Gradients and Fractional/Fractal Models at Micro/Nano Scales

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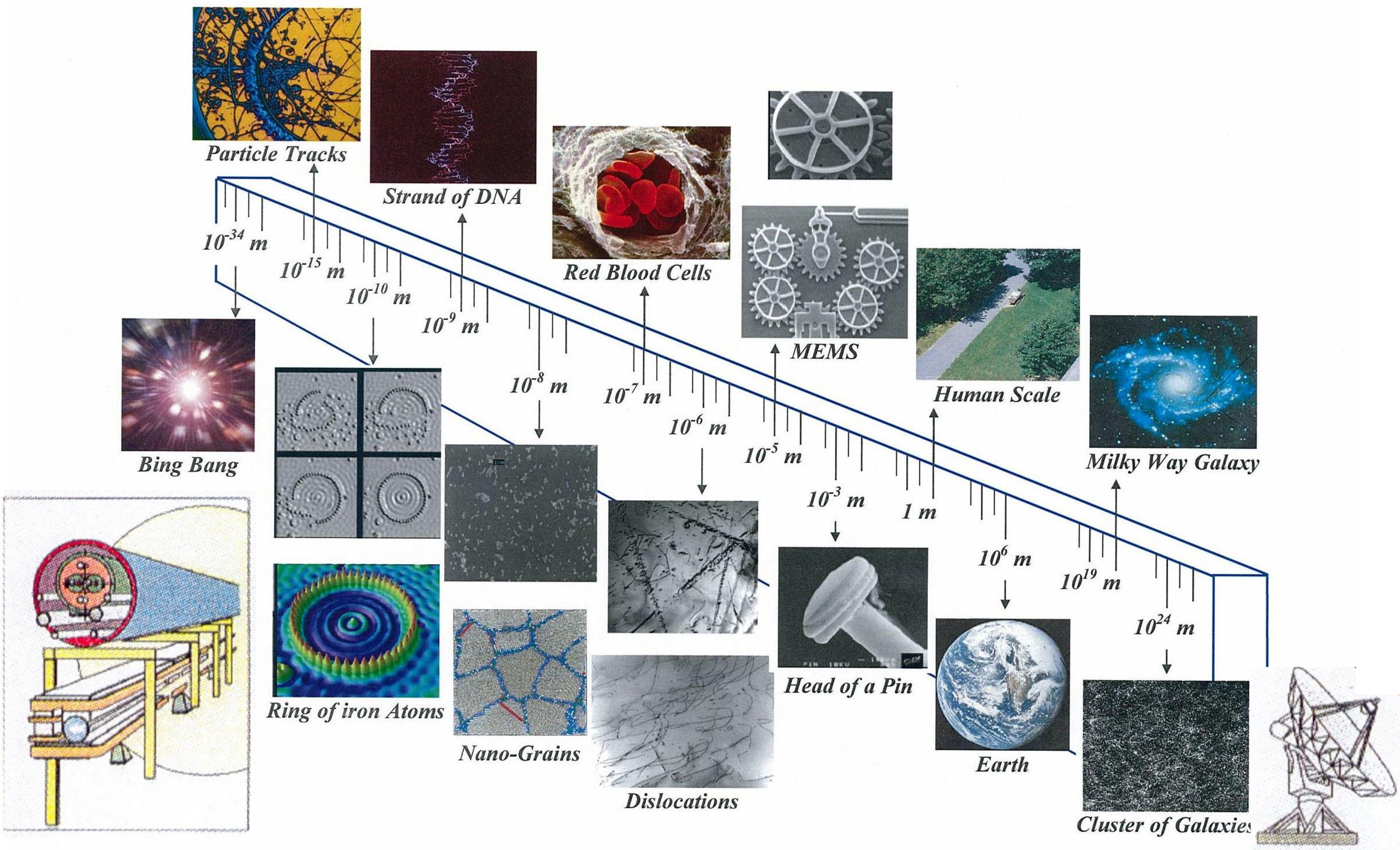
CONTENTS

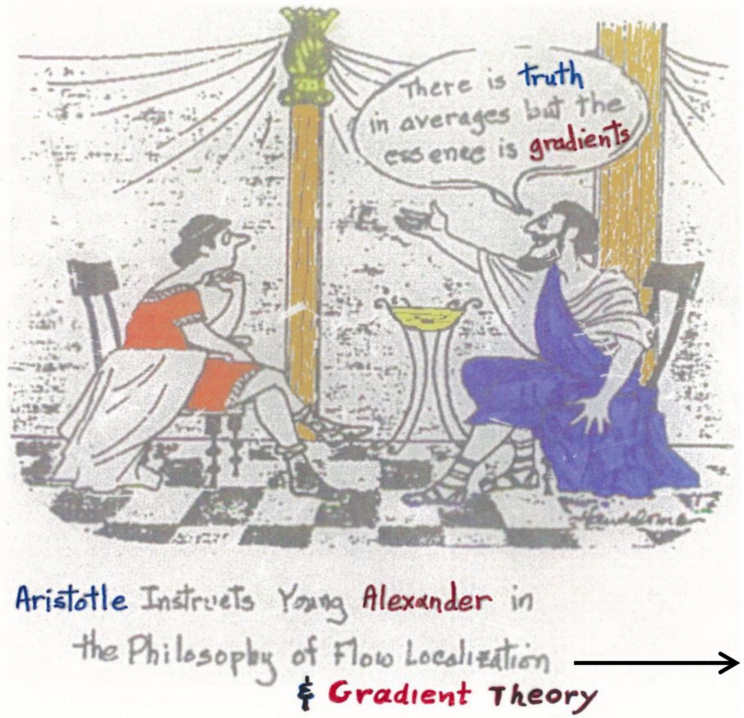
- **Gradients in Elasticity, Diffusion and Plasticity**
- **GradEla and Fractional/Fractal Dislocations and Cracks**
- **Higher-order Diffusion Theory**
- **Gradient Plasticity: Shear Bands and Size Effects**
- **Micro/Nanopillars Deformation**
- **Heterogeneity and Stochasticity**
- **No Equations – Tsallis q-statistics**

GRADIENT MECHANICS ACROSS SCALES, MATERIALS & PROCESSES

- **A Sense of Scale: $10^{-34} – 10^{24}$ m**



■ A Cartoon from Aristotle's 1990 Conference



ECA Gradient Models

- ***Gradient Elasticity (GradEla)***
- ***Gradient Plasticity (GradPla)***
- ***Gradient Diffusion (GradDif)***
- ***Gradient Dislocation Dynamics (GradDD)***

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

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]

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

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

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

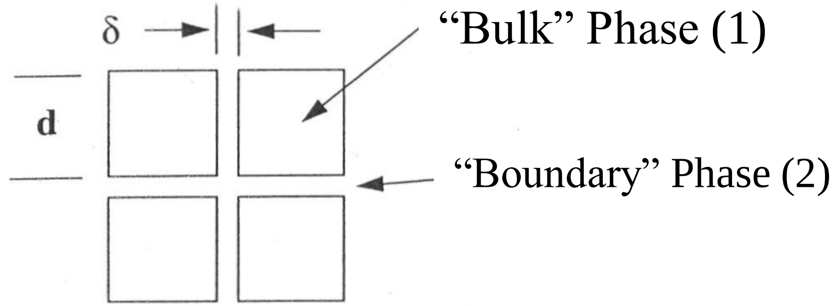
- ***Fick's Law:*** $\mathbf{j} = -D\nabla\rho$

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

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

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***

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

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

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

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

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

– ***Uncoupling*** $\Rightarrow$

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

- ## *Gradient Elasticity (GradEla)*

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*

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

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

■ A Note on Gradela Dislocation Nanomechanics

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

- ***Screw Dislocation***

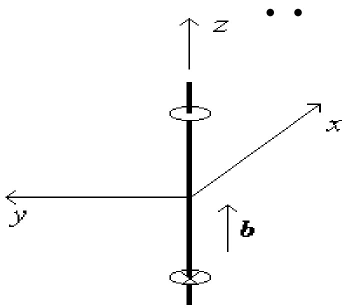
- Stress / Strain :

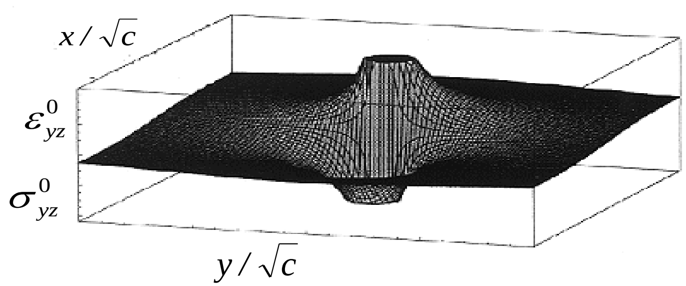
$$\begin{cases} \sigma_{xz} = \dfrac{Gb_z}{4\pi}\left[-\dfrac{y}{r^2} + \dfrac{y}{r\sqrt{c}}K_1\left(r/\sqrt{c}\right)\right]; \quad \sigma_{yz} = \ldots \\ \varepsilon_{xz} = \dfrac{b_z}{4\pi}\left[-\dfrac{y}{r^2} + \dfrac{y}{r\sqrt{c}}K_1\left(r/\sqrt{c}\right)\right]; \quad \varepsilon_{yz} = \ldots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

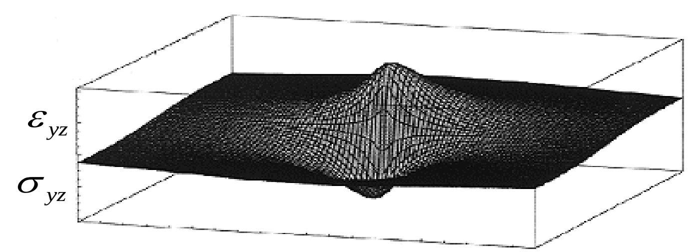
$$\therefore \quad \mathbf{r} \to \mathbf{0} \quad \Rightarrow \quad \mathbf{K_1}\left(\mathbf{r}/\sqrt{\mathbf{c}}\right) \to \frac{\sqrt{\mathbf{c}}}{\mathbf{r}} \quad \Rightarrow \quad \left(\boldsymbol{\sigma}_{\mathbf{xz}}, \boldsymbol{\varepsilon}_{\mathbf{yz}}\right) \to \mathbf{0}$$

- 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

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





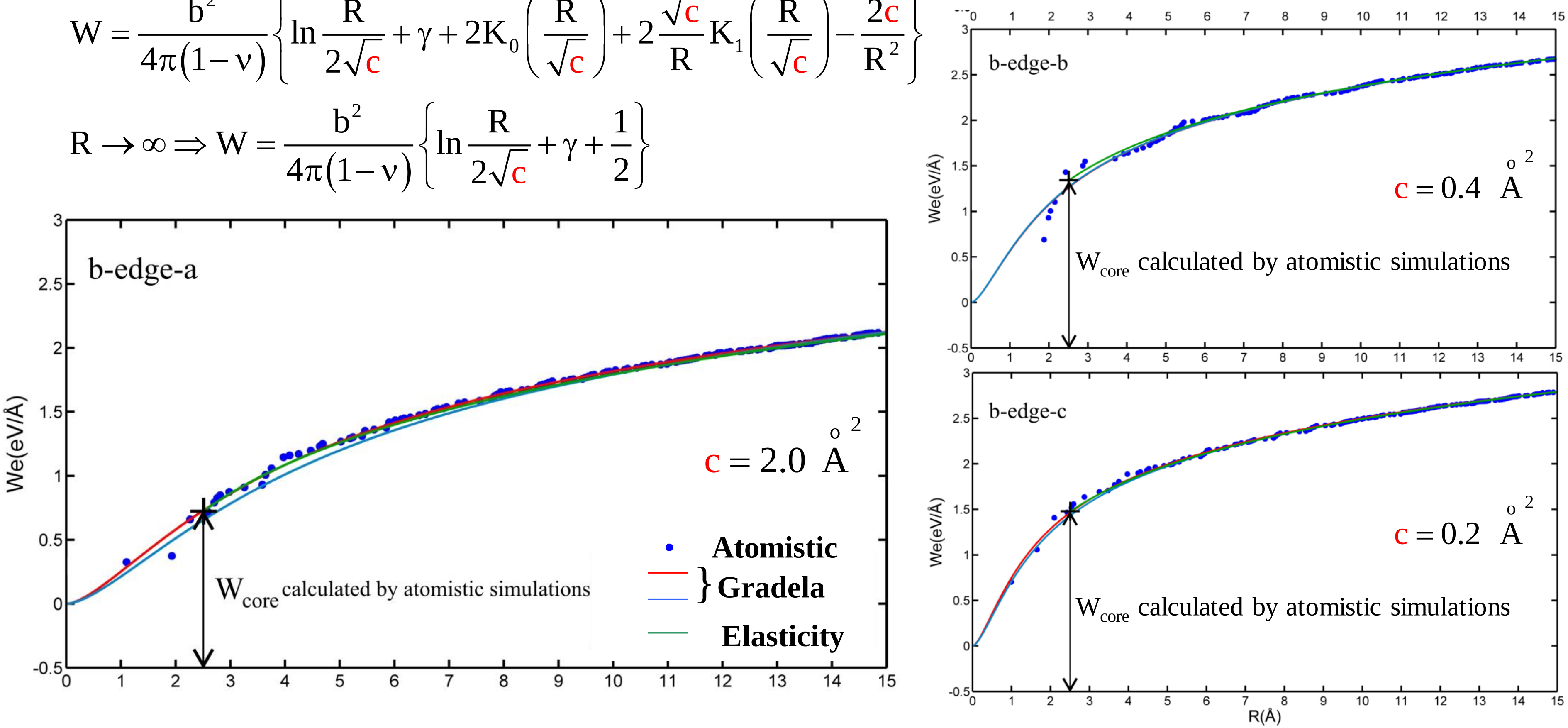


- Use these in simulations

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

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

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



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

Invariant Relations: $\frac{W_{core}\sqrt{c}}{r_0} = 0.33 \pm 0.008\frac{eV}{\mathring{A}}$; $\frac{W^g(b)\sqrt{c}}{b} = 0.3 \pm 0.008\frac{eV}{\mathring{A}}$

