Gradient and Fractional/Fractal Aspects of Material Modeling

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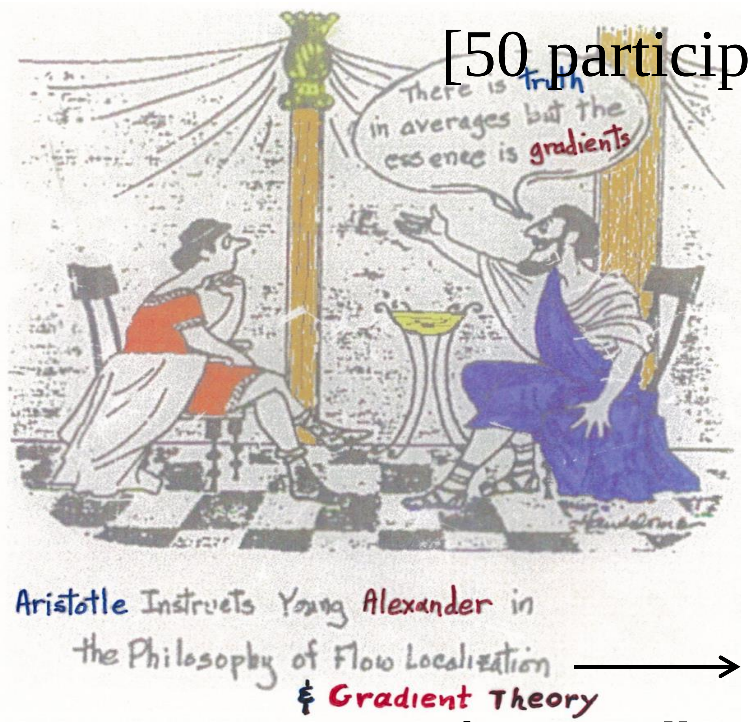
■ Appendix

A Cartoon from Aristotle's 1990 Conference

[50 participants from USSR]



→ *Owen Richmond (ALCOA) / Lev Pitaevskii (RAS)*

ECA Gradient Models

- ***Gradient Elasticity (GradEla)***
- ***Gradient Diffusion (GradDif)***
- ***Gradient Plasticity (GradPla)***

Note1: Quotation from Smalley (Nobel Prize 1996)

"*The Laws of **Continuum Mechanics** are amazingly robust for treating even intrinsically discrete objects only a few atoms in diameter*" [American Scientist **85**, 324-337, 1997]

Note2: ECA Modification (1984/87; 1992)

Gradient Continuum Mechanics [J. Eng. Mat. Tech. **106**, 326-330,1984; Int. J. Plast. **3**, 211-247, 1987; Int. J. Eng. Sci. **30**, 1279-1299, 1992]

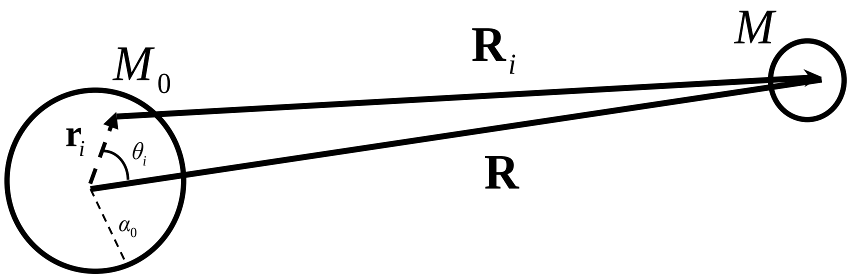
Note3: Gradient Gravitation Mechanics

Appendix: On Gradient Gravitation

■ Gradient Enhancement of Newton's Law

- ***Newton's Law***

$$\boldsymbol{F} = \frac{GM_0 M}{R^3}\boldsymbol{R} = \frac{GM_0 M}{R^2}\boldsymbol{e_R}; \quad \boldsymbol{e_R} = \frac{\boldsymbol{R}}{R}$$



- ***Distributed Mass***

$$M_0 = \sum_i m_i = \int_V \rho\, dV; \; \mathbf{f} = \sum_i \mathbf{f}_i = GM\sum_i \frac{m_i}{R_i^2}\boldsymbol{e}_{\boldsymbol{R}_i} = GM\int_V \frac{\rho(\mathbf{r}_i)}{R_i^2}\boldsymbol{e}_{\boldsymbol{R}_i}\, dV$$

- ***Radial Approximation***

$$\frac{\boldsymbol{e}_{\boldsymbol{R}_i}}{R_i^2} \approx \frac{1}{R^2}\left(\boldsymbol{e_R} - \frac{\mathbf{r}_i}{R}\right) \quad \Rightarrow \quad \mathbf{f} \approx \frac{GM}{R^2}\int_V \rho(\mathbf{r}_i)\left(\boldsymbol{e_R} - \frac{\mathbf{r}_i}{R}\right) dV$$

- ***Gradient Approximation***

$$\rho(\mathbf{r}_i) \approx \rho(0) + \mathbf{r}_i \cdot \nabla \rho(0) + \frac{1}{2}\left(\mathbf{r}_i \otimes \mathbf{r}_i\right) \cdot \nabla^{(2)} \rho(0) + \ldots$$

$$\mathbf{f} \approx \frac{GM}{R^2} \int_V \left[\rho(0) + \mathbf{r}_i \cdot \nabla \rho(0) + \frac{1}{2}\left(\mathbf{r}_i \otimes \mathbf{r}_i\right) \cdot \nabla^{(2)} \rho(0) \right] (\boldsymbol{e}_{\boldsymbol{R}} - \frac{\mathbf{r}_i}{R}) dV$$

– **Letting** $\mathbf{r}_i \to \mathbf{r};\ \rho(0) \to \rho_0$

$$\therefore \mathbf{f} = \frac{GMV}{R^2} \left\{ \underbrace{[\rho_0 + \ell^2 \nabla^2 \rho_0]}_{A} \boldsymbol{e}_{\boldsymbol{R}} - \underbrace{\frac{2\ell^2}{R} \nabla \rho_0}_{B} \right\}, \quad \ell^2 = \frac{\alpha_0^2}{10}$$

– **Letting** $\int_V \rho_0 dV = M_0$ **& since** $B \ll A$**, it follows**

$$\mathbf{f} \approx \left(1 + \ell^2 \nabla^2\right) \mathbf{F} \quad \Rightarrow \quad \left(1 - \ell^2 \nabla^2\right) \mathbf{f} \approx \mathbf{F}$$

- ***Nonlocal Interaction Kernel***

$$f_i(\mathbf{r}) = \int G_{ij}(\mathbf{r}-\mathbf{r}')F_j(\mathbf{r}')d^3\mathbf{r}'$$

$G_{ij}(\mathbf{r}-\mathbf{r}')$: Nonlocal Interaction Kernel

- ***Fourier Transform***

[redacted]

- ***Taylor Series Expansion***

$$\tilde{G}_{ij}(\mathbf{k}) \approx G_{ij}(0) + \alpha k^2 \delta_{ij},\ \alpha = \frac{d^2 G_{ij}(0)}{dk^2},\ k = \|\mathbf{k}\|$$

- ***FT Inversion***

$$\mathbf{f} = \left(1-\ell^2\nabla^2\right)\mathbf{F},\ \ell^2 = \mathrm{sgn}(\alpha)\left|d^2 G_{ij}(0)/dk^2\right|$$

Note: $G_{ij} = \frac{\delta_{ij}}{V} \Rightarrow \tilde{G}_{ij} \approx \delta_{ij}(1-l^2k^2) \Rightarrow \mathbf{f} = \left(1+\ell^2\nabla^2\right)\mathbf{F} \Rightarrow \left(1-\ell^2\nabla^2\right)\mathbf{f} = \mathbf{F}$

- ***Gradient Gravitational Force***

- ***Governing Equation***

$$\left(1-\ell^2\nabla^2\right)\mathbf{f}=\mathbf{F};\quad \mathbf{f}=F(r)\mathbf{e}_r\,;\,\mathbf{F}=\frac{A}{r^2}\mathbf{e}_r$$

$$F-\ell^2\left(\frac{\partial^2 F}{\partial r^2}+\frac{2}{r}\frac{\partial F}{\partial r}-\frac{2F}{r^2}\right)=\frac{A}{r^2}$$

- ***Solution (F → 0 for r → ∞)***

$$F=\frac{A}{r^2}\left(1+Be^{-r/\ell}\left(1+\frac{r}{\ell}\right)\right)$$

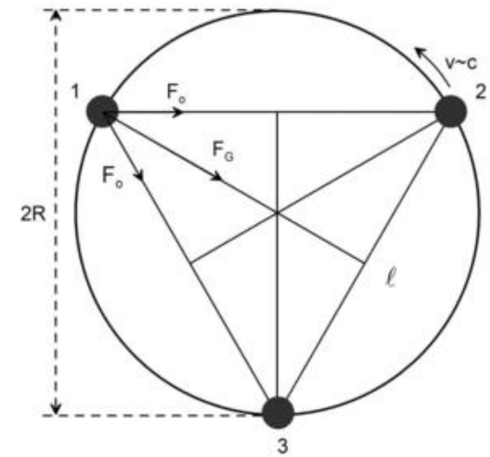
- ***Properties***
    - $r\to 0$ $\quad F=F_{SF}=\frac{AB}{r^2}\left(1-\frac{r^2}{2\ell^2}\right)\approx\frac{AB}{r^2}$ $\quad$ Strong Force?
    - $r\to\infty$ $\quad F=F_N\approx\frac{A}{r^2}$ $\quad$ Newtonian Force

- ***Note:*** $F_{SF}/F_N\approx B;\quad B\gg 1\Rightarrow F_{SF}\gg F_N$

- ***Determination of Parameters B and*** ℓ
  - ***For*** $\ell \sim r \quad F = \frac{A}{r^2}(1+\frac{2B}{e})$; for $F = F_{SF} \approx \frac{\hbar c}{r^2} \Rightarrow B \approx \frac{\hbar c}{A}$
  - ***For*** $r \ll \ell \quad F = \frac{A}{r^2}[1+B(1-\frac{r^2}{2\ell^2})] \approx \frac{AB}{r^2} \approx \frac{\hbar c}{r^2} \Rightarrow B = \frac{\hbar c}{A}$
  - ***For*** $r \gg \ell \quad F = \frac{A}{r^2}(1+Be^{-r/\ell}(1+\frac{r}{\ell})) \approx \frac{A}{r^2} \Rightarrow B$ undetermined
- ***Identification of*** ℓ
  - ***De Broglie/Relativistic*** $\quad \ell = \hbar / \gamma m_0 c \approx 6.309 \cdot 10^{-16} m$
  - ***Compton*** $\quad \ell = \hbar / m_p c \approx 2.1 \cdot 10^{-16} m$
  - ***Planck*** $\quad \ell = \sqrt{\hbar G / c^3} = 1.612 \cdot 10^{-35} m$
  - ***Schwarzschild*** $\quad \ell = 2Gm_p / c^2 = 4.48 \cdot 10^{-54} m$

Note: m_p: proton mass, m_0 : neutrino mass

■ Rotating Neutrino Model (RNM – Vayenas)



– ***De Broglie length:*** $\lambda = \dfrac{\hbar}{\gamma m_0 v}$

– ***Centrifugal Force:*** $F_C = \gamma m_0 \dfrac{v^2}{r} \approx \dfrac{\gamma m_0 c^2}{r}$

– ***Relativistic Neutrino Mass:*** $m_\nu = 3m = 3\gamma m_0$

– ***Lorentz factor γ:*** $\gamma = 1/\sqrt{1 - v^2/c^2}$

Bound RNM → Proton Mass m_p

– ***Proton Energy:*** $m_p c^2 = 3\gamma m_0 c^2 \rightarrow \gamma = m_p / 3m_0 = 7.818 \cdot 10^9$

- ***Gradient Gravitational Force***

$$F = \frac{A}{\sqrt{3}r^2}(1 + Be^{-r/\ell}(1 + \frac{r}{\ell})) = F_C = \frac{\gamma m_0 c^2}{r}; \quad A = G m_0^2 \gamma^2$$

- $r \approx \ell$:

$$B = \frac{\sqrt{3} e \gamma m_0 c^2 \ell}{2A}$$

- ***Parameter B ($\ell \sim \lambda$ …de Broglie/relativistic)***
- $\ell = \lambda$: $$B = \frac{\sqrt{3}e\gamma m_0 c^2 \lambda}{2A} = \frac{\sqrt{3}e}{2A}\frac{\gamma m_0 c^2 \hbar}{\gamma m_0 c} = \frac{\sqrt{3}e\hbar c}{2Gm_0^2\gamma^2}$$
- ***Gravitational Force***

$$F = \frac{Gm_0^2\gamma^2}{\sqrt{3}r^2}[1 + \frac{\sqrt{3}e\hbar c}{2Gm_0^2\gamma^2}e^{-r/\ell}(1+\frac{r}{\ell})]$$

$$B = \frac{\sqrt{3}e\hbar c}{2Gm_0^2\gamma^2} = 3.58\cdot 10^{39};\ \ell \approx \frac{\hbar}{\gamma m_0 c} = 6.32\cdot 10^{-16} m; F = 7.059\cdot 10^4\ \mathrm{N}$$

- ***Note: Vayenas Model***

$$F = \frac{Gm_0^2\gamma^6}{\sqrt{3}r^2} = F_C = \frac{\hbar c}{r^2}$$

$$\gamma = 3^{1/12} m_{Pl}^{1/3} m_0^{-1/3} = 7.382\cdot 10^9, \lambda = \frac{\hbar}{\gamma m_0 c} = 6.69\cdot 10^{-16}\,\mathrm{m},\ F = 7.059\cdot 10^4\ \mathrm{N}$$

Main Talk: Material Mechanics Models

■ A Unifying Ansatz

- ***Hooke's Law:*** $\boldsymbol{\sigma} = \lambda(tr\boldsymbol{\varepsilon})\mathbf{1} + 2G\boldsymbol{\varepsilon}$

$$\boldsymbol{\varepsilon} \to \frac{1}{V}\int_V G_{\boldsymbol{\varepsilon}}(|\mathbf{r}-\mathbf{r}'|)\boldsymbol{\varepsilon}(\mathbf{r}')\,dV \quad \Rightarrow \quad \boldsymbol{\varepsilon} \to \boldsymbol{\varepsilon} - l_\varepsilon^2\nabla^2\boldsymbol{\varepsilon}$$

$$\therefore \quad \boldsymbol{\sigma} = \lambda(tr\boldsymbol{\varepsilon})\mathbf{1} + 2G\boldsymbol{\varepsilon} - c\nabla^2\left[\lambda(tr\boldsymbol{\varepsilon})\mathbf{1} + 2G\boldsymbol{\varepsilon}\right] \;;\; c = l_\varepsilon^2$$

- ***Von-Mises Flow:*** $\tau = \kappa(\gamma) \;;\; \begin{cases} \tau = \frac{1}{2}\sqrt{\boldsymbol{\sigma}'\cdot\boldsymbol{\sigma}'} \;;\; \boldsymbol{\sigma}' = \boldsymbol{\sigma} - \frac{1}{3}(tr\boldsymbol{\sigma})\mathbf{1} \\ \gamma = \int \dot{\gamma}dt \;,\; \dot{\gamma} = \sqrt{2\dot{\boldsymbol{\varepsilon}}^p\cdot\dot{\boldsymbol{\varepsilon}}^p} \end{cases}$

$$\gamma \to \frac{1}{V}\int_V G_p(|\mathbf{r}-\mathbf{r}'|)\gamma(\mathbf{r}')\,dV \quad \Rightarrow \quad \gamma \to \gamma - l_p^2\nabla^2\gamma$$

$$\therefore \quad \tau = \kappa(\gamma) - c\nabla^2\gamma \;;\; c = l_p^2\kappa'(\gamma)$$

- ***Fick's Law:*** $\mathbf{j} = -D\nabla\rho$

$$\mathbf{j} \to \frac{1}{V}\int_V G_d(|\mathbf{r}-\mathbf{r}'|)\,\mathbf{j}(\mathbf{r}')\,dV \quad \Rightarrow \quad \mathbf{j} \to \mathbf{j} - l_d^2\nabla^2\mathbf{j}$$

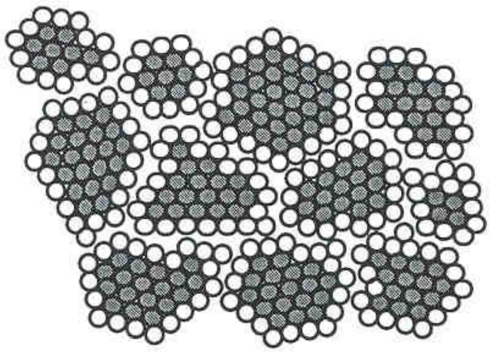
$$\therefore \quad \dot{\rho} + div\mathbf{j} = 0 \;\Rightarrow\; \dot{\rho} = D\nabla^2\rho - c\nabla^4\rho \;;\; c = l_d^2 D$$

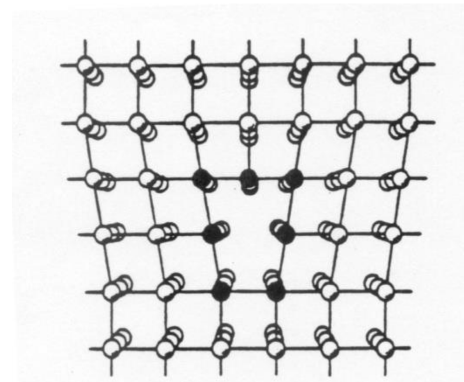
■ Motivation from Nanoscale Modeling – Nanomechanics

Traditional Polycrystals ……10 – 100 μm   Nanopolycrystals……………5 – 100 nm

Grain d

1-50 nm



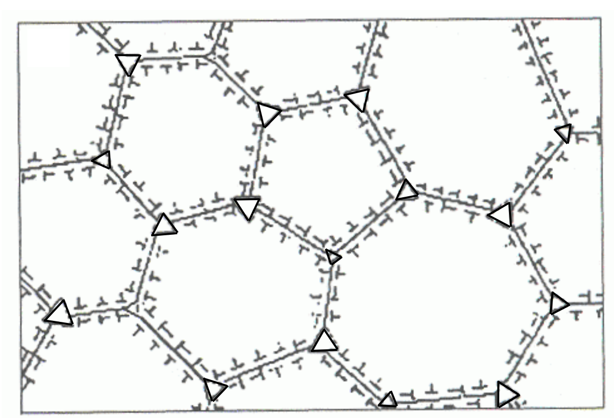


Core r_0

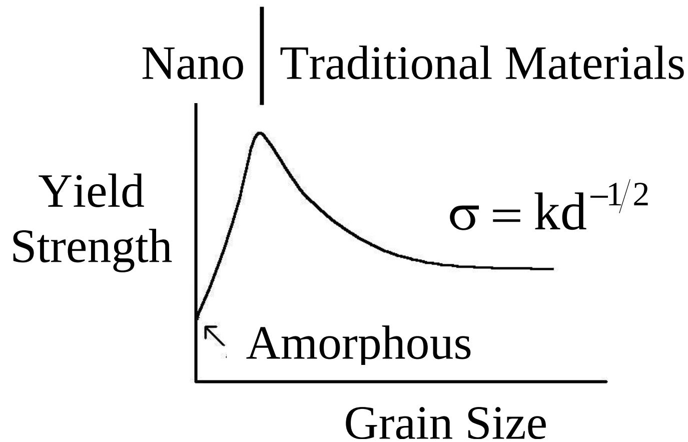
~1 nm

Grain size (d) of the same order as dislocation core (r_0)

10 nm grain size: 30% of atoms in the boundary



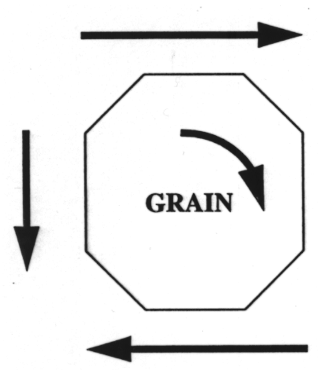
Plasticity Mechanisms ?

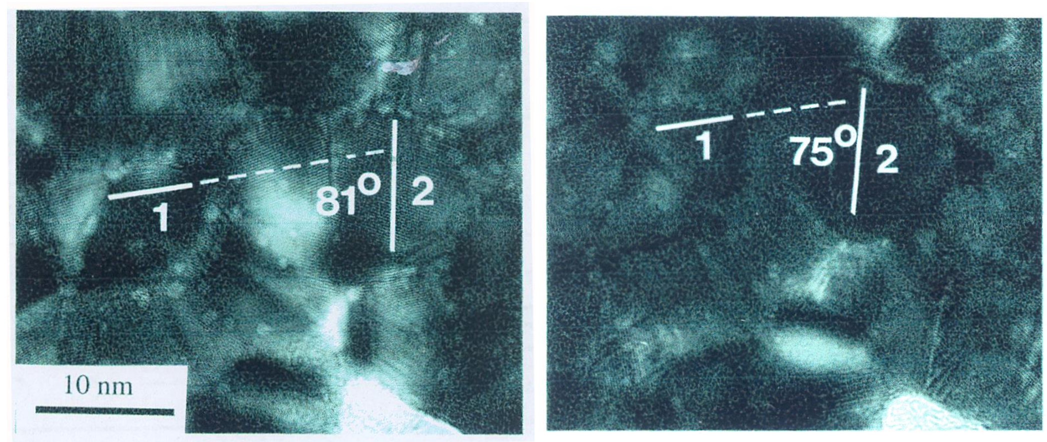


Inverse Hall-Petch Relation ?

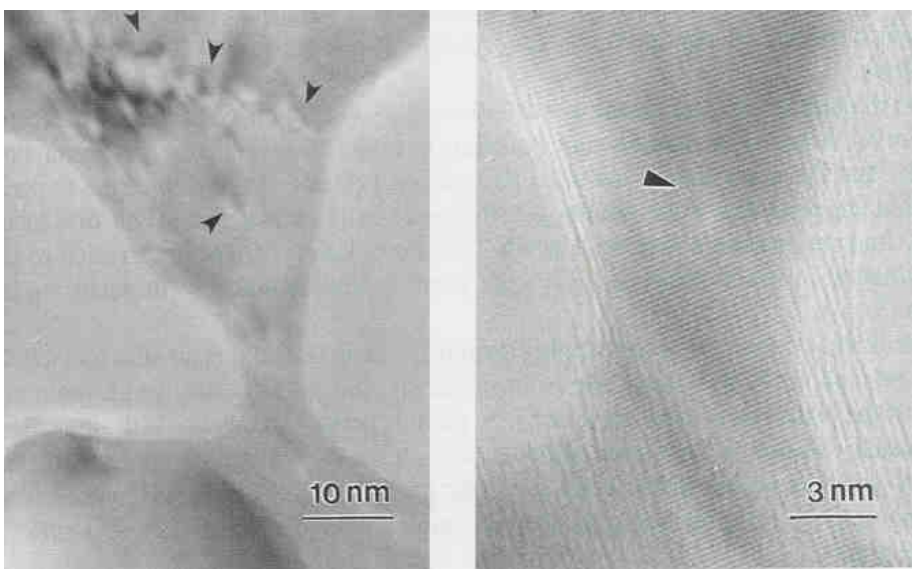
■ Early MTU Experimental Observations

• *Grain Boundary Sliding/ Grain Rotation*

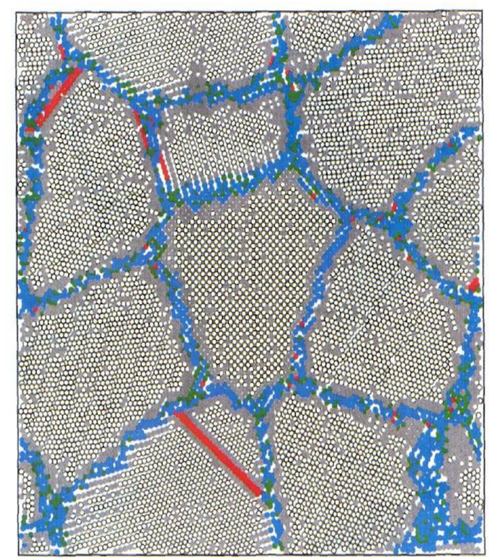




10 nm Au: 6-15 degrees relative grain rotation due to inhomogeneous GB sliding (unbalanced shear stress)



100 nm Ag film



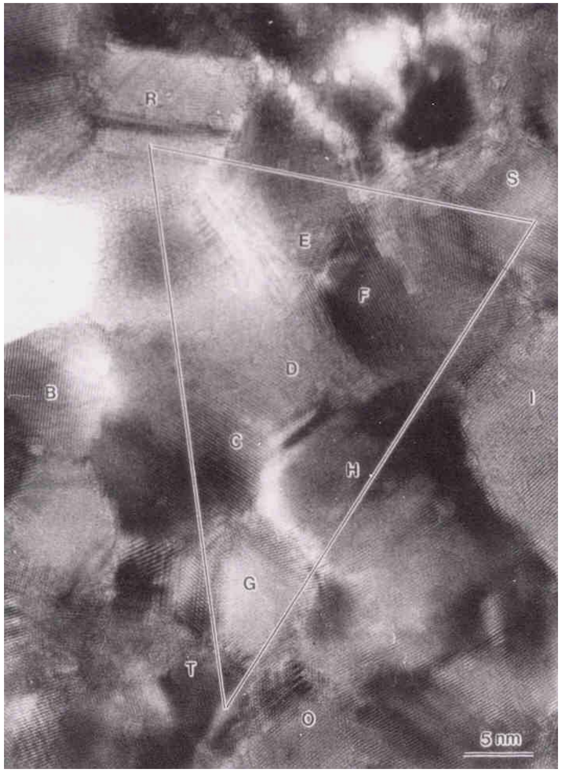
~12 nm Ni nanopolycrystals

- ***Grain Rotation / Dislocation Emergence***

Elementary Rosette Analysis

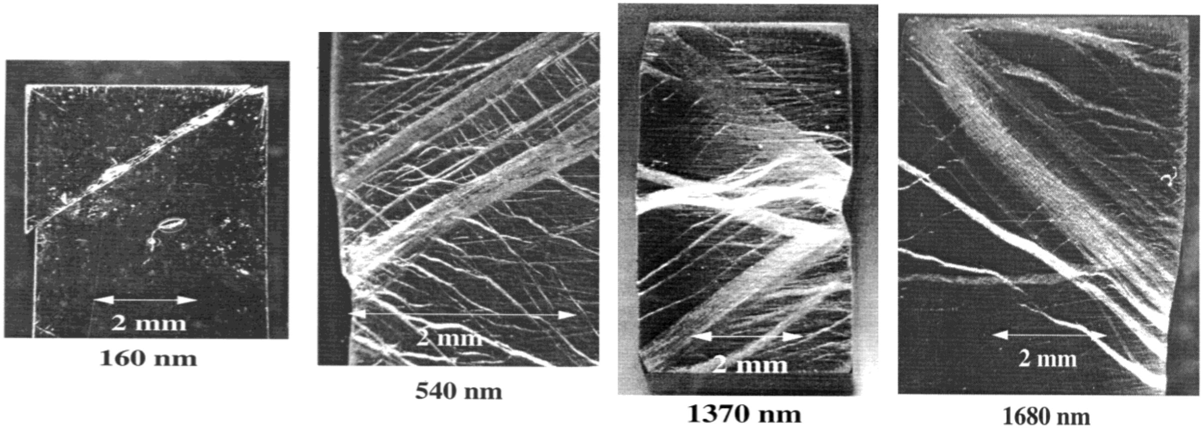
	Triangle angles (deg)			Triangle lengths (nm)		
Step	α	β	γ	a	b	c
Start	89	36	55	22.2	27.7	16.4
1	91	35	54	22.6	27.9	17.4
2	96	36	48	23.4	31.2	18.9
3	102	33	45	21.7	32.0	18.0

Strain Tensor $$\boldsymbol{\varepsilon} = \begin{bmatrix} 0.05 & -0.11 & 0 \\ -0.11 & 0.16 & 0 \\ 0 & 0 & -0.24 \end{bmatrix} \quad \varepsilon_{eff} = 20\ \%$$



TEM Strain Rosette

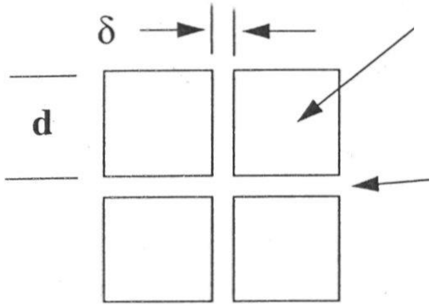
- ***Multiple Shear Banding***



Optical micrographs showing deformation and fracture behavior under compression of nanostructured Fe-10% Cu alloy for different grain sizes.

