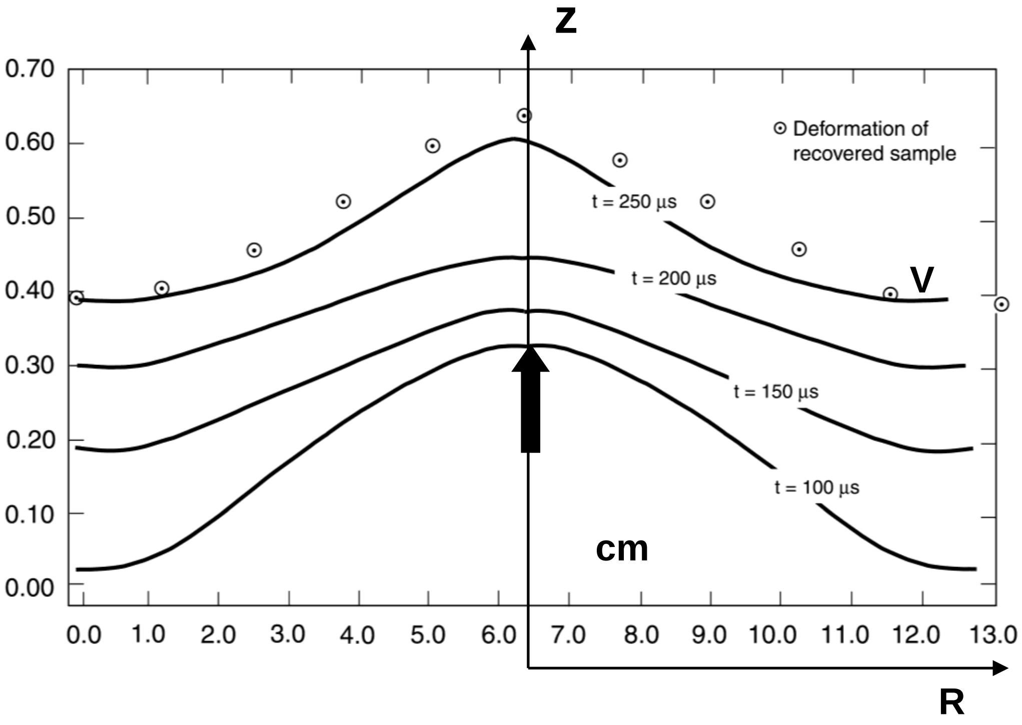


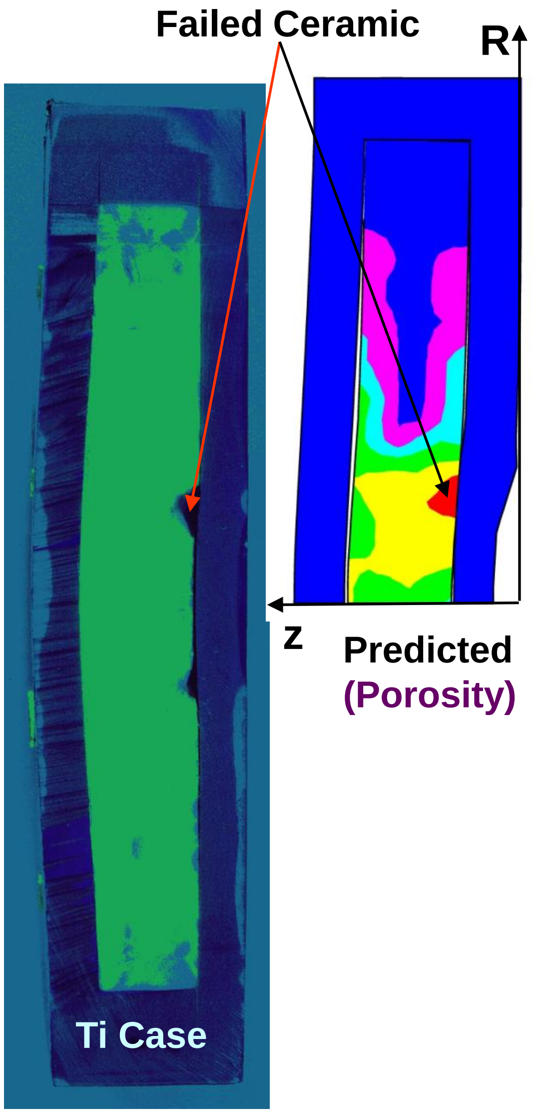
**Calculated**

EOS!