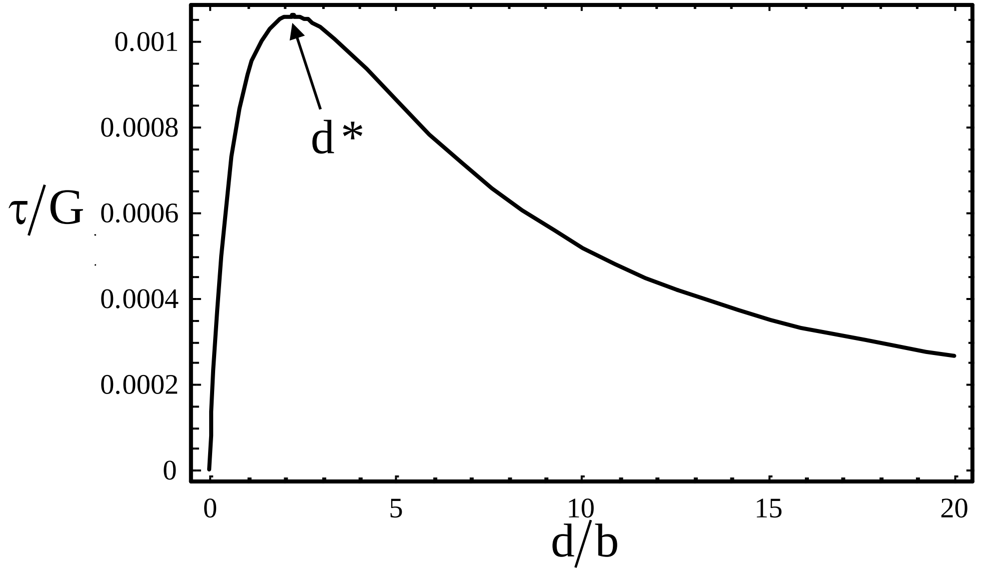
• *Image Force – Inverse Hall Petch Behavior*

- *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 $\perp$* $\left(\mathbf{b} = \mathrm{b}\,\mathbf{e}_{\mathbf{x}}\right)$

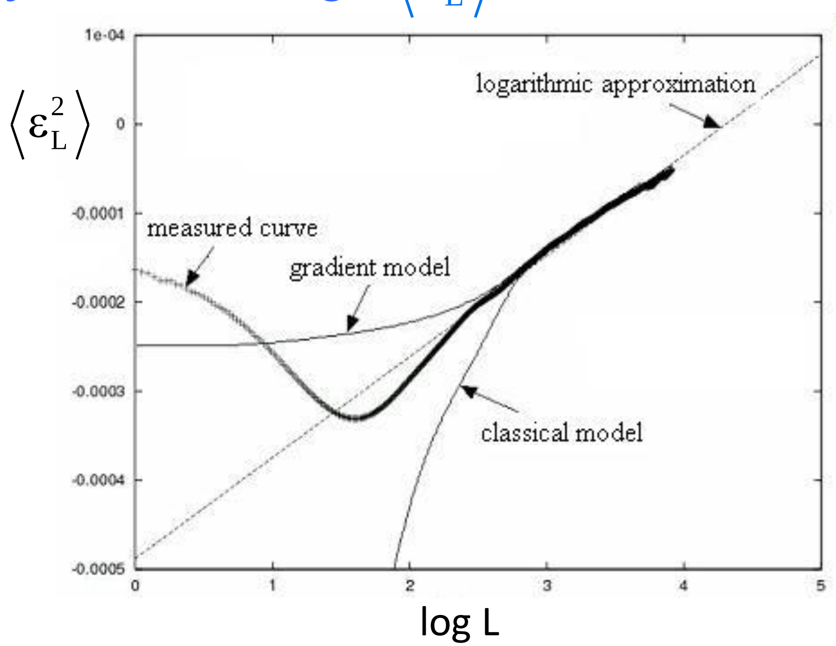
According to Gradela (e.g. ECA 2003) the ε_{xx} component of the strain tensor corresponding to an edge dislocation with Burgers vector $\mathbf{b} = \mathrm{b}\,\mathbf{e}_{\mathbf{x}}$ is

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

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* $\left\langle \varepsilon_L^2 \right\rangle$



■ A Note on Gradela Fracture Mechanics (Mode III)

- ***Gradela Mode III Crack Problem***

  - ***Gradela:*** $(1-c\Delta)\boldsymbol{\sigma}_{ij} = \boldsymbol{\sigma}_{ij}{}^{\mathbf{0}}$ & $(1-c\Delta)\boldsymbol{\varepsilon}_{ij} = \boldsymbol{\varepsilon}_{ij}{}^{\mathbf{0}}$; $\boldsymbol{\sigma}^{\mathbf{0}} = \lambda\, \mathrm{tr}\boldsymbol{\varepsilon}^{\mathbf{0}}\,\mathbf{1} + 2\mu\boldsymbol{\varepsilon}^{\mathbf{0}}$

    as before through Ru-Aifantis thm.

  Target: Non-Singular Stresses/Strain Estimation at the crack tip

  - ***Boundary Conditions***

    Far field coincidence of stresses: $\lim_{\mathbf{r}\to\infty} \boldsymbol{\sigma}_{ij} = \boldsymbol{\sigma}_{ij}{}^{\mathbf{0}}$

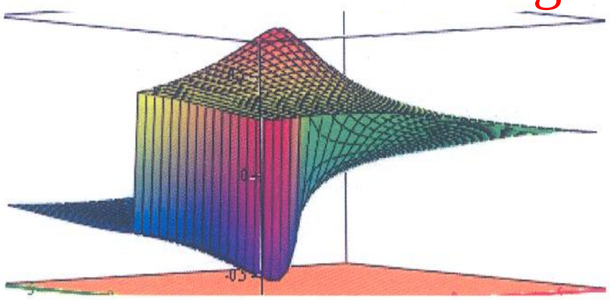
    Vanishing of stresses at the origin: $\lim_{\mathbf{r}\to 0} \boldsymbol{\sigma}_{ij} = 0$

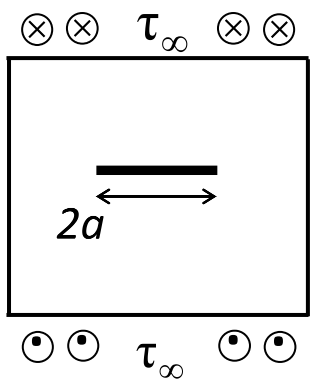
    Zero tractions on crack surfaces: $\sigma_{zy}(x, 0^{\pm}) = 0 \quad ; \quad |x| \leq a$

• *Nonsingular Stress Distribution in Mode III*

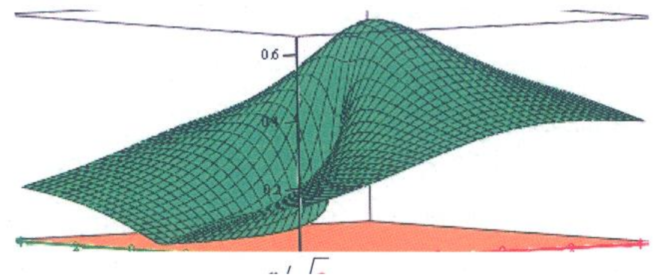
$$\sigma_{xz} = -\frac{K_{III}}{\sqrt{2\pi r}}\left[\sin\frac{\theta}{2}\left(1-\exp\left[-r/\sqrt{c}\right]\right)\right] \qquad \sigma_{yz} = \frac{K_{III}}{\sqrt{2\pi r}}\left[\cos\frac{\theta}{2}\left(1-\exp\left[-r/\sqrt{c}\right]\right)\right]$$

Gradient Stress non-singular

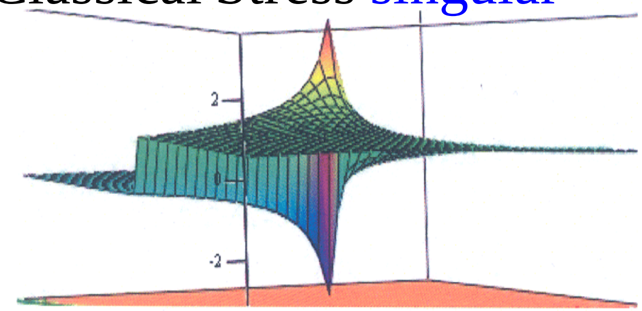




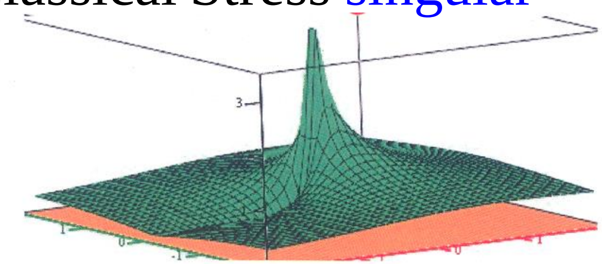
Gradient Stress non-singular



Classical Stress singular



Classical Stress 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)** $K_{III} = \tau_\infty\sqrt{\pi a}$

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

■ Fractional GradEla Dislocations

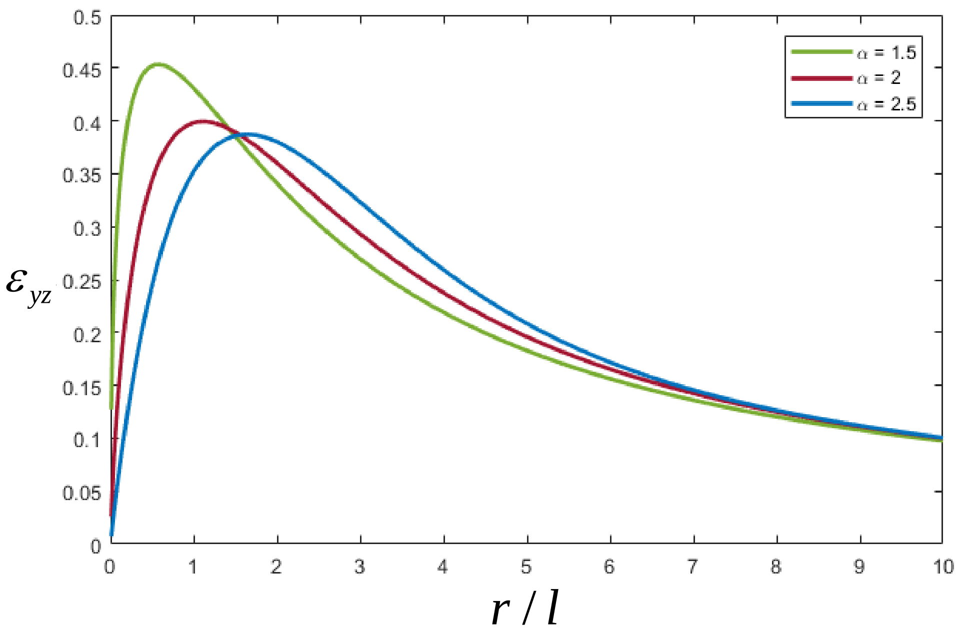
- ***Ru-Aifantis thm:*** $\boldsymbol{\varepsilon} + l^{\alpha}(-\Delta)^{\alpha/2}\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^{0}$; $\quad l = c^{1/\alpha}$

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

- ***Riesz Laplacian:*** $((-\Delta)^{\alpha/2}\varepsilon_{ij})(\mathbf{r}) = \mathcal{F}^{-1}(|\mathbf{k}|^{\alpha}\varepsilon_{ij}(\mathbf{k}))(\mathbf{r}).$ *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 $\alpha \to 2$: $K_{\alpha}(r)\big|_{\alpha\to 2} \to K_1(r)$

i.e. previous GradEla Solution

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

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

■ 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***

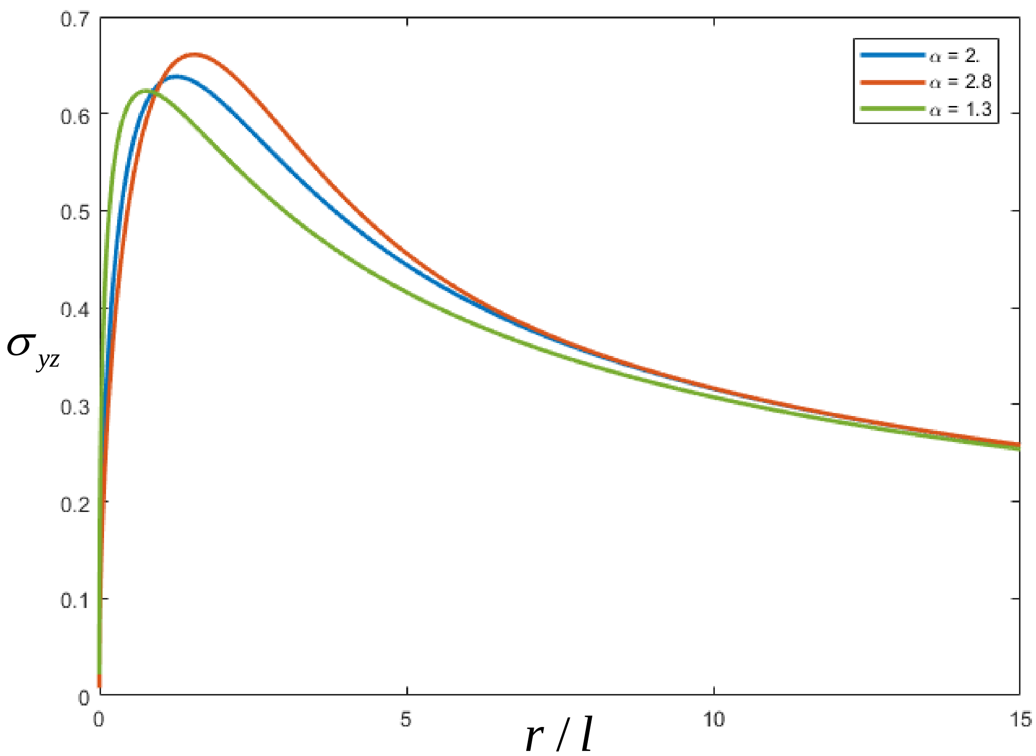
$$\sigma_{xz} = \sigma_{xz}^0 - f(r)\sin\frac{\theta}{2} \qquad \sigma_{yz} = \sigma_{yz}^0 + f(r)\cos\frac{\theta}{2}$$