I. Gradient Elasticity (GradEla)

■ Motivation from Nanopolycrystal Elasticity



– ***"Bulk" phase and "boundary" phase*** *occupy the same material point and interact via an internal body force*

– ***Equilibrium***

$$div\boldsymbol{\sigma}_1 = \hat{\mathbf{f}}, \quad div\boldsymbol{\sigma}_2 = -\hat{\mathbf{f}} \text{ ....} \textit{for each phase} \;;\; \hat{\mathbf{f}} \text{ ...... interaction force}$$

$$div\boldsymbol{\sigma} = 0, \quad \boldsymbol{\sigma} = \boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2 \text{ ....} \textit{total stress}$$

– ***Elasticity:*** *Each phase obeys Hooke's Law and the internal body force (interaction force) is proportional to the difference of the individual displacements*

$$\boldsymbol{\sigma}_i = \lambda(tr\boldsymbol{\varepsilon}_i)\mathbf{1} + 2G\boldsymbol{\varepsilon}_i \,, \quad \boldsymbol{\varepsilon}_i = \frac{1}{2}\left[\nabla\mathbf{u}_i + \left(\nabla\mathbf{u}_i\right)^T\right]; \quad i = 1, 2$$

$$\hat{\mathbf{f}} = \alpha(\mathbf{u}_1 - \mathbf{u}_2)\,; \quad \hat{\mathbf{f}} \to \hat{\mathbf{f}} + \hat{\mathbf{T}}_{12}\,; \quad \hat{\mathbf{T}}_{12} \text{ ...} \textit{interaction stress}$$

– ***Uncoupling*** $\Rightarrow$

$$G\nabla^2\mathbf{u} + (\lambda + G)\,grad\,div\mathbf{u} - c\nabla^2\left[G\nabla^2\mathbf{u} + (\lambda + G)\,grad\,div\mathbf{u}\right] = \mathbf{0}$$

- ***GradEla Constitutive Eq.***

The above implies the following gradient-elasticity relation

$$\boldsymbol{\sigma} = \lambda(tr\boldsymbol{\varepsilon})\mathbf{I} + 2G\boldsymbol{\varepsilon} - c\nabla^2\left[\lambda(tr\boldsymbol{\varepsilon})\mathbf{I} + 2G\boldsymbol{\varepsilon}\right]$$

i.e. *elasticity of nanopolycrystals depends on higher – order gradients in strain or the Laplacian of Hookean stress*

- ***Ru-Aifantis Theorem***

$$\boldsymbol{u} - c\nabla^2\boldsymbol{u} = \boldsymbol{u}_0 \quad \Rightarrow \quad \boldsymbol{\varepsilon} - c\nabla^2\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_0 \quad \cdots$$

$\left(\boldsymbol{u},\boldsymbol{\varepsilon}\right)$ ... *Gradela solution ;* $\left(\boldsymbol{u}_0,\boldsymbol{\varepsilon}_0\right)$ ... *classical elasticity solution*

i.e. Inhomogeneous Helmholtz Equation: Solutions known

- ***Note:*** *The above reduction of GradEla solutions to corresponding (known) classical elasticity solutions for traction bvp's is analogous to a similar reduction for higher-order diffusion theory (GradDif), as will be shown later.*

■ Gradela Dislocation Mechanics

- ***Gradient Elasticity/GradEla*** $\Rightarrow \ (1-c\nabla^2)\begin{bmatrix}\sigma_{ij}\\ \varepsilon_{ij}\end{bmatrix}=\begin{bmatrix}\sigma^0_{ij}\\ \varepsilon^0_{ij}\end{bmatrix}$ ... Ru-Aifantis

- ***Screw Dislocation***

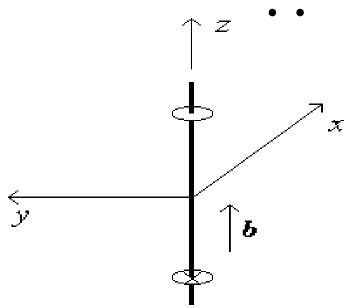
- Stress / Strain :

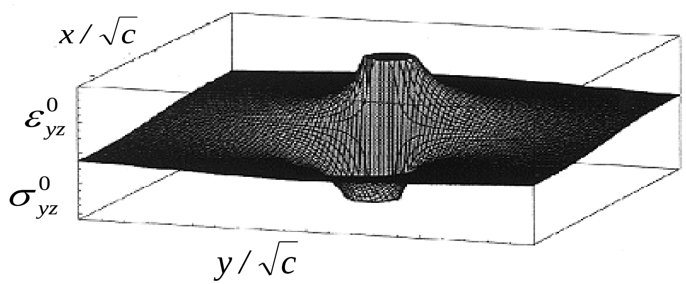
$$\begin{cases}\sigma_{xz}=\dfrac{Gb_z}{2\pi}\left[-\dfrac{y}{r^2}+\dfrac{y}{r\sqrt{c}}K_1\left(r/\sqrt{c}\right)\right]; \qquad \sigma_{yz}=\ldots\\[2ex] \varepsilon_{xz}=\dfrac{b_z}{4\pi}\left[-\dfrac{y}{r^2}+\dfrac{y}{r\sqrt{c}}K_1\left(r/\sqrt{c}\right)\right] \ ; \qquad \varepsilon_{yz}=\ldots\end{cases}$$

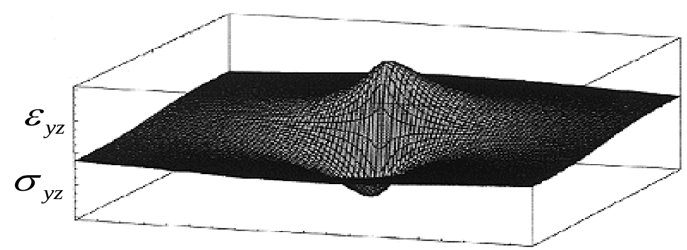
$$\therefore \quad \mathbf{r}\to\mathbf{0} \quad \Rightarrow \quad \mathbf{K_1}\left(\mathbf{r}/\sqrt{\mathbf{c}}\right)\to\frac{\sqrt{\mathbf{c}}}{\mathbf{r}} \quad \Rightarrow \quad \left(\boldsymbol{\sigma}_{\mathbf{xz}},\boldsymbol{\varepsilon}_{\mathbf{yz}}\right)\to\mathbf{0}$$

- Self – energy : $W_s=\dfrac{Gb_z^2}{4\pi}\left\{\gamma^E+\ln\dfrac{R}{2\sqrt{c}}\right\}$ ... $\gamma^E=0.577$; Euler constant

$$\therefore \quad \mathbf{r}\to\mathbf{0} \quad \Rightarrow \quad \textbf{no need for ad hoc dislocation core } \mathbf{r_0}$$





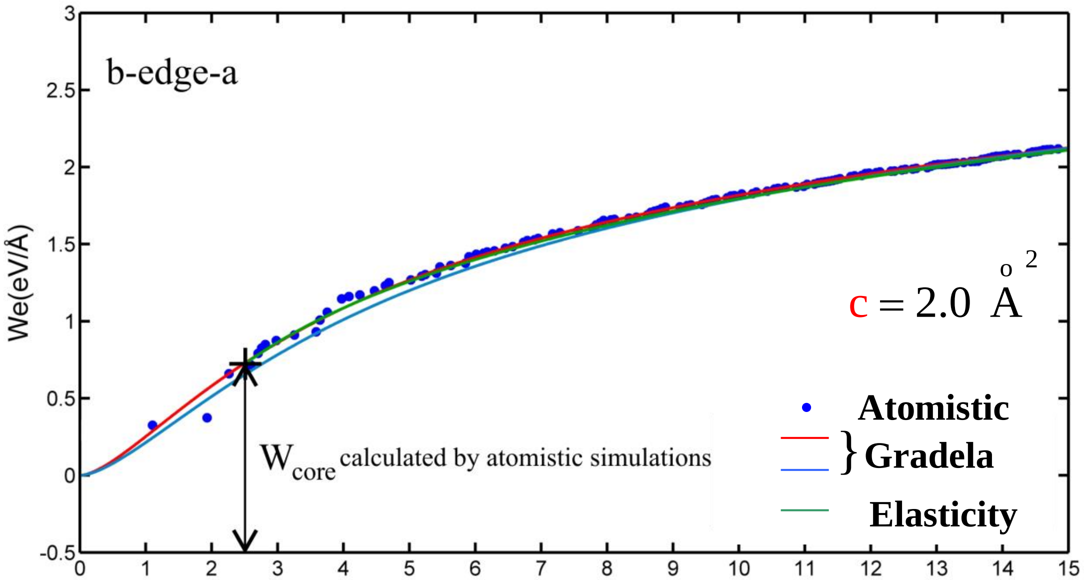


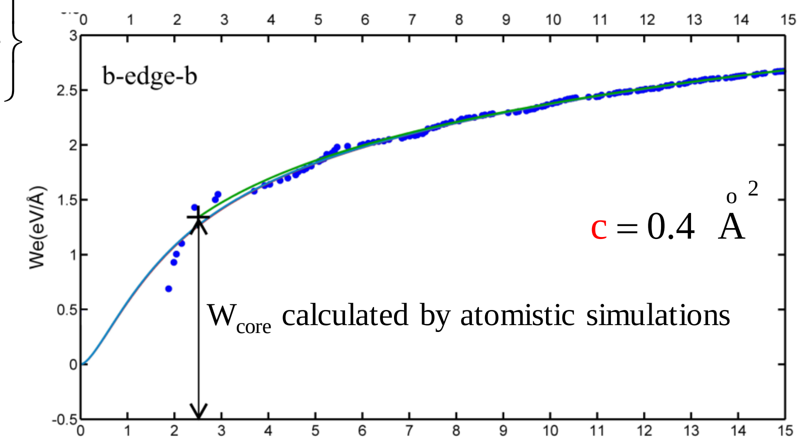
- Use these in simulations

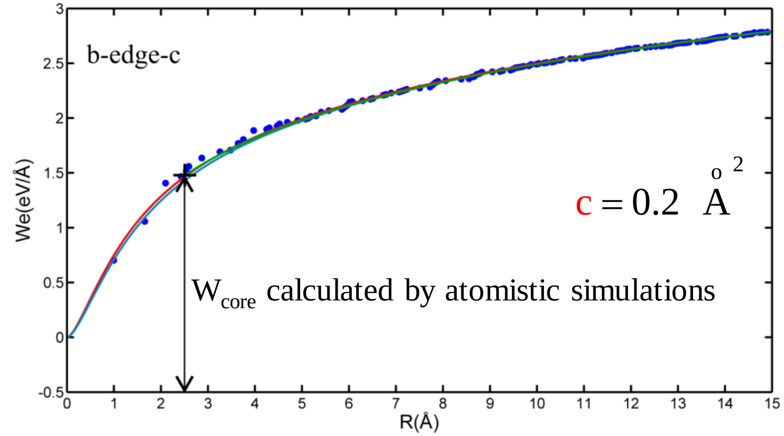
• *Comparison with MD Simulations (Stilliger – Weber Potential)*

$$W=\frac{b^2}{4\pi(1-\nu)}\left\{\ln\frac{R}{2\sqrt{c}}+\gamma+2K_0\left(\frac{R}{\sqrt{c}}\right)+2\frac{\sqrt{c}}{R}K_1\left(\frac{R}{\sqrt{c}}\right)-\frac{2c}{R^2}\right\}$$

$$R\to\infty\Rightarrow W=\frac{b^2}{4\pi(1-\nu)}\left\{\ln\frac{R}{2\sqrt{c}}+\gamma+\frac{1}{2}\right\}$$







$$\sqrt{c}=0.2-2.2\quad \mathring{A}$$

Invariant Relations: $\frac{W_{core}\sqrt{c}}{r_0}=0.33\pm0.008\frac{eV}{\mathring{A}}$; $\frac{W^g(b)\sqrt{c}}{b}=0.3\pm0.008\frac{eV}{\mathring{A}}$

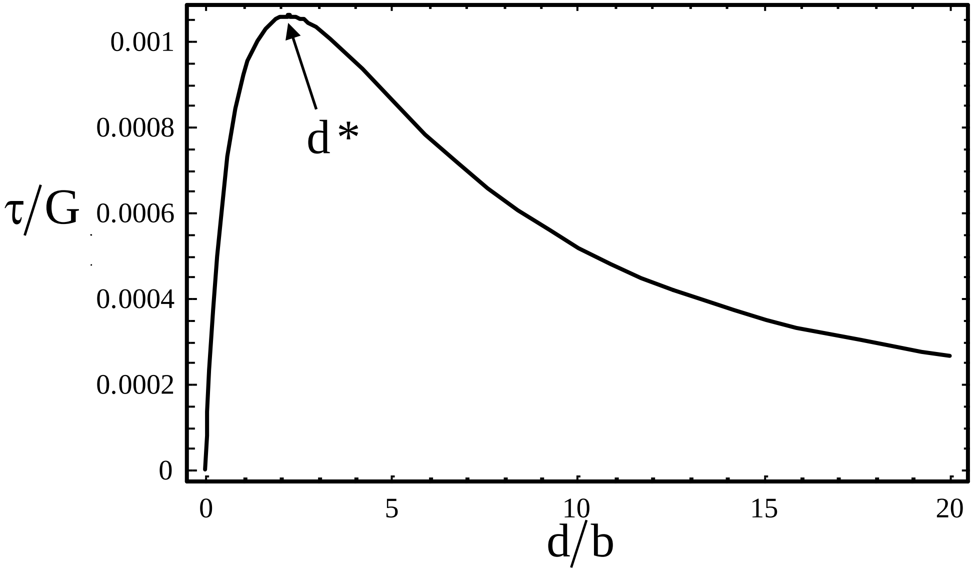
- ***Image Force – Inverse Hall Petch Behavior***

  - *Self -energy:* $$W = \frac{Gb^2}{2\pi}\left[\ln\frac{R}{2\sqrt{c}} + \gamma^E + K_0\left(\frac{R}{\sqrt{c}}\right)\right]$$

  - *Image Stress:* $$\tau = \frac{Gb}{2\pi}\left[\frac{1}{d} - \frac{1}{2\sqrt{c}}K_1\left(\frac{d}{2\sqrt{c}}\right)\right]$$

derived by differentiation and evaluation at $R = d/2$ (d … grain diameter)

- stress to move a dislocation situated at the center of a grain of diameter d



$d^* \approx 9$ nm

i.e. d^* critical grain size for inverse Hall-Petch behavior

• *X-ray Line Profile Analysis*

- *Gradela Soltn for ε_{xx} of edge $\perp$* $(\mathbf{b} = b\,\mathbf{e}_x)$

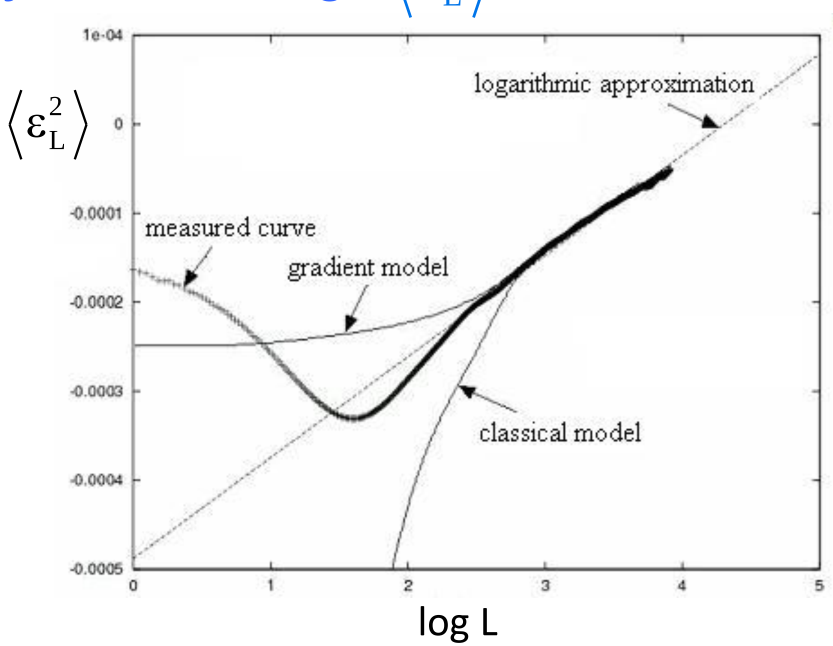
According to Gradela (e.g. ECA 2003) the ε_{xx} component of the strain tensor corresponding to an edge dislocation with Burgers vector $\mathbf{b} = b\,\mathbf{e}_x$ is

$$\varepsilon_{xx} = -\frac{b}{4\pi(1-\nu)}\frac{(1-2\nu)r^2 + 2x^2}{r^4} + \frac{b}{2\pi(1-\nu)}y\left[\left(y^2 - \nu r^2\right)\Phi_1 + \left(3x^2 - y^2\right)\Phi_2\right]$$

where

$$\Phi_1 = \frac{1}{r^3\sqrt{c}}K_1\left(r/\sqrt{c}\right), \quad \Phi_2 = \frac{1}{r^4}\left[\frac{2c}{r^2} - K_2\left(r/\sqrt{c}\right)\right], \quad r^2 = x^2 + y^2$$

- *The first results for calculating* $\langle \varepsilon_L^2 \rangle$

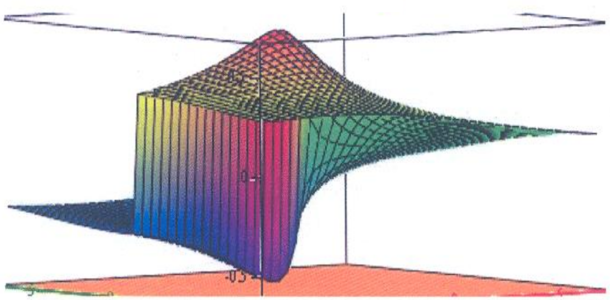


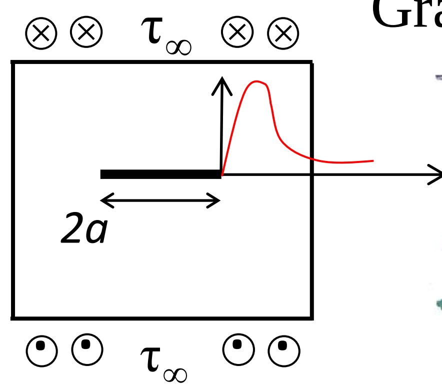
■ GradEla Fracture Mechanics

- ***GradEla:*** $(1-c\Delta)\boldsymbol{\sigma}_{ij} = \boldsymbol{\sigma}_{ij}^{\mathbf{0}}$ & $(1-c\Delta)\boldsymbol{\varepsilon}_{ij} = \boldsymbol{\varepsilon}_{ij}^{\mathbf{0}}$; $\boldsymbol{\sigma}^{\mathbf{0}} = \lambda\, \mathrm{tr}\boldsymbol{\varepsilon}^{\mathbf{0}}\mathbf{1} + 2\mu\boldsymbol{\varepsilon}^{\mathbf{0}}$
- ***Bc's:*** $\lim_{\mathbf{r}\to\infty} \boldsymbol{\sigma}_{ij} = \boldsymbol{\sigma}_{ij}^{\mathbf{0}}$; $\lim_{\mathbf{r}\to 0} \boldsymbol{\sigma}_{ij} = 0$; $\sigma_{zy}(x, 0^{\pm}) = 0$; $|x| \le a$
- ***Mode III:***

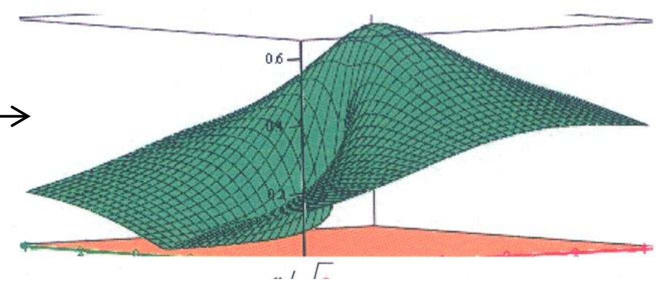
$$\sigma_{xz} = -\frac{K_{III}}{\sqrt{2\pi r}}\left[\sin\frac{\theta}{2}\left(1-\exp\left[-r/\sqrt{c}\right]\right)\right] \qquad \sigma_{yz} = \frac{K_{III}}{\sqrt{2\pi r}}\left[\cos\frac{\theta}{2}\left(1-\exp\left[-r/\sqrt{c}\right]\right)\right]$$

Gradient Stress non-singular





Gradient Stress non-singular



Note: $\left(1-e^{-r/\sqrt{c}}\right)\Big/\sqrt{r}$ max at $r \cong 1.25\sqrt{c}$

$$\therefore \sigma_{yz}^{max} = \sigma_{xz}^{max} \cong 0.254\frac{K_{III}}{\sqrt[4]{c}} \cong \frac{K_{III}}{4\sqrt[4]{c}}$$ **(Stress Fracture Criterion)** $K_{III} = \tau_\infty\sqrt{\pi a}$

- ***Mode I: Stresses (Non-Separable)***

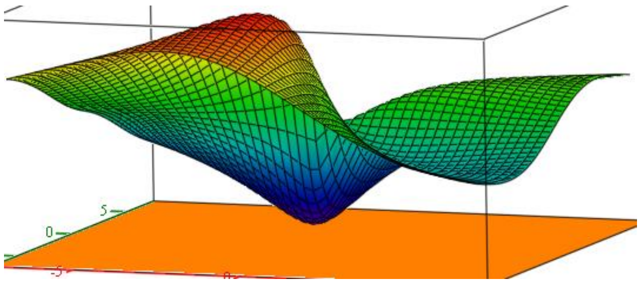
$$\sigma_{xx} = \frac{K_I}{4\sqrt{2\pi r}}\left[3\cos\frac{\theta}{2}\left(1-e^{-\frac{r}{\sqrt{c}}}\right)+\cos\frac{5\theta}{2}\left\{1-\frac{6c}{r^2}+2e^{-\frac{r}{\sqrt{c}}}\left(\frac{3c}{r^2}+\frac{3\sqrt{c}}{r}+1\right)\right\}\right]$$

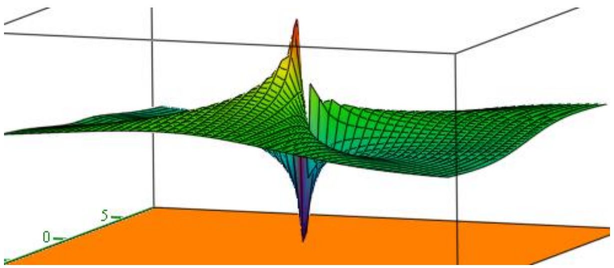
$$\sigma_{yy} = -\frac{K_I}{4\sqrt{2\pi r}}\left[5\cos\frac{\theta}{2}\left(-1+e^{-\frac{r}{\sqrt{c}}}\right)+\cos\frac{5\theta}{2}\left\{1-\frac{6c}{r^2}+2e^{-\frac{r}{\sqrt{c}}}\left(\frac{3c}{r^2}+\frac{3\sqrt{c}}{r}+1\right)\right\}\right]$$

$$\sigma_{zz} = \frac{2K_I\nu}{\sqrt{2\pi r}}\cos\frac{\theta}{2}\left(1-e^{-\frac{r}{\sqrt{c}}}\right)$$

$$\sigma_{xy} = \frac{K_I}{4\sqrt{2\pi r}}\left[\sin\frac{\theta}{2}\left(-1+e^{-\frac{r}{\sqrt{c}}}\right)+\sin\frac{5\theta}{2}\left\{1-\frac{6c}{r^2}+2e^{-\frac{r}{\sqrt{c}}}\left(\frac{3c}{r^2}+\frac{3\sqrt{c}}{r}+1\right)\right\}\right]+\sigma_{hom}$$

$$\sigma_{hom} = \frac{K_I}{2\sqrt{2\pi}}\frac{3y}{\pi c^{1/4}}\int_{-\infty}^{0}\frac{|s|^{-5/2}-\frac{e^s}{\sqrt{-s}}[\frac{1}{2}-\frac{1}{s}+\frac{1}{s^2}]}{\sqrt{(x-s\sqrt{c})^2+y^2}}K_1\left(\sqrt{(\frac{x}{\sqrt{c}}-s)^2+(\frac{y}{\sqrt{c}})^2}\right)ds$$





- ***Mode I: Stresses – Simplified Separable Expressions***

$$\sigma_{xx}^{sim} = \frac{K_I}{\sqrt{2\pi r}}\left[\cos(\frac{\theta}{2})\left(1-\sin(\frac{\theta}{2})\sin(\frac{3\theta}{2})\right)\right](1-e^{-\frac{r}{\sqrt{c}}})$$

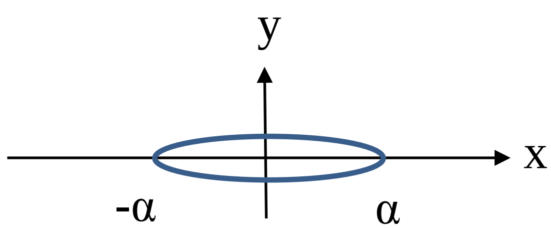
$$\sigma_{yy}^{sim} = \frac{K_I}{\sqrt{2\pi r}}\left[\cos(\frac{\theta}{2})\left(1+\sin(\frac{\theta}{2})\sin(\frac{3\theta}{2})\right)\right](1-e^{-\frac{r}{\sqrt{c}}})$$

$$\sigma_{xy}^{sim} = \frac{K_I}{\sqrt{2\pi r}}\left(\sin(\frac{\theta}{2})\cos(\frac{\theta}{2})\cos(\frac{3\theta}{2})\right)(1-e^{-\frac{r}{\sqrt{c}}})$$

$$\sigma_{zz}^{sim} = \frac{2\nu K_I}{\sqrt{2\pi r}}\cos(\frac{\theta}{2})(1-e^{-\frac{r}{\sqrt{c}}})$$

■ A Note on COD: Ru-ECA

- Central Crack



$$u_{+} - u_{-} = \delta(x); \quad |x| \le \alpha, \quad y = 0$$

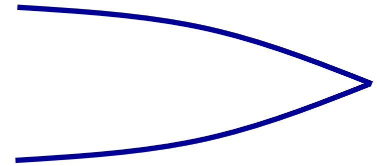
$$\Rightarrow \delta(x) - c\delta''(x) = \delta^{0}(x); \quad \delta = \text{COD}$$

- Soltn: $\delta(x) = -\frac{1}{\sqrt{c}}\int_{0}^{x} \text{sh}\left(\frac{x-s}{\sqrt{c}}\right)\delta^{0}(s)\,ds + c_1 e^{s/\sqrt{c}} + c_2 e^{-s/\sqrt{c}}$

$$\text{with} \quad \delta^{0}(x) = b\sqrt{\alpha^2 - x^2}; \quad b = \tau_0/G \quad \& \quad \delta(-\alpha) = \delta(\alpha) = 0$$

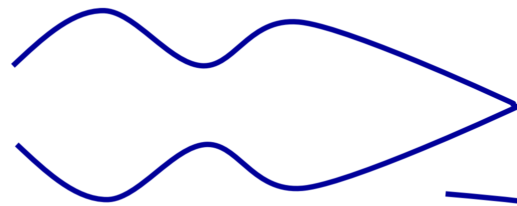
$$\Rightarrow \delta(x) = \frac{b}{\sqrt{c}}\left[\frac{\text{sh}\left((\alpha+x)/\sqrt{c}\right)}{\text{sh}\left(2\alpha/\sqrt{c}\right)}\int_{-\alpha}^{\alpha} \text{sh}\left((\alpha-s)/\sqrt{c}\right)\sqrt{\alpha^2 - s^2}\,ds - \int_{-\alpha}^{x} \text{sh}\left((x-s)/\sqrt{c}\right)\sqrt{\alpha^2 - s^2}\,ds\right]$$

$\therefore \quad \delta'(\pm\alpha) \neq (0,\infty), \quad \delta''(\pm\alpha) = 0 \quad \Rightarrow$