# Modeling Damage and Failure of Ceramic Armor

## Comparison





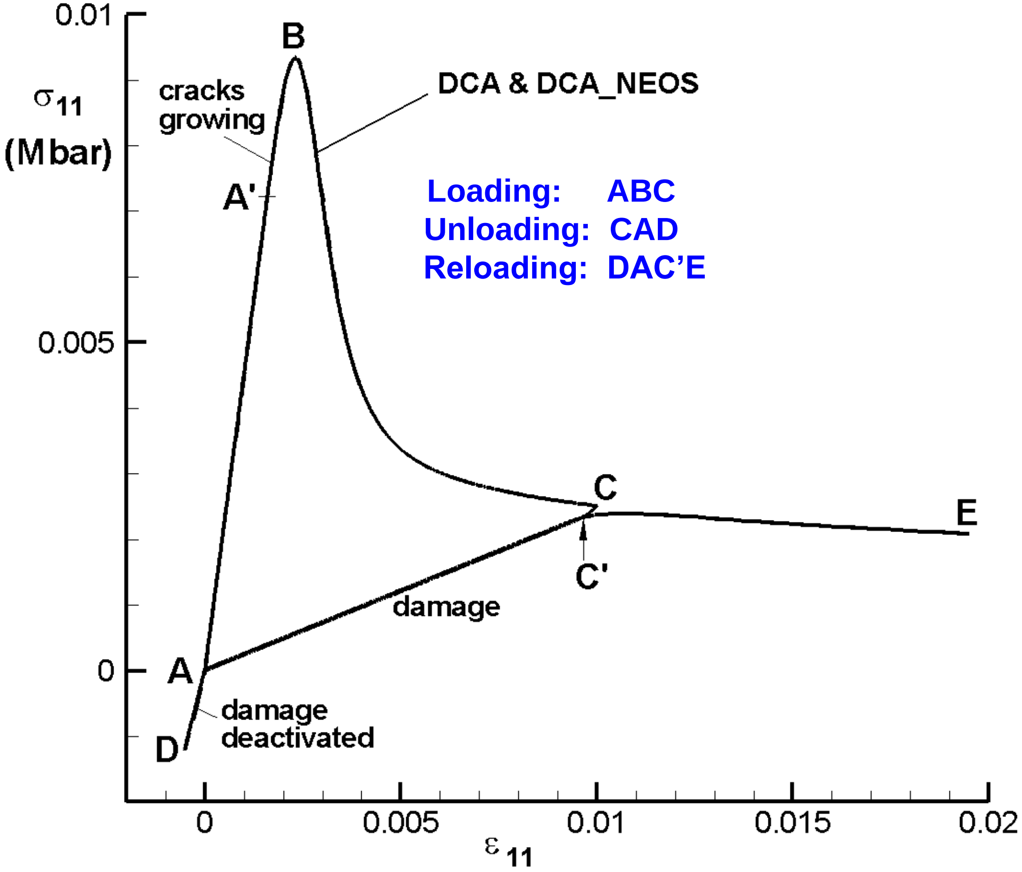
**Predicted**
**(Porosity)**

**Sectioned Post-Mortem sample**

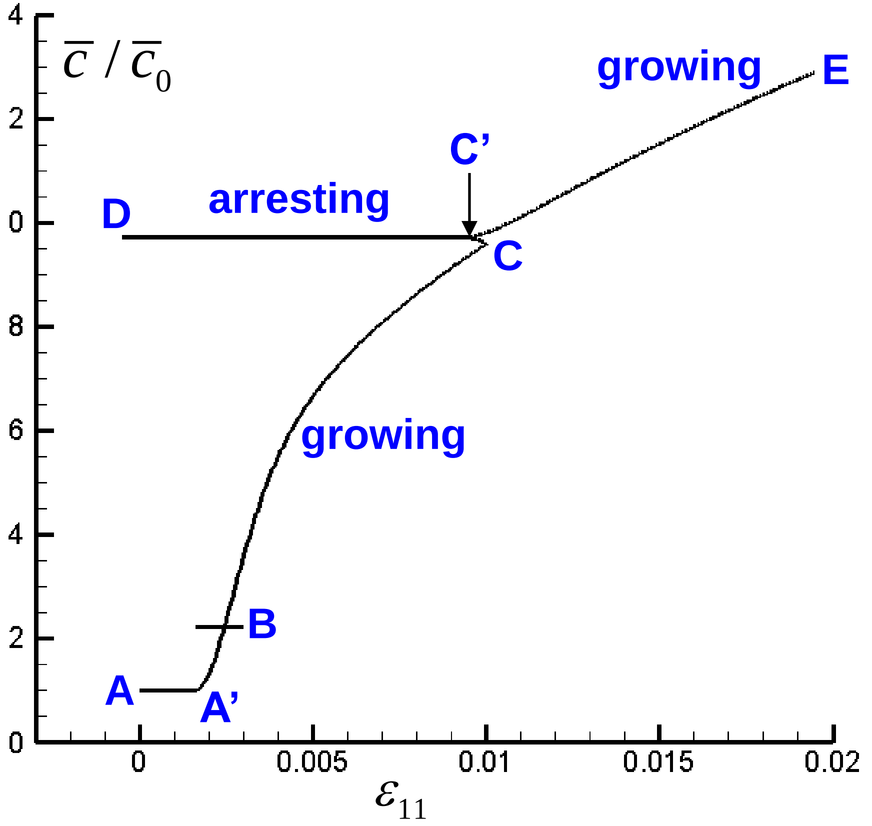
- **Model calculation matches the deformed profile**

- **Calculated location of failure (maximum porosity) agrees with the post-mortem observation**

