ON GRADIENT MICRO/NANOMECHANICS

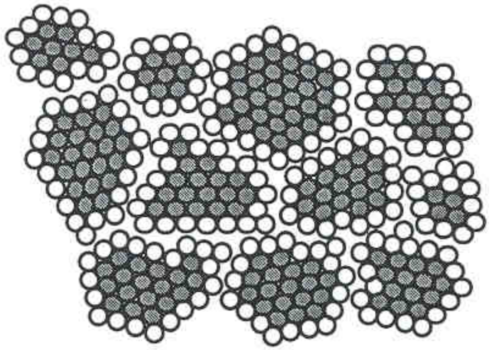
NANOELASTICITY, NANOPLASTICITY, NANODIFFUSION

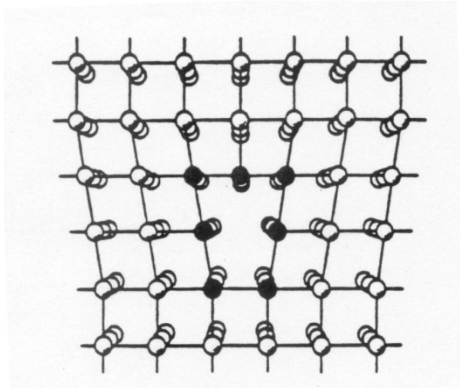
■ Grain Configuration at the Nanoscale

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

Grain d

1-50 nm



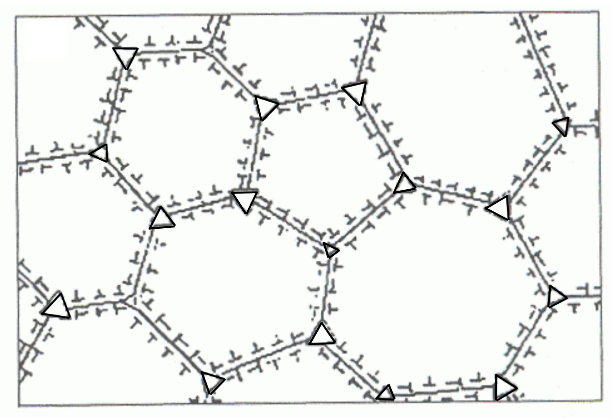


Core r_0

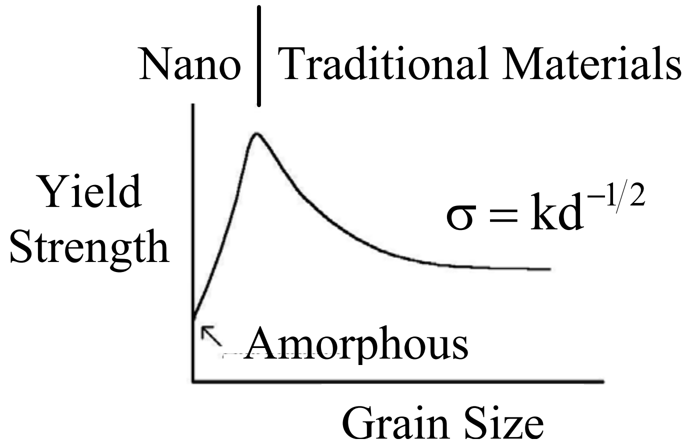
~1 nm

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

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



Plasticity Mechanisms ?

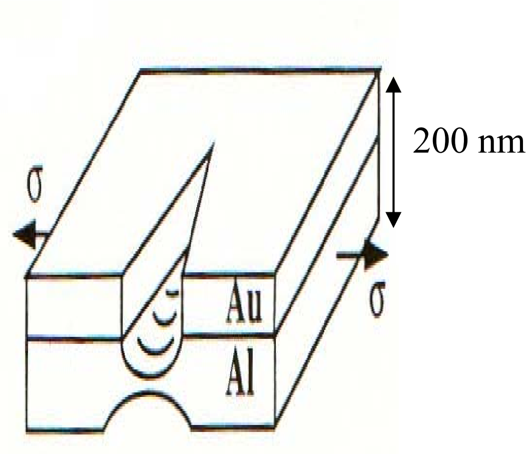


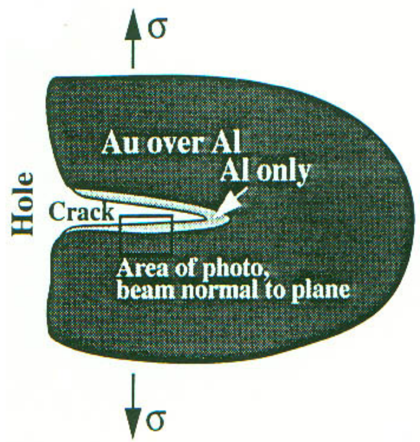
Inverse Hall-Petch Relation ?