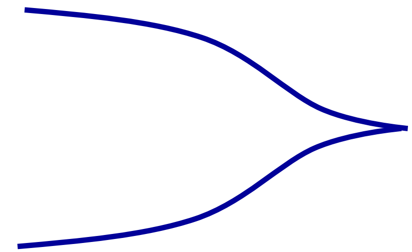
wedge-like

- $c < 0 \quad \Rightarrow$



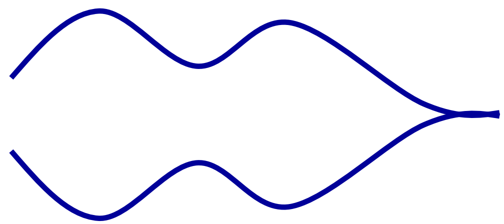
oscillatory-like

- Other BCs $\quad \delta'(\pm\alpha) = 0$

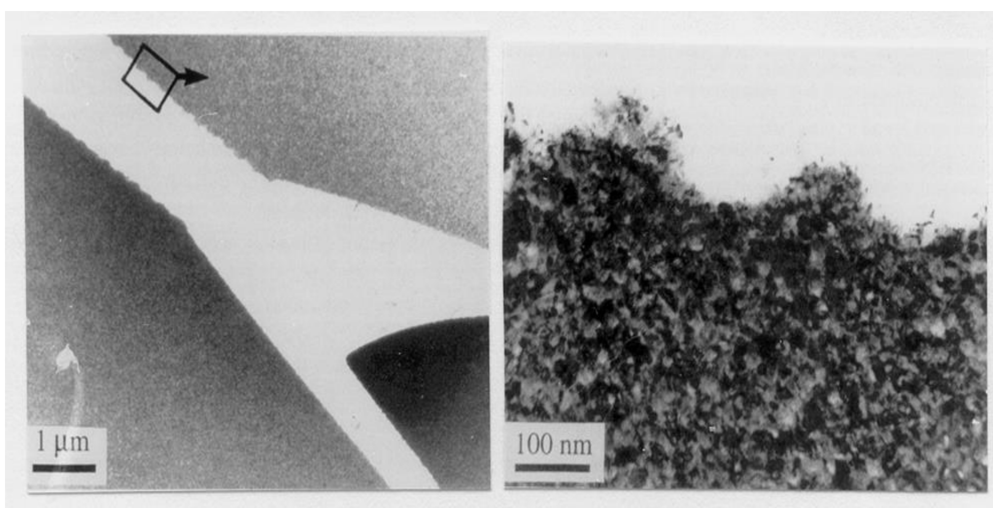


cusp-like

- $c < 0$

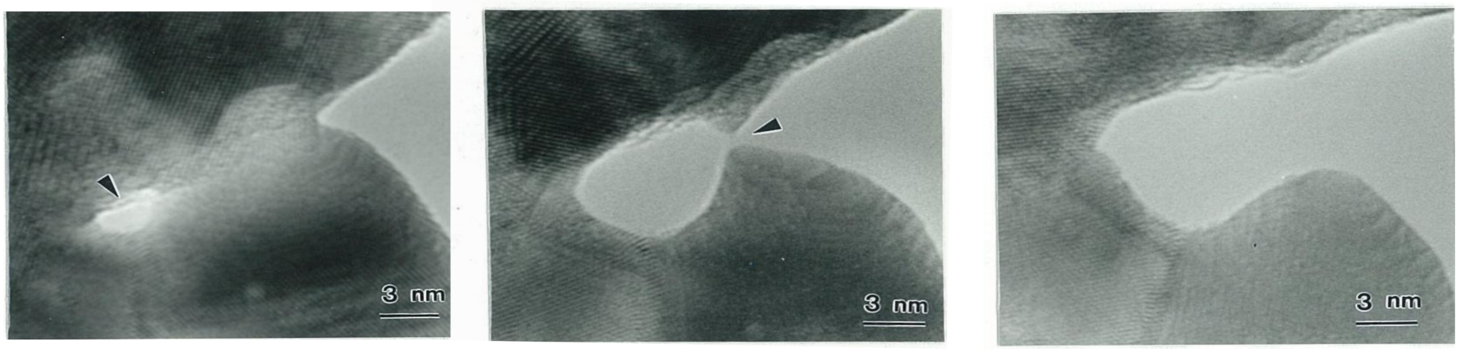


oscillatory

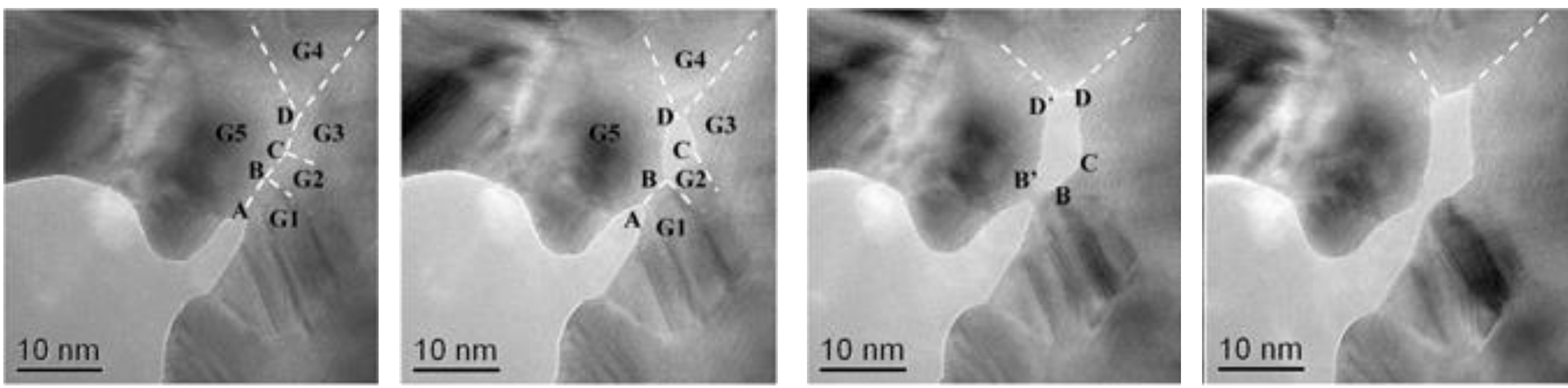


25 nm Au on C:
Periodic Crack
profiles and
bifurcation

- ***Crack Propagation mechanism: Nanovoid Nucleation at the Tip***



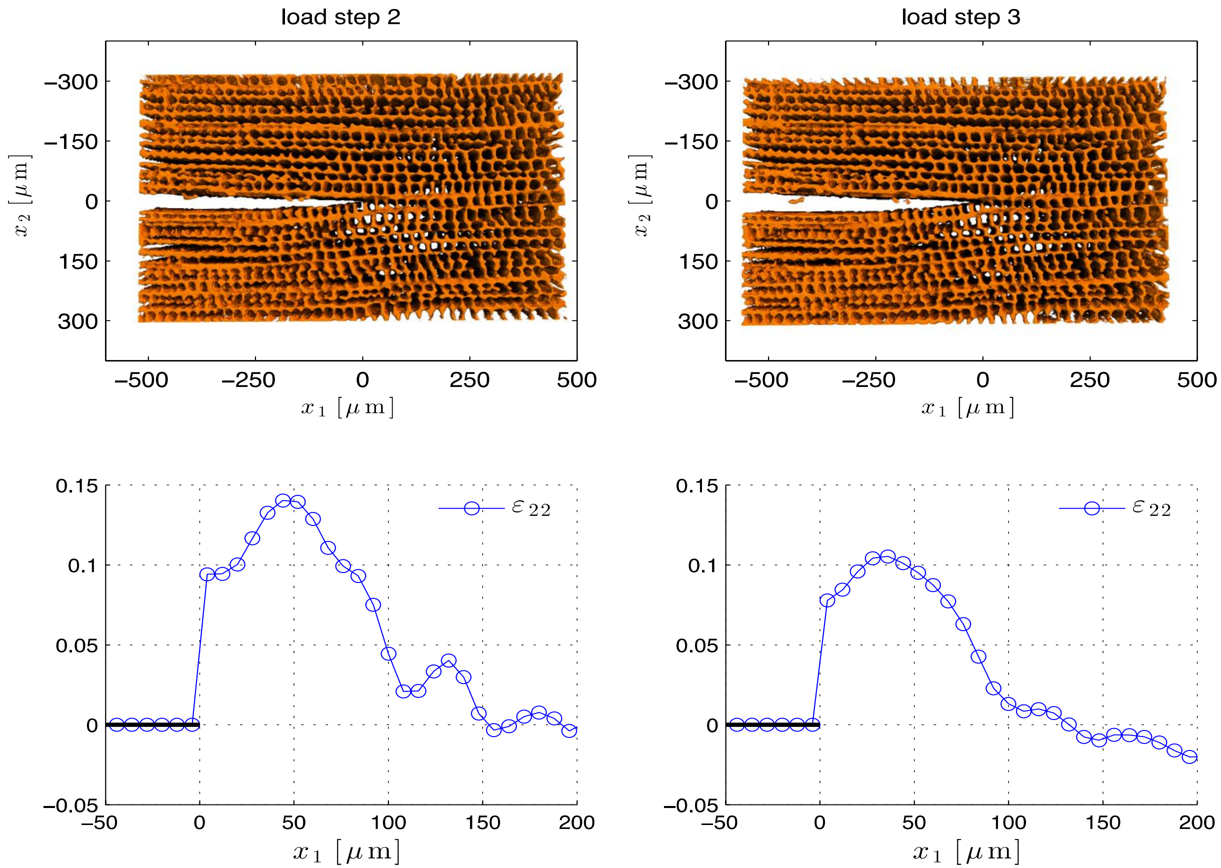
8 nm Au on C: Nanocrack growth via nanopore/nanovoid formation/nucleation at triple GB junction
[Miligan/Hackney/Ke/Aifantis Nanostr. Mat. 1993]



[Wei et al, Science / Scripta Met., 2011/2014]

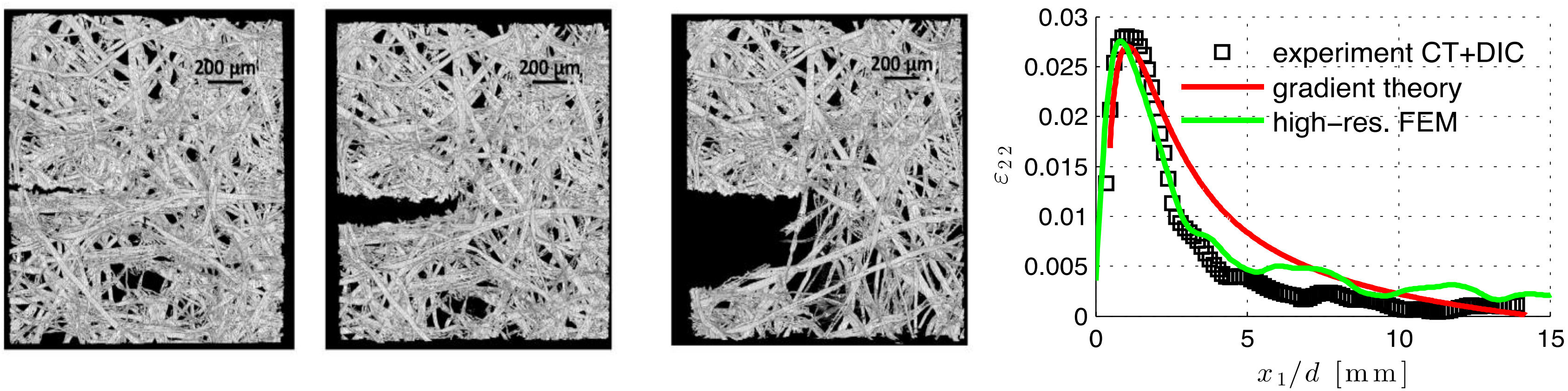
■ More on Crack Tips: Isaksson et al

• *Experiments on Wood*



Upper row: Parts of reconstructed images of wood in the radial plane. Note the edge crack, extending from the left in two scan steps. Lower row: estimated strain fields along the crack plane, evaluated from the images obtained in the aforementioned scans using the digital image correlation algorithm. The tip is always positioned at $x_1 = 0$, i.e. the origin moves when the crack grows. The strains have manually been put to zero at $x_2 = 0$ and $x_1 < 0$.

• *Experiments on Paper*



(a) **(b)** **(c)** **(d)**

Reconstructed cross section from a X-ray CT scan of a growing crack in a fibre material at ESRF (a-c). CT/DIC-estimated strains along the crack plane in front of the tip. Observe the non-singular strain and that the maximum is located ahead of the tip at approximately the average cell diameter d. Also shown are the strains computed by a high-resolution FE model and the enhanced gradient theory (d).

■ Application to Environmental Cracking

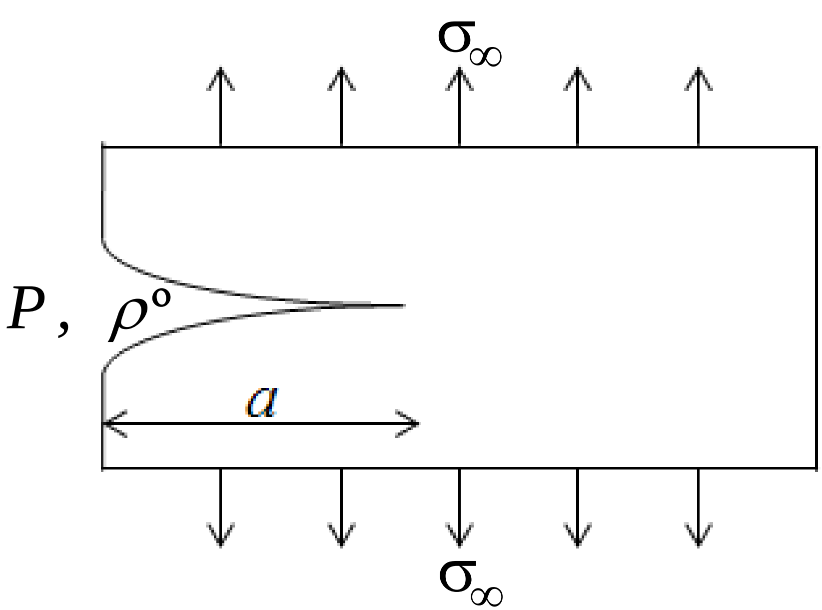
- ***Hydrogen Atmosphere:***

$$Pressure\ :\ P_{H_2} \equiv P \quad ; \qquad Concentration\ :\ \rho_H \equiv \rho$$

- ***Stress – Assisted Diffusion***

$$\frac{\partial \rho}{\partial t} = D^* \nabla^2 \rho - M^* \nabla \sigma \cdot \nabla \rho \quad ; \quad \sigma \equiv tr\boldsymbol{\sigma} = \sigma_{ii}$$

$$D^* = D + N\sigma, \quad M^* = M - N$$



$$\rho \ , \ \sigma$$

$$\sigma_{ij} = C \frac{K_I}{\sqrt{2\pi r}} f_{ij}(\theta) \ ; \ K_I = \sigma_\infty \sqrt{\pi a}$$

$$\rho^o = const\sqrt{P}$$

- ***Steady State:***

$$\rho = \rho^{o}\left(1 + \frac{N}{D}\sigma\right)^{\frac{M}{N}}$$

$$N \rightarrow 0 \quad \Rightarrow \quad \rho = \rho^{o} e^{\frac{M\sigma}{D}} \quad \text{...Cottrell's Relation}$$

- *Chemical Fracture Criterion (Threshold)*

$$\rho\Big|_{r = r_C} = \rho_{crit} \quad \Rightarrow \quad P = \overset{o}{P} K_I^{-2\frac{M}{N}}$$

- *Chemical Fracture Criterion (Kinetics)*

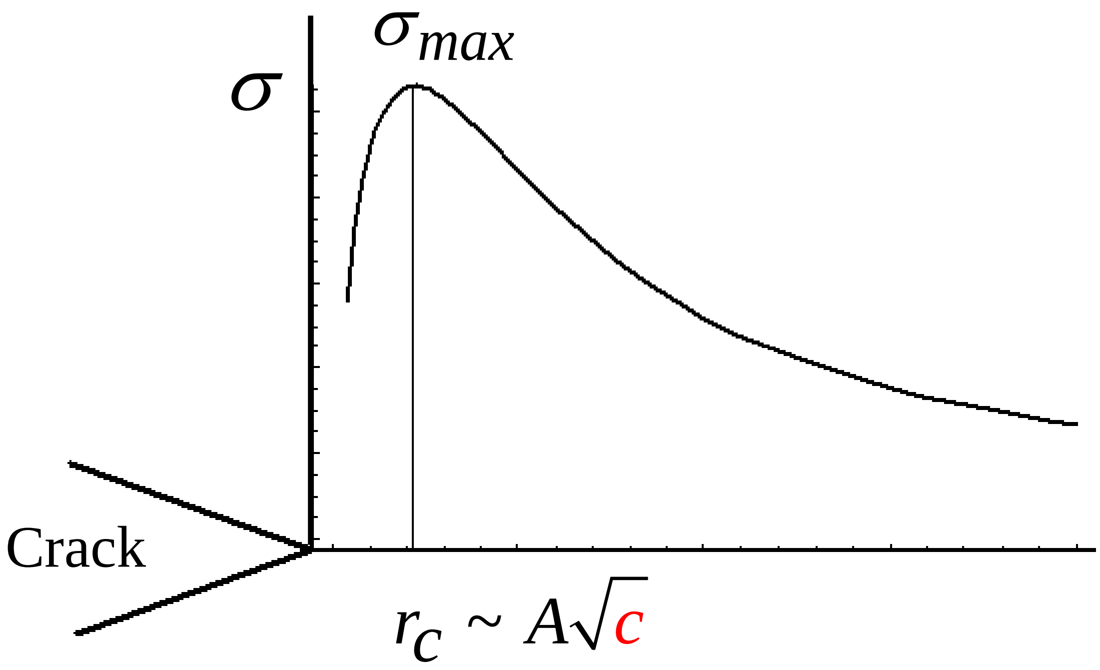
$$V = const\, \rho\Big|_{r = r_C} \quad \Rightarrow \quad V = \overset{o}{V} K_I^{\frac{M}{N}}$$

- *Combined Criterion:*

$$V = \overset{o}{V}\sqrt{P}\left(1 + \frac{CN}{D\sqrt{r_C}}\right)^{\frac{M}{N}}$$

- ***Problem: Determination of r_c***

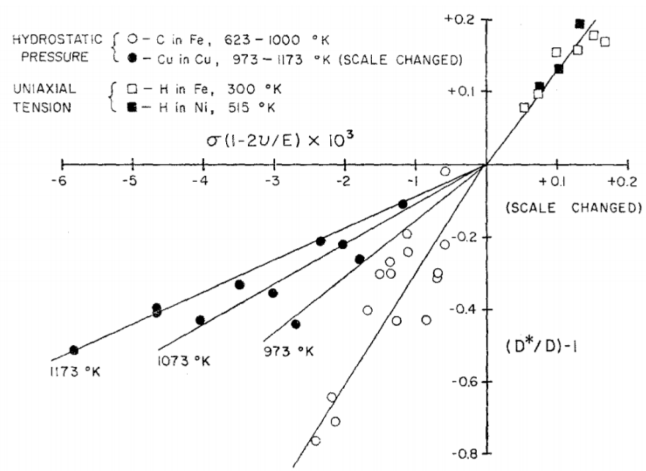
  - *Empirical Estimate:* $r_c \sim d$ *grain size*
  - *Gradela*

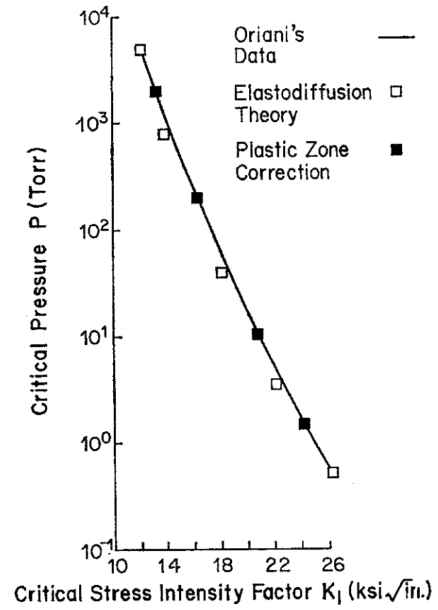


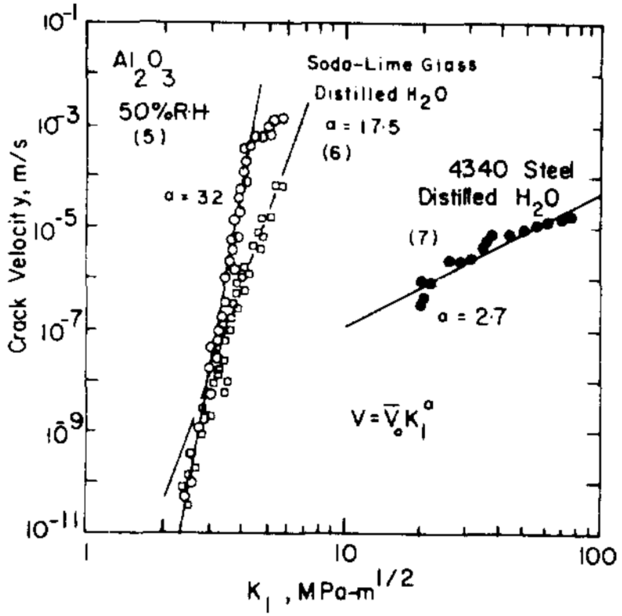
$$\sigma \sim \frac{K_I}{\sqrt{2\pi r}}\left(1 - e^{-r/\sqrt{c}}\right)$$

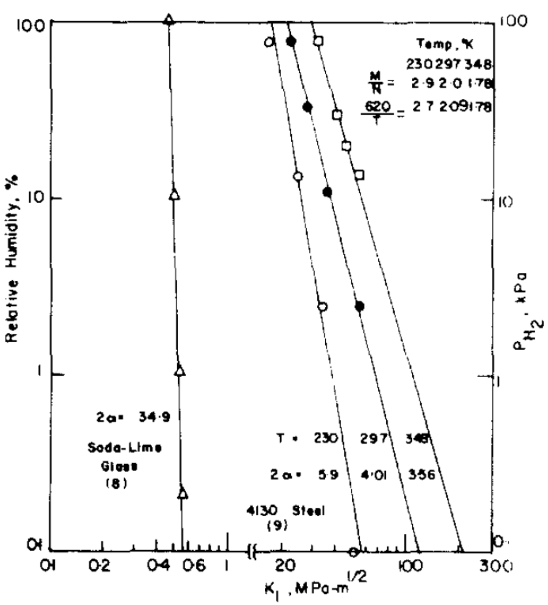
$$\sigma_{max} \;\; at \;\; r = r_c \sim A\sqrt{c}$$

- ***Comparison with Experiments***









■ Models for Fractional/Fractal GradEla Generalizations

$$\sigma_{ij} = \left(\lambda\varepsilon_{kk}\delta_{ij} + 2\mu\varepsilon_{ij}\right) - \ell_s^2 \Delta \left(\lambda\varepsilon_{kk}\delta_{ij} + 2\mu\varepsilon_{ij}\right)$$

- $$\sigma_{ij} = \left(\lambda\varepsilon_{kk}\delta_{ij} + 2\mu\varepsilon_{ij}\right) - \ell_s^2(\alpha)(-\Delta)^{\alpha/2} \left(\lambda\varepsilon_{kk}\delta_{ij} + 2\mu\varepsilon_{ij}\right)$$

$(-\Delta)^{\alpha/2}$... Fractional Laplacian in **Riesz** form

$$((-\Delta)^{\alpha/2}\varepsilon_{ij})(\mathbf{r}) = \mathcal{F}^{-1}(|\mathbf{k}|^{\alpha}\,\varepsilon_{ij}(\mathbf{k}))(\mathbf{r})$$

- $$\sigma_{ij} = \left(\lambda\varepsilon_{kk}\delta_{ij} + 2\mu\varepsilon_{ij}\right) - \ell_F^2(D)\Delta^D \left(\lambda\varepsilon_{kk}\delta_{ij} + 2\mu\varepsilon_{ij}\right)$$

Δ^D... fractal Laplacian ; D... volumetric fractal dimension;

$$\Delta^D \varphi(r) = \mathrm{Div}^D \mathrm{Grad}^D \varphi = \frac{\partial^2 \varphi}{\partial r^2} + \frac{D-1}{r}\frac{\partial \varphi}{\partial r} \quad ; \quad \varphi = \varphi(r) \text{ scalar}$$

$$\Delta^D \mathbf{u}(r) = \mathrm{Grad}^D\, \mathrm{Div}^D \mathbf{u} = \left(\frac{\partial^2 u}{\partial r^2} + \frac{D-1}{r}\frac{\partial u}{\partial r} - \frac{D-1}{r^2} u \right) \mathbf{e}_r \quad ; \quad \mathbf{u} = u(r)\mathbf{e}_r \text{ vector}$$

- **Note:** $\varphi(r) = \dfrac{\mu b_z \Gamma(D/2)}{2\pi^{D/2}} r^{2-D}$ stress fct for screw dislocation

■ Fractional GradEla Dislocations

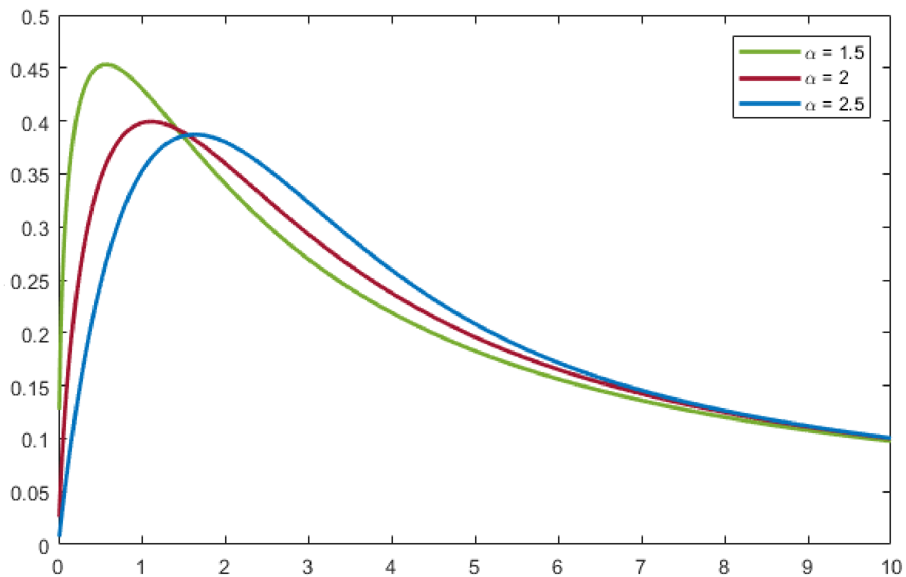
- ***Ru-Aifantis thm:*** $\boldsymbol{\varepsilon} + l^{\alpha}(-\Delta)^{\alpha/2}\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^{0}$; $\quad l = c^{1/\alpha}$

$\boldsymbol{\varepsilon}$ ... *fractional GradEla strain ;* $\boldsymbol{\varepsilon}^{0}$ *...classical strain*

$$((-\Delta)^{\alpha/2}\varepsilon_{ij})(\mathbf{r}) = \mathcal{F}^{-1}(|\mathbf{k}|^{\alpha}\varepsilon_{ij}(\mathbf{k}))(\mathbf{r}). \quad \textit{Fourier form}$$

- ***Screw Dislocation/Nonsingular Strain fields***

$$\varepsilon_{xz} = \frac{b_z}{4\pi}\left[-\frac{y}{r^2} + \frac{y}{rl}K_{\alpha}\left(\frac{r}{l}\right)\right] \quad ; \quad \varepsilon_{yz} = \frac{b_z}{4\pi}\left[\frac{x}{r^2} - \frac{x}{rl}K_{\alpha}\left(\frac{r}{l}\right)\right]$$



$$K_{\alpha}(r) = \int_0^{\infty}\frac{k^2 J_1(kr)}{k^{2-\alpha}[1+k^{\alpha}]}dk$$

Note $\alpha \to 2:\quad K_{\alpha}(r)\big|_{\alpha\to 2} \to K_1(r)$

i.e. previous GradEla Solution

Note $r \to 0 \quad K_{\alpha}(r)\big|_{r\to 0} \to \frac{1}{r}$

$\varepsilon_{xz}, \varepsilon_{yz} \to 0,\ $ *not* ∞

- ***Note: Solution is tentative***

■ Fractional GradEla Cracks

- ***Ru-Aifantis thm:*** $\boldsymbol{\sigma} + l^{\alpha}(-\Delta)^{\alpha/2}\boldsymbol{\sigma} = \boldsymbol{\sigma}^0$

  $\boldsymbol{\sigma}$ *... fractional GradEla stress field ;* $\boldsymbol{\sigma}^0$ *...classical stress field*

- ***Riesz Laplacian:*** $((-\Delta)^{\alpha/2}\sigma_{ij})(\mathbf{r}) = \mathcal{F}^{-1}(|\mathbf{k}|^{\alpha}\sigma_{ij}(\mathbf{k}))(\mathbf{r}).$

  Convolution $((-\Delta)^{\alpha/2}\sigma_{ij})(\mathbf{r}) = -(\frac{1}{\gamma_\alpha}\frac{1}{|\mathbf{r}|^{\alpha}} * [\Delta\sigma_{ij}(\mathbf{r})])(\mathbf{r})$