# *Uniaxial Strain* – Cyclic loading Tension/Compression- I

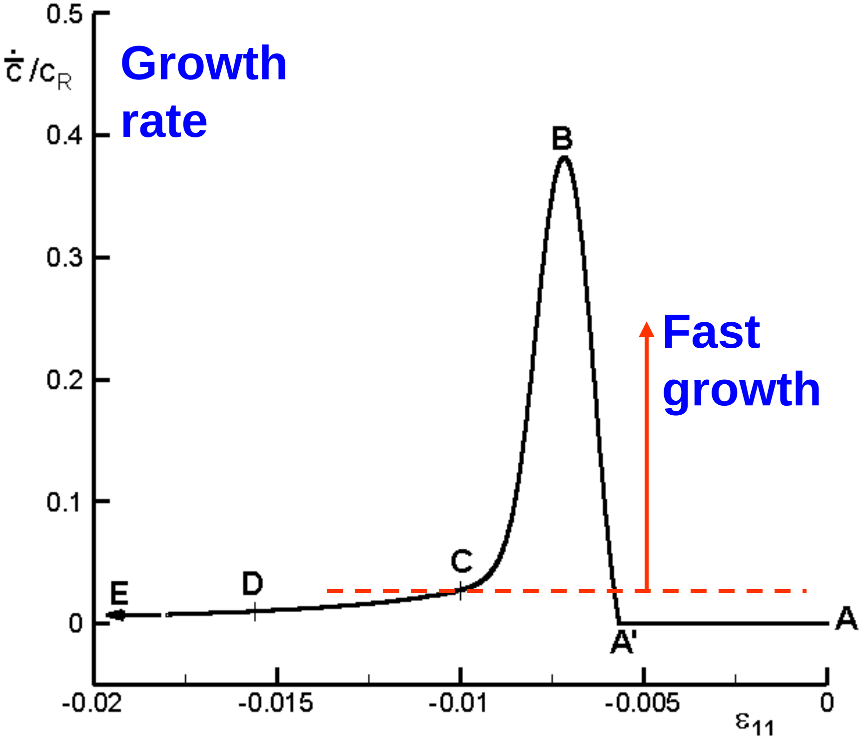


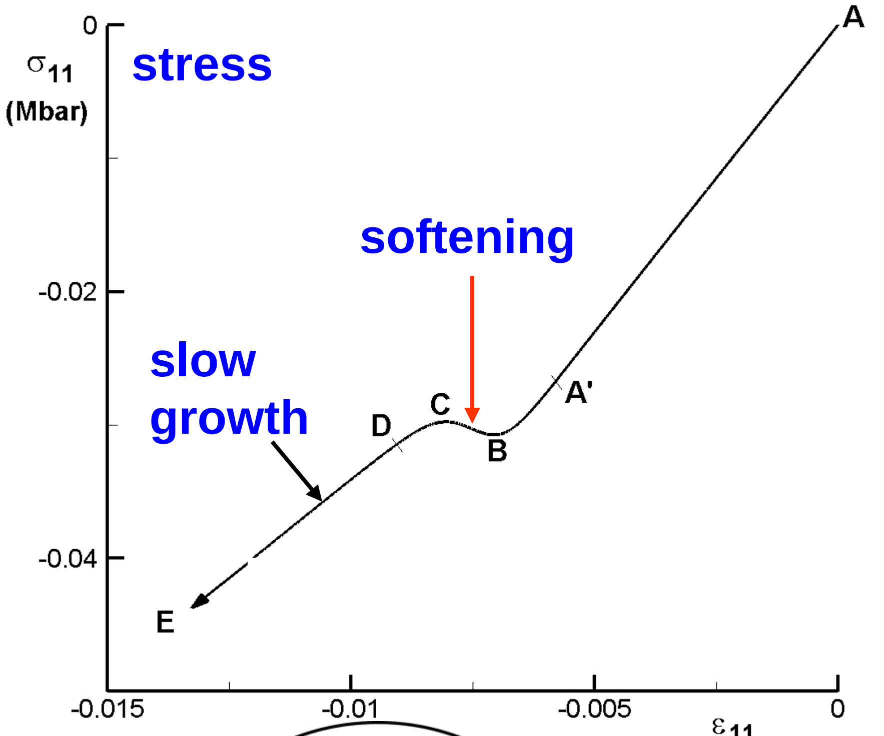
Stress-strain



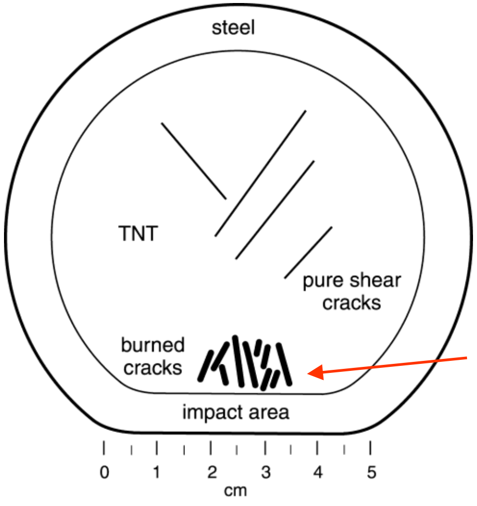
Evolution of crack size

# Crack growth under *Uniaxial* strain compression



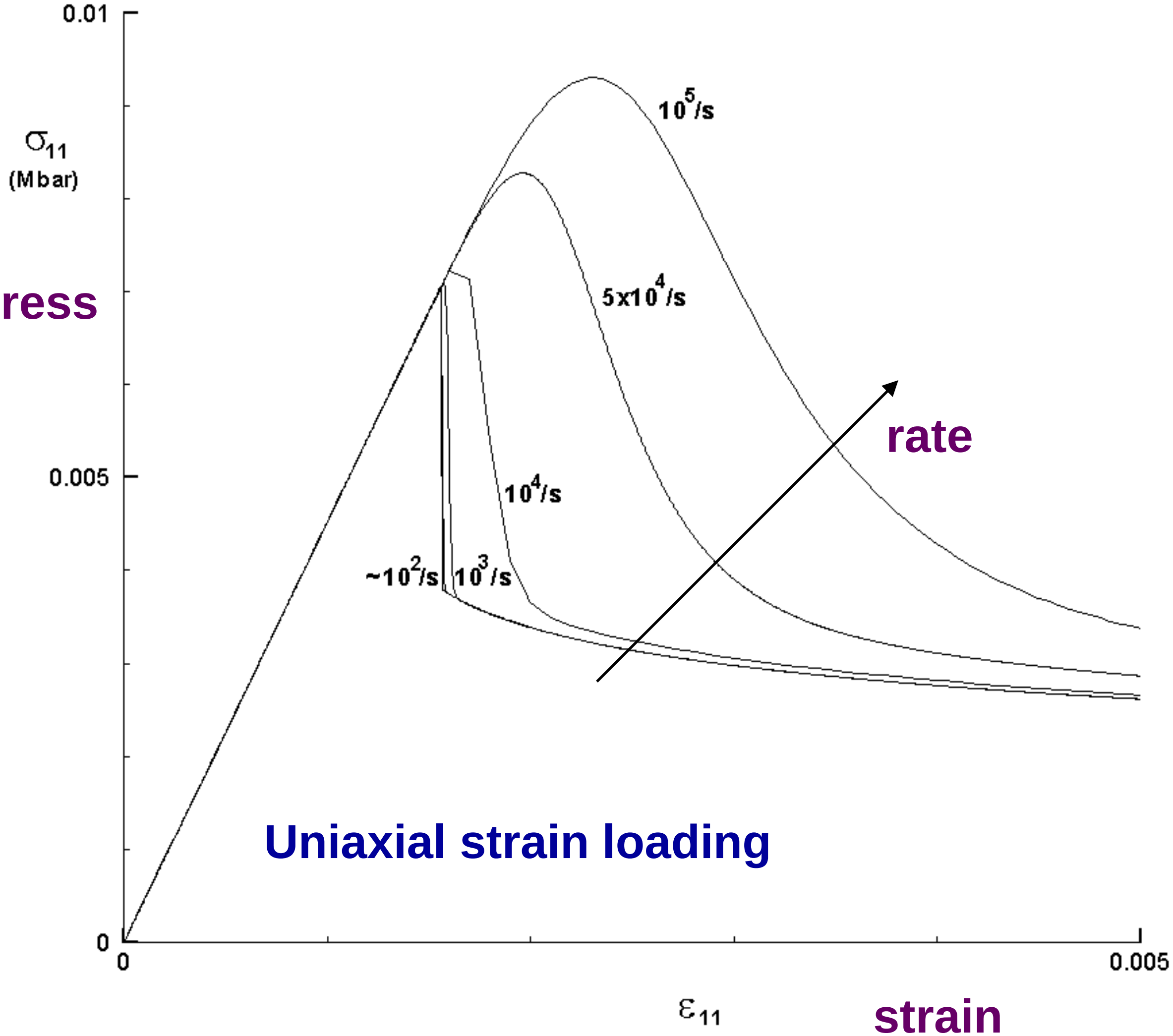


- Cracks becomes un*stable*
when shear overcomes friction;
- Damage accumulates over a period;
- Stabilized as friction (pressure) takes over



Growth of shear Cracks

# Rate Effects



Stress

rate

Uniaxial strain loading

strain

# Summary/Discussions

- **SCRAM: three-dimensional framework for anisotropic damage & failure of *brittle* materials. It also models the *initiation* of chemical reactions (*explosion*) of energetic materials.**

- **DCA: based on SCRAM model but is significantly simpler. It emphasizes on the growth of dominate (critical) crack. No chemical reactions.**

- **Many challenges exists both in fundamental understanding of the response of brittle materials under high rate conditions and in the representation in analysis (*continuum-level*) codes.**

# Extra: Supporting Modeling

# ISO-SCM Model (Addessio-Johnson)

- A continuum damage model based on Dienes' SCM work.
- Key assumptions/limitations: distribution of cracks remain isotropic. Damage is also isotropic.
- The size distribution remains exponential (Seaman et al, SRI), with the mean crack size (damage) evolving with loading.
- Simple damage surface based on averaging the instability conditions over all crack orientations. Damage surface is discontinuous at $p=0$.
- The crack strain is a simple function of stress and mean crack size. Crack opening strain accounted for $p<0$ (tension) only.

# Crack Shear and Opening

- **Exponential crack size (radius) distribution (Seaman et al, SRI):**

$$n(c,\mathbf{n},t)=\frac{N_0(\mathbf{n})}{\bar{c}(\mathbf{n},t)}\exp(-\frac{c}{\bar{c}(\mathbf{n},t)})$$

$N_0(\mathbf{n})=N_0$ **Initial crack number density (# per unit vol.); isotropic**

$\bar{c}(\mathbf{n},t)$: **Average radius of the cracks with normal (n)**

- **SCRAM accounts for material anisotropy by allowing each direction has its own mean size:** $\bar{c}(\mathbf{n},t)$ **depends on the crack normal (n)**

- **ISO-SCM (Visco-Scram, etc): the cracks remain isotropic:**

$$\bar{c}(\mathbf{n},t)=\bar{c}$$

**Crack shear strain:** $\boxed{\boldsymbol{\varepsilon}_c^s(\boldsymbol{\sigma},\bar{c})=\beta_1 d(\bar{c})\boldsymbol{\sigma}^d}$ **For any** $p$

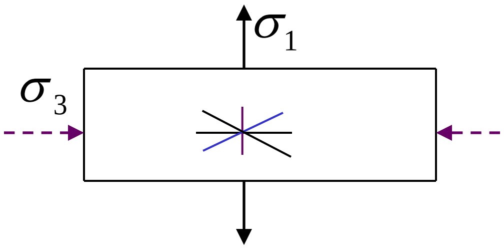
**Crack opening strain:** $\boldsymbol{\varepsilon}_c^o(\boldsymbol{\sigma},\bar{c})=(2-\nu)\beta_1 d(\bar{c})\left(\boldsymbol{\sigma}-\frac{3}{2}p\mathbf{i}\right)$ **For** $p<0$

$\boldsymbol{\varepsilon}_c^o(\boldsymbol{\sigma},\bar{c})=0$ **For** $p\geq 0$

$$\beta_1=\frac{64}{5G}\frac{1-\nu}{2-\nu};\qquad d(\bar{c})\equiv N_0\bar{c}^3$$ **-damage**

# Dominant Crack Model (DCA)

## - Crack Opening strain



**Mixed stress states:** $\sigma_1 > 0; \sigma_3 < 0$

**Only the directions with** $\sigma_n \equiv \mathbf{n} \bullet \boldsymbol{\sigma}\mathbf{n} > 0$ **should contribute**

**ISO-SCM:**

$$p = -\frac{\sigma_1 + \sigma_2 + \sigma_3}{3}$$

$p < 0$, **All directions contribute** $\qquad \boldsymbol{\varepsilon}_c^o(\boldsymbol{\sigma}, \bar{c}) = 2\beta_1 D(\bar{c})\left(\boldsymbol{\sigma} + \frac{1}{2} tr(\boldsymbol{\sigma})\mathbf{i}\right)$