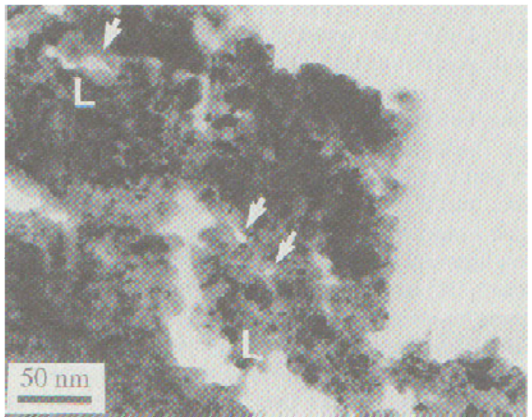
■ Improved/Engineered Properties: Examples

Property	*Material*	*Bulk*	*Nano*
Density (g/cc)	Fe	7.5	6
Modulus (GPa)	Pd	123	88
Fracture Stress (GPa)	Fe	0.7	8
E_a for Self-diffusion (eV)	Cu	2.0	0.64

■ In-situ TEM Strain Tests/MTU Early Observations



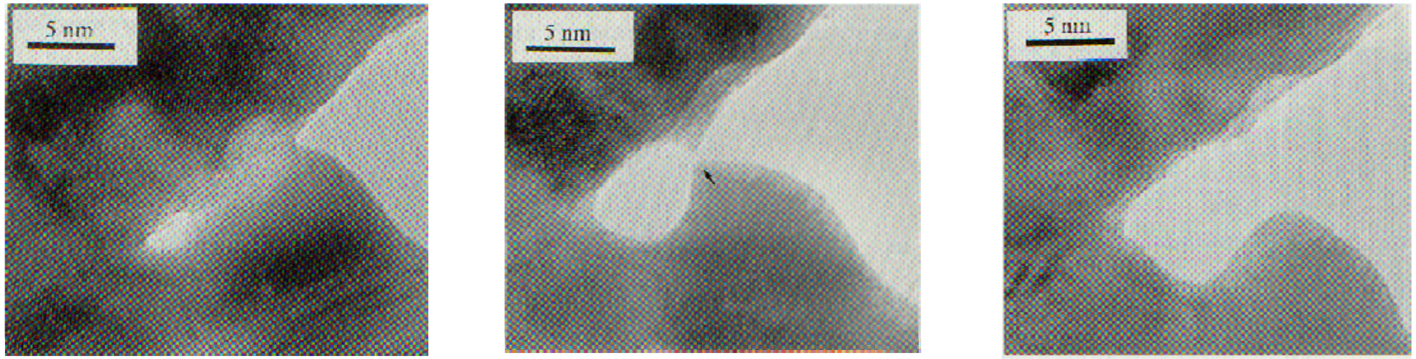




Schematics

8 nm Au on Al: Nanovoid Coalescense

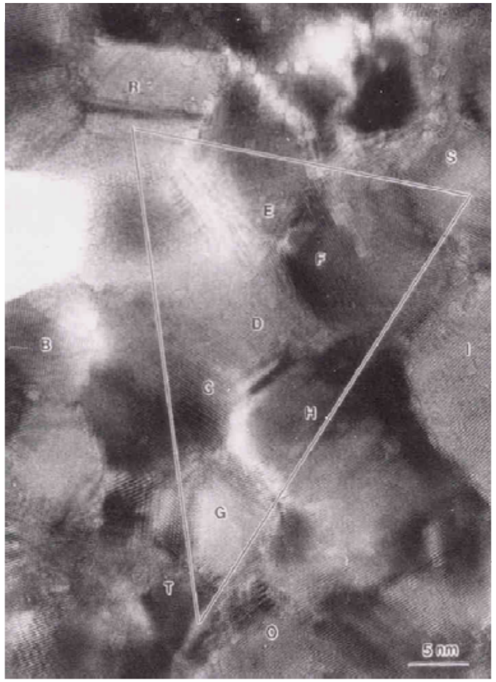
- ***Nanovoid Nucleation***



8 nm Au on C: Nanocrack growth via nanopore formation

25 nm Au on C: Periodic Crack profiles and bifurcation

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



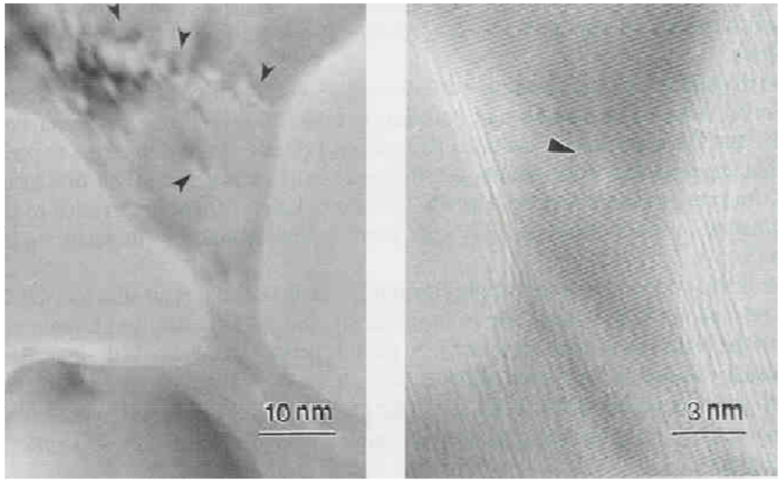
10 nm Au: 6-15 degrees relative grain rotation

Elementary Rosette Analysis

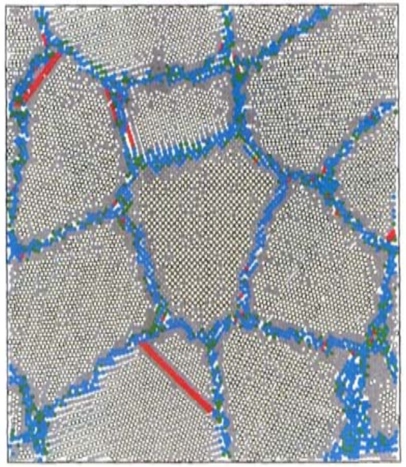
	Triangle angles (deg)			Triangle lengths (nm)		