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

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

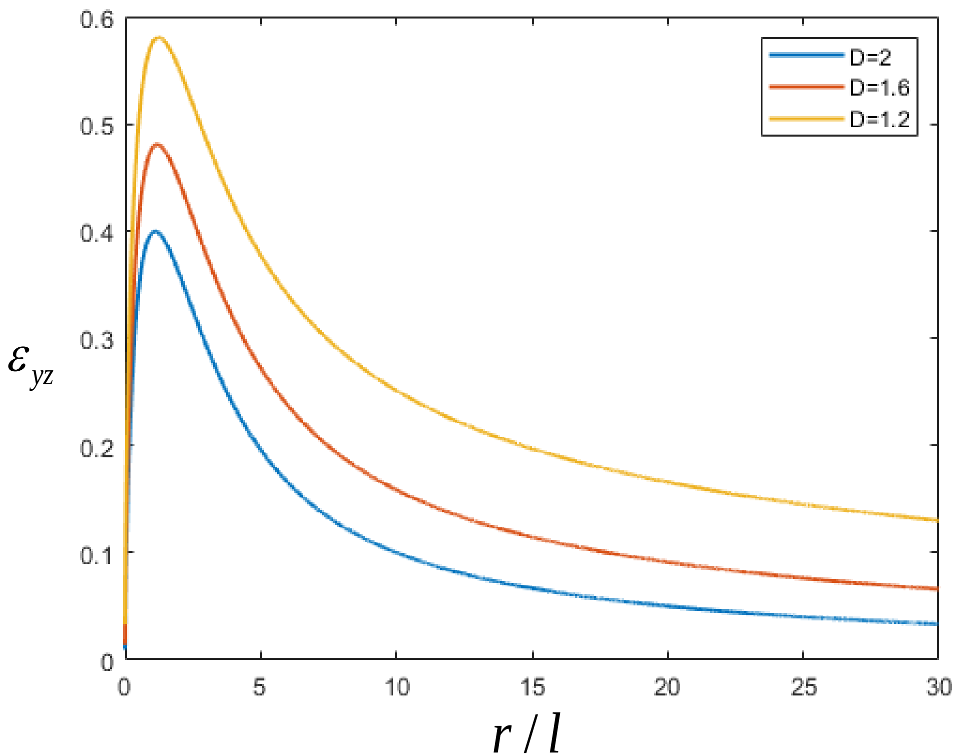
■ Fractal GradEla Dislocations

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

  $\boldsymbol{\varepsilon}$ *... 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 $D \to 2: \; K_{D/2}(r)\big|_{D\to 2} \to K_1(r)$

i.e. previous GradEla Solution

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

$\varepsilon_{xz}, \varepsilon_{yz} \to 0$, *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:** $\{\mathbf{T}, \hat{\mathbf{f}}\} \rightarrow \{\rho, \nabla\rho;\, \dot{\rho}, \nabla\nabla\rho \,...\}$

- **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:*** $\mathbf{T} = -(\pi\rho + \overline{\pi}\dot{\rho} - \pi^{*}\nabla^{2}\rho)\mathbf{1} \;\; ; \;\; \hat{\mathbf{f}} = \alpha \mathbf{j} \;\Rightarrow$

•***Governing Eq:*** $\dot{\rho} + \tau\ddot{\rho} = D\nabla^{2}\rho + \overline{D}\nabla^{2}\dot{\rho} - D^{*}\nabla^{4}\rho \qquad (\tau = 1/\alpha)$

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*

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

$$\rho_2 = \;\; \ldots$$

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

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

• *Higher-order Diffusion Equation*

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

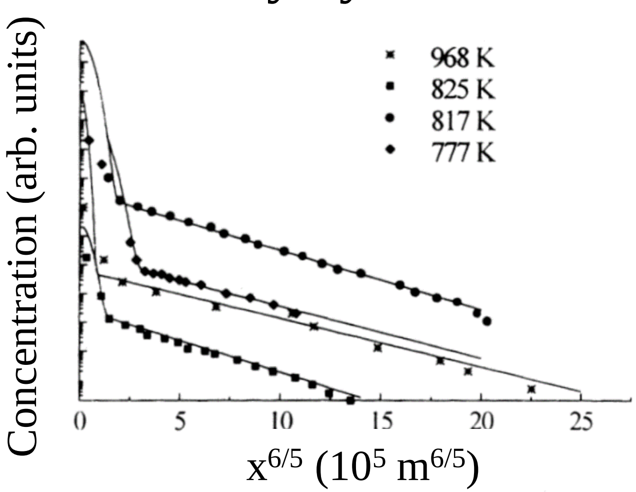
$$\dot{\rho} + \tau\ddot{\rho} = D\nabla^2\rho + \bar{D}\nabla^2\dot{\rho} - \mathrm{D}^*\nabla^4\rho$$

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

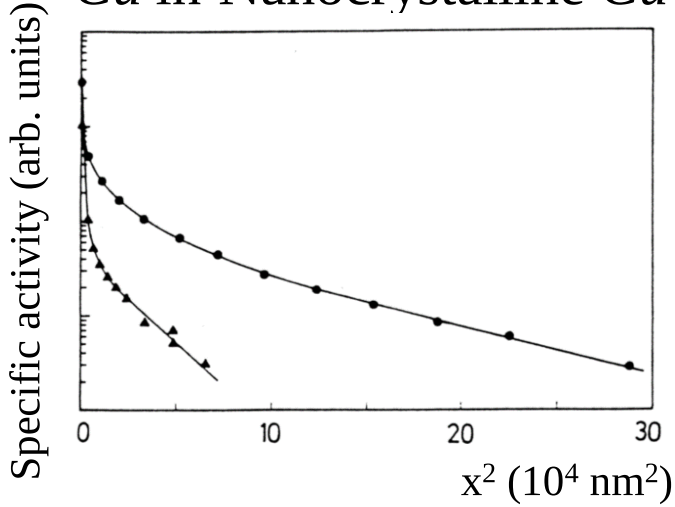
$$\left[t \to \infty \Rightarrow \dot{\rho} = D\nabla^2\rho \;;\; D = D_{eff} = \frac{\kappa_2}{\kappa_1 + \kappa_2} D_1 + \frac{\kappa_1}{\kappa_1 + \kappa_2} D_2 = f\,D_1 + (1 - f)D_2 \right]$$

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

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

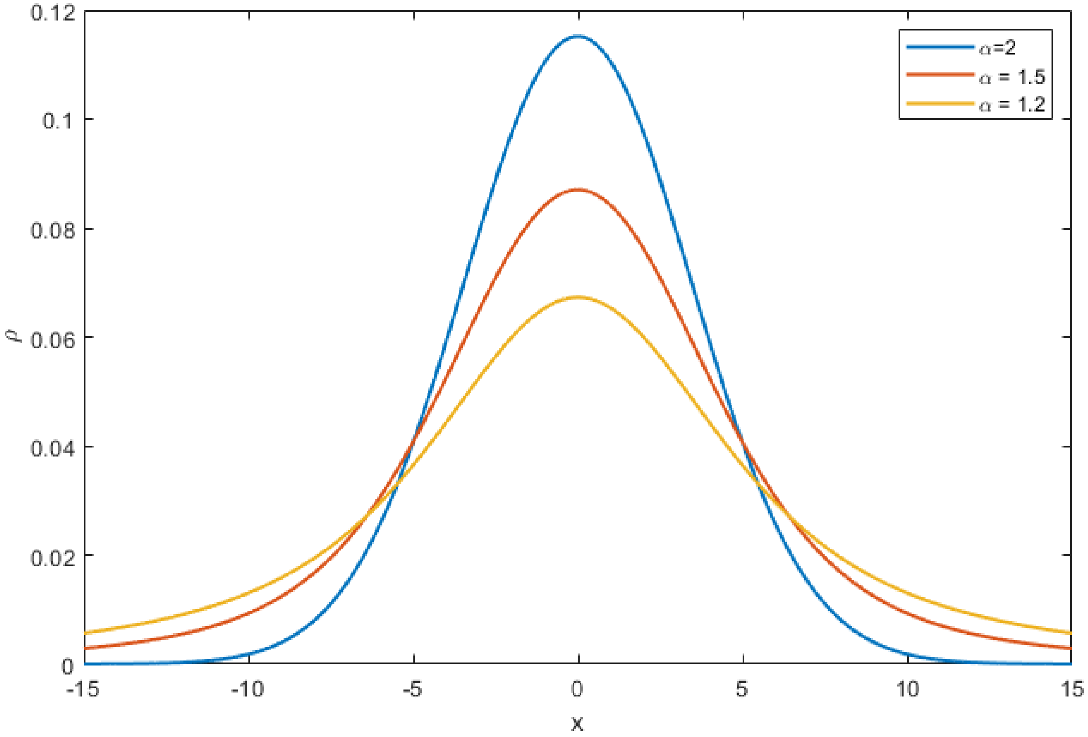
$$G_{\alpha}(x,t) = \frac{1}{\alpha(4\pi)^{1/2}(D_{\alpha}t)^{1/\alpha}}\mathrm{H}_{1,2}^{1,1}\left[\frac{|x|}{2(D_{\alpha}t)^{1/\alpha}}\right] \quad ; \quad \mathrm{H}_{1,2}^{1,1} = \mathrm{H}_{1,2}^{1,1}\Big|_{(0,2^{-1});(2^{-1},2^{-1})}^{1-\alpha^{-1},\alpha^{-1}}$$

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

• *Profiles of fundamental solution*

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

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



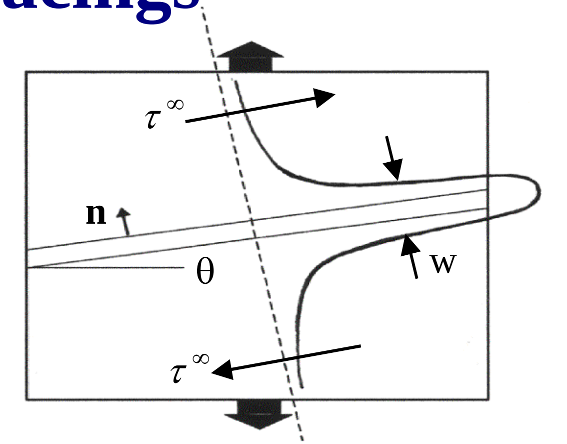
III. Gradient Plasticity

■ Capturing Shear Band Widths & Spacings

- ***Constitutive Equation***

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

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



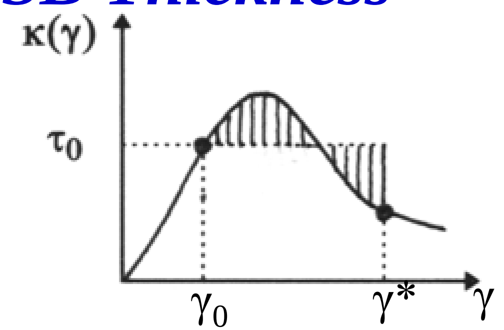
- ***Linear Stability / SB Orientation***

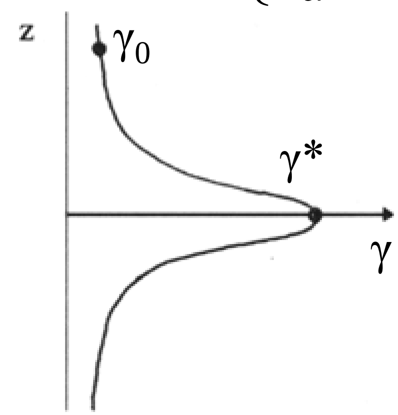
$$\mathrm{v} = \mathrm{L}_\infty \mathrm{x} + \tilde{\mathrm{v}} e^{iqz+\omega t} ; \quad \omega > 0 \quad (\& \omega_{\max}) \quad \to \quad \theta_{cr} = \frac{\pi}{4} \quad \& \quad \begin{cases} h_{cr} = 0 \\ q_{cr} = 0 \end{cases}$$

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

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

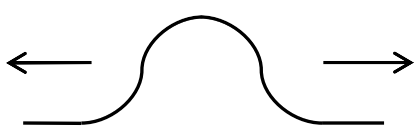
$$\gamma \equiv \int \dot{\gamma}\, dt$$





- ***Front Propagation***

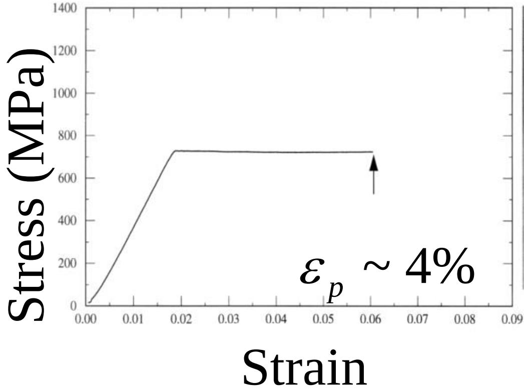
Similar Procedure

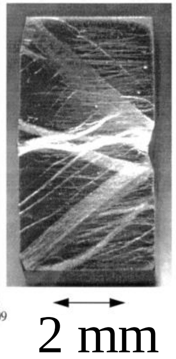


■ Multiple Shear Banding

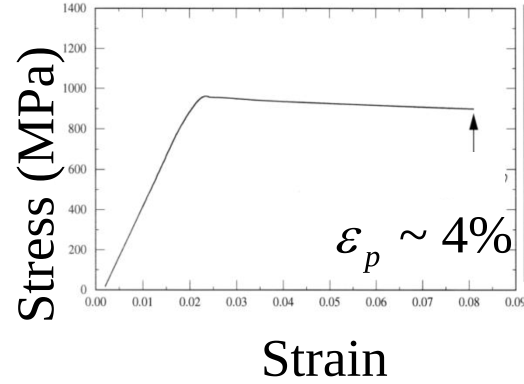
- Compression of Bulk Nanostructured Fe – 10% Cu Polycrystals (UFGs)