- ***Separable Solutions/Ansatz***

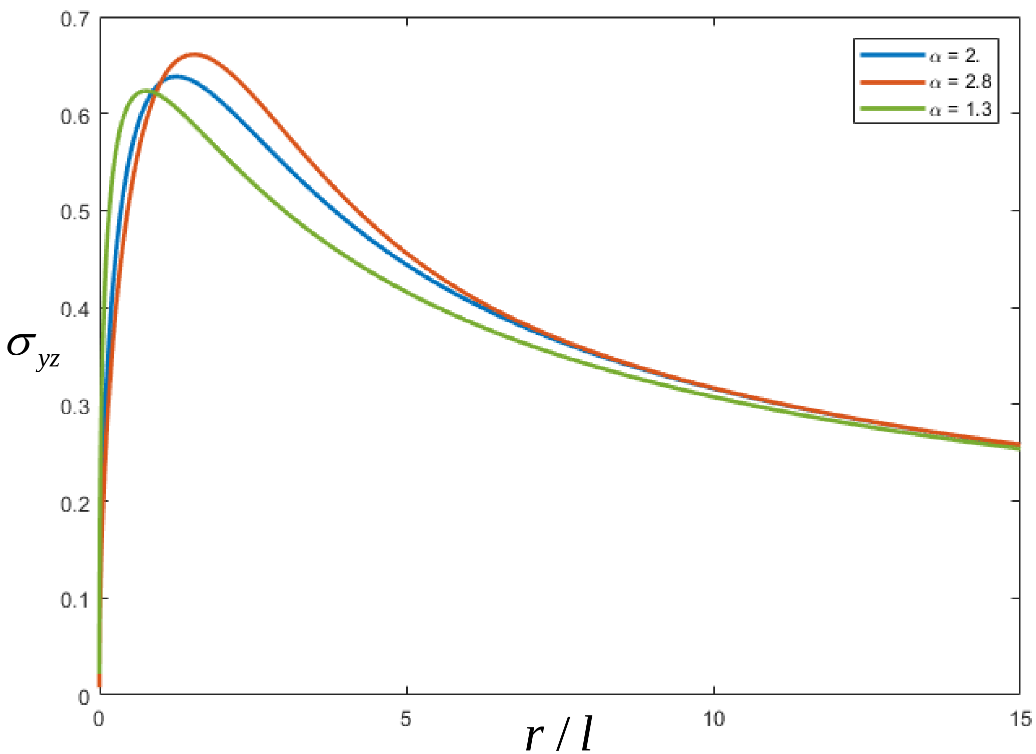
$$\sigma_{xz} = \sigma_{xz}^0 - f(r)\sin\frac{\theta}{2} \qquad \sigma_{yz} = \sigma_{yz}^0 + f(r)\cos\frac{\theta}{2}$$

$$\therefore\ \sigma_{xz}^0 = -\frac{K_{III}}{\sqrt{2\pi r}}\sin\frac{\theta}{2} \qquad \sigma_{yz}^0 = \frac{K_{III}}{\sqrt{2\pi r}}\cos\frac{\theta}{2}$$

• Nonsingular Stress Distribution for Mode III

$$\sigma_{xz}(r,\theta) = -\frac{K_{III}}{\sqrt{2\pi r}}[1-\sqrt{\frac{2r}{\pi l}}K_{\alpha}(\frac{r}{l})]\sin\frac{\theta}{2}; \quad \sigma_{yz}(r,\theta) = \frac{K_{III}}{\sqrt{2\pi r}}[1-\sqrt{\frac{2r}{\pi l}}K_{\alpha}(\frac{r}{l})]\cos\frac{\theta}{2}$$

GradEla $$\sigma_{yz}(r,\theta) = -\frac{K_{III}}{\sqrt{2\pi r}}[1-e^{-r/l}]\sin\frac{\theta}{2}; \quad \sigma_{yz}(r,\theta) = \frac{K_{III}}{\sqrt{2\pi r}}[1-e^{-r/l}]\cos\frac{\theta}{2}$$



$$K_{\alpha}(r) = \int_0^{\infty}\frac{k^{3/2}J_{1/2}(kr)}{k^{2-\alpha}[1+k^{\alpha}]}dk.$$

Note: $\alpha \to 2: \ K_{\alpha}(r) \to \sqrt{\frac{\pi}{2r}}e^{-r}$

Note: $r \to 0: \ K_{\alpha}(r) \to \sqrt{\frac{\pi}{2r}}$

• Note: Solution is tentative

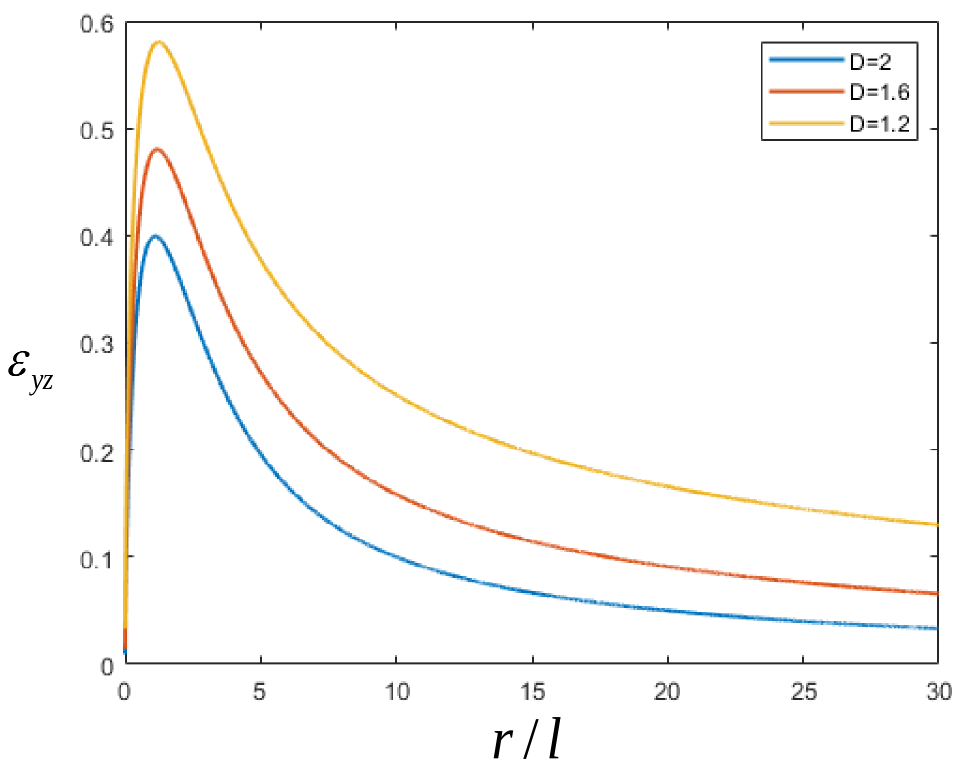
■ Fractal GradEla Dislocations

- ***Ru-Aifantis thm:*** $\boldsymbol{\varepsilon} - l_D^2 \Delta^D \boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^0 \ ; \quad l_D = c^{1/2}$

  $\boldsymbol{\varepsilon}$ *... fractal GradEla strain ;* $\boldsymbol{\varepsilon}^0$ *...classical strain*

- ***Screw Dislocation/Nonsingular Strain fields***

$$\tilde{\varepsilon}_{xz} = [-\frac{y}{r^D} + \frac{2^{1-D/2} y}{\Gamma(D/2) r^{D/2} l_D^{D/2}} K_{D/2}\left(\frac{r}{l_D}\right)] \ ; \ \tilde{\varepsilon}_{yz} = [\frac{x}{r^D} - \frac{2^{1-D/2} x}{\Gamma(D/2) r^{D/2} l_D^{D/2}} K_{D/2}\left(\frac{r}{l_D}\right)]$$



$$\varepsilon_{xz} = \frac{b_z \Gamma(D/2)}{4\pi^{D/2}} \tilde{\varepsilon}_{xz} \ ; \ \varepsilon_{yz} = \frac{b_z \Gamma(D/2)}{4\pi^{D/2}} \tilde{\varepsilon}_{yz}$$

Note D: fractal dimension; $1 < D < 2$

Note $D \to 2: \quad K_{D/2}(r)\big|_{D\to 2} \to K_1(r)$

i.e. previous GradEla Solution

Note $r \to 0 \quad K_{D/2}(r)\big|_{r\to 0} \to \frac{\Gamma(D/2)}{2^{1-D/2} r^{D/2}}$

$\varepsilon_{xz}, \varepsilon_{yz} \to 0, \quad$ *not* ∞

II. Higher-order Diffusion (GradDif)

- **Mass & Momentum Balances:** $\dot{\rho} + \mathrm{div}\,\mathbf{j} = 0\,; \quad \mathrm{div}\,\mathbf{T} = \hat{\mathbf{f}}$

  $\mathbf{T}$ ... stress of diffusing species $\quad \hat{\mathbf{f}}$ ... diffusive force (Maxwell)

  $\partial_t \mathbf{j} = \partial \mathbf{j} / \partial t \approx \rho \dot{\mathbf{v}}$...inertia is neglected in r.h.s. of momentum balance

  $\hat{\mathbf{f}}$ ... internal body force for the interaction of diffusive species with surrounding solid matrix

- **Gradient Constitutive Eqs:** $\{\mathbf{T}, \hat{\mathbf{f}}\} \rightarrow \{\rho, \nabla\rho; \dot{\rho}, \nabla\nabla\rho \ldots\}$

- **Diffusion Classes/Non-universality of Fick's Law**

  - $\mathbf{T} = -\pi\rho\mathbf{1} \quad \hat{\mathbf{f}} = \alpha\mathbf{j} \quad \Rightarrow \quad \dot{\rho} = D\nabla^2\rho \qquad (D \equiv \pi/\alpha)$

    Fick's equation ... parabolic

  - $\mathbf{T} = -\pi\rho\mathbf{1} - \bar{\pi}\dot{\rho}\mathbf{1} \quad \hat{\mathbf{f}} = \alpha\mathbf{j} \Rightarrow \dot{\rho} = D\nabla^2\rho + \bar{D}\nabla^2\dot{\rho} \qquad (\bar{D} \equiv \bar{\pi}/\alpha)$

    Barenblatt's equation ... pseudoparabolic

  - $\mathbf{T} = -\pi\rho\mathbf{1} + \pi^*\nabla^2\rho\mathbf{1} \quad \hat{\mathbf{f}} = \alpha\mathbf{j} \Rightarrow \dot{\rho} = D\nabla^2\rho - D^*\nabla^4\rho \qquad (D^* \equiv \varepsilon/\alpha)$

    Cahn – Hilliard equation $\quad (D < 0, D^* > 0)$
    uphill diffusion / spinodal decomposition

■ Higher-order Diffusion Theory

- ***Balance Laws:*** $\dot{\rho} + \mathrm{div}\mathbf{j} = 0 \quad ; \quad \mathrm{div}\mathbf{T} = \hat{\mathbf{f}} + \partial_t \mathbf{j} \;\; , \;\; \mathbf{j} \sim \rho\mathbf{v}$ ... inertia
- ***Constitutive Eqs:*** $\mathbf{T} = -(\pi\rho + \bar{\pi}\dot{\rho} - \pi^* \nabla^2 \rho)\mathbf{1} \;\; ; \;\; \hat{\mathbf{f}} = \alpha\mathbf{j} \;\Rightarrow$
- ***Governing Eq:*** $\dot{\rho} + \tau\ddot{\rho} = D\nabla^2\rho + \bar{D}\nabla^2\dot{\rho} - D^*\nabla^4\rho \qquad (\tau = 1/\alpha)$

Note1: This is the diffusion equation which can also be derived for a composite medium containing two phases with diffusion of Fick type taking place in each phase and with a mass exchange term introduced to model the jumps of diffusion species from one phase to another.

Note2: This is shown in the next slide for diffusion in nanopolycrystals with one phase identified with the bulk of nanocrystals and the other phase identified with the grain boundaries between the nanocrystals.

■ 2ble Diffusivity/Nanopolycrystals/Micro-Nanodiffusion

$$\dot{\rho}_i + \mathrm{div}\mathbf{j}_i = \hat{\mathrm{c}}_i, \quad \mathrm{div}\mathbf{T}_i = -\hat{\mathbf{f}}_i \;\; ; \;\; \{\mathbf{T}_i,\ \hat{\mathbf{f}}_i,\ \hat{\mathrm{c}}_i\} \longrightarrow \{\rho_i,\ \mathbf{j}_i,\ \ldots\}; \;\; i = 1,2$$

• *Simplest Model/Fick type*

$$\mathbf{T}_i = -\pi_i \rho_i \mathbf{1} \quad ; \quad \hat{\mathbf{f}}_i = \alpha_i \mathbf{j}_i \quad ; \quad \hat{\mathrm{c}}_i = (-1)^i [\kappa_1 \rho_1 - \kappa_2 \rho_2], \quad D_i = \pi_i / \alpha_i$$

$$\dot{\rho}_1 = \mathrm{D}_1 \nabla^2 \rho_1 - (\kappa_1 \rho_1 - \kappa_2 \rho_2) \quad , \quad \dot{\rho}_2 = \mathrm{D}_2 \nabla^2 \rho_2 + (\kappa_1 \rho_1 - \kappa_2 \rho_2)$$

• *Solution*

$$\rho_1 = e^{-\kappa_1 t} \mathrm{h}_1(\mathrm{x}, \mathrm{D}_1 \mathrm{t}) + \frac{\sqrt{\kappa_2}}{\mathrm{D}_1 - \mathrm{D}_2} e^{\lambda t} \int_{D_2 t}^{D_1 t} e^{-\mu \xi} [\mathrm{A}_1 \mathrm{h}_1(x,\xi) + \mathrm{A}_2 \mathrm{h}_2(x,\xi)] \mathrm{d}\xi$$

$$\rho_2 = \quad \ldots$$

$$\dot{\mathrm{h}}_\alpha = \nabla^2 \mathrm{h}_\alpha \quad ; \quad \mathrm{A}_1 = \sqrt{\kappa_1} \left(\frac{\xi - \mathrm{D}_2 \mathrm{t}}{\mathrm{D}_1 \mathrm{t} - \xi} \right)^{1/2} \mathrm{I}_1(\eta) \quad ; \quad \mathrm{A}_2 = \sqrt{\kappa_2} \mathrm{I}_2(\eta)$$

$$\lambda = \frac{\kappa_1 D_2 - \kappa_2 D_1}{D_1 - D_2} \quad , \quad \mu = \frac{\kappa_1 - \kappa_2}{D_1 - D_2} \quad , \quad \eta = \frac{2\sqrt{\kappa_1 \kappa_2}}{D_1 - D_2} [(D_1 t - \xi)(\xi - D_2 t)]^{1/2}$$

• *Higher-order Diffusion Equations*

It turns out that uncoupling of the 2ble Diffusivity Eqs yields

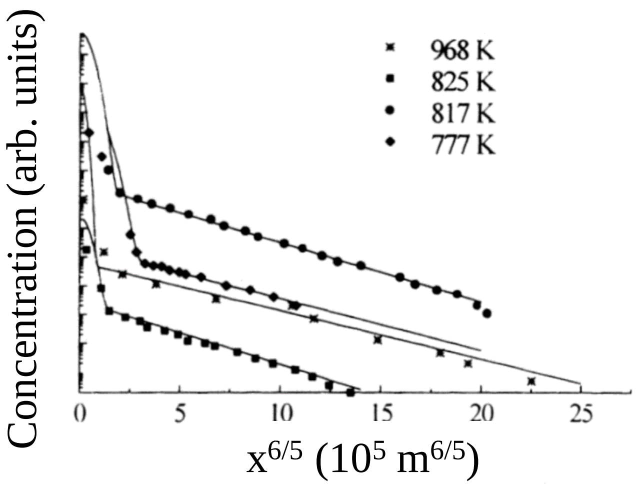
$$\dot{\rho} + \tau\ddot{\rho} = D\nabla^2\rho + \bar{D}\nabla^2\dot{\rho} - D^*\nabla^4\rho$$

$$\tau = (\kappa_1 + \kappa_2)^{-1} \ , \ D = \tau(\kappa_1 D_2 + \kappa_2 D_1) \ , \ \bar{D} = \tau(D_1 + D_2) \ , \ D^* = \tau D_1 D_2$$

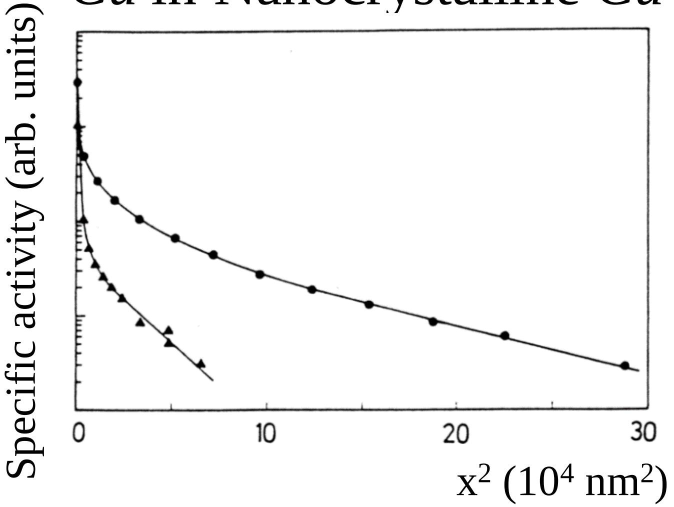
$$\left[t \to \infty \Rightarrow \ \dot{\rho} = D\nabla^2\rho \ ; \ D = D_{eff} = \frac{\kappa_2}{\kappa_1 + \kappa_2} D_1 + \frac{\kappa_1}{\kappa_1 + \kappa_2} D_2 = f\,D_1 + (1 - f)D_2 \right]$$

- *Diffusion Penetration Profiles*

^{64}Cu in Polycrystalline Cu



^{67}Cu in Nanocrystalline Cu



- *Special Case* $(\tau = \bar{D} = 0)$ $\dot{\rho} = D\nabla^2\rho - D^*\nabla^4\rho$ ... Cahn-Hilliard type

- *Fractional Generalization:* $\dot{\rho} = D\nabla^2\rho + D_\alpha \nabla \cdot \left\{ (-\Delta)^{\alpha/2} \nabla\rho \right\} \ ; \ D_\alpha = D l^\alpha$

■ Higher-order Fractional Diffusion

- ***Fractional GradDif:*** $\dot{\rho} + div\mathbf{j} = 0 \quad ; \quad \mathbf{j} = -D\nabla\left[\rho + l^{\alpha}(-\Delta)^{\alpha/2}\rho\right]$

- ***Governing Equation:*** $\dot{\rho} = D\Delta\rho + D_{\alpha}\nabla\cdot\left\{(-\Delta)^{\alpha/2}\nabla\rho\right\} \;\; ; \;\; D_{\alpha} \sim D l_d^{\alpha}$

- ***Riesz Laplacian:*** $((-\Delta)^{\alpha/2}\rho)(\mathbf{r}) = \mathcal{F}^{-1}(|\mathbf{k}|^{\alpha}\rho(\mathbf{k}))(\mathbf{r})$ ... as before

- ***Fundamental Solution:*** $\rho(x,t) = \dfrac{1}{(4\pi D t)^{1/2}}\int_{-\infty}^{\infty} G_{\alpha+2}(x',t)\, e^{-(x-x')^2/4Dt} dx'$

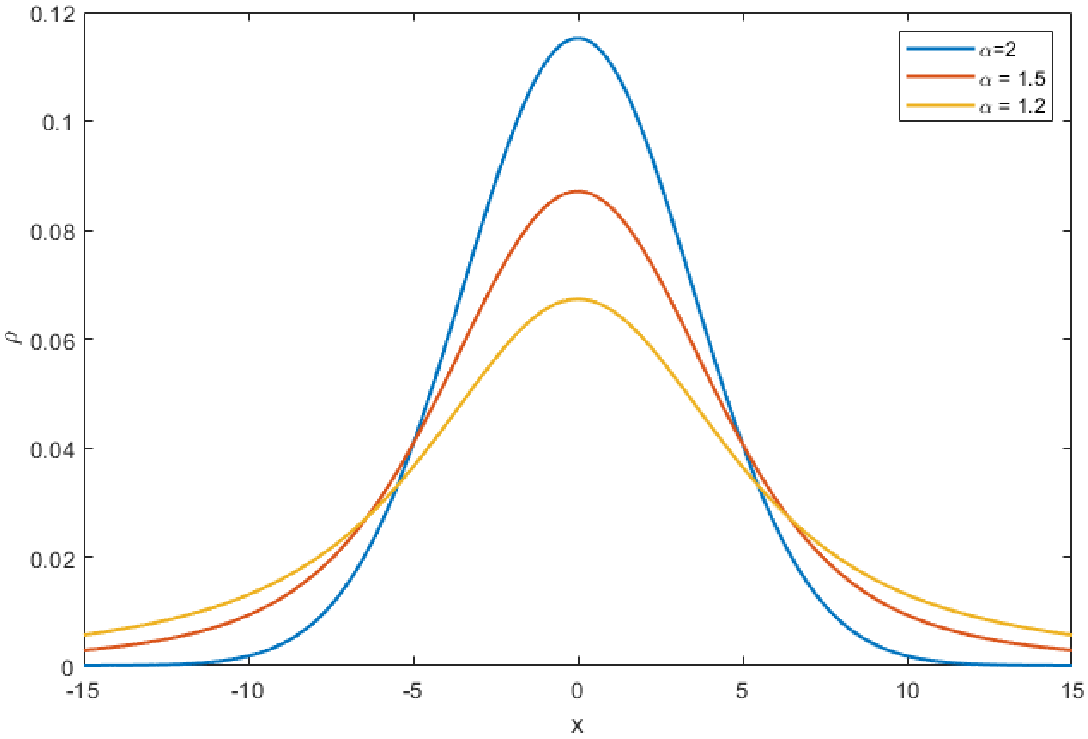
$$G_{\alpha}(x,t) = \frac{1}{\alpha(4\pi)^{1/2}(D_{\alpha}t)^{1/\alpha}} \mathrm{H}_{1,2}^{1,1}\left[\frac{|x|}{2(D_{\alpha}t)^{1/\alpha}}\right] \quad ; \quad \mathrm{H}_{1,2}^{1,1} = \mathrm{H}_{1,2}^{1,1}\Big|_{(0,2^{-1});(2^{-1},2^{-1})}^{1-\alpha^{-1},\alpha^{-1}}$$

$$= \frac{2}{\alpha(4\pi)^{1/2}(D_{\alpha}t)^{1/\alpha}} {}_1\Psi_1\left[-\frac{|x|^2}{4(D_{\alpha}t)^{2/\alpha}}\right] \quad ; \quad {}_1\Psi_1(z) = \sum_{\nu=0}^{\infty}\frac{\Gamma(\alpha^{-1}+2\nu\alpha^{-1})}{\Gamma(2^{-1}+\nu)}\frac{(-z)^{\nu}}{\nu!}$$

• *Profiles of Fractional Fundamental Solution*

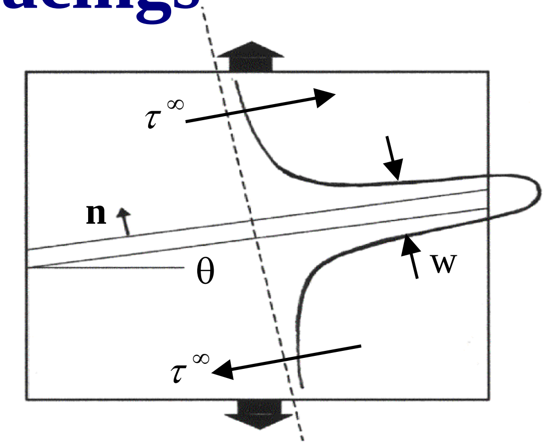
- $l^{\alpha} = 0 \quad \Rightarrow \quad \rho(x,t) = \frac{1}{(4\pi D t)^{1/2}} e^{-(x-x')^2/4Dt}$

- $l^{a} \neq 0 \ , \ \alpha \neq 2 \quad \Rightarrow \quad \rho(x,t) = \frac{1}{(4\pi D t)^{1/2}} \int_{-\infty}^{\infty} G_{\alpha+2}(x',t) e^{-(x-x')^2/4Dt} dx'$



III. Gradient Plasticity (GradPla)

■ Capturing Shear Band Widths & Spacings



- ***Constitutive Equation***

$$\mathbf{S}' = -p\mathbf{1} + 2\mu\mathbf{D} \quad ; \quad \mathbf{D} \approx \dot{\boldsymbol{\varepsilon}}^p$$

$$\mu = \frac{\tau}{\dot{\gamma}} \quad , \quad \begin{cases} \tau \equiv \sqrt{\frac{1}{2}\mathbf{S}'\cdot\mathbf{S}'} \\ \dot{\gamma} \equiv \sqrt{2\mathbf{D}\cdot\mathbf{D}} \end{cases} ; \quad \tau = \kappa(\gamma) - c\nabla^2\gamma$$

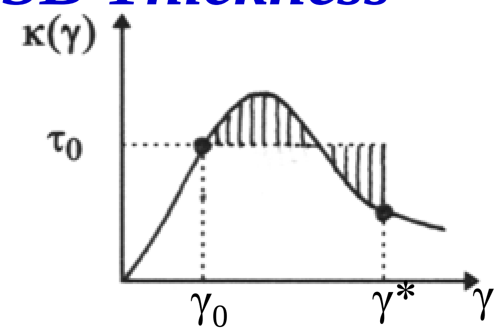
- ***Linear Stability / SB Orientation***

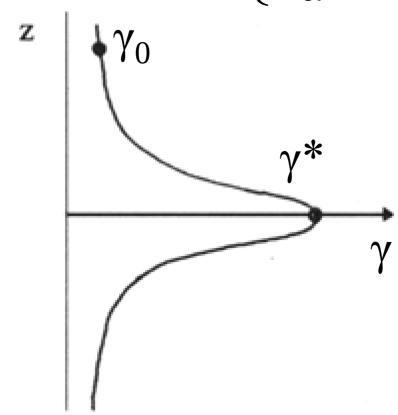
$$\mathrm{v} = \mathrm{L}_\infty \mathrm{x} + \tilde{\mathrm{v}}\mathrm{e}^{\mathrm{iqz}+\omega \mathrm{t}} ; \quad \omega > 0 \quad (\&\omega_{\max}) \quad \to \quad \theta_{cr} = \frac{\pi}{4} \quad \& \quad \begin{cases} h_{cr} = 0 \\ q_{cr} = 0 \end{cases}$$

- ***Nonlinear Solution / SB Thickness***

$$c\gamma_{zz} = \kappa(\gamma) - \tau_0$$

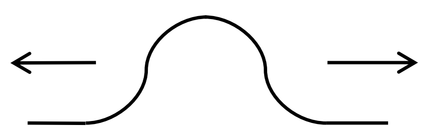
$$\gamma \equiv \int \dot{\gamma}\, dt$$





- ***Front Propagation***

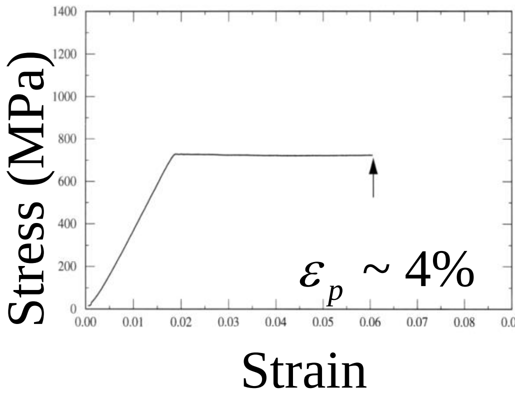
Similar Procedure

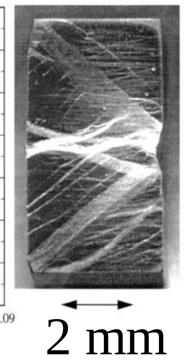


■ Multiple Shear Banding

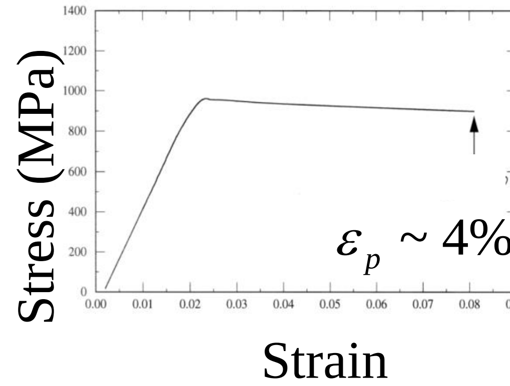
- Compression of Bulk Nanostructured Fe – 10% Cu Polycrystals (UFGs)