$p \geq 0$, **No direction contributes** $\qquad \boldsymbol{\varepsilon}_c^o(\boldsymbol{\sigma}, \bar{c}) = \mathbf{0}$

**"Improved":**

$$\boxed{\boldsymbol{\varepsilon}_c^o(\boldsymbol{\sigma}, \bar{c}) = 2\beta_1 D(\bar{c})\mathbf{P}^+\left(\mathbf{P}^d + \frac{5}{2}\mathbf{P}^{sp}\right)\mathbf{P}^+\boldsymbol{\sigma}}$$

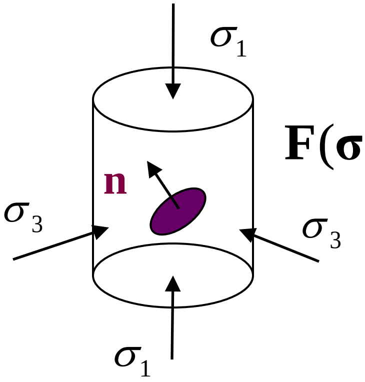
**Projection operators:** $\mathbf{P}^{sp} = \frac{1}{3}\mathbf{i} \otimes \mathbf{i} \quad \mathbf{P}^d = \mathbf{I} - \mathbf{P}^{sp} \qquad \mathbf{P}^+ \equiv \mathbf{Q}^+ \wedge \mathbf{Q}^+$

**Positive spectral tensor:** $\mathbf{Q}^+ \equiv \sum_{i=1,3} H[\sigma_i]\mathbf{e}_i \otimes \mathbf{e}_i$

$$\left.\begin{array}{l} \sigma_1 > \sigma_3 > 0 \\ 0 > \sigma_1 > \sigma_3 \end{array}\right\} \Rightarrow$$ **ISO-SCM!**

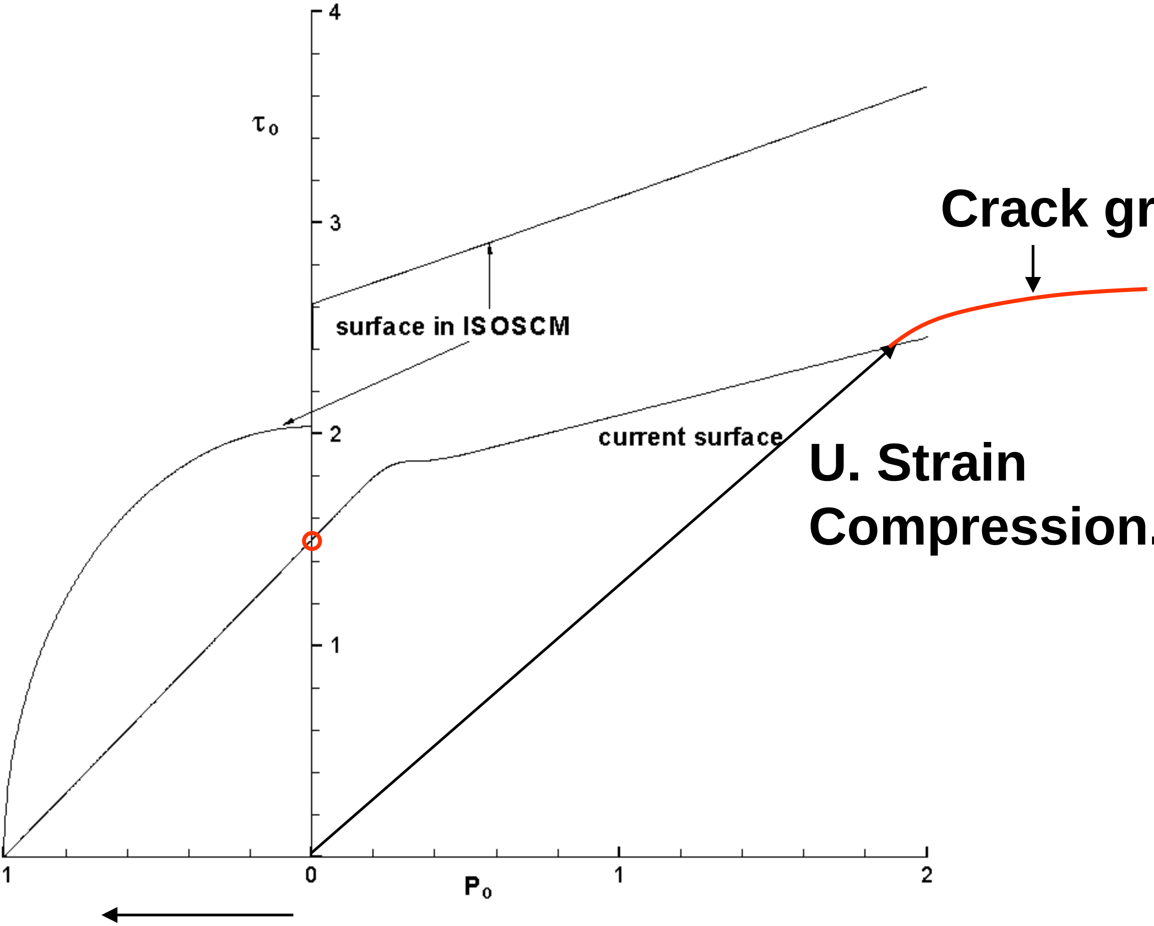
**Only tensile principal stresses contribute to open strain**

# Comparison of the Damage Surfaces



$$\mathbf{F}(\boldsymbol{\sigma},\bar{\mathbf{c}}) \equiv g(\boldsymbol{\sigma},\mathbf{n}^{c},\bar{\mathbf{c}})/2\gamma - 1 \Rightarrow$$

**Dam. Surf.** $\mathbf{F}(\boldsymbol{\sigma},\bar{\mathbf{c}}) = \mathbf{0}$



**Crack growth**

**U. Strain Compression.**

**Tensile**

**New damage surface is similar to that in ISO-SCM, but it is continuous.**

# Evolution equation for damage (Crack growth rate)

**Dam. Surf.** $F(\boldsymbol{\sigma},\bar{c})=0$

**Damage increases for stress state outside the surface** $(\mathbf{F}(\boldsymbol{\sigma},\bar{\mathbf{c}})>\mathbf{0})$:

**Dynamic crack growth (Freund, 1990):**

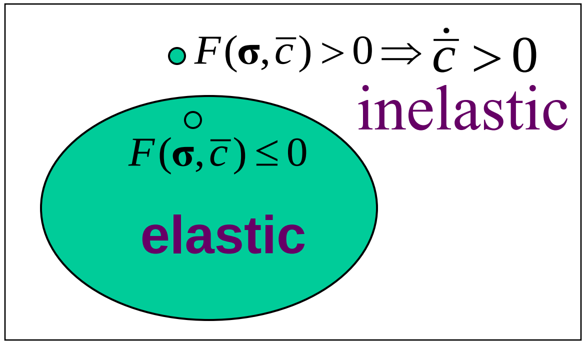
$$\dot{\bar{c}}=\dot{c}_{\max}\left(1-\frac{2\gamma}{g(\boldsymbol{\sigma},\mathbf{n}^{c},\bar{c})}\right)$$

$\dot{c}_{\max}$ : **Terminal growth speed (Rayleigh wave speed)**

**Damage function is also based on** $g(\boldsymbol{\sigma},\mathbf{n}^{c},\bar{c}):\left(F(\boldsymbol{\sigma},\bar{c})\equiv\frac{g(\boldsymbol{\sigma},\mathbf{n}^{c},\bar{c})}{2\gamma}-1\right)$