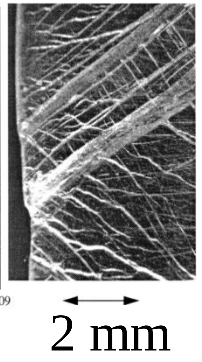
d ~1370 nm, σ_y ~750 MPa
angle ~ 49^0





d ~540 nm, σ_y ~960 MPa
angle ~ 49^0





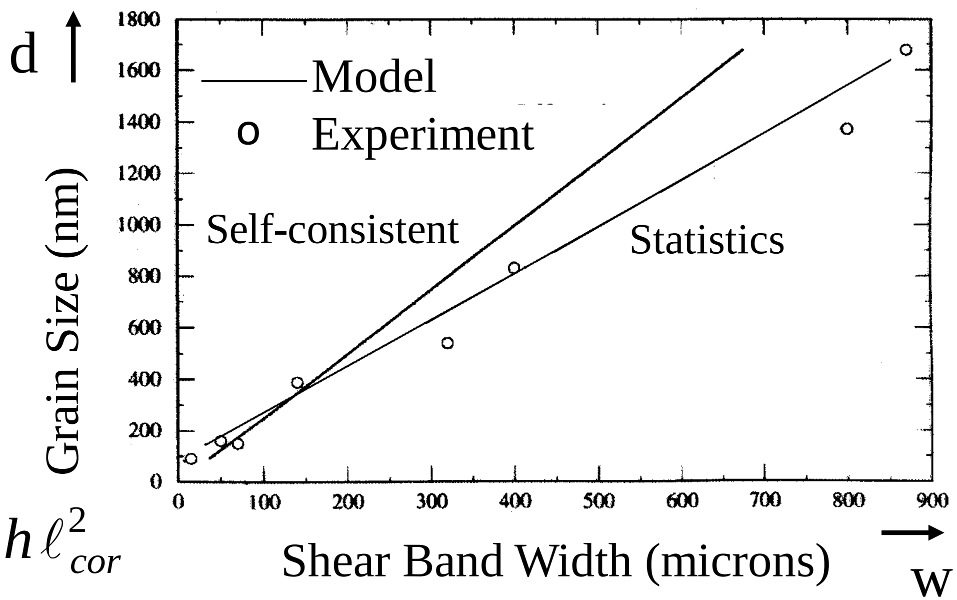
- Shear band width analysis

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

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

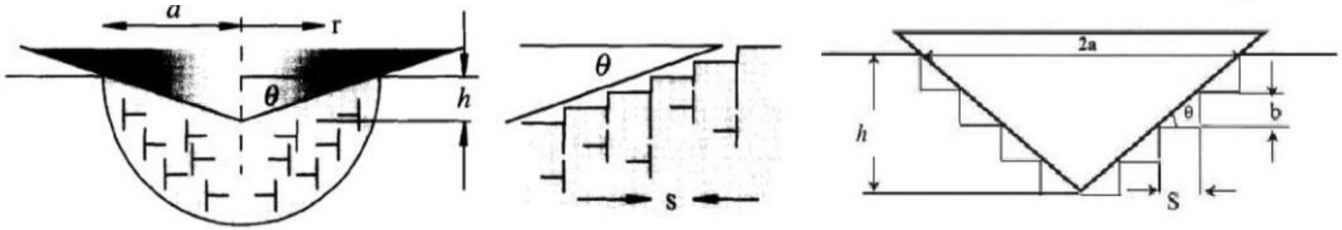
$$\beta = \alpha G \frac{7-5\nu}{15(1-\nu)}$$

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



■ 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)***

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

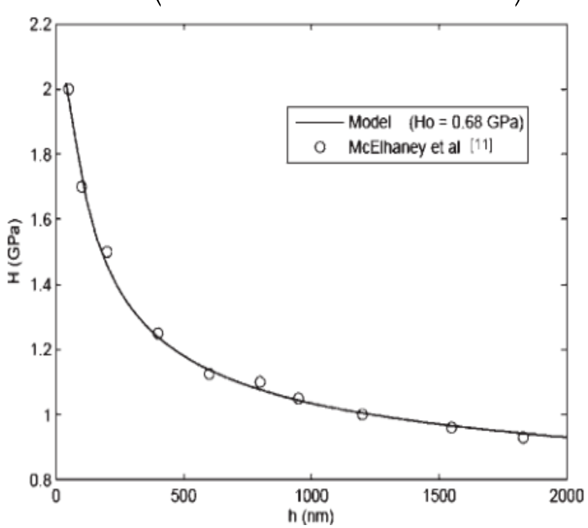
- ***Aifantis (1984)***

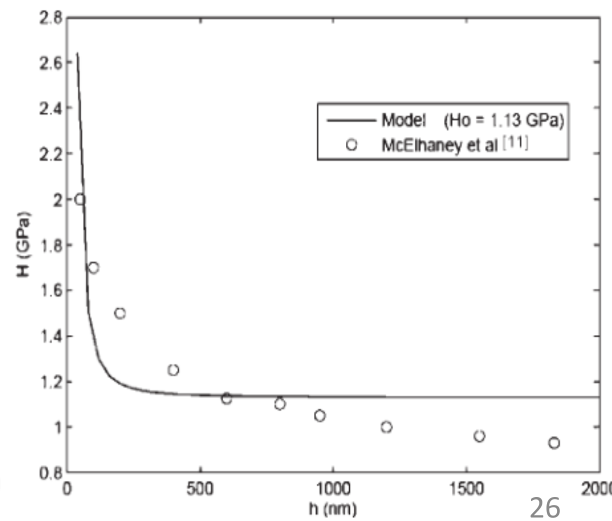
$$\tau = \tau_0\left(1 + c_1\left|\nabla\gamma\right|^{1/2} - c_2\nabla^2\gamma\right)$$

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

l_1, l_2 : internal lengths

h : indentation depth



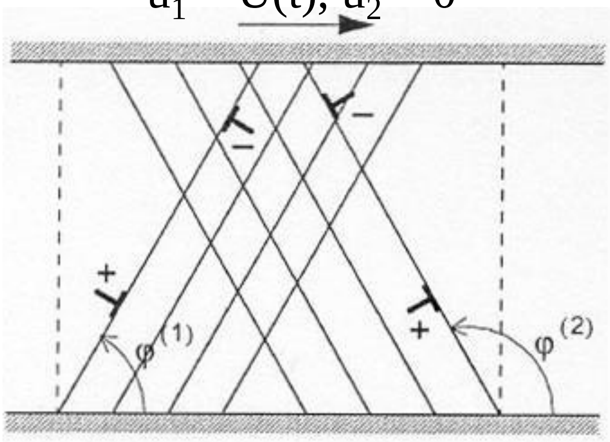


■ A Note on Plastic Boundary Layers

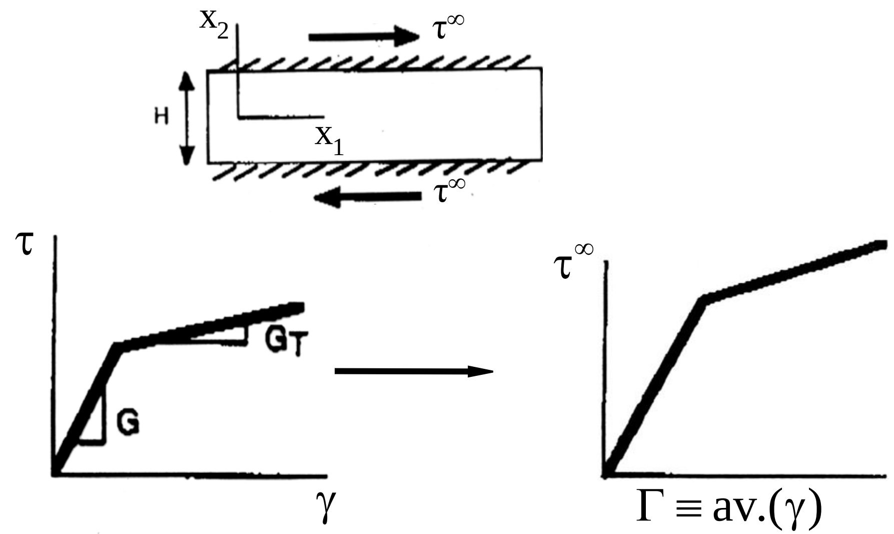
- ***Fleck/Van Der Giessen/Needleman (2000)***

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

$u_1 = U(t),\ u_2 = 0$



$u_1 = 0,\ u_2 = 0$

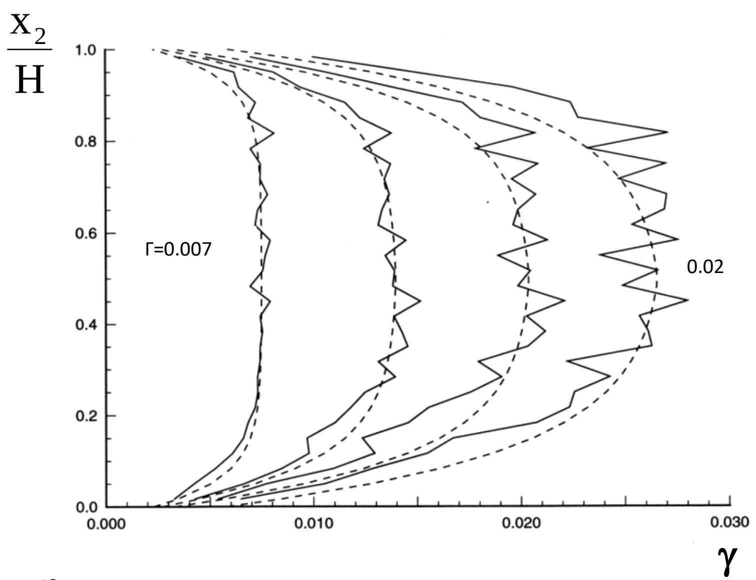


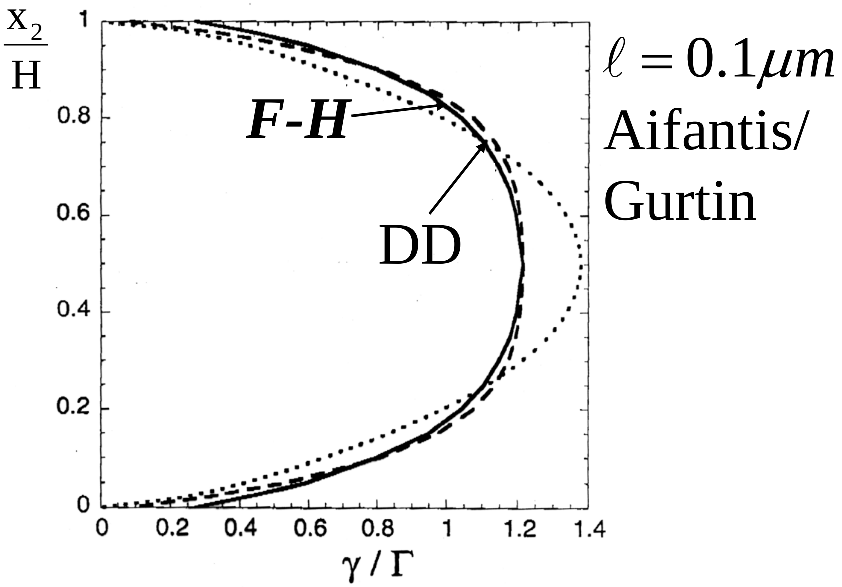
- ***Aifantis (1984) / Gurtin (2000)***

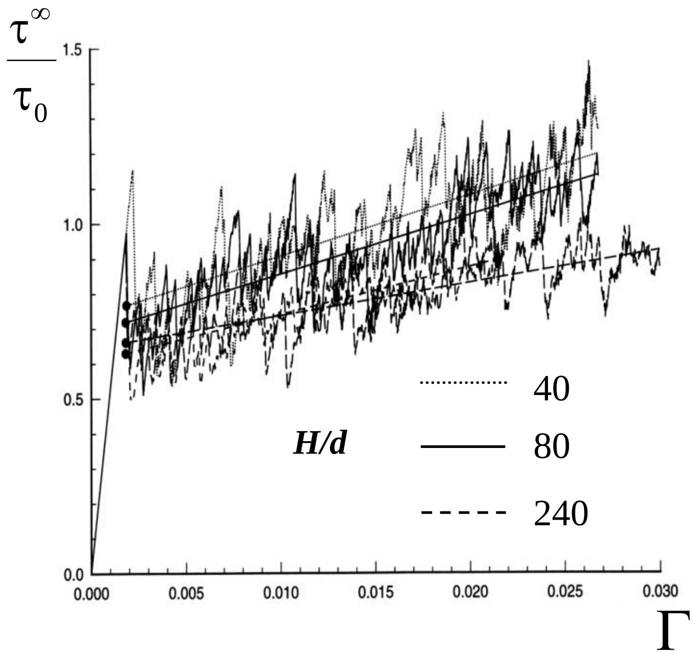
$$\tau = \tau_0 + G_T\gamma - G_T\ell^2\nabla^2\gamma = \tau^\infty \quad \Rightarrow \quad \gamma = \frac{\tau^\infty}{G} + \frac{\tau^\infty - \tau_0}{G_T}\left[1 - \frac{\cosh(x_2/\ell)}{\cosh(H/\ell)}\right]$$