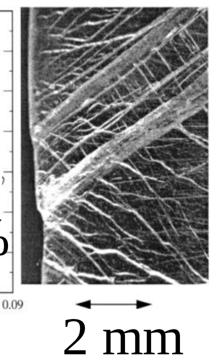
d ~1370 nm, σ_y ~750 MPa
angle ~ 49^0





d ~540 nm, σ_y ~960 MPa
angle ~ 49^0





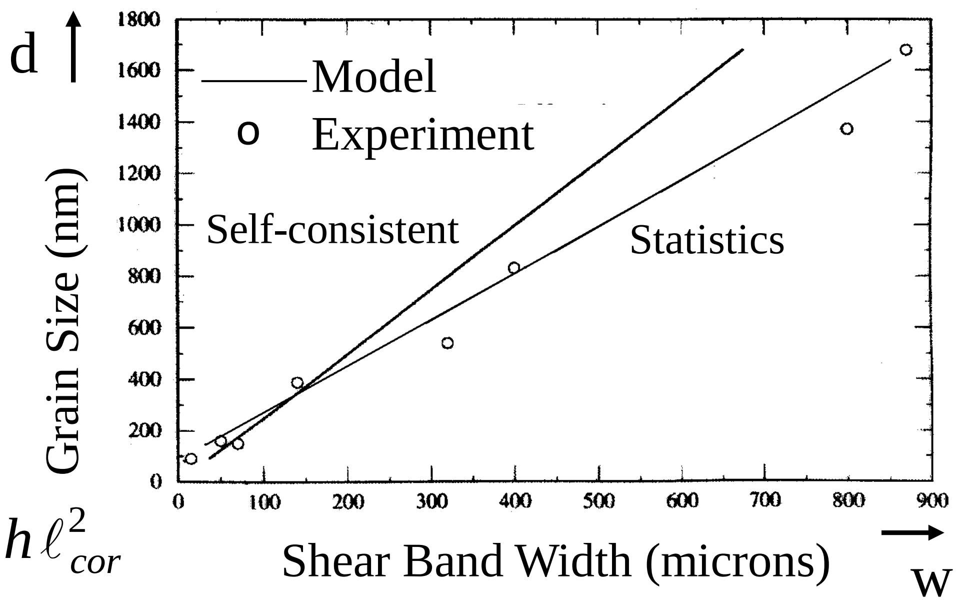
- Shear band width analysis

$$\tau = \kappa(\gamma) - c\nabla^2\gamma$$

$$w \sim \sqrt{c}\,; \qquad c \sim d^2\,(\beta + h)$$

$$\beta = \alpha G \frac{7-5\nu}{15(1-\nu)}$$

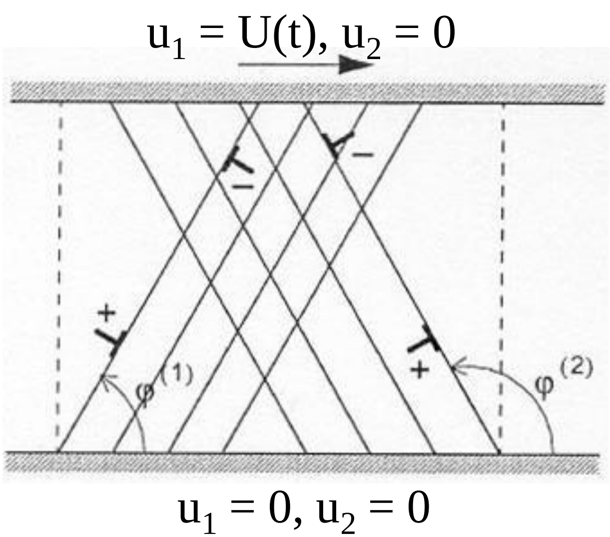
$$c = -h\left(\left.\frac{\partial^2 \Lambda(r)}{\partial r^2}\right|_{r=0}\right)^{-1}, \quad w \sim \sqrt{c}, \;\; c \sim h\,\ell_{cor}^2$$

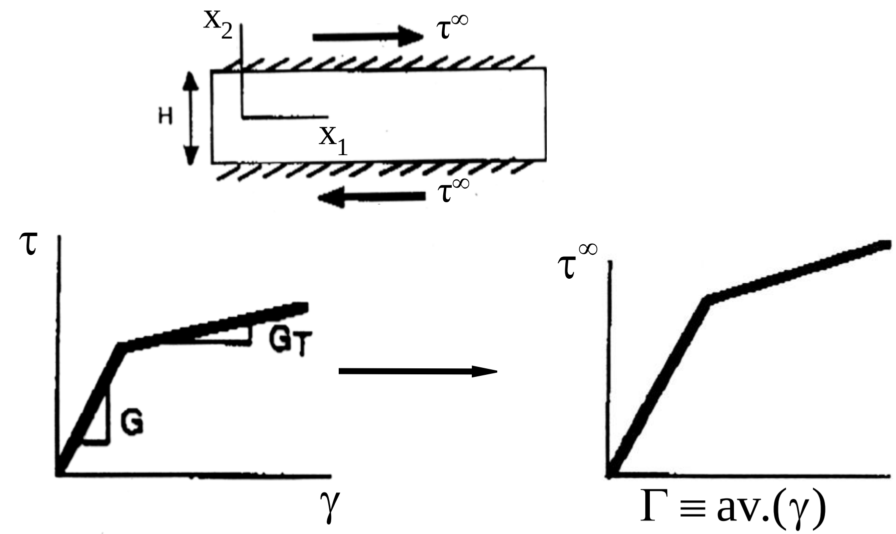


■ Plastic Boundary Layers

- ***Fleck/Van Der Giessen/Needleman (2000)***

Discrete Dislocations (DD) Fleck-Hutchinson (F-H)



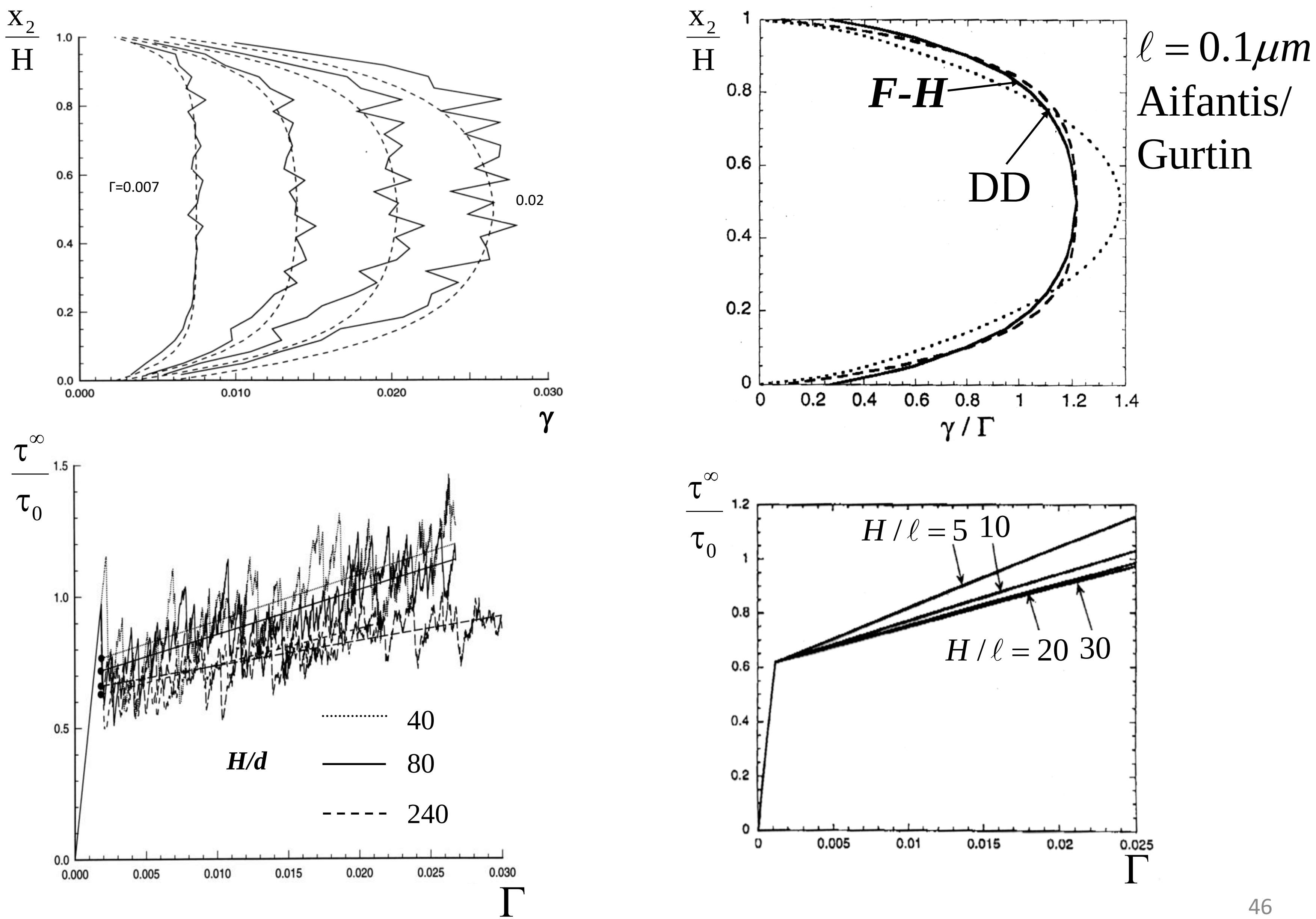


- ***Aifantis (1984) / Gurtin (2000)***

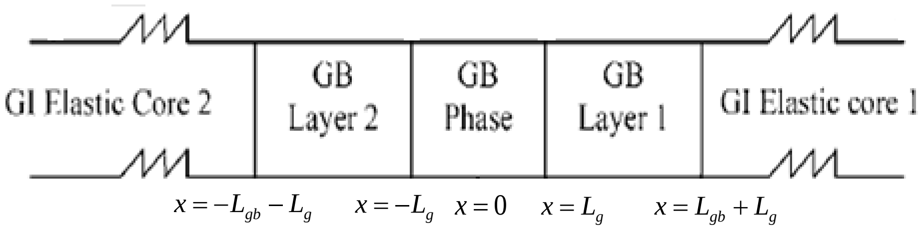
$$\tau = \tau_0 + G_T\gamma - G_T\ell^2\nabla^2\gamma = \tau^\infty \quad \Rightarrow \quad \gamma = \frac{\tau^\infty}{G} + \frac{\tau^\infty - \tau_0}{G_T}\left[1 - \frac{\cosh(x_2/\ell)}{\cosh(H/\ell)}\right]$$

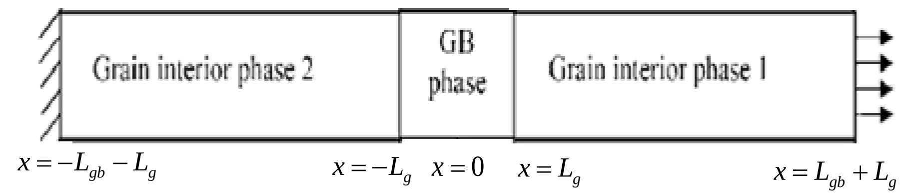
$$\Gamma = \frac{1}{H}\int_{-H/2}^{H/2}\gamma(x_2)dx_2 = \frac{\tau^\infty}{G} + \frac{\tau^\infty - \tau_0}{G_T}\left(1 - \frac{2\ell}{H}\tanh\frac{H}{2\ell}\right)$$

• *Plastic Strain Profiles / Size Effects*



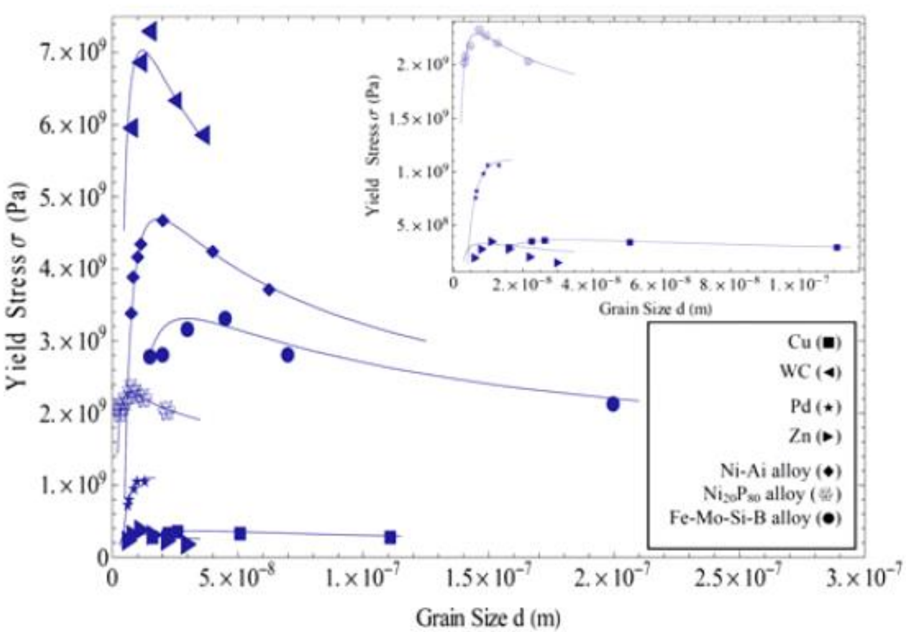
■ Inverse H-P Relation (Kat. Aifantis)

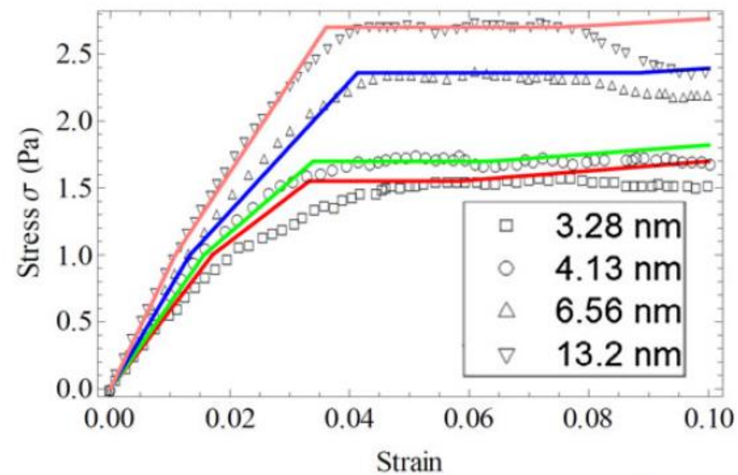




Unit cell model for GB & GI (elastic core + GB layer) phases: Inverse H-P and size-dependent stress-strain curves

$$\bar{\sigma}=\sigma_0+\frac{k}{\sqrt{d}}+\frac{\gamma_{gb}}{2ad};\quad d_c=\left(\gamma_{gb}/ak\right)^2$$

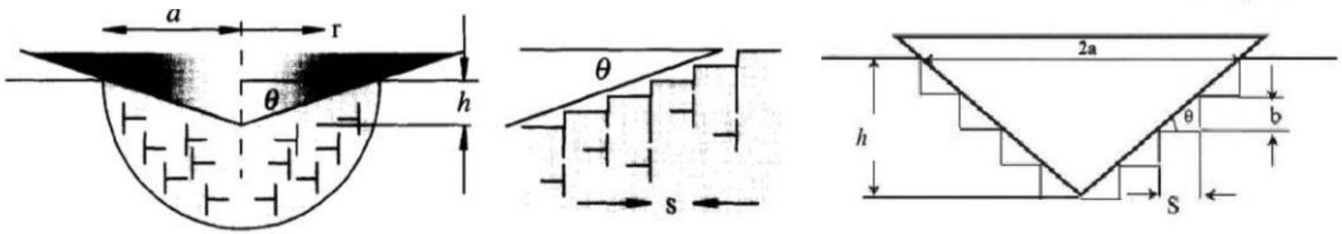




	L_g = 3.28 nm	L_g = 4.13 nm	L_g = 6.56 nm	L_g = 13.2 nm	
σ^0_{gb} (GPa)	1	1	1	1	
σ^0_g (GPa)	1.55	1.70	2.36	2.70	
E_g (GPa)	E_{gb} (GPa)	L_{gb} (nm)	ℓ_{gb} (nm)	β_{gb} (GPa)	β_g (GPa)
127	27	1.5	1	10	2

■ Nanoindentation –A Simplified Analysis

- ***Schematics***



$$\varepsilon^p = \frac{h}{a} = \tan\theta$$

$$\left|\nabla\varepsilon^p\right| = \frac{\varepsilon^p}{a} = \frac{h}{a^2} = \frac{\tan^2\theta}{h}$$

$$\nabla^2\varepsilon^p = \frac{\varepsilon^p}{a^2} = \frac{h}{a^3} = \frac{\tan^3\theta}{h^2}$$

- ***Fleck-Hutchinson-Ashby (1994) / Gao-Nix (1998)***

$$\rho_{GND} \sim \nabla\gamma \xrightarrow{Taylor} \tau = \tau_0\left(1 + \frac{\rho_{GND}}{\rho_S}\right)^{1/2}$$

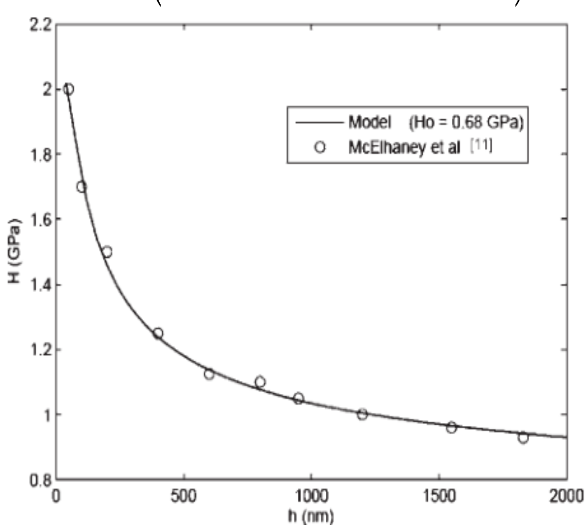
- ***Aifantis (1984)***

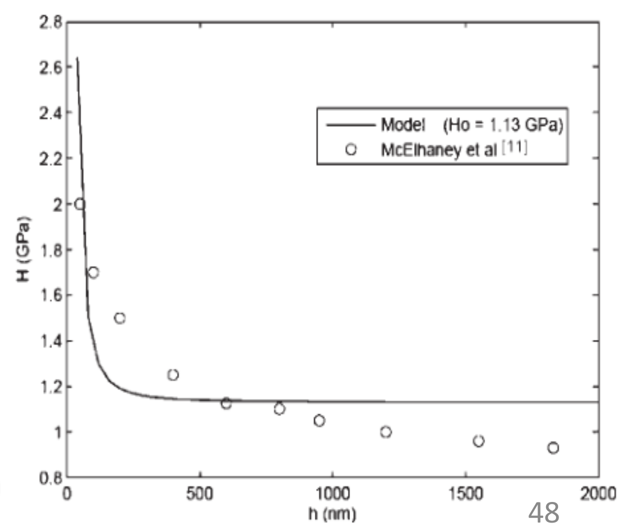
$$\tau = \tau_0\left(1 + c_1\left|\nabla\gamma\right|^{1/2} - c_2\nabla^2\gamma\right)$$

$$H = H_0\left[1 + \left(\frac{l_1}{h}\right)^{1/2} - \left(\frac{l_2}{h}\right)^2\right]$$

l_1, l_2 : internal lengths

h : indentation depth





■ A Note on Consistency with Continuum Thermodynamics

Thermodynamics applied to gradient theories :
The theories of Aifantis and Fleck & Hutchinson and their generalization
[*J. Mech. Phys. Sol.* **57**, 405-421 (2009)]

M.E. Gurtin/Carnegie-Mellon & L. Anand/MIT

Abstract : We discuss the physical nature of flow rules for rate-independent (gradient) plasticity laid down by Aifantis and Fleck and Hutchinson. As central results we show that:

- the flow rule of Fleck and Hutchinson is incompatible with thermodynamics unless its nonlocal term is dropped.
- If the underlying theory is augmented by a general defect energy dependent on γ^p and $\nabla\gamma^p$, then compatibility with thermodynamics requires that its flow rule reduce to that of Aifantis.

Refs

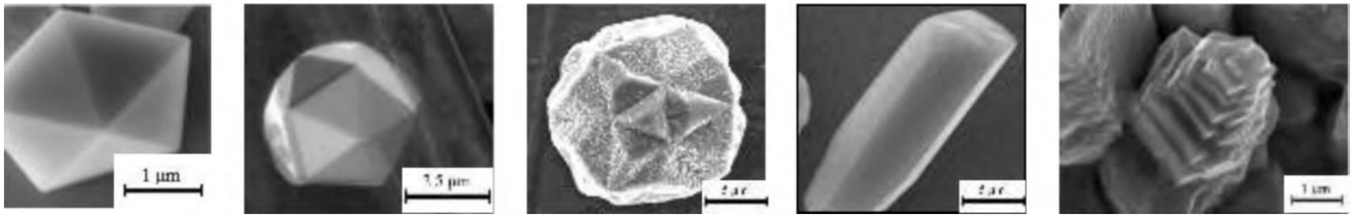
• E.C. Aifantis, On the microstructural origin of certain inelastic models, *Trans. ASME, J. Engng. Mat. Tech.* **106**, 326-330 (1984).

• E.C. Aifantis, The physics of plastic deformation, *Int. J. Plasticity* **3**, 211-247 (1987).

• N.A. Fleck and J.W. Hutchinson, A reformulation of strain gradient plasticity, *J. Mech. Phys. Solids* **49**, 2245-2271 (2001).

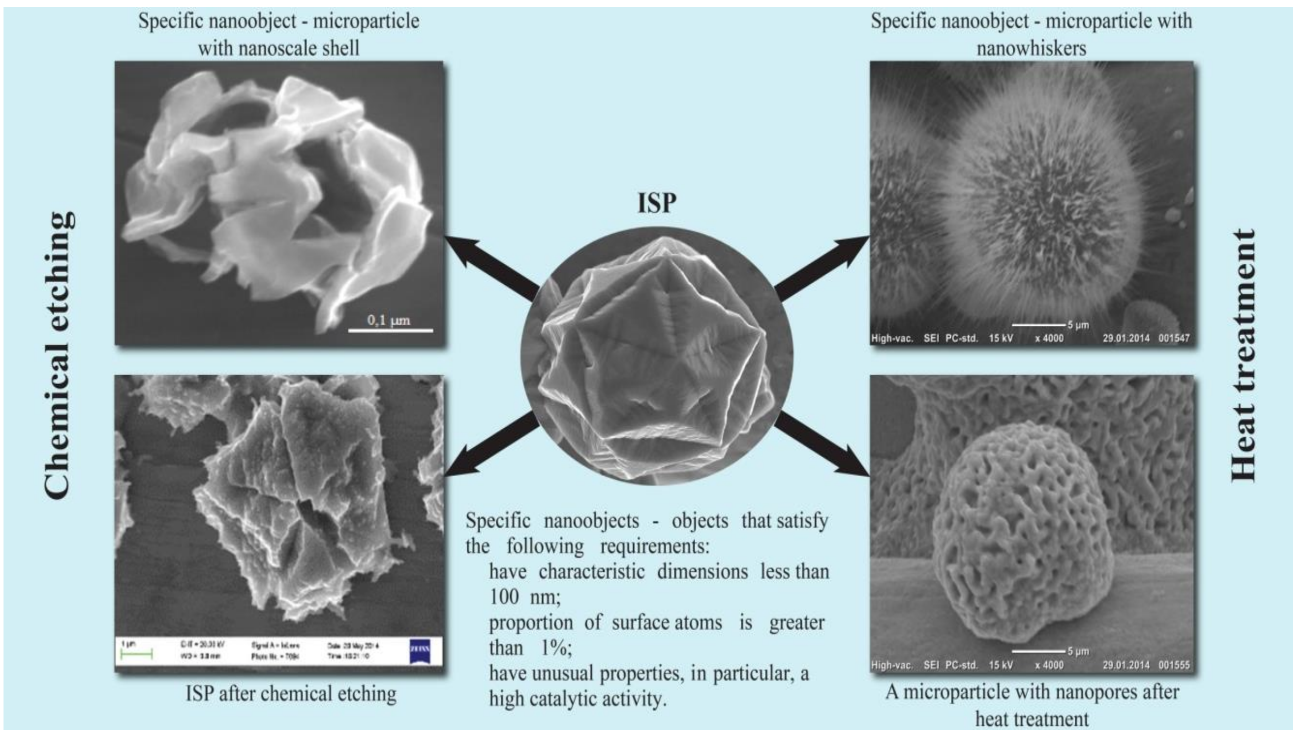
IV. Disclinated Micro Crystals (DMC): Void Formation

■ Fabrication/Electrodeposition & Observations/Morphology



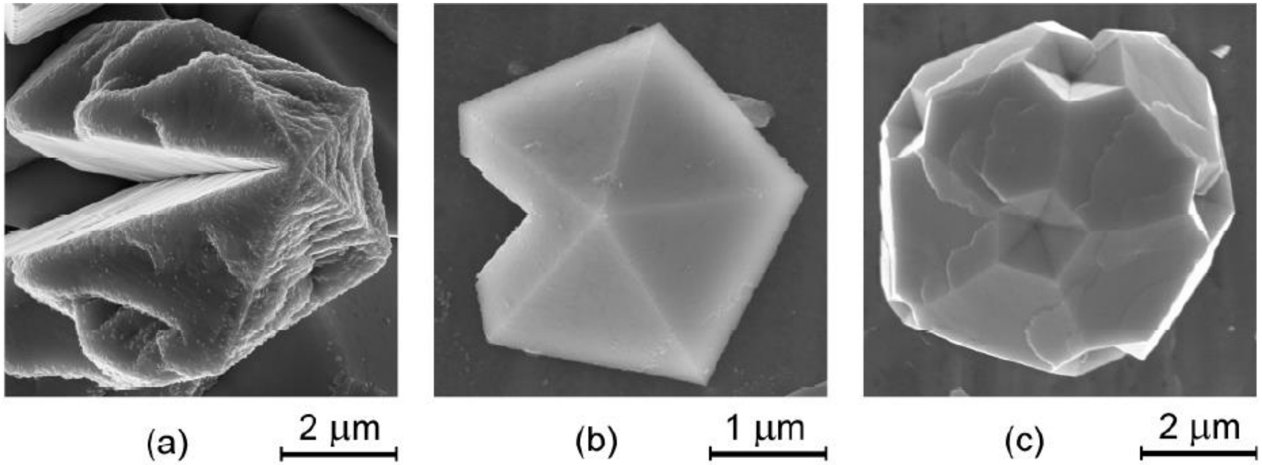
(a) (b) (c) (d) (e)

Copper pentagonal particles and crystals: ***(a)*** *decahedral small particles (DSPs);* ***(b)*** *icosahedral small particles (ISPs);* ***(c)*** *stellated pentagonal polyhedral (SPP);* ***(d)*** *pentagonal whiskers (PWs);* ***(e)*** *pentagonal pyramids (PPs).*

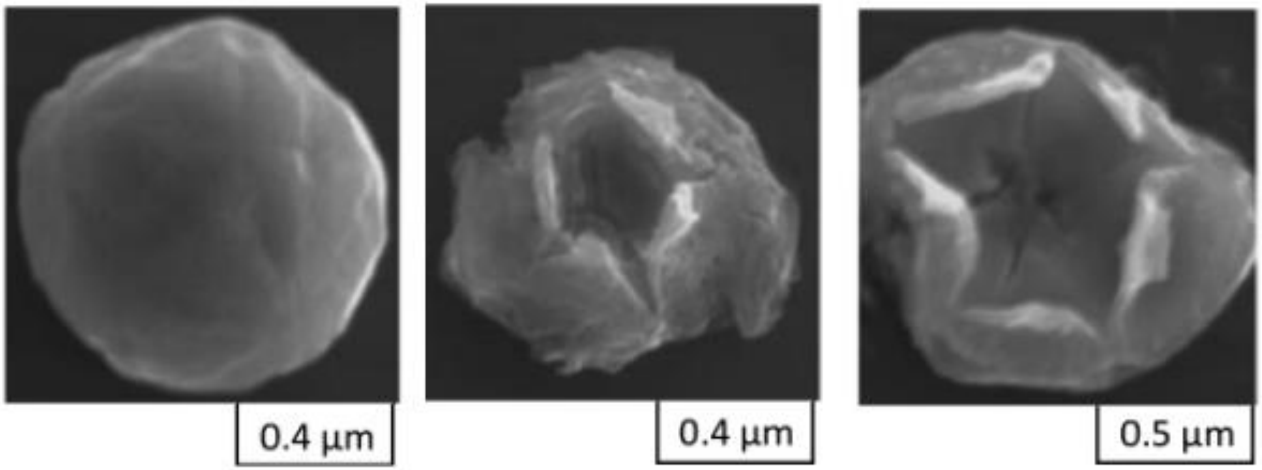


Preparation of the developed surface of icosahedral small particles.

■ Stress Relaxation in DMC



*Examples of relaxation processes in DMCs observed in electrodeposition experiments: **(a)** opening of a gap instead of TB (CuDMC); **(b)** formation of an open sector outside TBs (AgDMC); **(c)** faceting surface around the disclination axis (Ag DMC)*



ISP Copper Micro-object before and after being subjected to chemical etching. The existence of an internal void is revealed.