**Crack growth is related to the damage function:**

$$\boxed{\dot{\bar{c}}=\dot{c}_{\max}\left(1-\frac{1}{1+\left\langle F(\boldsymbol{\sigma},\bar{c})\right\rangle}\right)}$$



# Stress-strain Relationship

**Given a total (applied) strain rate, we need to update stress and damage.**

**Recall:**

$$\boldsymbol{\varepsilon} = \left(\mathbf{C}^m + \mathbf{D}(\bar{c})\right)\boldsymbol{\sigma}$$

**Damage:**

$$\mathbf{D}(\bar{c}) = \beta^e N_0 \bar{c}^3 \left( \frac{3}{2-\nu}\mathbf{P}^d + \mathbf{P}^+ \left( \mathbf{P}^d + \frac{5}{2}\mathbf{P}^{sp} \right) \mathbf{P}^+ \right)$$

**Rate form:**

$$\dot{\boldsymbol{\varepsilon}} = \mathbf{C}^m \dot{\boldsymbol{\sigma}} + \left[ \mathbf{D}(\bar{c})\dot{\boldsymbol{\sigma}} + \dot{\mathbf{D}}(\bar{c})\boldsymbol{\sigma} \right] = \mathbf{C}^m \dot{\boldsymbol{\sigma}} + \left[ \underbrace{\dot{\boldsymbol{\varepsilon}}^c}_{\text{Stationary}} + \underbrace{\dot{\boldsymbol{\varepsilon}}^{gr}}_{\text{Crack growth}} \right] \quad \textbf{(1)}$$

**strain rate due to crack growth:**

$$\boxed{\dot{\boldsymbol{\varepsilon}}_c^{gr} = \dot{\mathbf{D}}(\bar{c})\boldsymbol{\sigma} = \left(3\dot{\bar{c}}/\bar{c}\right)\mathbf{D}(\bar{c})\boldsymbol{\sigma}}$$

**Stress rate:**

$$\dot{\boldsymbol{\sigma}} = -\dot{P}\mathbf{i} + \dot{\mathbf{s}}$$

coupling

**Deviatoric rate:**

$$\mathbf{P}^d \,\text{Eq.(1)} \Rightarrow \quad \frac{1}{2G_s}\dot{\mathbf{s}} + \mathbf{P}^d \mathbf{D}(\bar{c})\left(\dot{\mathbf{s}} - \boxed{\dot{P}\mathbf{i}}\right) + \dot{\bar{c}}\frac{3}{\bar{c}}\mathbf{P}^d \mathbf{D}(\bar{c})\left(\mathbf{s} - \boxed{P\mathbf{i}}\right) = \dot{\mathbf{e}} \quad \textbf{(2a)}$$

$$\dot{P}\,?$$

**Deganis, L.E. and Q.H. Zuo (2011), JAP, 109, 073504**

# Volumetric Response

**Pressure in the porous (voided) material**

$$P(\phi,\rho,e)=(1-\phi)P_s(\rho_s,e_s)$$

**Mie-Gruneisen equation of state (Addessio and Johnson, 1990)**

**The porosity:**

$$\phi\equiv\frac{V_v}{V_s+V_v}$$

**Pressure in the solid:**

$$P_s(\rho_s,e_s)=P_H(\mu_s)\left(1-\frac{1}{2}\Gamma_s\mu_s\right)+\Gamma_s\rho_s e_s$$

**Hugoniot Pressure:**

$$P_H(\mu_s)=c_v\mu_s+\boxed{d_v\mu_s^2+s_v\mu_s^3}$$

**Nonlinear effect**

**Compression ratio:**

$$\mu_s\equiv\frac{\rho_s}{\rho_{s0}}-1$$

**Porosity evolution:**

$$\boxed{\dot\phi=(1-\phi)\left(\dot\varepsilon_{kk}^{c}+\dot\varepsilon_{kk}^{gr}\right)}$$

**TEPLA model:**

$$\dot\phi=(1-\phi)\dot\varepsilon_{kk}^{p}$$

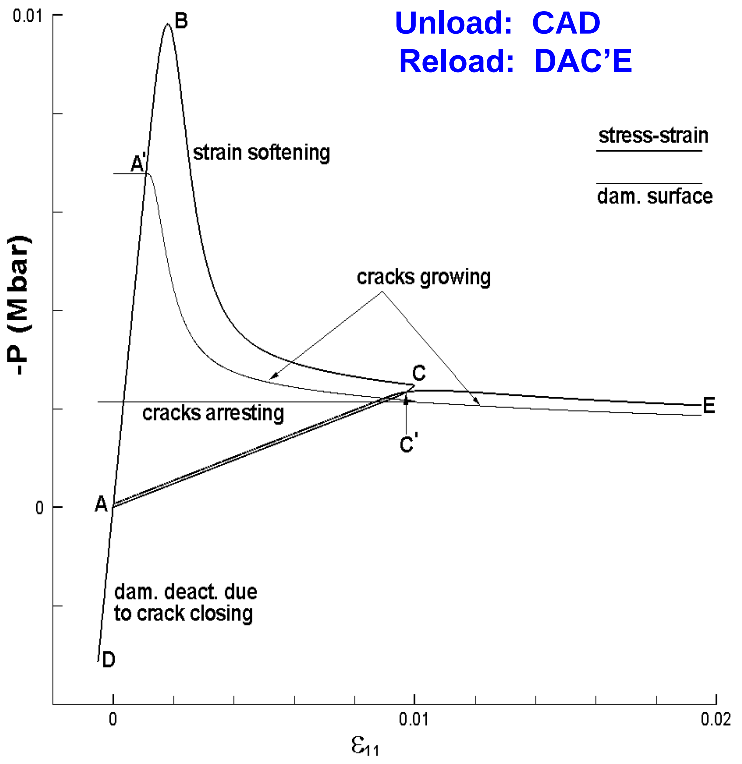
**Rate form:**

$$\boxed{\dot P(\phi,\rho,e)=-B\dot\varepsilon_{kk}+\alpha\left(\dot\varepsilon_{kk}^{c}+\dot\varepsilon_{kk}^{gr}\right)+\Gamma_s\mathbf{s}:\dot{\mathbf{e}}}\quad\text{(2b)}$$