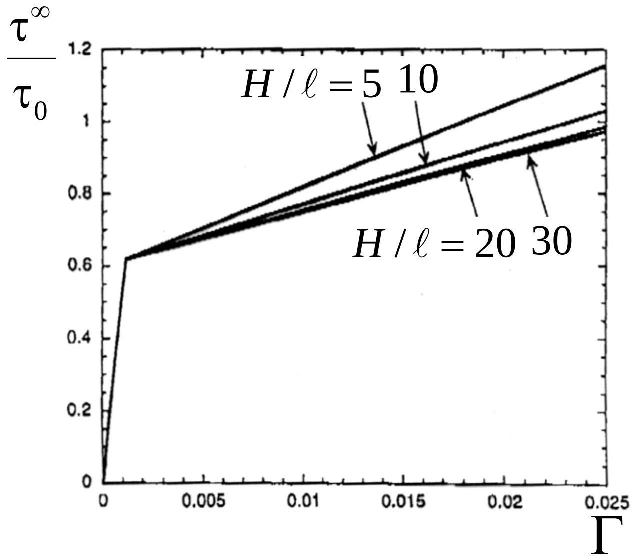
$$\Gamma = \frac{1}{H}\int_{-H/2}^{H/2} \gamma(x_2)dx_2 = \frac{\tau^\infty}{G} + \frac{\tau^\infty - \tau_0}{G_T}\left(1 - \frac{2\ell}{H}\tanh\frac{H}{2\ell}\right)$$

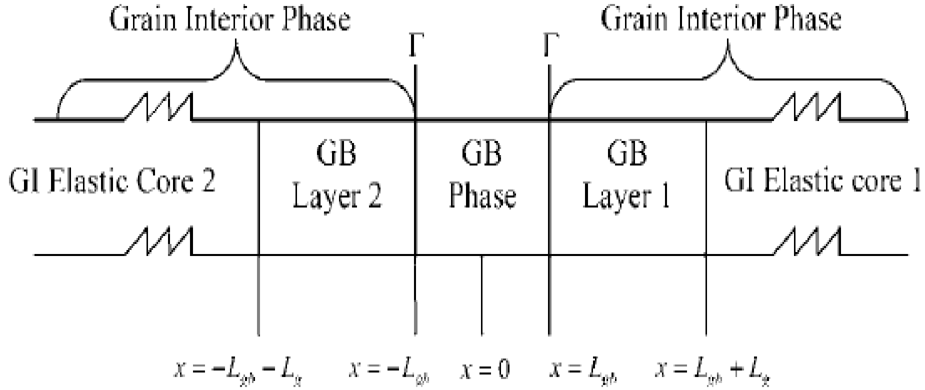
- ***Plastic Strain Profiles / Size Effects***



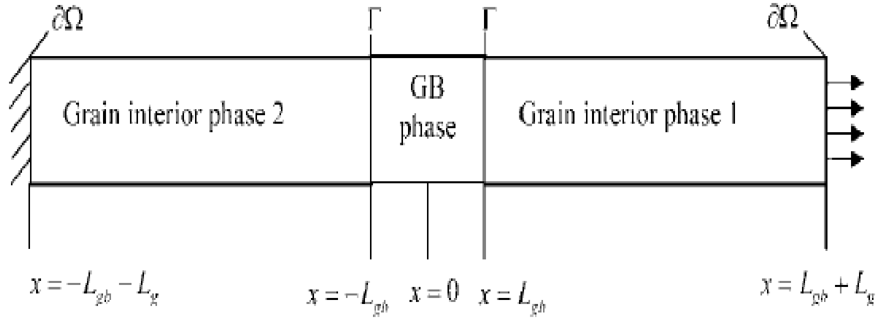






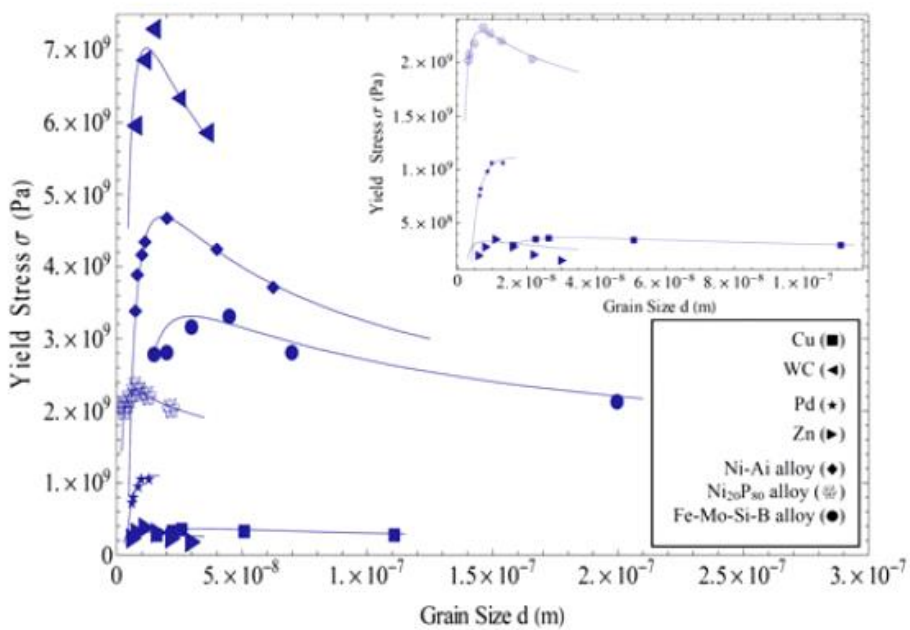


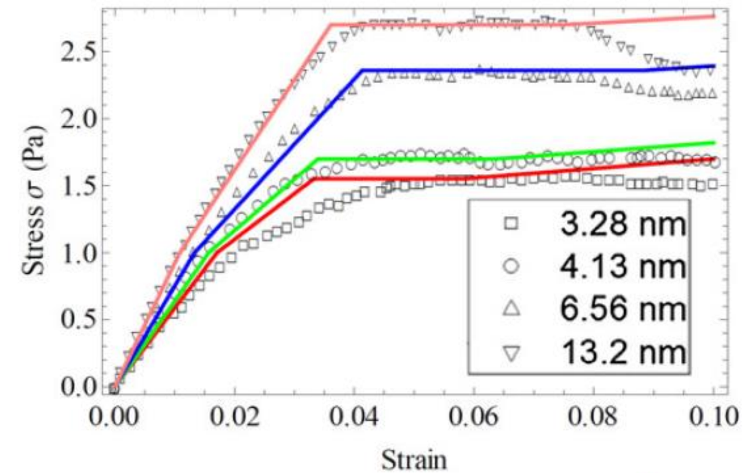
Unit cell model with GB phase, GI phase comprised of GI-GB layers, and elastic GI cores



Unit cell consisting of a GB and a GI phase, for size-dependent stress-strain prediction

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





	$L_g =$ 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

■ 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:

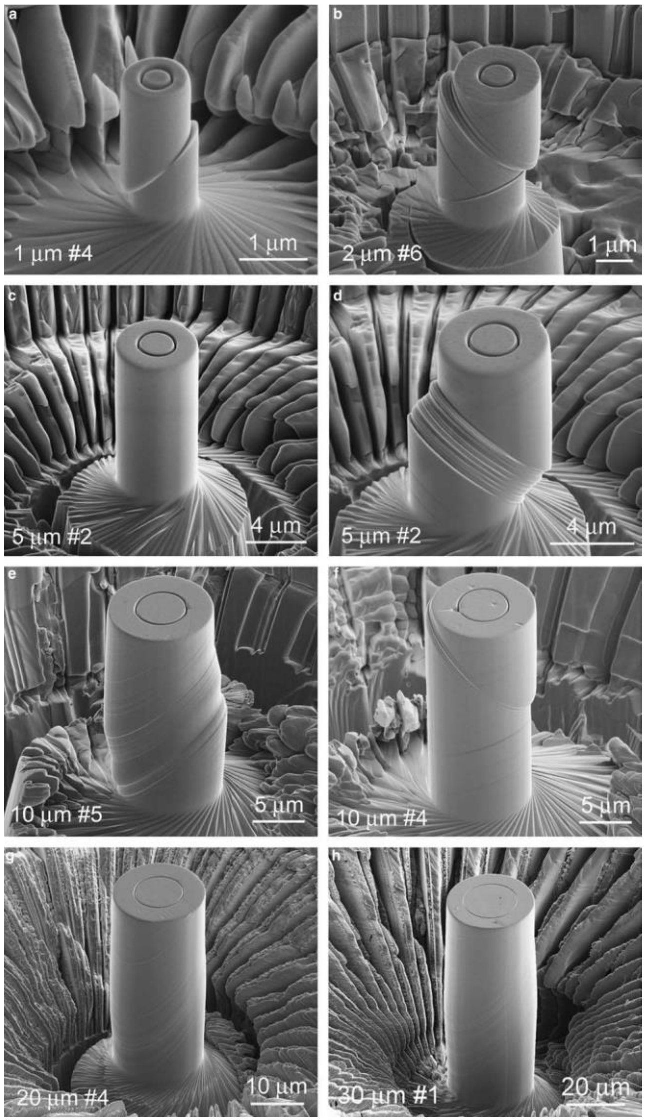
- the flow rule of Fleck and Hutchinson is incompatible with thermodynamics unless its nonlocal term is dropped.
- If the underlying theory is augmented by a general defect energy dependent on γ^p and $\nabla\gamma^p$, then compatibility with thermodynamics requires that its flow rule reduce to that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

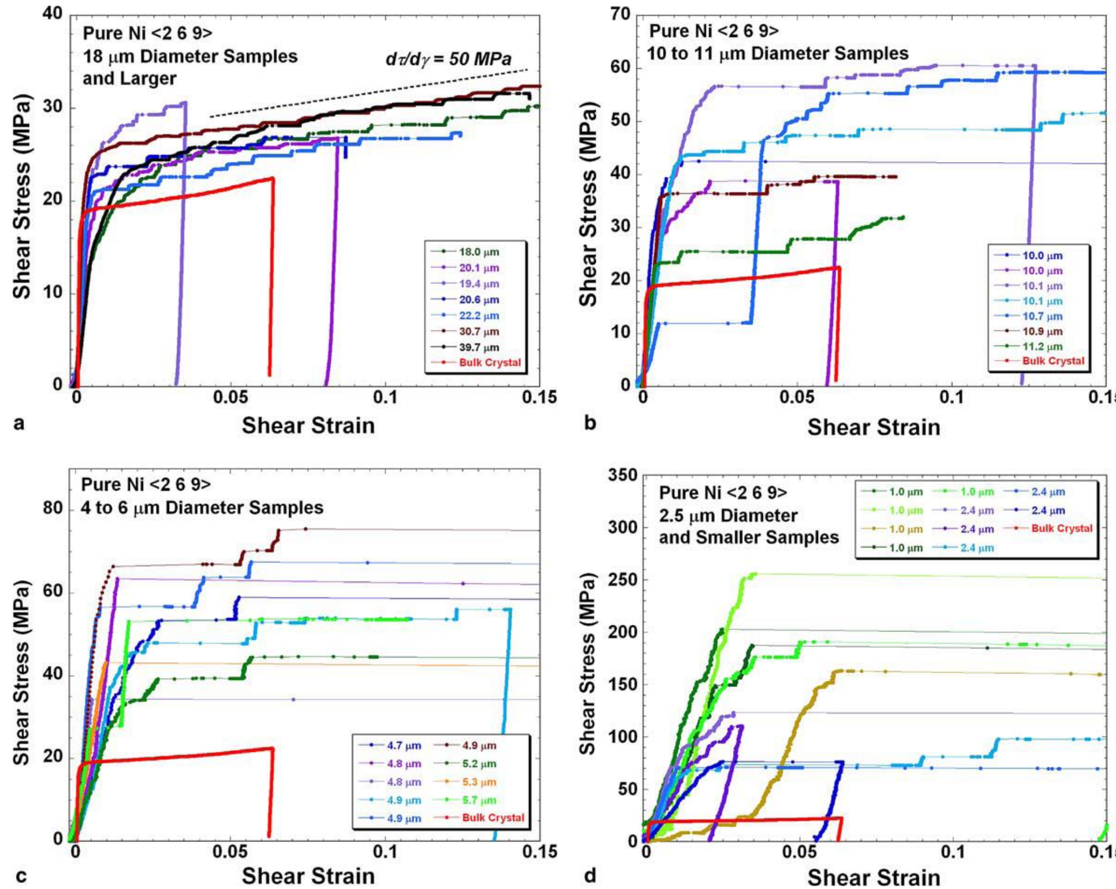
Refs

- 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).