- Internal Stress: Disclination in a hollowed sphere $\left(R_1, R_0\right)$
- Mechanical Stability: Minimize (elastic + surface) energy: E_{ISP}

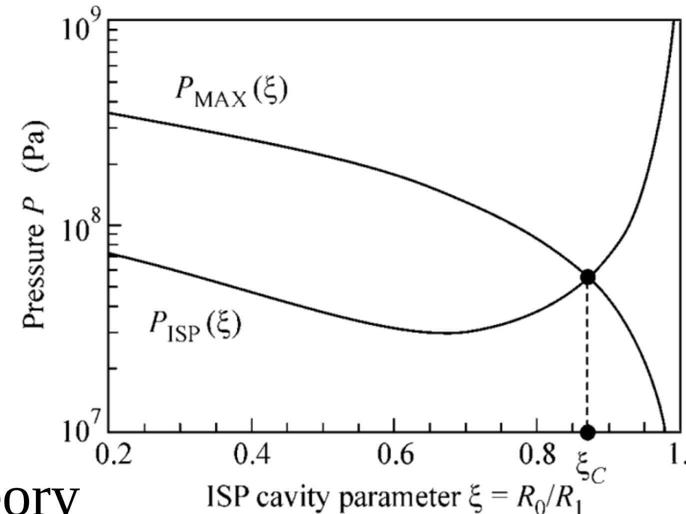
■ Modeling Efforts I / Elastic Disclination

- $$E_{ISP} = \underbrace{4\pi\gamma\left(R_0^2 + R_1^2\right)}_{\text{surface energy}} + \underbrace{\frac{8\pi G\kappa^2(1+\nu)}{27(1-\nu)}\left[R_1^3 - R_0^3 - \frac{9R_0^3R_1^3}{R_1^3 - R_0^3}\left(\ln\frac{R_0}{R_1}\right)^2\right]}_{\text{stored elastic energy}}$$

γ (=0.1 Ga, a lattice spacing) - surface energy; (G,ν) - elastic constants

κ (=0.12) - disclination strength

- $P_{ISP} \le P_{\max}$ ... fracture criterion
- $P_{ISP} = \dfrac{E_{ISP}}{V}$ ... thermodynamic approx.
- $P_{\max} = \dfrac{2\sigma(R_1 - R_0)}{R_0}$ ... thin cell elastic theory



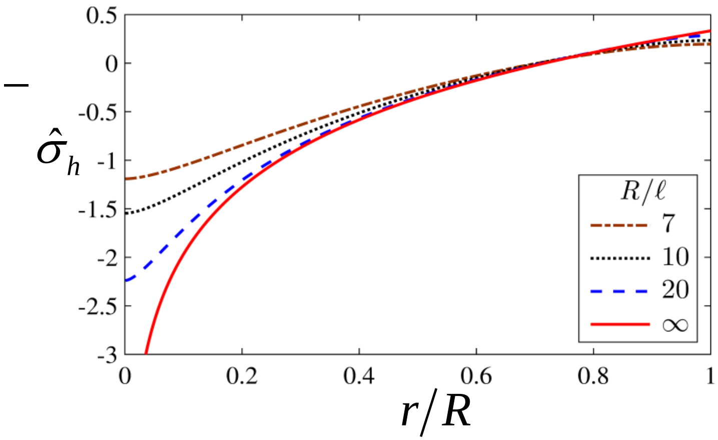
$$\therefore\ P_{ISP} = \frac{3Ga(1+\xi^2)}{10R_1(1-\xi^3)} + \frac{2G\kappa^2(1+\nu)}{9(1-\nu)}\left[1 - \frac{9\xi^3\ln^2\xi}{(1-\xi^3)^2}\right]; \quad P_{\max} = \frac{2\sigma(R_1 - R_0)}{R_1} = 2\sigma(1-\xi)$$

σ : fracture stress, $\xi = R_0/R_1$

■ Modeling Efforts II / Gradela Disclination

- ***Hydrostatic stress***

$$\sigma_h = \frac{1}{3}\mathrm{tr}(\boldsymbol{\sigma}) = \frac{4G\kappa}{3}\frac{1+\nu}{1-\nu}\left[\frac{1}{3} + \ln\left(\frac{r}{R}\right) + \frac{\ell}{r}\cosh\left(\frac{r}{\ell}\right)\mathrm{Shi}\left(\frac{r}{\ell}\right) - \frac{\ell}{r}\sinh\left(\frac{r}{\ell}\right)\left(C_1 + \mathrm{Chi}\left(\frac{r}{\ell}\right)\right)\right]$$

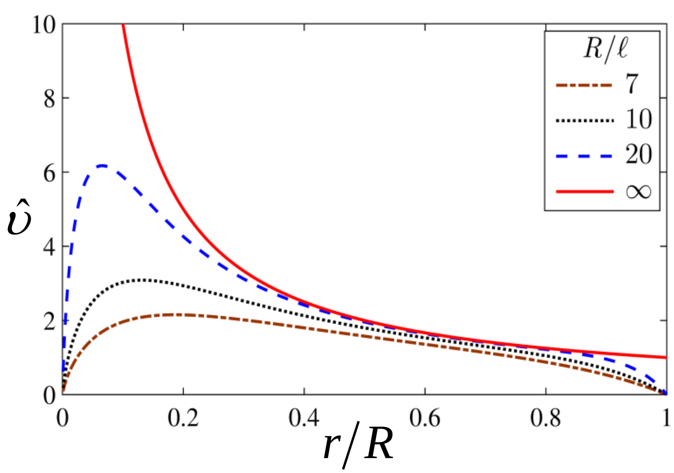


- ***Vacancy Drift Velocity υ***

$$\upsilon = (D / k_B T) F \;\; ; \;\; F = -(\delta\Omega)\frac{\partial \sigma_h}{\partial r}$$ ... driving force, $(\delta\Omega)$ ... local volume change

$$\upsilon = -\frac{D_o(\delta\Omega)}{k_B T}\frac{4G\kappa}{3}\frac{1+\nu}{1-\nu}\exp\left(\frac{-Q}{k_B T}\right)\frac{1}{r}\left\{1 + \sqrt{\frac{\pi r}{2\ell}}\left[I_{-3/2}\left(\frac{r}{\ell}\right)\mathrm{Shi}\left(\frac{r}{\ell}\right) - I_{3/2}\left(\frac{r}{\ell}\right)\left(C_1 + \mathrm{Chi}\left(\frac{r}{\ell}\right)\right)\right]\right\}$$

$D = D_o \exp(-Q / k_B T)$; Q: activation energy

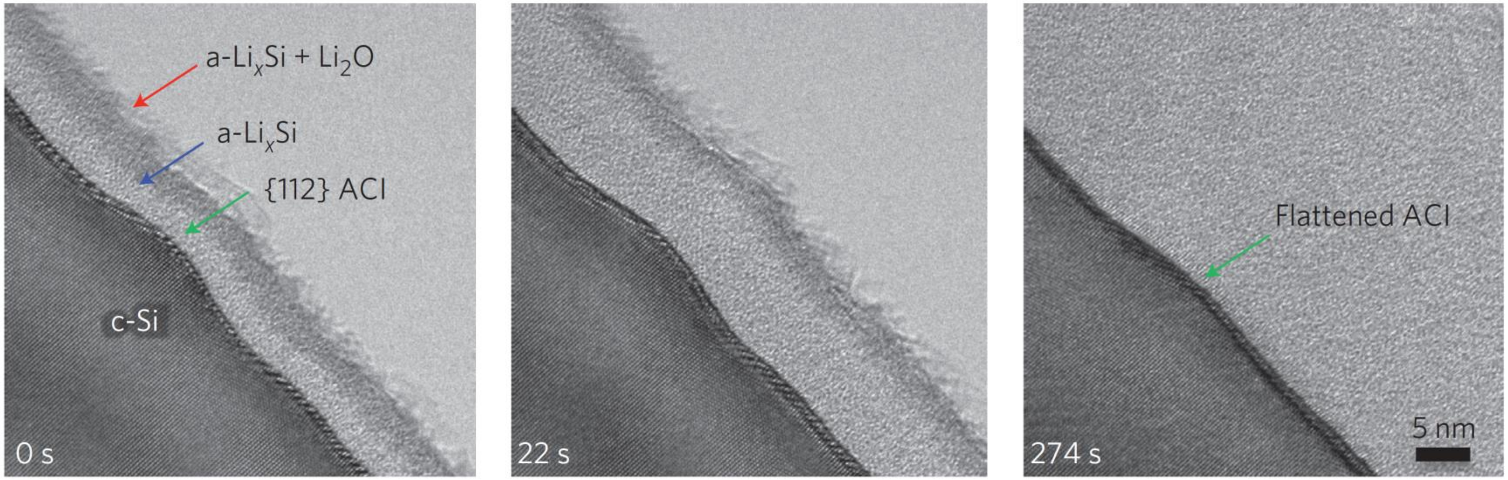


Effect of the stress gradient internal length ℓ on the drift velocity of vacancies at the initial stages of the void formation. Dimensionless parameters are used:

$$\hat{\upsilon} = -\exp(Q / k_B T)\left[3Rk_B T(1-\nu) / 4G\kappa D_o(\delta\Omega)(1+\nu)\right]\upsilon$$

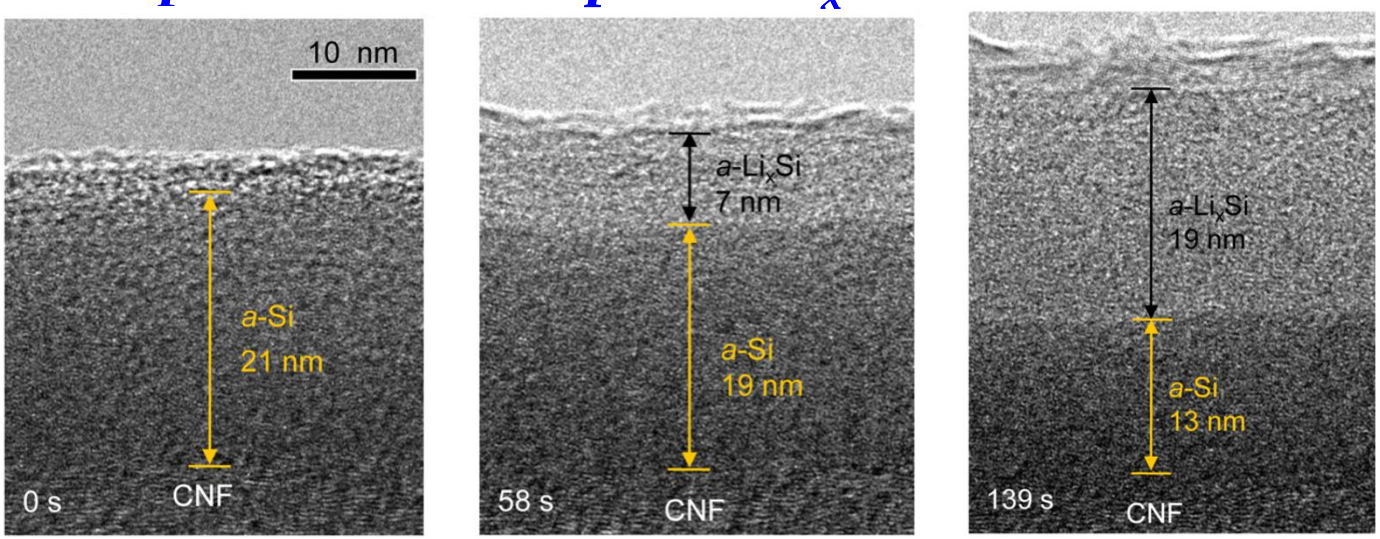
V. Li-ion Anodes (LiBs): Two-phase Lithiation

- ***Crystalline Si / Amorphous LixSi***



Migration of {112} Amorphous / Crystalline Interface (ACI) during lithiation. (*Xiao Hua Liu et al*, *2012*).

- ***Amorphous Si / Amorphous Li_xSi***



Migration of the Interface during lithiation of an a-Si surface layer covering a carbon nanofiber (CNF). (*Jiang Wei Wang et al*, *2013*).

Note: Average interface velocity $\upsilon \sim 3.6$ nm/min

- ***Chemomechanical Constitutive and Balance Eqs***
  - ***Gradient Chemoelastic Stress***

$$\boldsymbol{\sigma} = 2G\boldsymbol{\varepsilon} + \lambda(\mathrm{tr}\,\boldsymbol{\varepsilon})\mathbf{1} - \ell_\varepsilon^2 \nabla^2 \left[2G\boldsymbol{\varepsilon} + \lambda(\mathrm{tr}\,\boldsymbol{\varepsilon})\mathbf{1}\right] - (2G + 3\lambda) M_o \rho \mathbf{1}$$

  - ***Gradient Chemical Potential***

$$\mu = \mu^0 + RT\left[\ln\left(\frac{\rho}{1-\rho}\right) + \alpha(1-2\rho)\right] - \kappa\nabla^2\rho - \Omega_{Li}\sigma_h$$

(λ, G) ... Lamé consts; R ... gas const; T ... abs.temperature
M_o ... chem.expansion (misfit strain) coeff; $(\kappa, \ell_\varepsilon)$ ... gradient coeffs;
$\Omega_{Li} = 3M_o / C_{\max}$ ... partial molar volume

  - ***Quasistatic Mechanical Equilibrium:*** $\mathrm{div}\,\boldsymbol{\sigma} = 0$

  - ***Diffusion:*** $\dfrac{\partial\rho}{\partial t} + \mathrm{div}\,\bar{\boldsymbol{j}} = 0\,;\qquad \bar{\boldsymbol{j}} = \dfrac{\boldsymbol{j}}{c_{\max}} = -\dfrac{D_o}{RT}\rho(1-\rho)\nabla\mu$

$$\rho = C/C_{\max} \quad (0 \le \rho \le 1)$$

• Lithiation Modeling of Si / Radial Symmetry

$$\operatorname{div}\boldsymbol{\sigma} = 0 \;\Rightarrow\; \sigma_h = -\frac{4G(2G+3\lambda)}{3(2G+\lambda)} M_o \rho + f(t); \qquad \begin{cases} f(t) \ldots \text{arbitrary} \\ \text{(it depends on mech. BC's)} \end{cases}$$

$$\therefore \quad \bar{\mu} = \ln\left(\frac{\rho}{1-\rho}\right) + \alpha(1-2\rho) + \beta\rho - \ell_\rho^2 \nabla^2 \rho = g(\rho) - \ell_\rho^2 \nabla^2 \rho$$

Dimensionalization: $\bar{\mu} := \dfrac{\mu - \mu^0 - \Omega_{Li} f(t)}{RT}; \quad \beta := \dfrac{4G(2G+3\lambda)M_o^2}{(2G+\lambda)RTC_{\max}}; \quad \ell_\rho = \sqrt{\dfrac{\kappa}{RT}}$

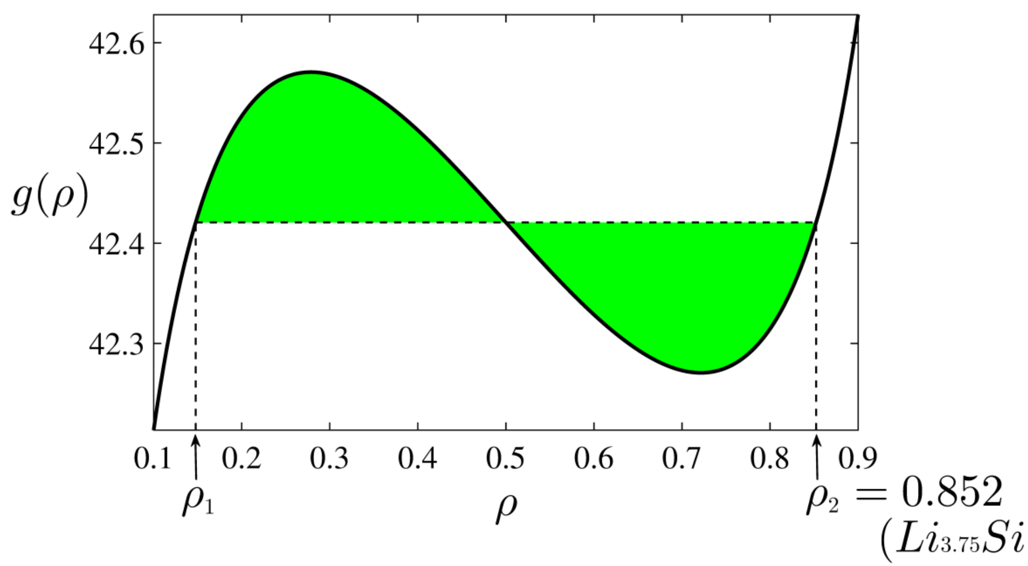
– Evaluation of Parameters

- 310% free expansion at max lithiation ($Li_{4.4}Si$, $\rho = 1$) $\Rightarrow M_o \cong 0.5874$

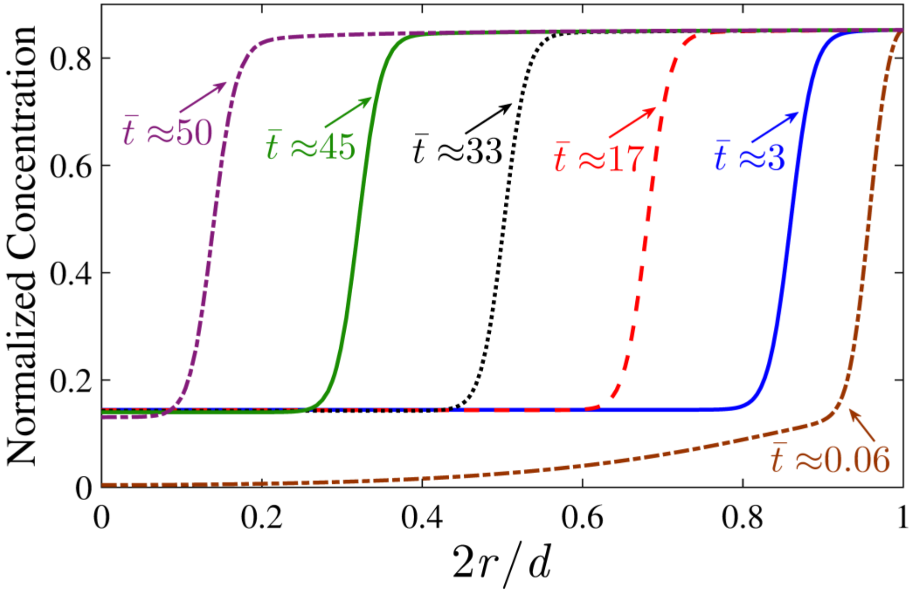
- Experiments suggest:

  Li-rich phase $= Li_{3.75}Si$

  $\Rightarrow \alpha \cong 44.9$

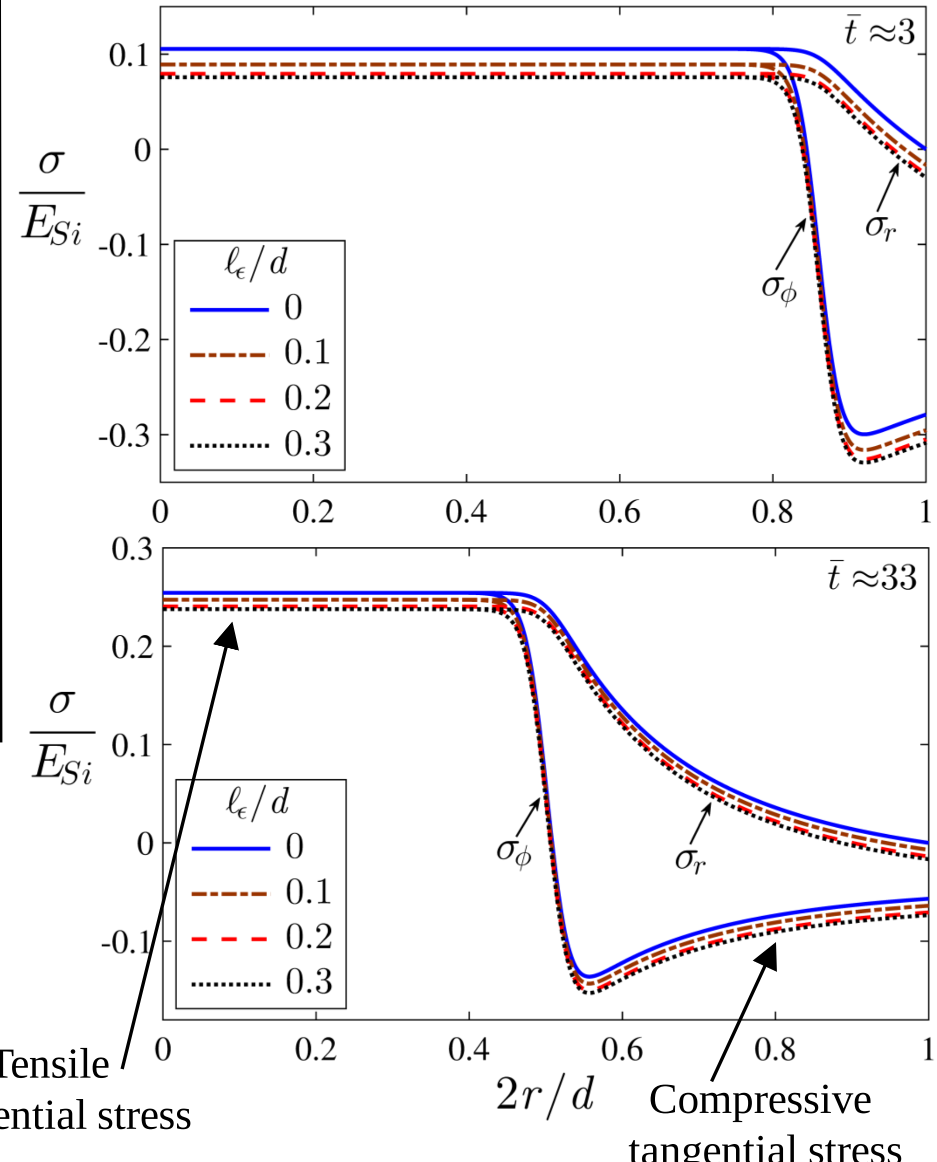


– Li Concentration Profiles



$$\bar{t} = \frac{4D_o t}{d^2} \ \ldots \ \text{normalized time}$$

– Stress Profiles

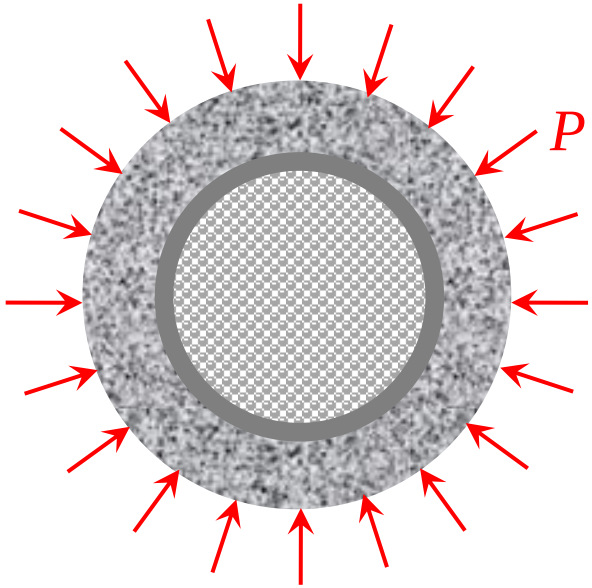


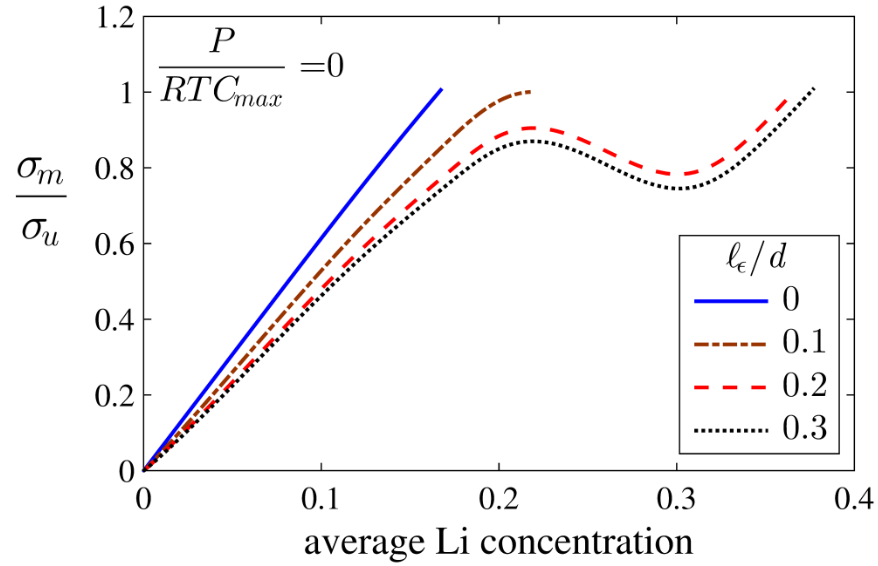
$$\frac{\sigma_u}{E_{Si}} \approx 0.07 \ \ldots \ \text{normalized ultimate stress}$$

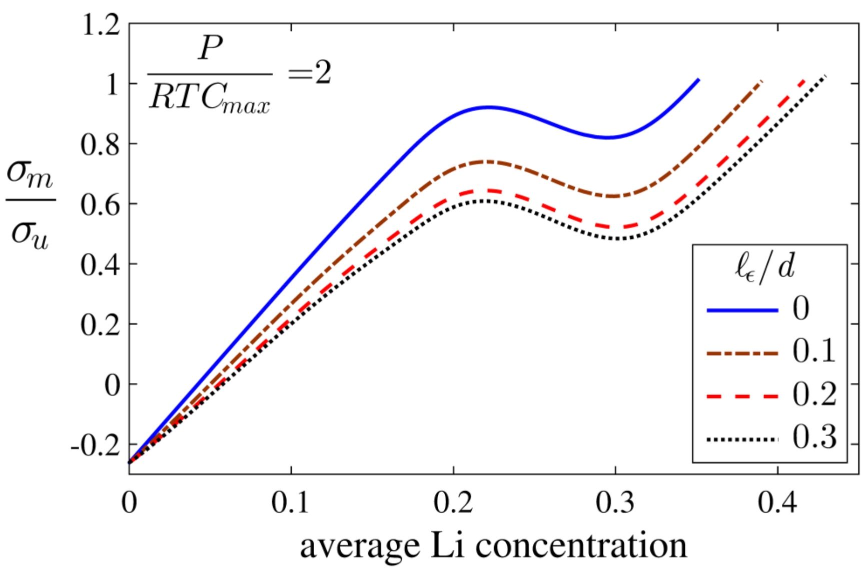
Relatively high stresses ⇒ **Failure** at early stages of interface migration

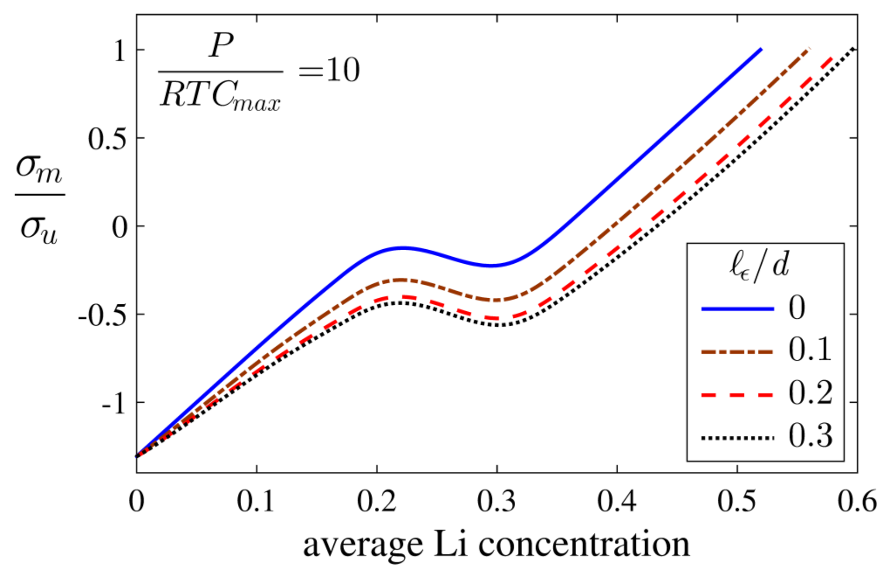
Note: Predicted interface $\upsilon \sim 1.1$ nm/min, i.e. 3 times smaller than experiments
($d = 140$ nm, $D_0 = 10^{-16}$ m^2/sec, $\ell_\varepsilon \approx \ell_\rho$)