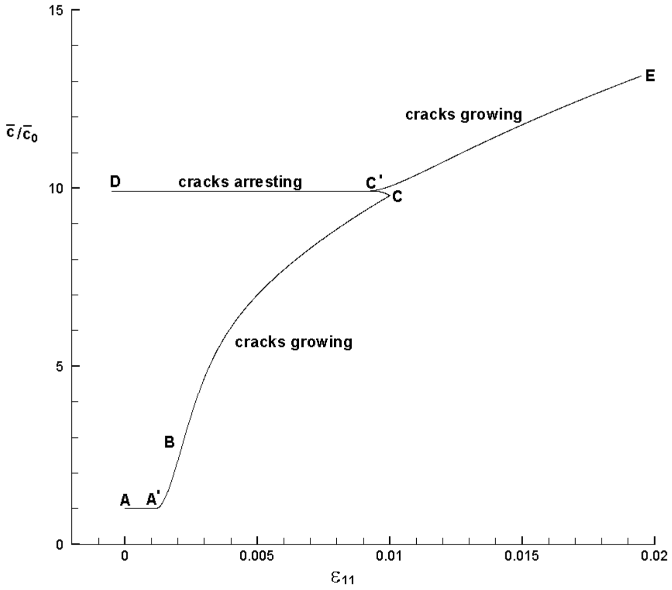
**stationary**

# Vol. Tension/Compression

**Load: ABC**
**Unload: CAD**
**Reload: DAC'E**

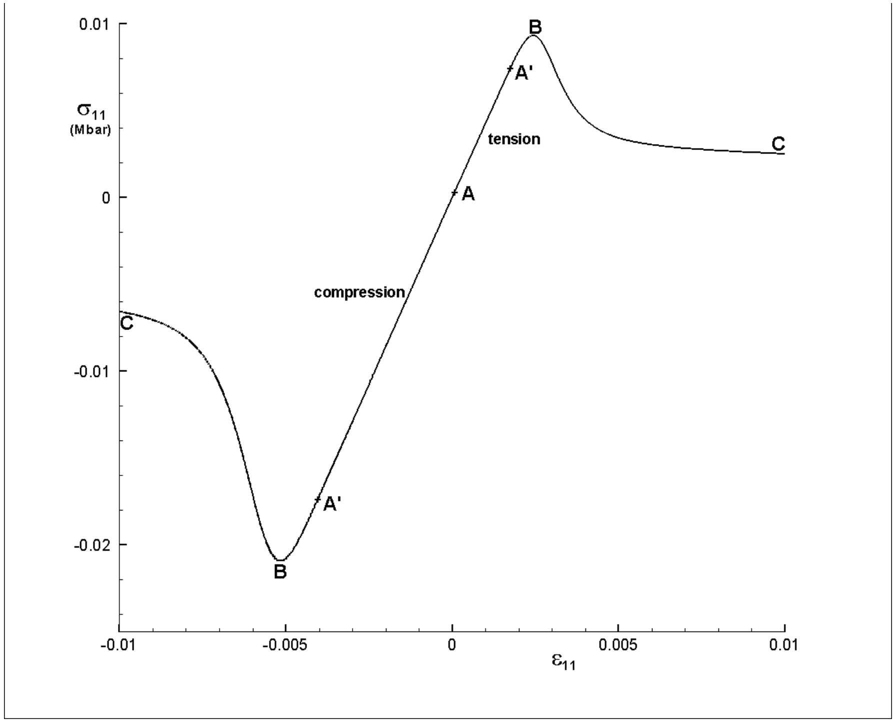


**Pressure-strain**



**Evolution of damage**

# Uniaxial (stress) tension and compression

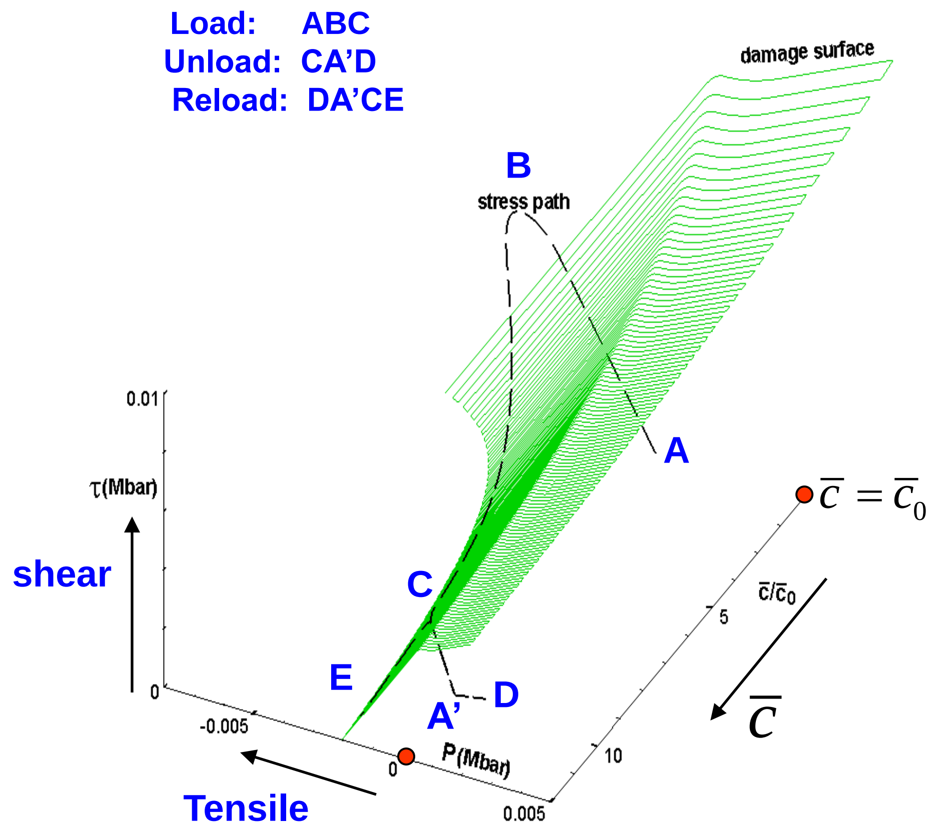


Stress-strain

**Compression is much stronger than tension**

$$\sigma_c / \sigma_t = 2\sqrt{1-\nu/2}\left(\sqrt{\mu^2+1}+\mu\right)$$

# Damage Surface and Stress path



**The damage surface is continuous;**

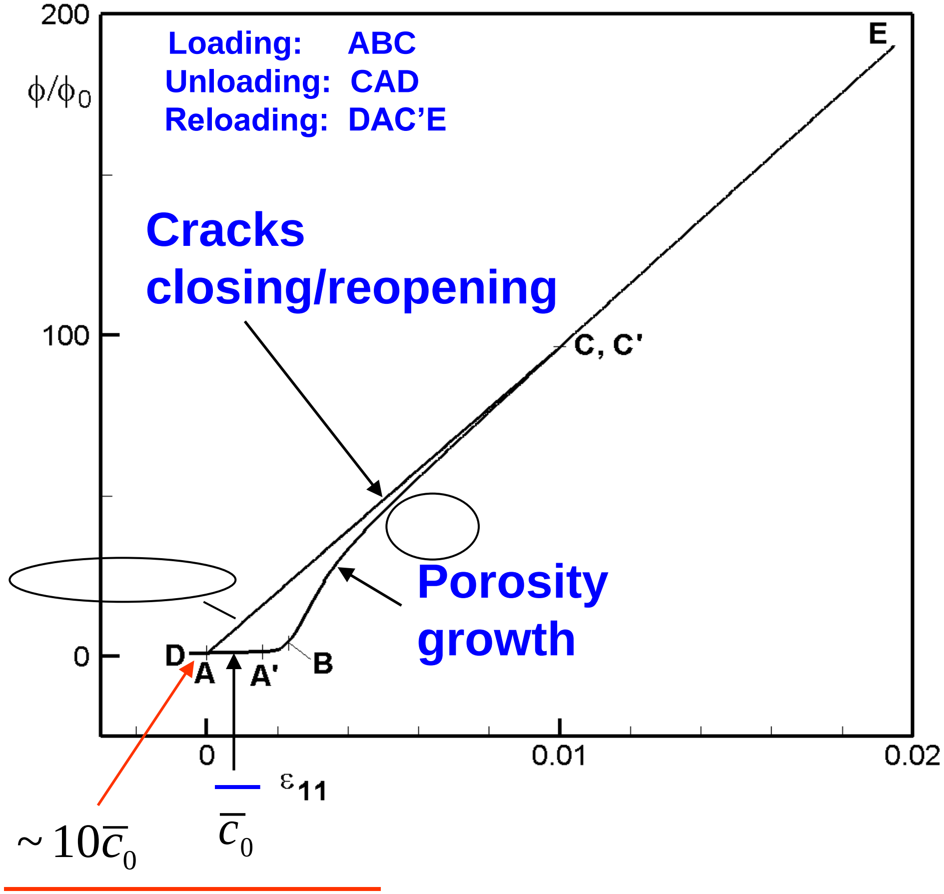
**Size of the damage surface (in stress space) shrinks as cracks grow;**