APPENDIX A: Size Effects in 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

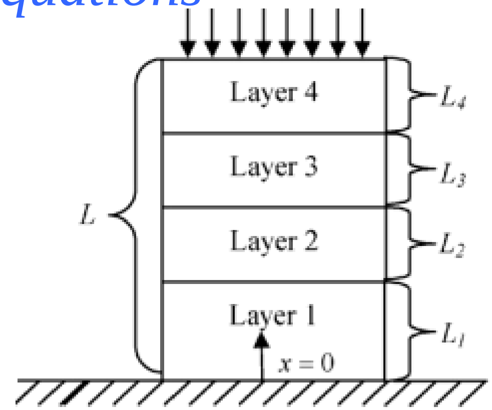
- ***Serrated Plastic Flow: The Gradient-Stochastic Model***

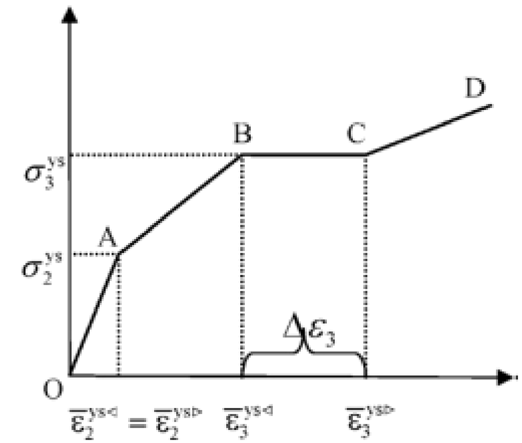
- *Governing Deterministic Equations*

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

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

(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

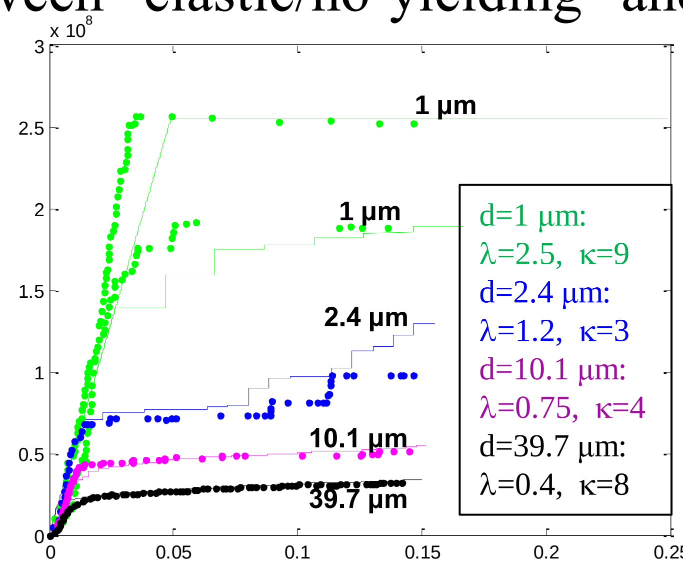
- *Introducing Stochasticity*

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

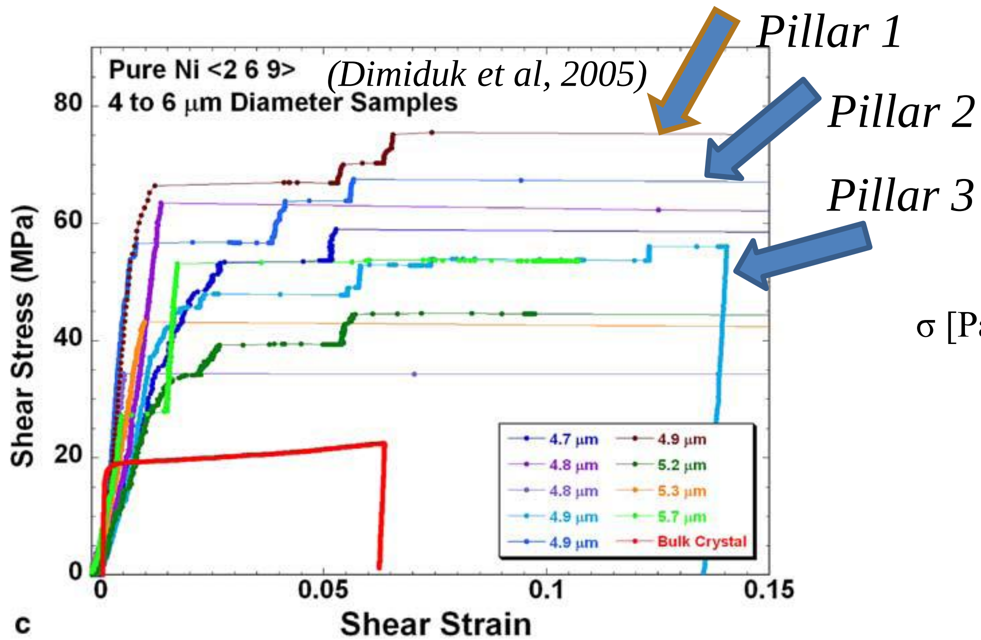
$$PDF(\delta) = \frac{k}{\lambda}\left(\frac{\delta}{\lambda}\right)^{k-1} e^{-(\delta/\lambda)^k};$$

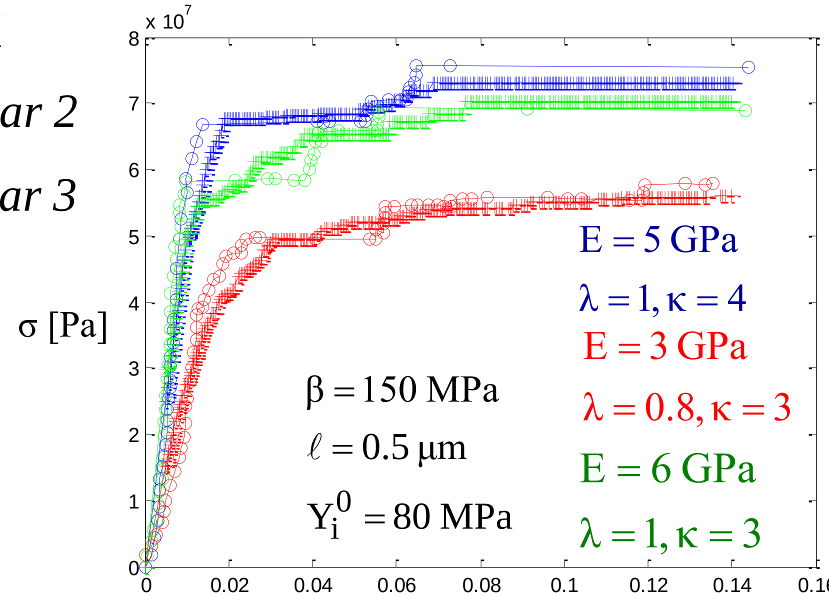
$$\bar{\delta} = \lambda\Gamma\left[1+(1/k)\right], \quad \left\langle \delta^2 \right\rangle = \lambda^2\Gamma\left[1+(k)\right] - \bar{\delta}^2$$

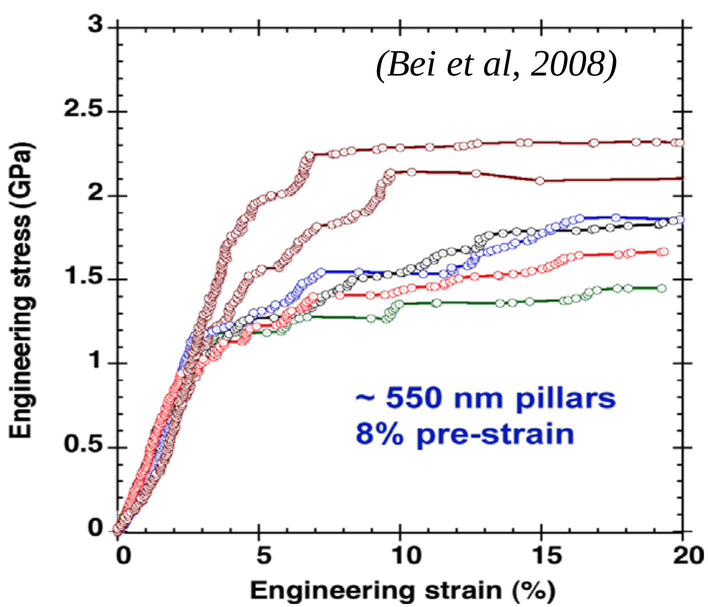
k/λ : shape/scale parameters

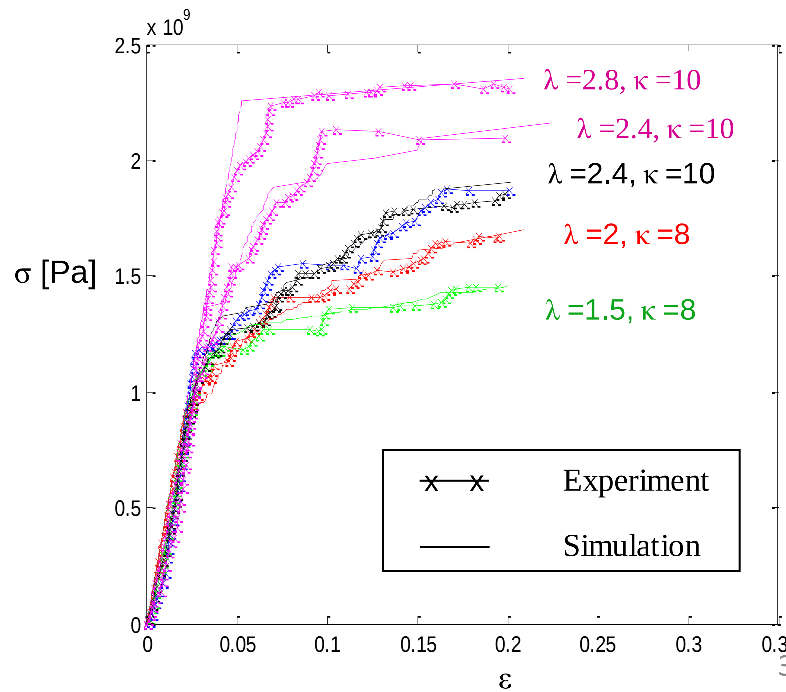


• *Random Response of Same Diameter Micropillars*









■ 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

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

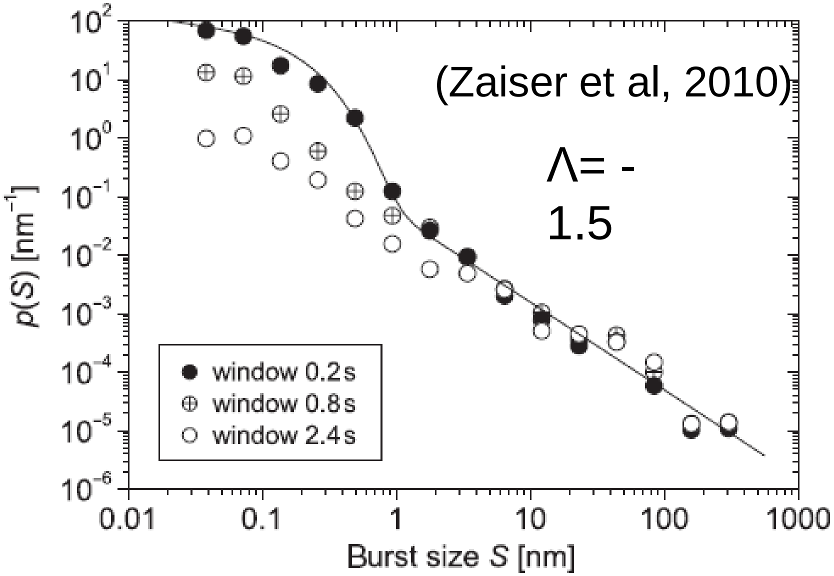
Burst size relation to local yield stress

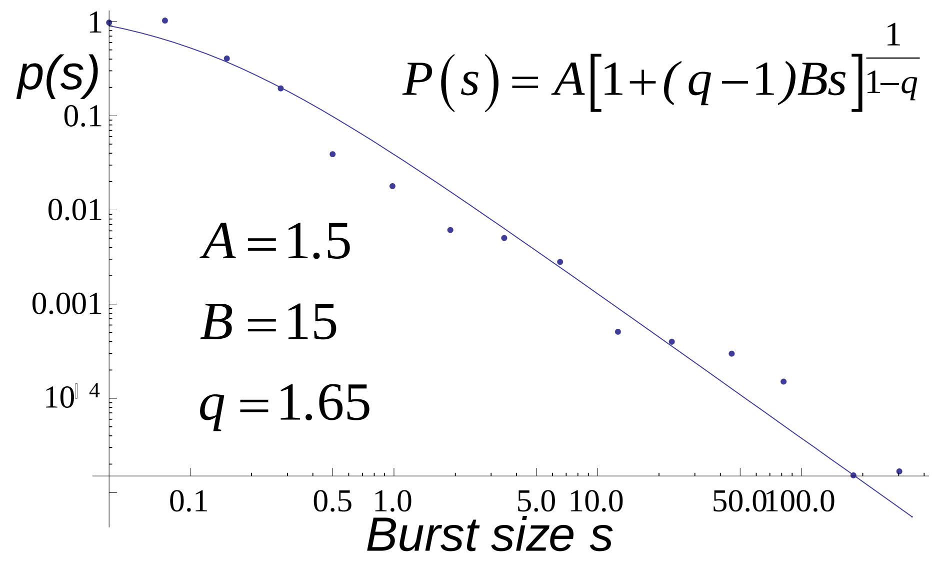
$$s=nL\varepsilon_y^{loc}=nL\frac{\sigma_y^{loc}}{E}; \quad P\left(\sigma_y^{loc}\right)\equiv P\left(\varepsilon_y^{loc}\right) \quad (L\text{: cell size})$$

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

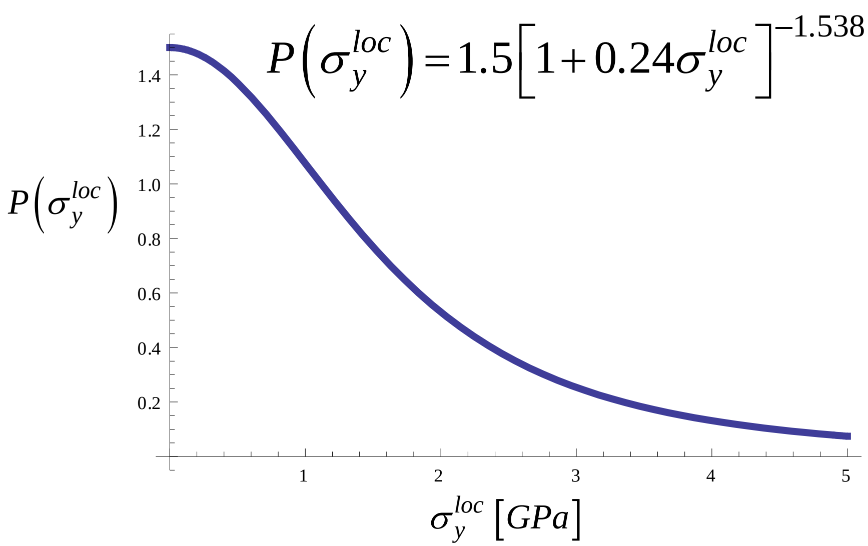
$$\therefore \quad P\left(\sigma_y^{loc}\right)=A\left[1+(q-1)Bs_b\left(\frac{\sigma_y^{loc}}{\sigma_y^b}\right)^2\right]^{1/(1-q)}$$