– *Failure Suppression by External Pressure*



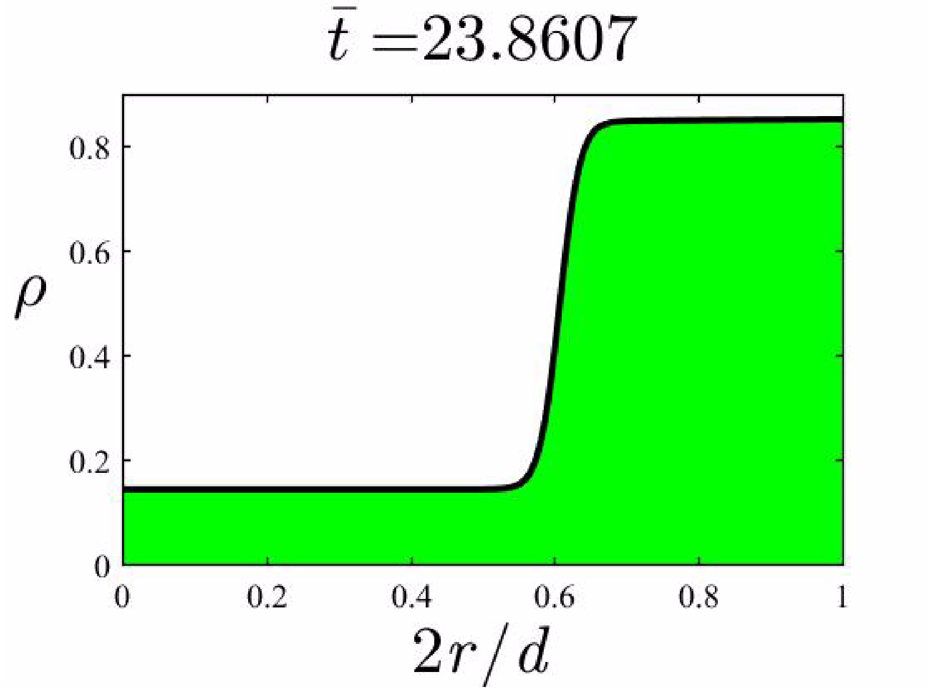


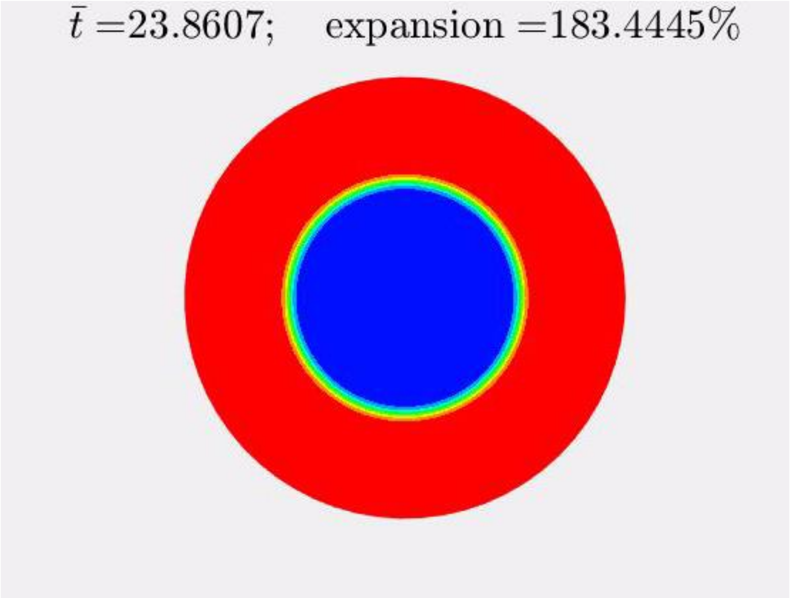


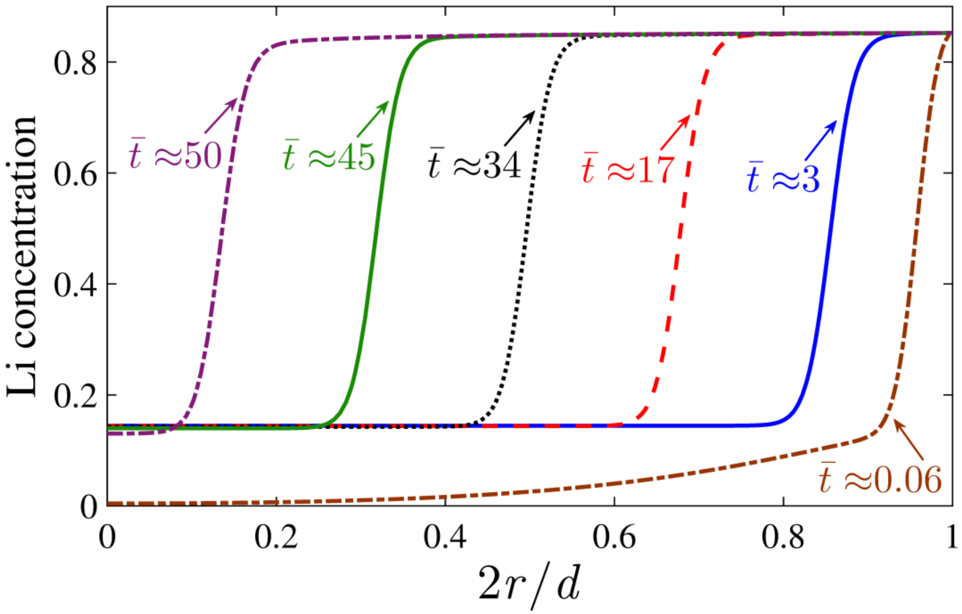


- Larger pressure ⇒ Higher lithiation without failure
- Gradela predicts higher lithiation without failure

– Evolution of Li Concentration Profiles







$\bar{t} = \dfrac{4D_o t}{d^2}$ ... normalized time

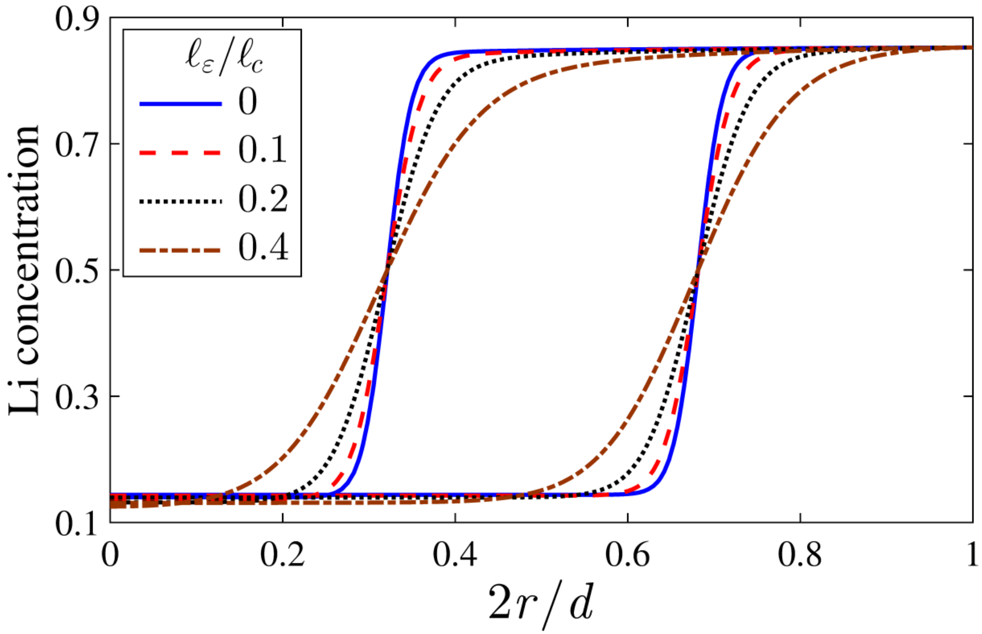
$\bar{v} \cong 0.0132$ ... average normalized interface velocity

For $d = 140$ nm & $D_o \cong 10^{-16}$ m^2/sec

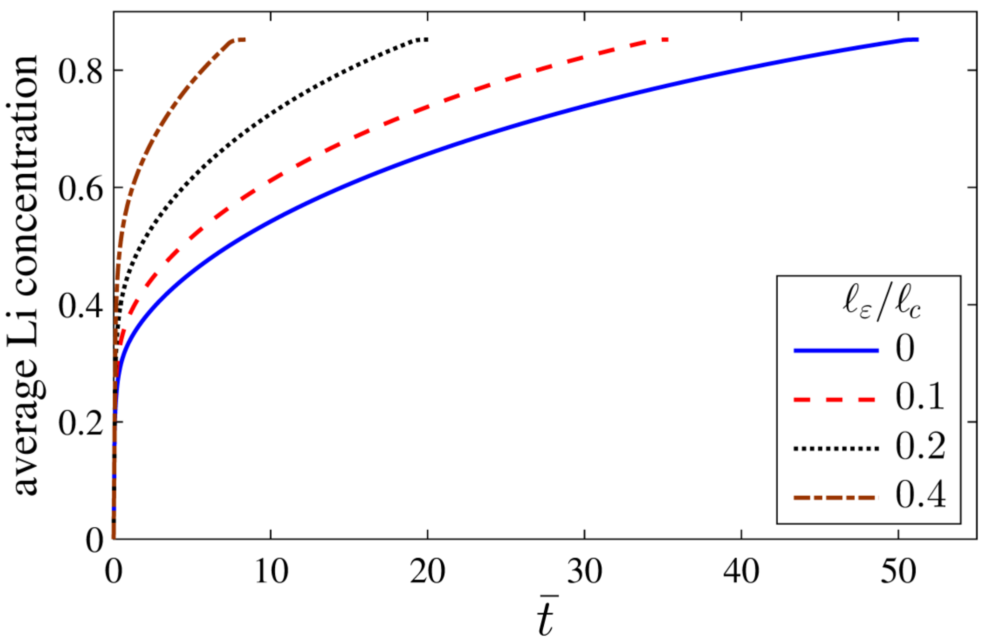
$\Rightarrow v \cong 1.1$ nm/min

i.e. ~3-4 times smaller w.r. experiments

– *Effect of Strain Gradient Length Scale on Li Concentration*



As ℓ_ε increases a more diffused interface is obtained

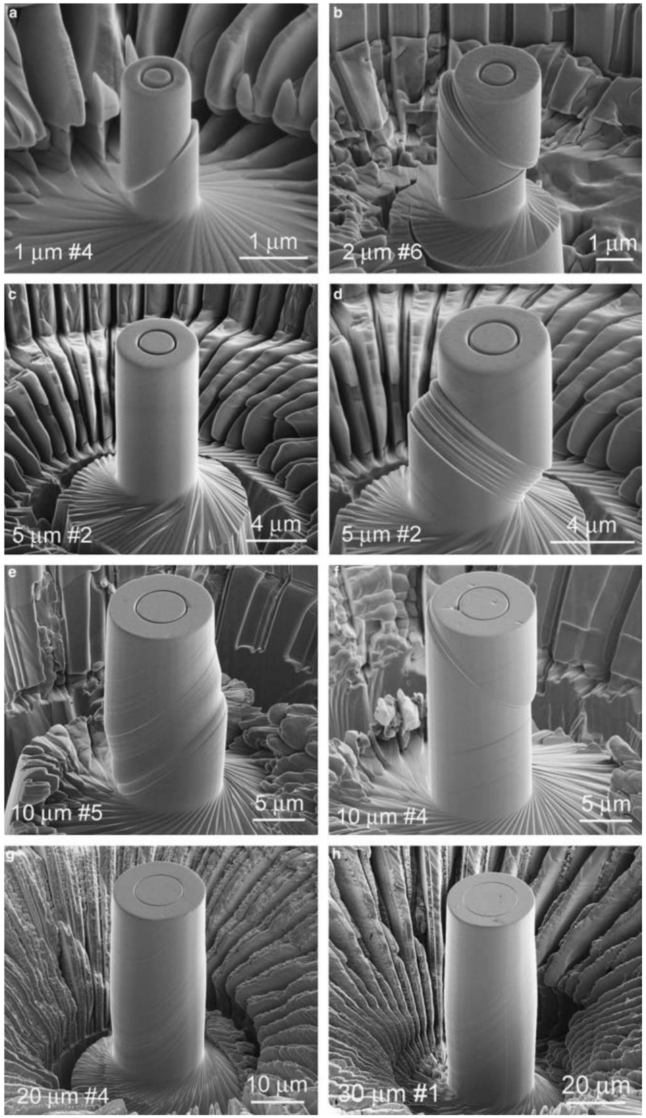


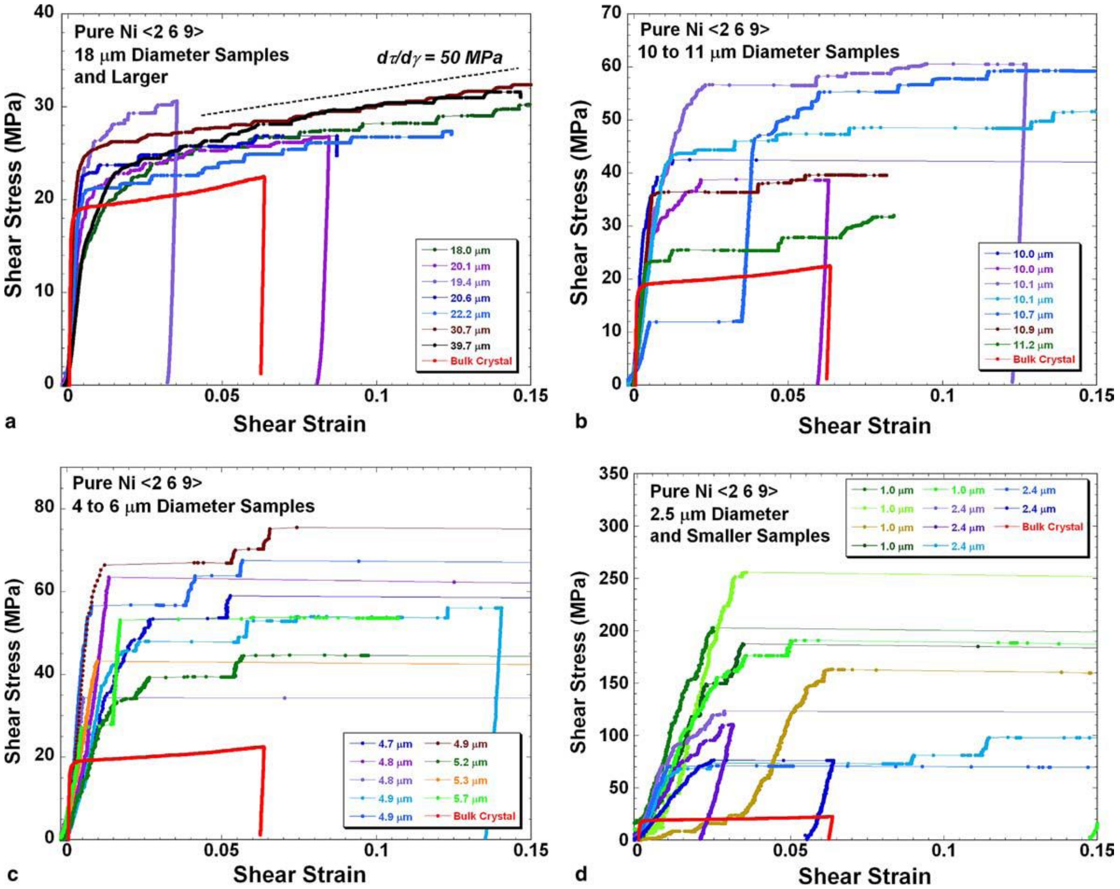
Lithiation rate, hence interface velocity increase with ℓ_ε. Experimental values are approximated for $\ell_\varepsilon / \ell_c = 0.3 - 0.4$

ADDENDUM: Intermittency & Micro/Nano Pillars

❑ Nanoplasticity [Gradient Plasticity at the Nanoscale]

■ Discontinuous/Intermittent Plasticity [Gradient Stochastic Models]





Nix et al, *Science* 2004;

Dimiduk et al, *Acta Mater.* 2005;

Dimiduk et al, *Science* 2006

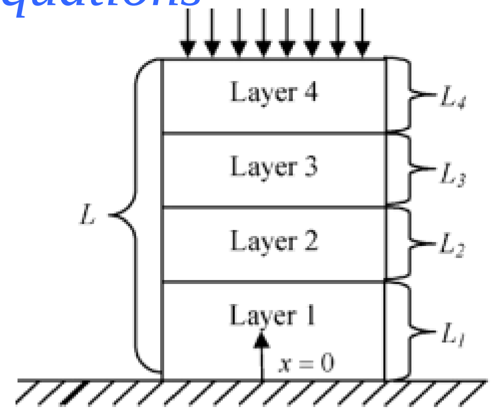
- ***Serrated Plastic Flow: The Gradient-Stochastic Model***

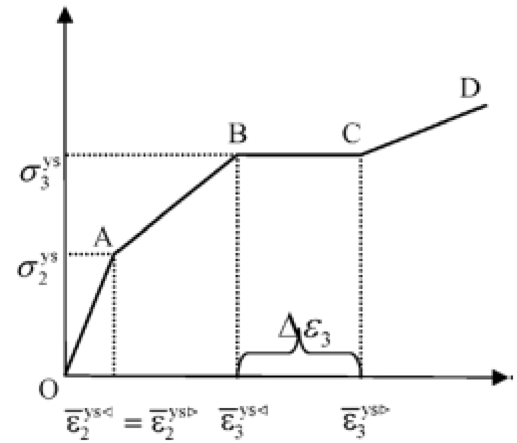
- *Governing Deterministic Equations*

$$\sigma_i = E_i(\varepsilon_i - \varepsilon_i^p),$$

$$\beta_i \varepsilon^p - \beta_i \ell_i^2 \frac{d^2\varepsilon_i^p}{dx^2} = (\sigma_0 - Y_i)$$

(Zhang and K.E. Aifantis, 2011)





- *Serrations*

Strain bursts ($\Delta\varepsilon$) are obtained due to the occurrence of discontinuity of the hyperstress $\tau = \beta\ell^2(d^2\varepsilon^p / dx^2)$ between "elastic/no-yielding" and "plastic/yielding" layers

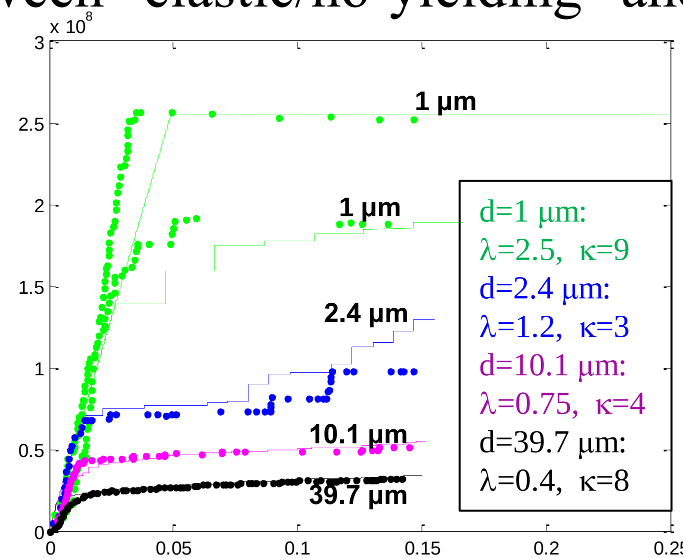
- *Introducing Stochasticity*

$$Y_i = Y^0 + Y_i^{weib} = (1+\delta)Y^0$$

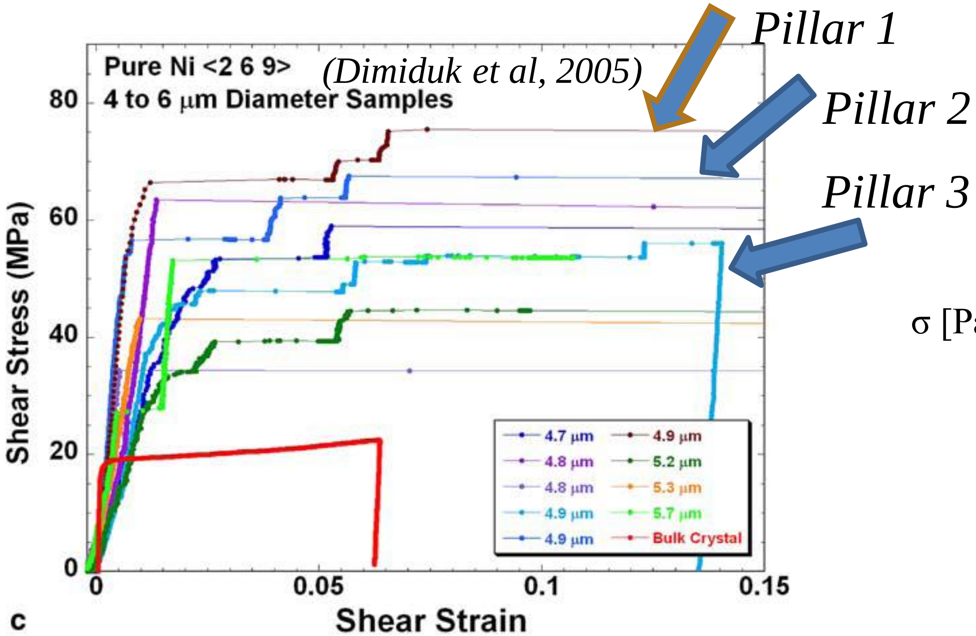
$$PDF(\delta) = \frac{k}{\lambda}\left(\frac{\delta}{\lambda}\right)^{k-1} e^{-(\delta/\lambda)^k};$$

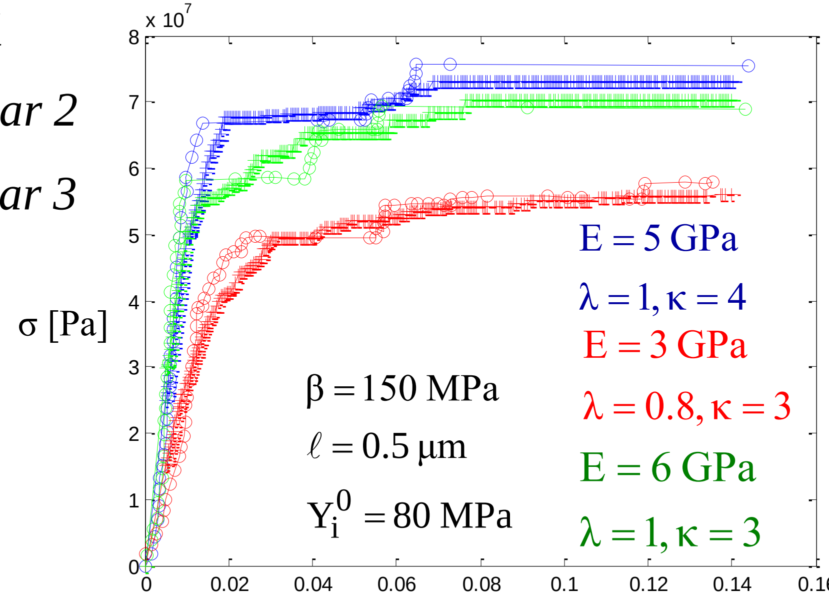
$$\bar{\delta} = \lambda\Gamma\left[1+(1/k)\right], \quad \langle \delta^2 \rangle = \lambda^2\Gamma\left[1+(k)\right] - \bar{\delta}^2$$

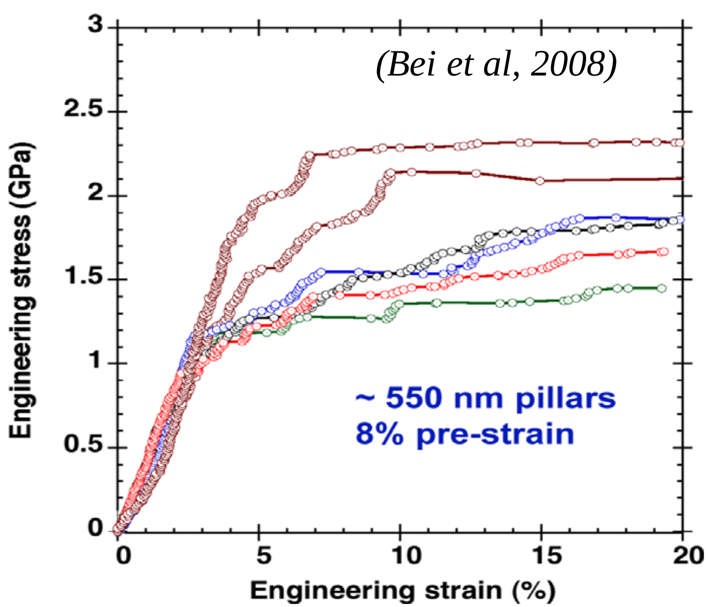
k/λ : shape/scale parameters

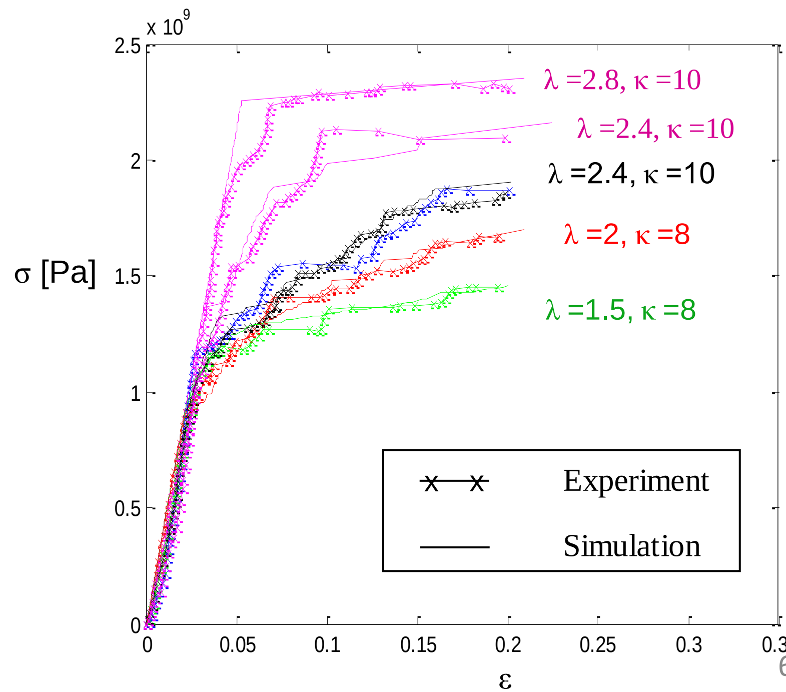


• *Random Response of Same Diameter Micropillars*









■ Stochasticity: Information from Entropy

- ***Tsallis q-Entropy***

$$S_q(P) = \frac{1}{q-1}\left[1 - \sum_I \left(P(I)\right)^q\right]; \quad q \neq 1 \ : \quad \text{entropic index}$$

- Maximum entropy principle leads to q-exponential distribution

$$\therefore \quad P\left(I\right) = A\left[1 + B(q-1)I\right]^{1/(1-q)} \quad \ldots \ [\text{instead of } P\left(I\right) \sim I^{\Lambda}\ ]$$

Note: *Using the Tsallis entropy formulation the "events" with high probability but low intensity are **not** ignored, as is the case with power-law formulations*

- ***Extracting Information on Randomness / PDF***

Probability of bursts of size s

$$P\left(s\right) = A\left[1 + (q-1)Bs\right]^{\frac{1}{1-q}}$$

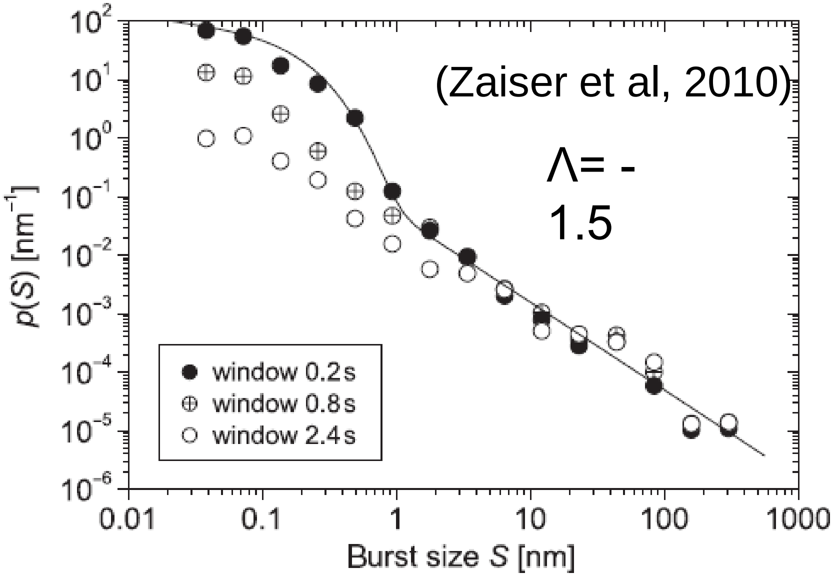
Burst size relation to local yield stress

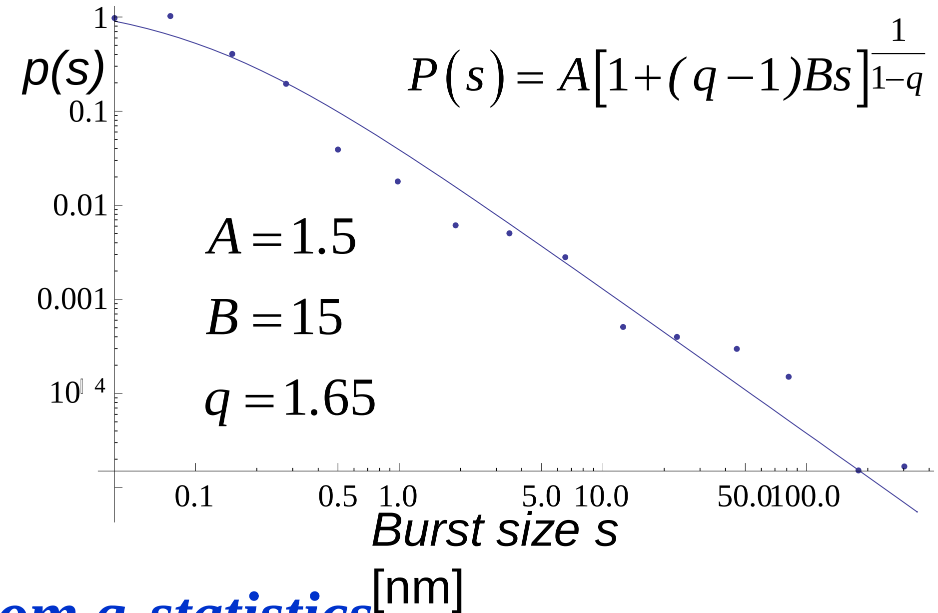
$$s = nL\varepsilon_y^{loc} = nL\,\frac{\sigma_y^{loc}}{E}; \quad P\left(\sigma_y^{loc}\right) \equiv P\left(\varepsilon_y^{loc}\right) \quad (L\text{: cell size})$$