**Stress path is above the damage surface, due to rate effects;**

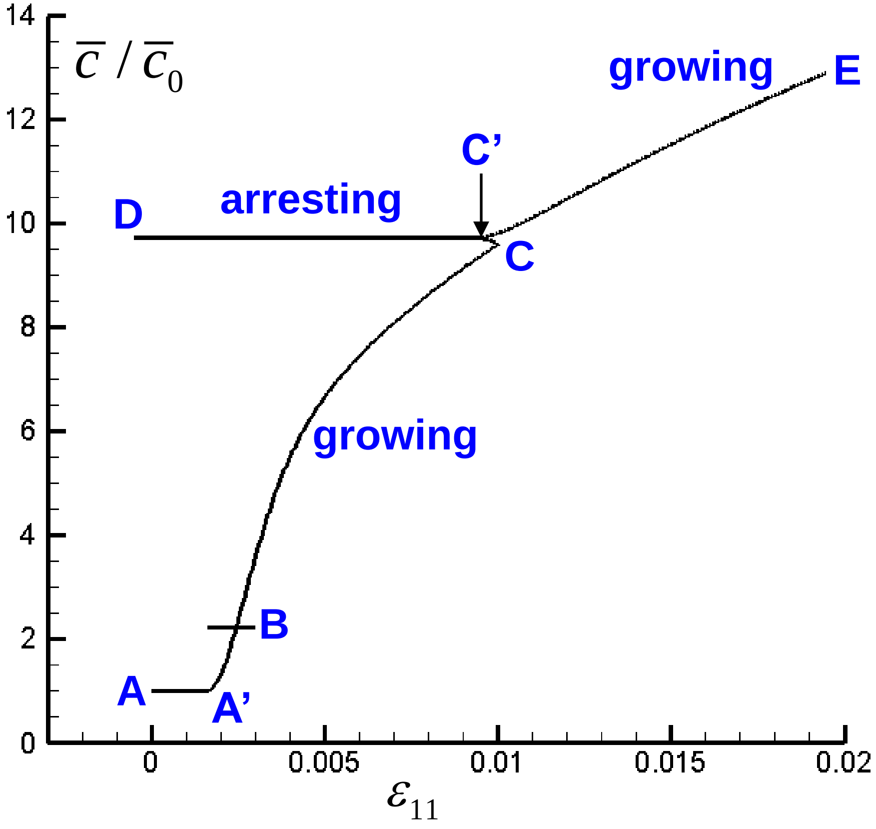
**Pronounced strain softening right after the stress peak.**