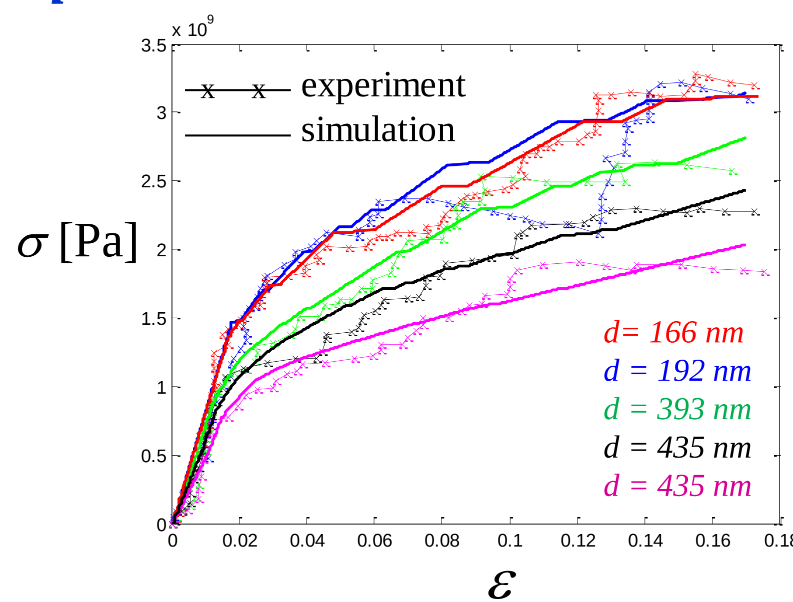
• ***Strain bursts in Mo micropillars under compression***



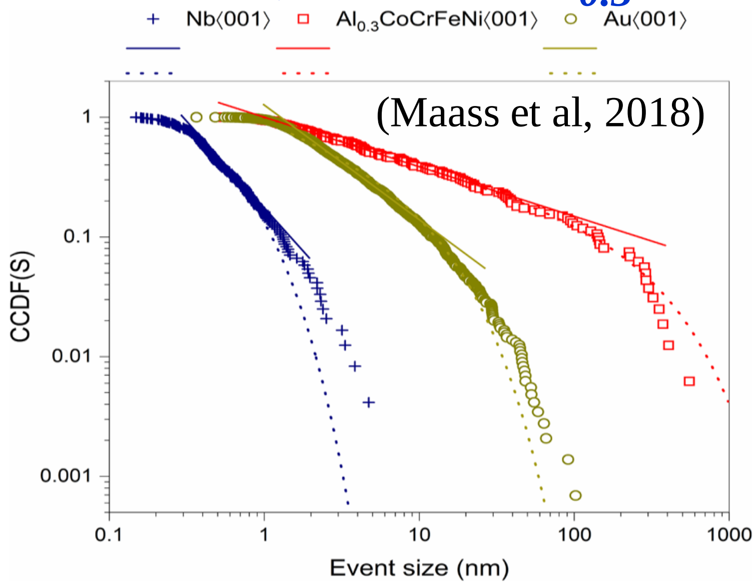


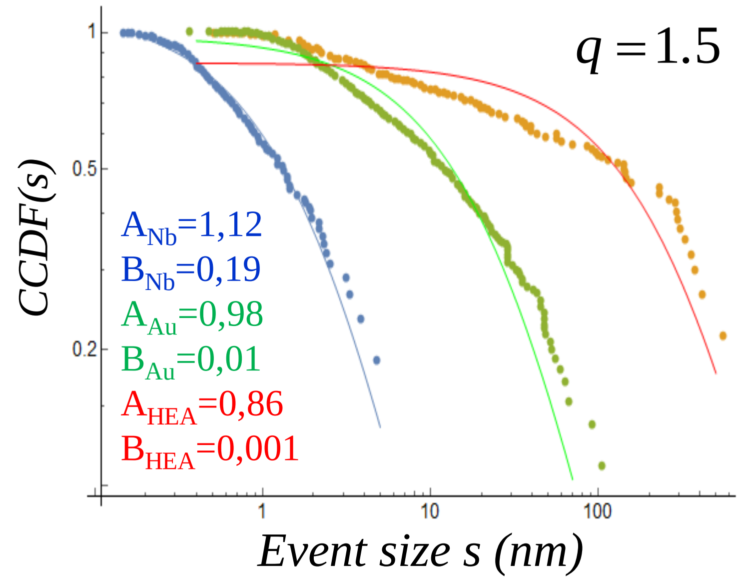
• ***CA simulations with input from q-statistics***





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

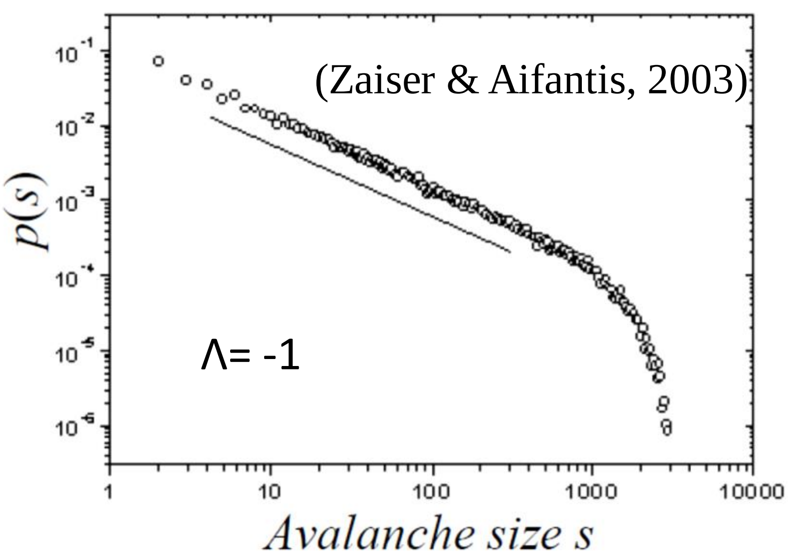


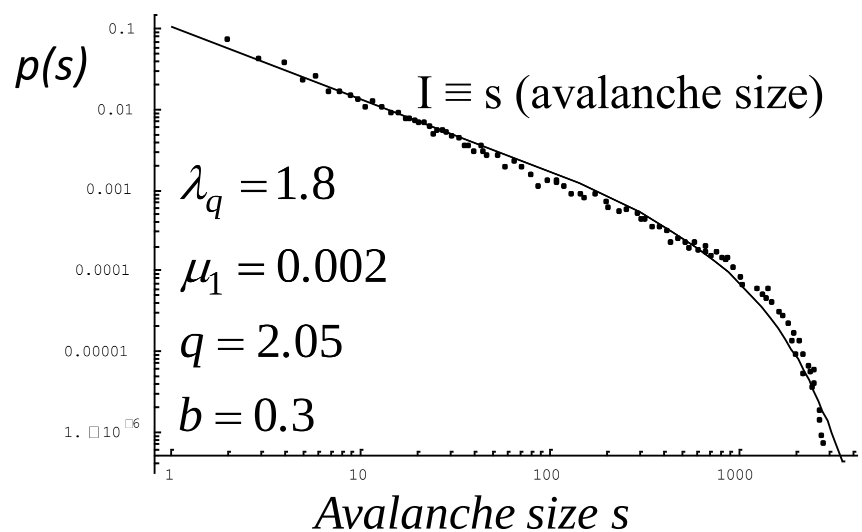


• Slip Avalanches

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

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

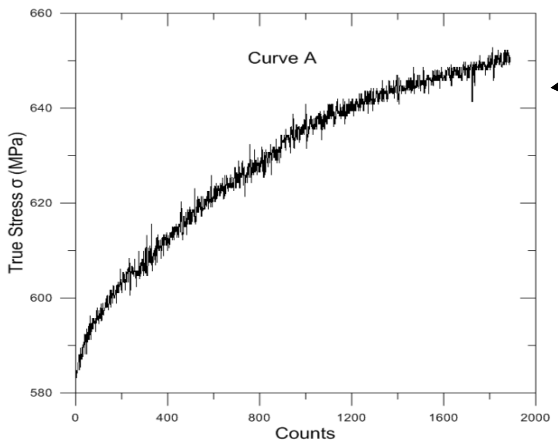




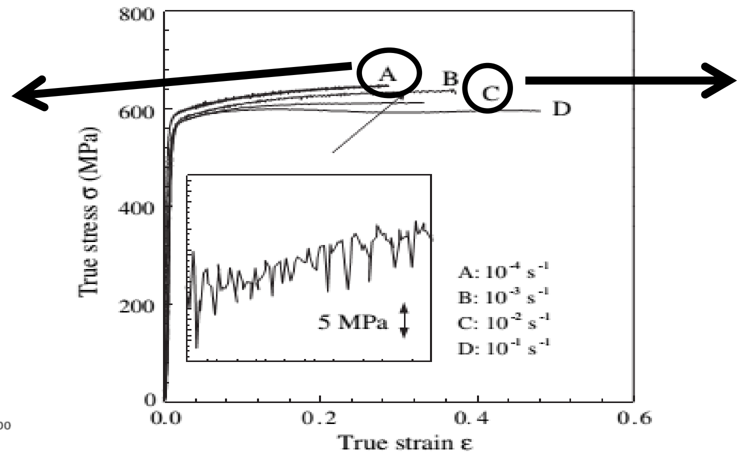
APPENDIX B: No Equations – Tsallis Statistics

■ Serrated Plastic Flow & Multiple Shear Banding in UFGs

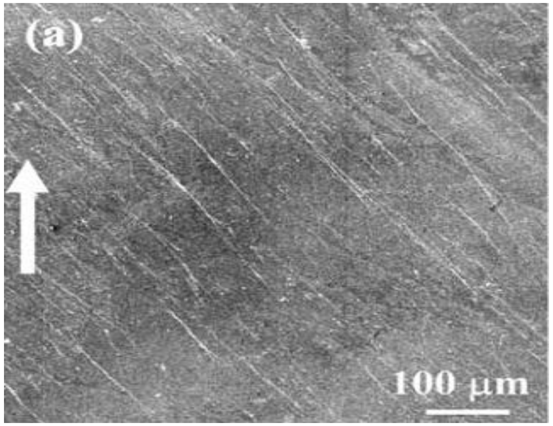
(Fan *et al*. Scripta/Acta Materialia 2005/2006)



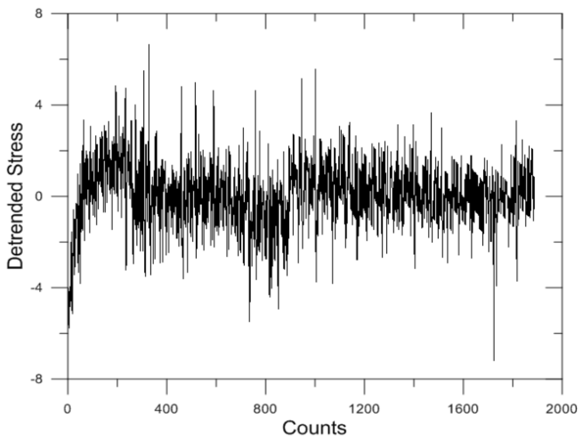
Low $\dot{\varepsilon}$ (10^{-4} s^{-1}) – Serrations



σ-*ε* curves (compression)



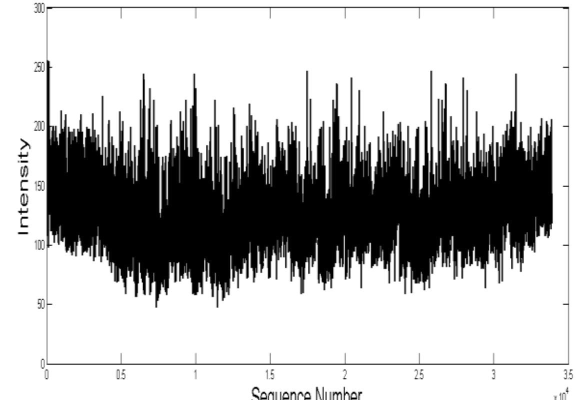
High $\dot{\varepsilon}$ (10^{-2} s^{-1})
Shear Bands (SEM)



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

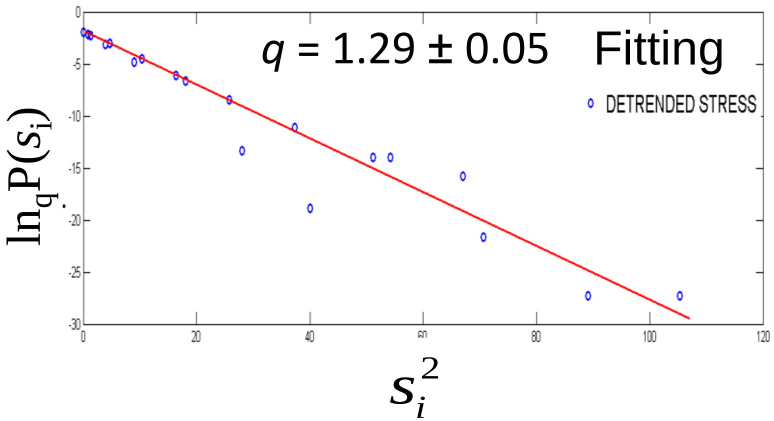
[2D → 1D: Space Filling Curve Method (Morton, 1966)]