Bursts from n "sites" $\quad s^b = \varepsilon_y^b L = \left(\sigma_y^b / E\right)L \quad (s_b$ *: smallest burst,* σ_y^b *: yield stress of a "site")*

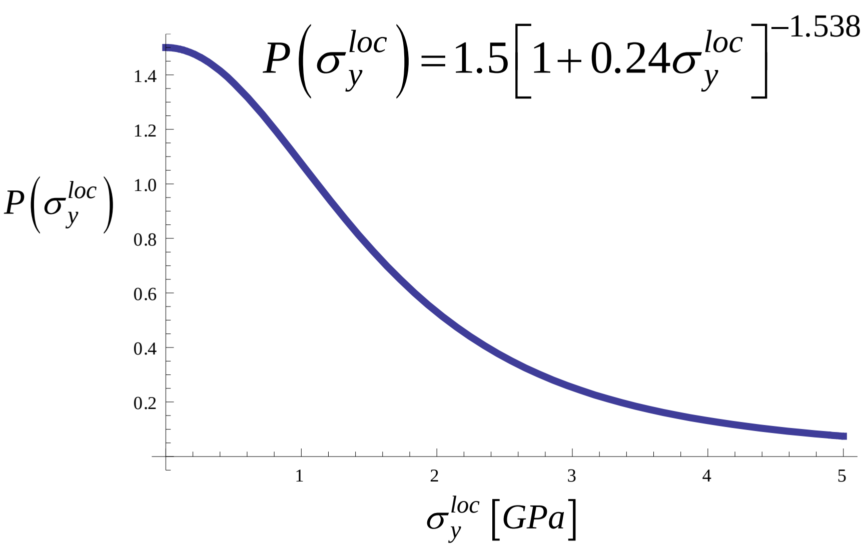
$$\therefore \quad P\left(\sigma_y^{loc}\right) = A\left[1 + (q-1)Bs_b\left(\frac{\sigma_y^{loc}}{\sigma_y^b}\right)^2\right]^{1/(1-q)}$$

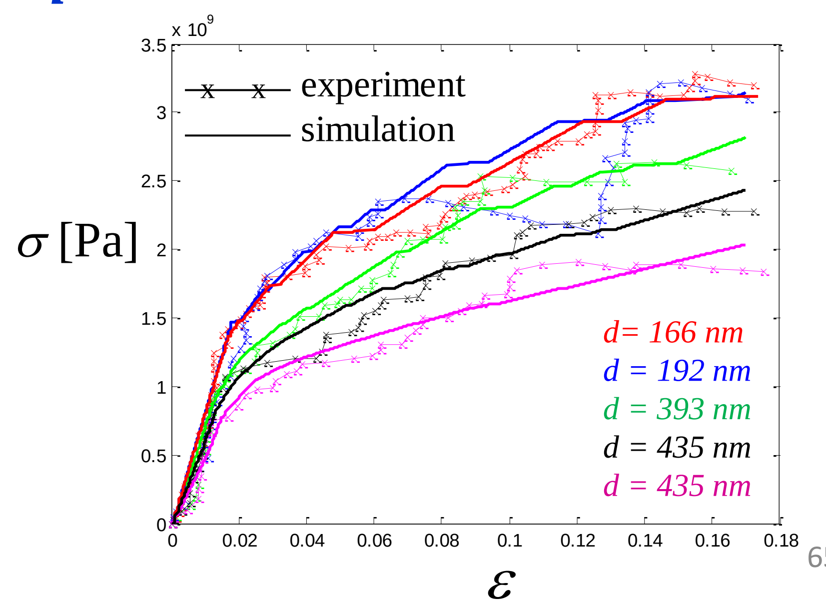
• *Strain bursts in Mo micropillars under compression*





• *CA simulations with input from q-statistics*

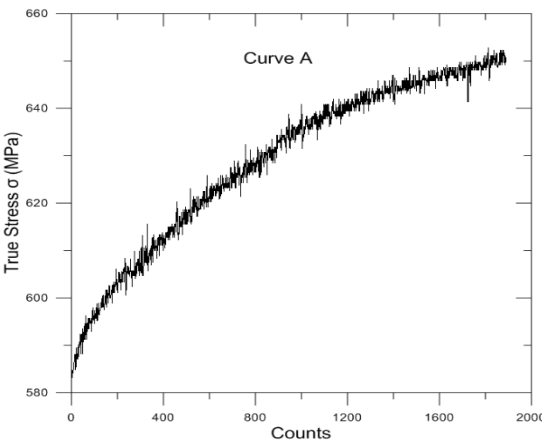




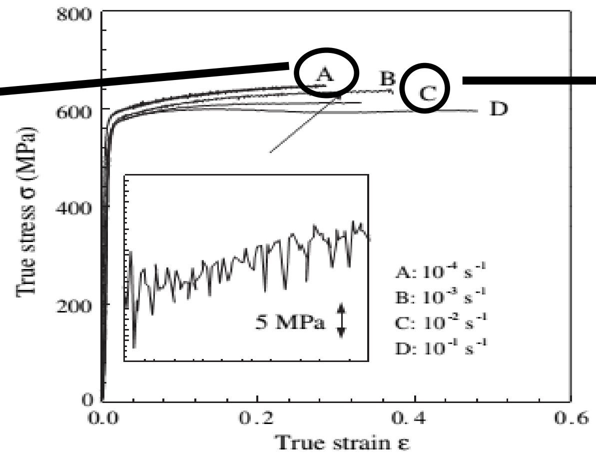
■No Equations – Tsallis q-Statistics

- ***Serrated Plastic Flow & Multiple Shear Banding in UFGs***

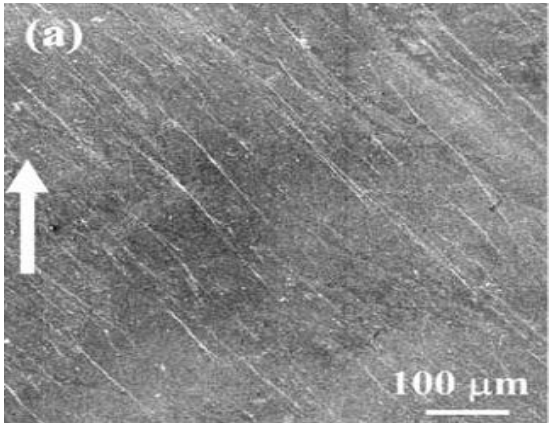
(Fan *et al*. Scripta/Acta Materialia 2005/2006)



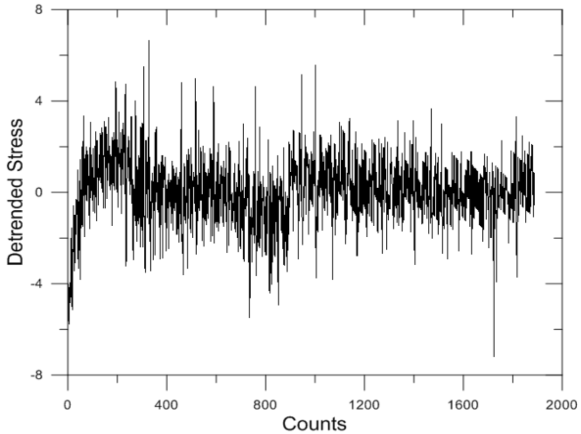
Low $\dot{\varepsilon}$ (10^{-4} s^{-1}) – Serrations



σ-ε curves (compression)



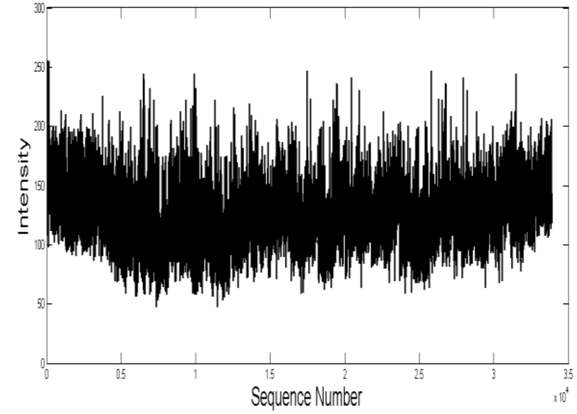
High $\dot{\varepsilon}$ (10^{-2} s^{-1})
Shear Bands (SEM)



Stress Drops time series

[Remove hardening effect (slope)]

Bimodal Grain Size Distribution
UFG matrix: 197 nm
Coarse grains : 3.1 μm (10 %)



Intensity series for Shear Band Distribution

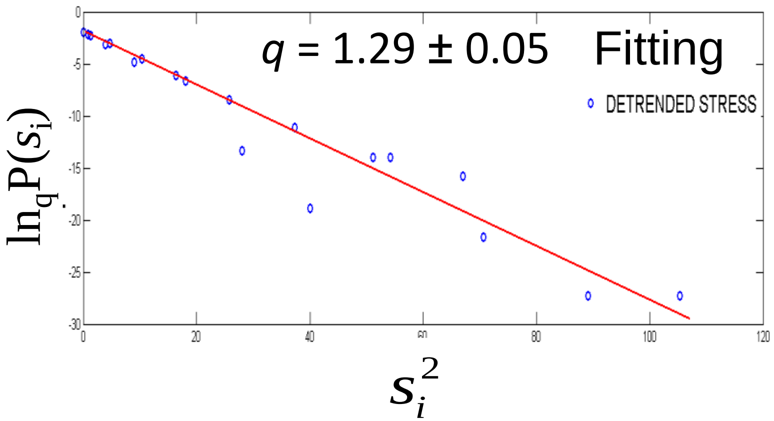
[2D → 1D: Space Filling Curve Method (Morton, 1966)]

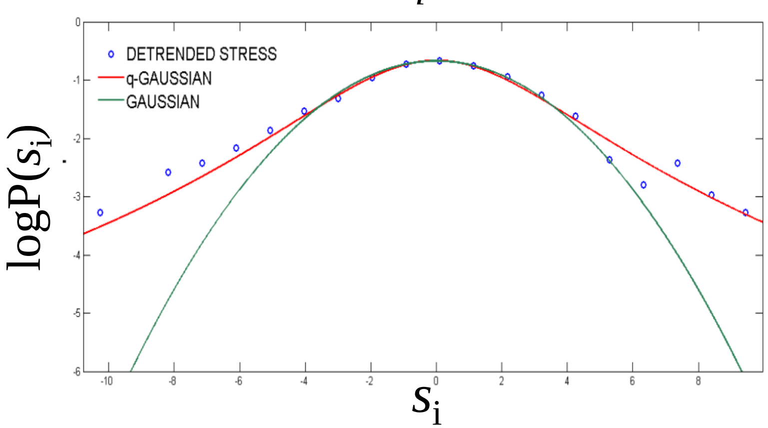
• Serrations

•*Tsallis q- Gaussian:* $P(s) = p_0[1+(q-1)\beta_q(s)^2]^{1/(1-q)}$

•*Fitting:* $\ln_q(P(s_i))$ vs s_i^2

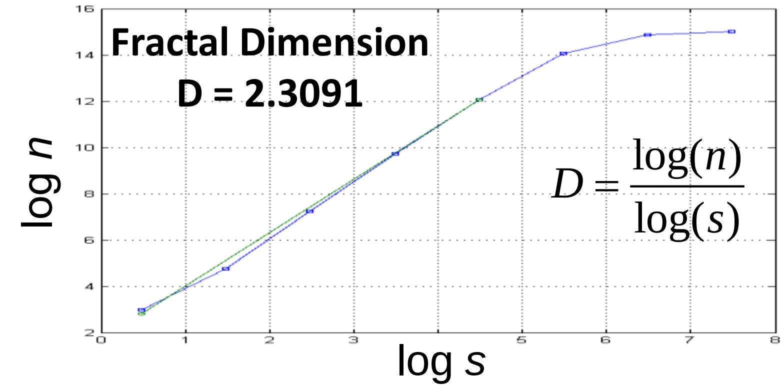
•*Power Law Tail (q>1):* $P(|s|) \sim |s|^{-2/(q-1)}$

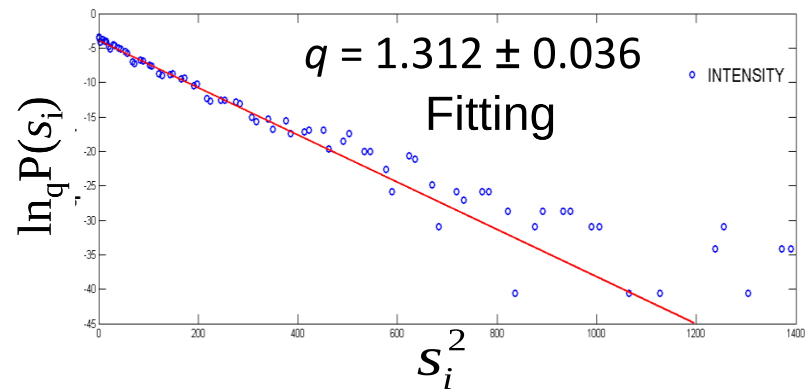


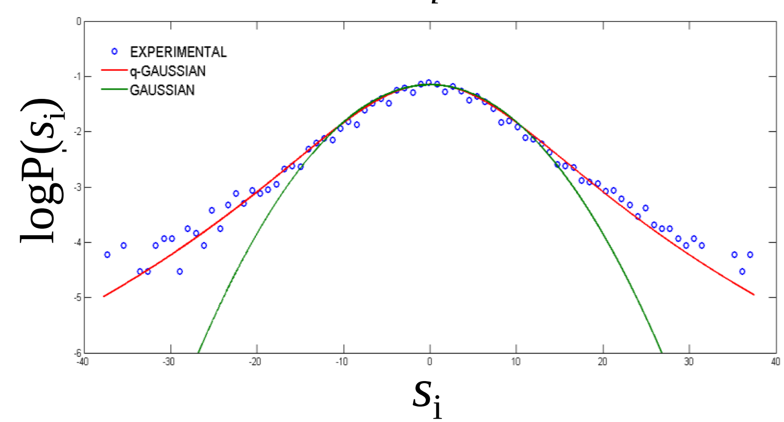


$q > 1 \longrightarrow$
- Non-Gaussian Statistics
- Tsallis Nonextensive Statistics,
- Temporal Long range correlations

• Shear Band Fractality





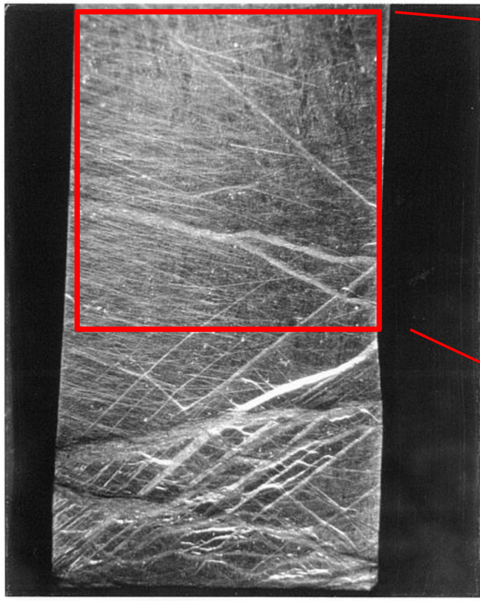


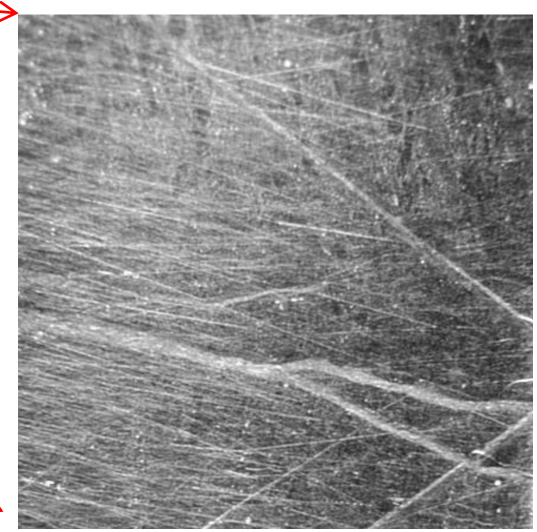
$D > 2 \longrightarrow$ Fractal Geometry of Shear Band network

$q > 1 \longrightarrow$
- Non-Gaussian Pixels Distributions
- Spatial Long range correlations

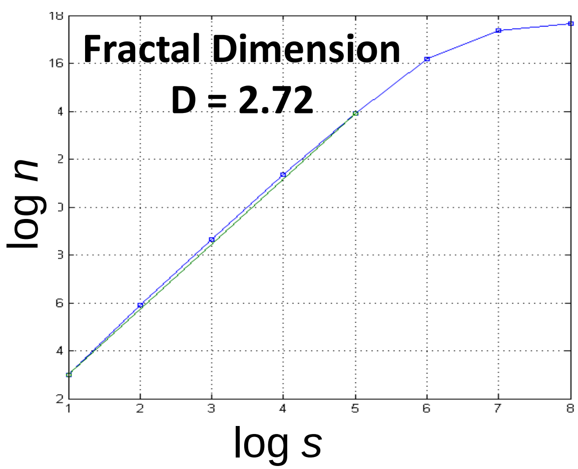
• Shear Band Fractality in Fe – 10% Cu UFG Alloy

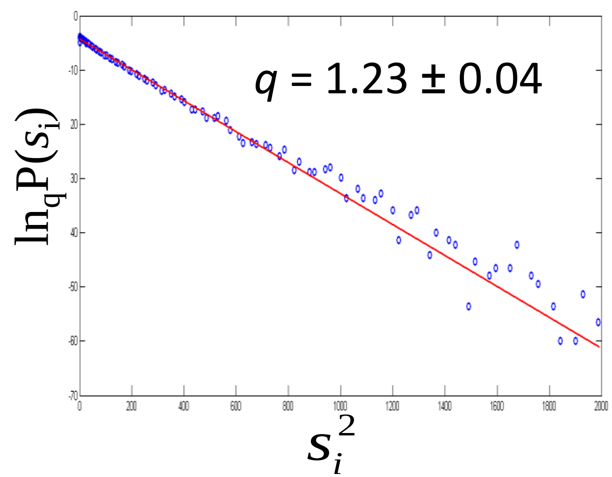
(Carsley *et al*. Metall. Mater. Trans 1998)

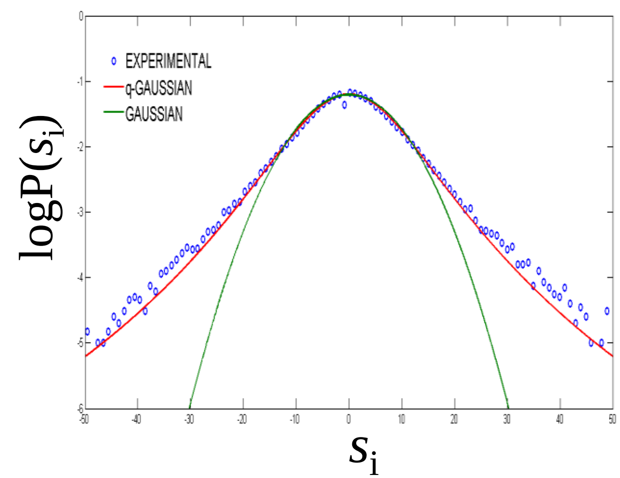




Shear Bands



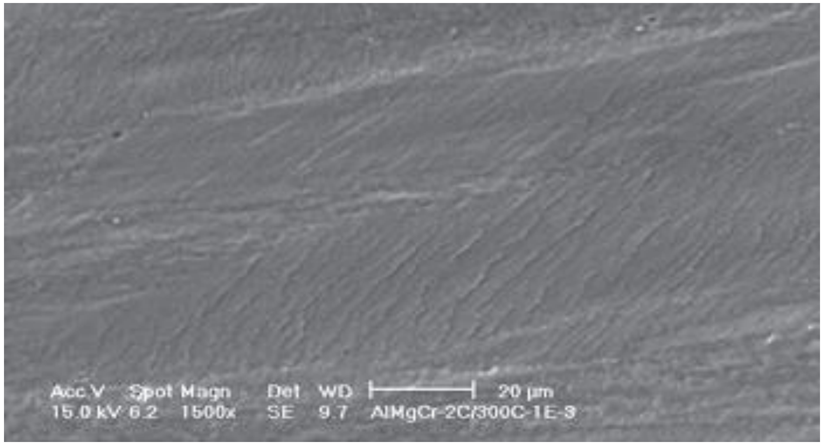




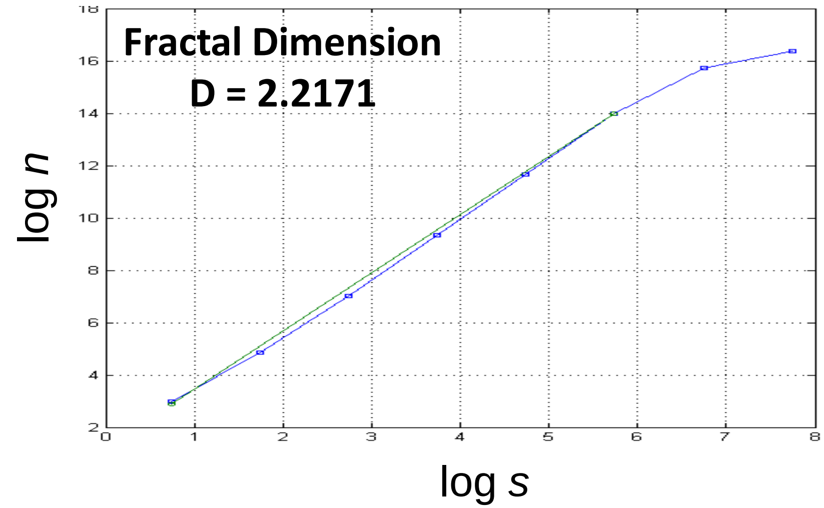
$D > 2 \longrightarrow$ Hierarchical Fractal Shear Band network || $D = 2 \rightarrow$ No Fractality; $D = 3 \longrightarrow$ Extreme Fractality

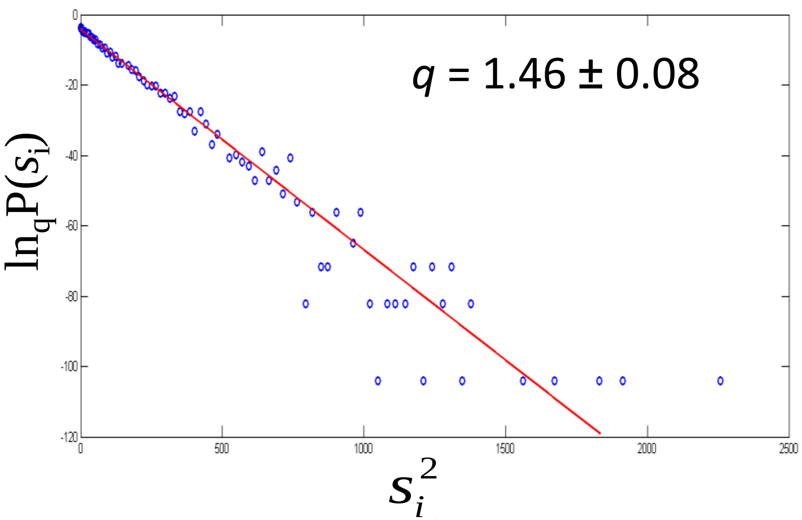
$q > 1 \longrightarrow$ { Non-Gaussian Pixels Distributions; Spatial Long range correlations } || $q = 1 \rightarrow$ { Gaussian Pixels Distributions; Spatial short range correlations }

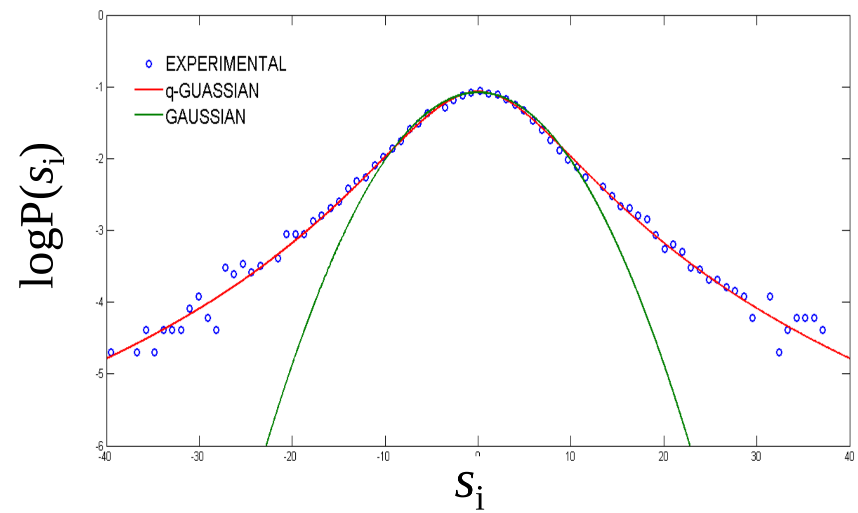
• Shear Band Fractality in Al – 5%Mg - 1.2% Cr ECAP Alloy



Shear Bands
(Eddahbi *et al*. J. Matchar. 2012)







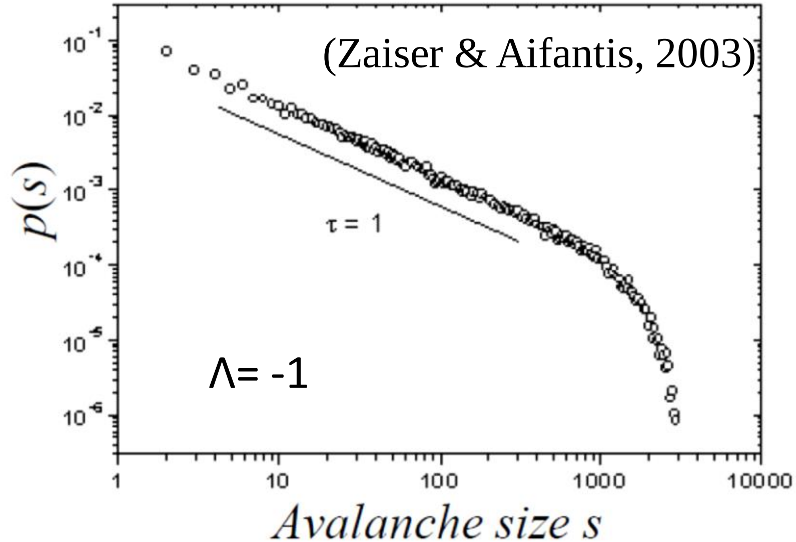
$D > 2$ ⟶ Hierarchical Fractal Shear Band network

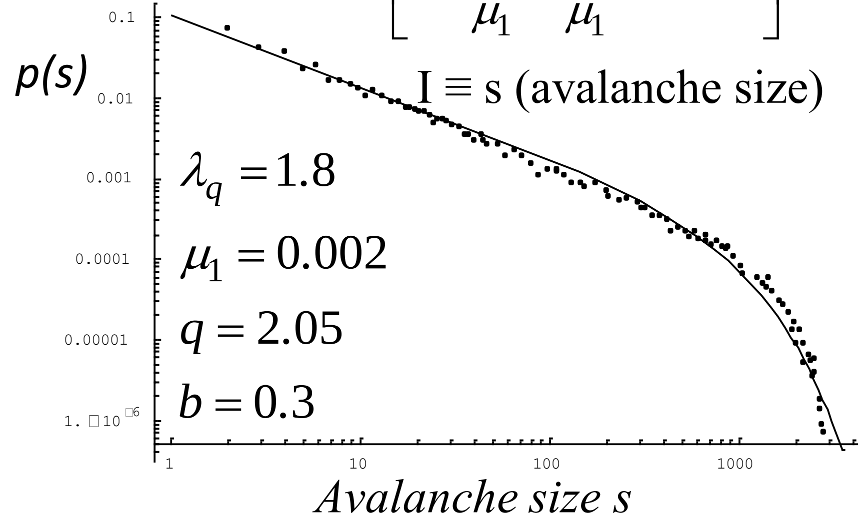
$q > 1$ ⟶ { Non-Gaussian Pixels Distributions; Spatial Long range correlations }

• *Slip Avalanches*

$$\frac{d\xi}{dt} = -\mu_r \xi^r - (\lambda_q - \mu_r)\xi^q \quad ; \quad r = 1 \text{ and } q > 1$$

$$\xi = \frac{b}{\left[1 - \frac{\lambda_q}{\mu_1} + \frac{\lambda_q}{\mu_1} e^{(q-1)\mu_1 t}\right]^{\frac{1}{q-1}}}$$





• *Bursts in Nb, Au and $Al_{0.3}$CoCrFeNi (HEA) micropillars compression*