**Uniaxial (strain) Tension loading**

# Cyclic loading - II

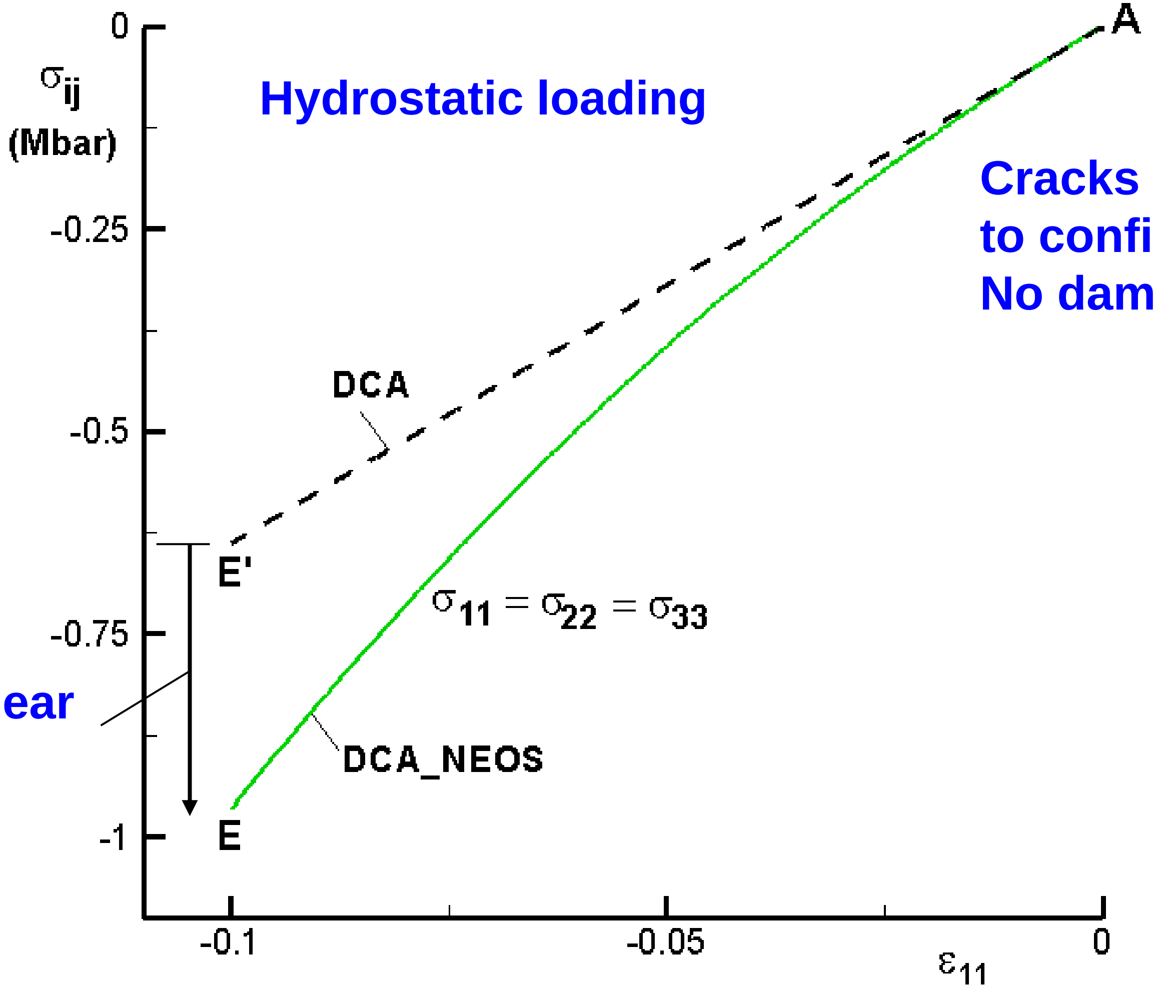


Evolution of porosity



Evolution of crack size

# Large strain (10%) compression: *Hydrostatic* Loading

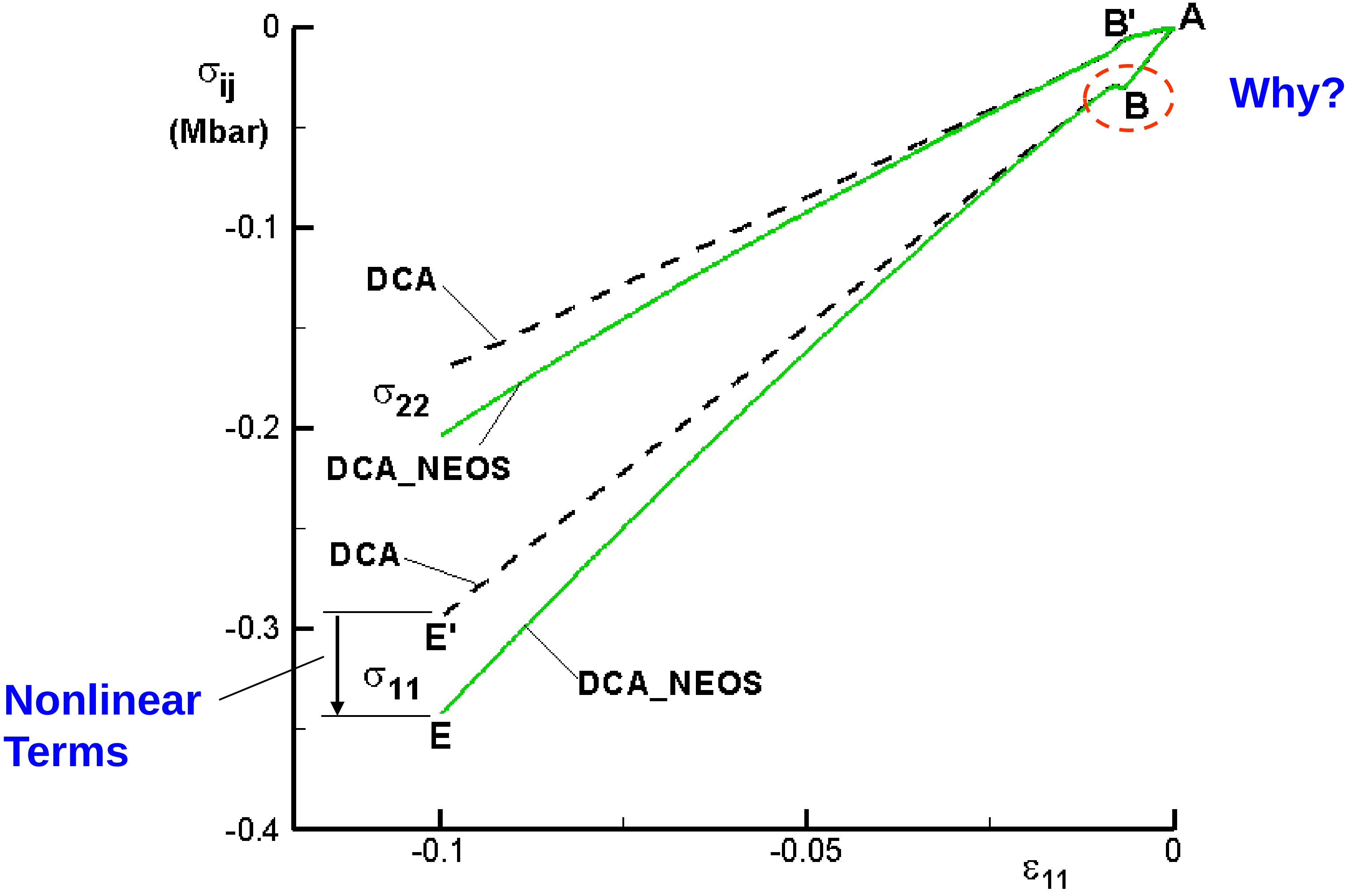


**Hydrostatic loading**

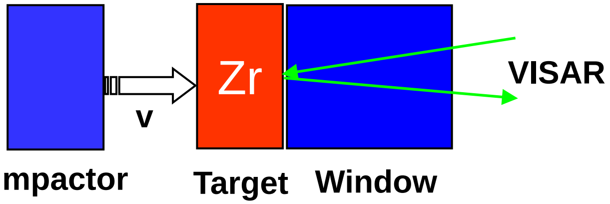
**Cracks remain stable due to confinement:**
**No damage accumulation**

**Nonlinear Terms**

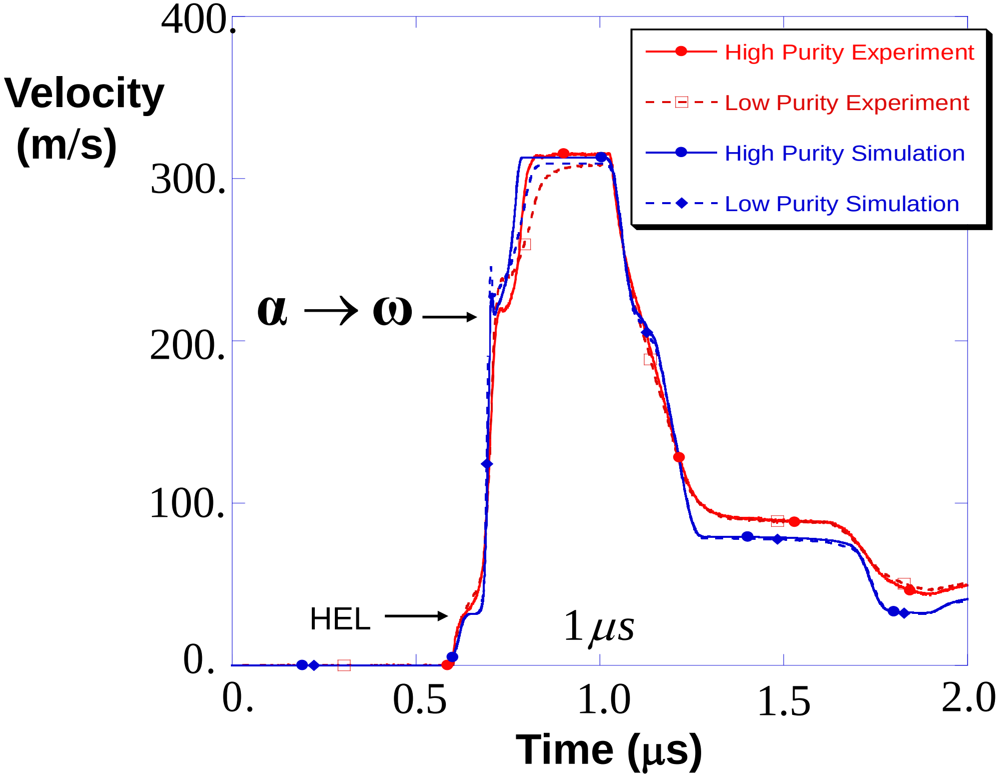
# Large strain compression:
# *Uniaxial* strain



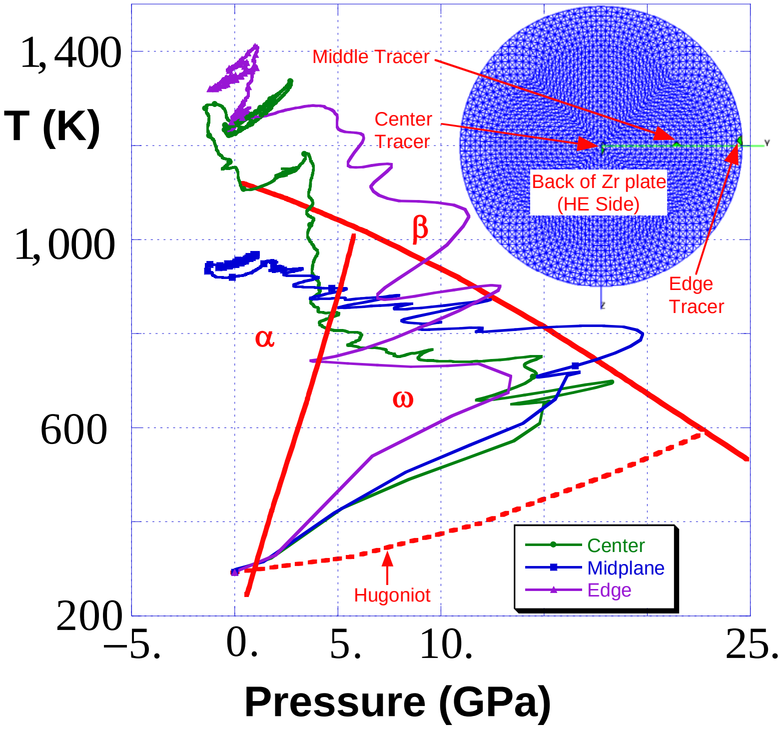
# Multiphase Plasticity Model for Zirconium



**sapphire impactor; v=658 m/s**



## The phase diagram of Zr



**That the material experiences all three phases can have important implications…**