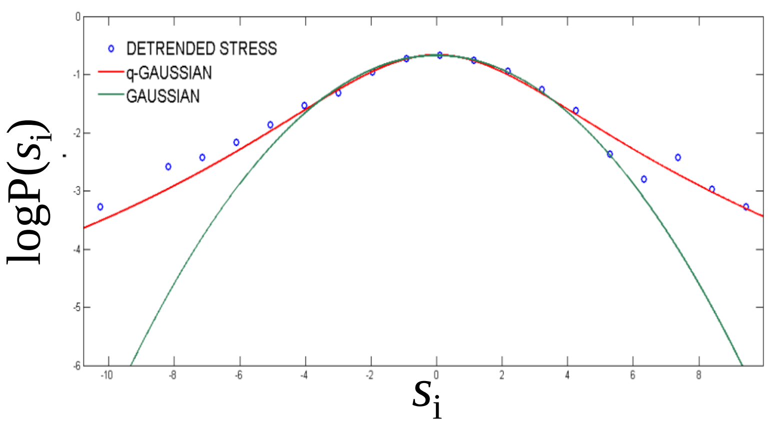
■ Serrations

•*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

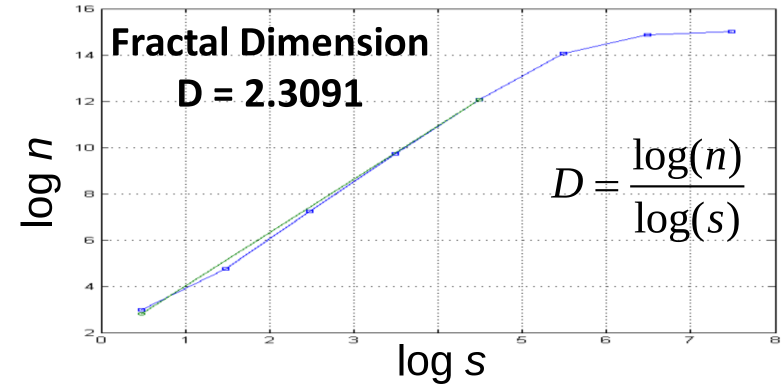
•*Power Law Tail (q>1):* $P(|s|) \sim |s|^{-2/(q-1)}$

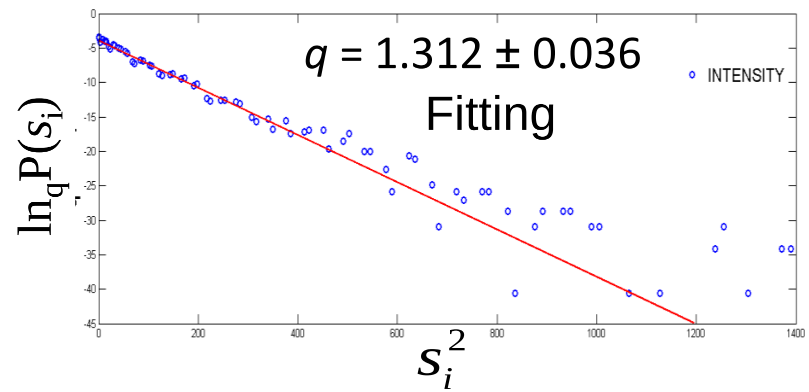


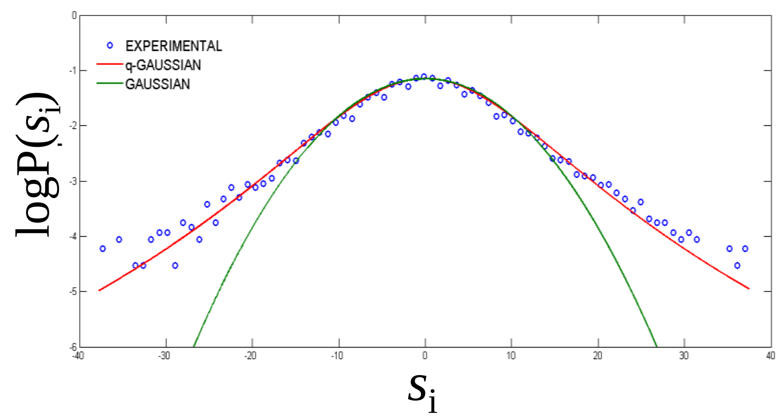


$q > 1 \longrightarrow$ {
Non-Gaussian Statistics
Tsallis Nonextensive Statistics,
Temporal Long range correlations

■ Shear Band Fractality





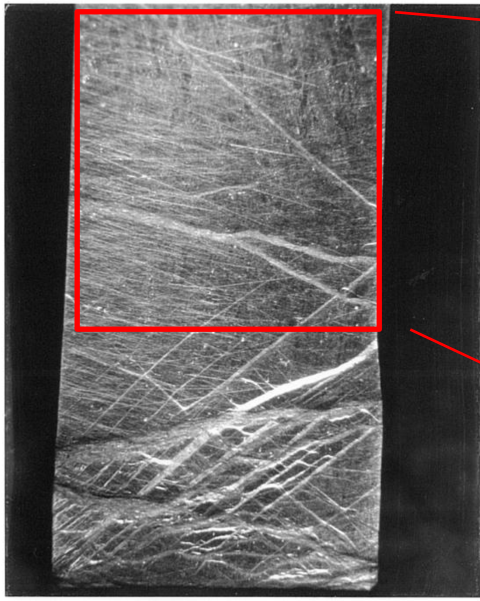


$D > 2 \longrightarrow$ Fractal Geometry of Shear Band network

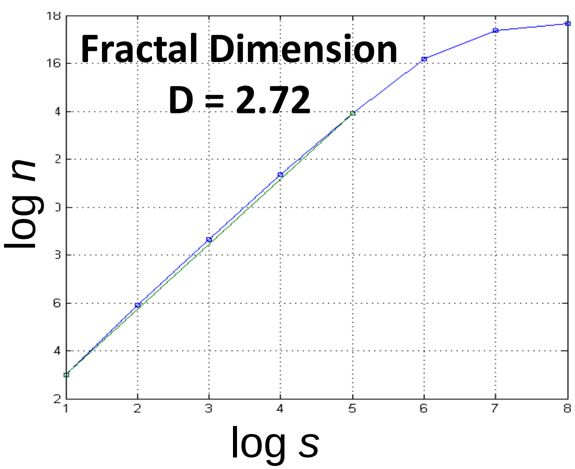
$q > 1 \longrightarrow$ {
Non-Gaussian Pixels Distributions
Spatial Long range correlations

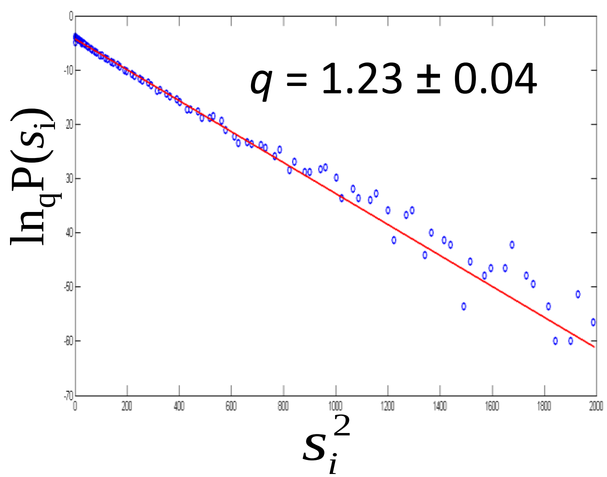
■ Shear Band Fractality in Fe – 10% Cu UFG Alloy

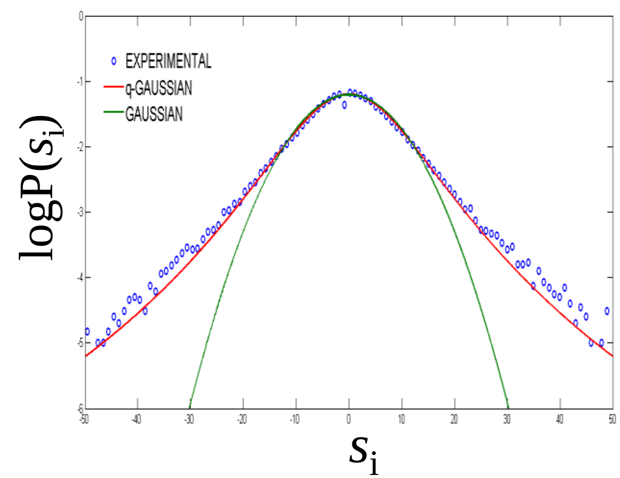
(Carsley *et al*. Metall. Mater. Trans 1998)



Shear Bands



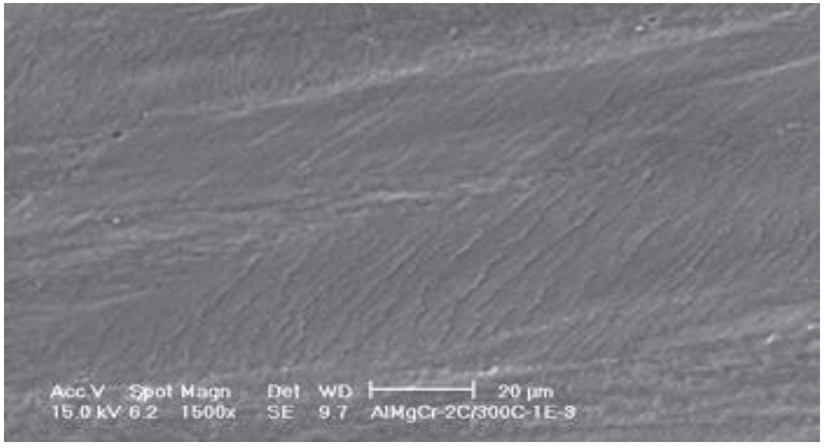




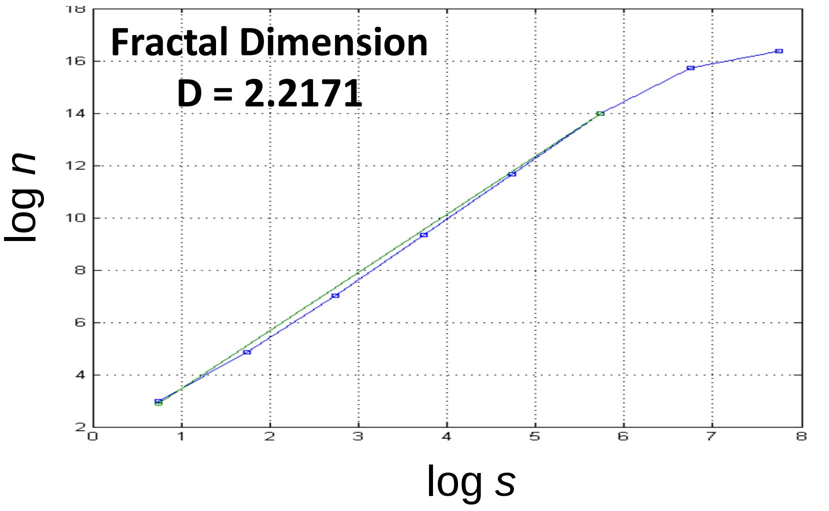
$D > 2 \longrightarrow$ Hierarchical Fractal Shear Band network ‖ $D = 2 \rightarrow$ No Fractality; $D = 3 \longrightarrow$ Extreme Fractality

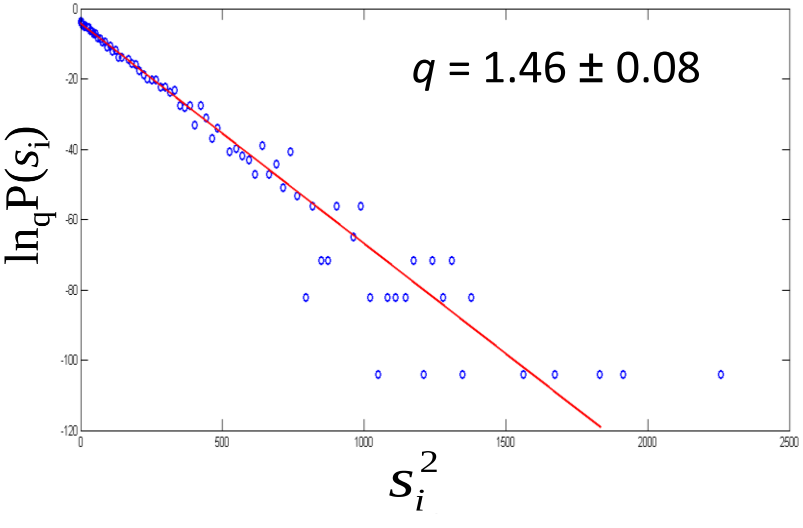
$q > 1 \longrightarrow$ { Non-Gaussian Pixels Distributions; Spatial Long range correlations ‖ $q = 1 \longrightarrow$ { Gaussian Pixels Distributions; Spatial short range correlations

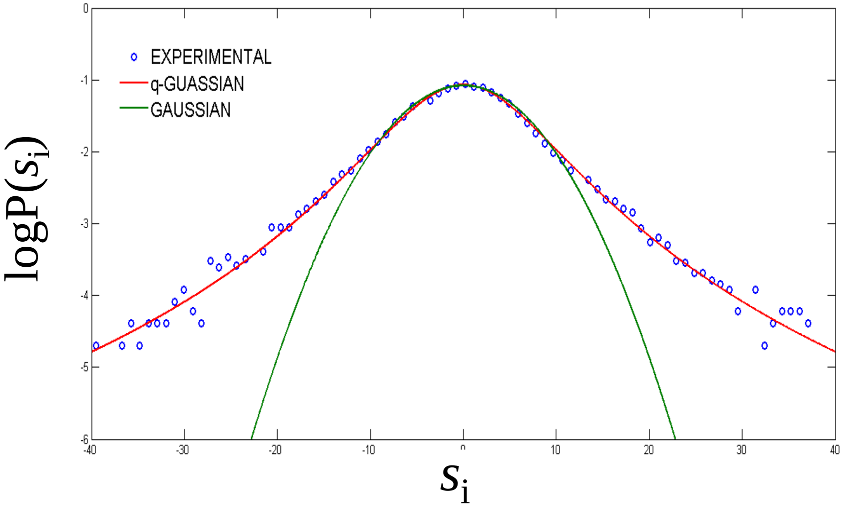
■ Shear Band Fractality in Al – 5%Mg - 1.2% Cr ECAP Alloy



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







$D > 2 \longrightarrow$ Hierarchical Fractal Shear Band network

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