Step	α	β	γ	a	b	c
Start	89	36	55	22.2	27.7	16.4
1	91	35	54	22.6	27.9	17.4
2	96	36	48	23.4	31.2	18.9
3	102	33	45	21.7	32.0	18.0

Strain Tensor

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



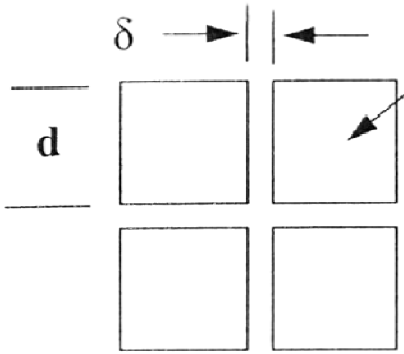
100 nm Au film



~12 nm Ni nanopolycrystals

■ Initial Simple-minded Models

- ***Continuum Two-Phase Model***



"Bulk" Phase, Hall – Petch relation

$$\sigma_G = \sigma_0 + \frac{k}{\sqrt{d}}$$

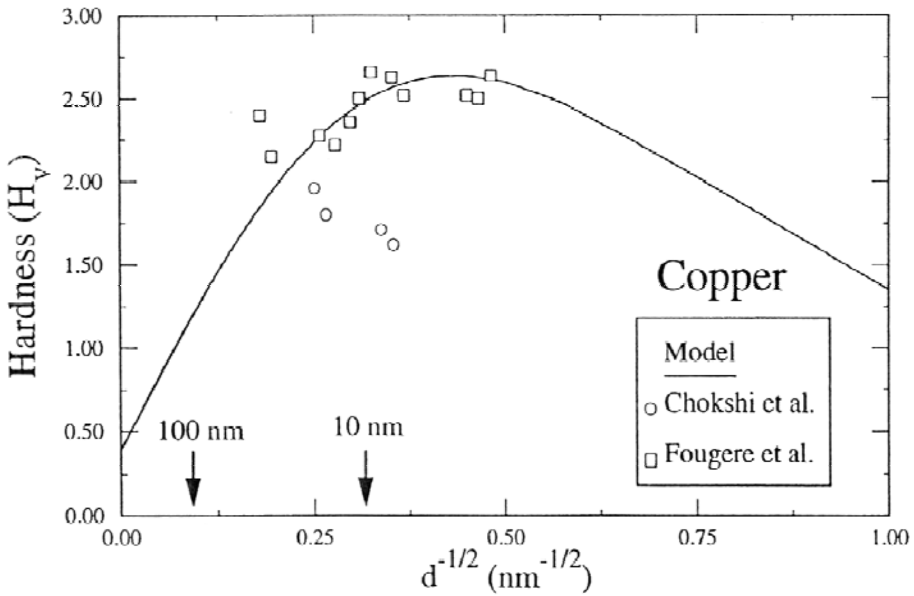
"Boundary" Phase, Constant strength related to amorphous material or grain boundary sliding (σ_{GB})

- Volume Fraction

$$f = \frac{d^3}{(d+\delta)^3}$$

- Rule of Mixtures

$$\sigma = f\sigma_G + (1-f)\sigma_{GB}$$



•Continuum Model predicts behavior of NanoCrystalline Materials

•Continuum Model can sort out conflicting Materials Science data

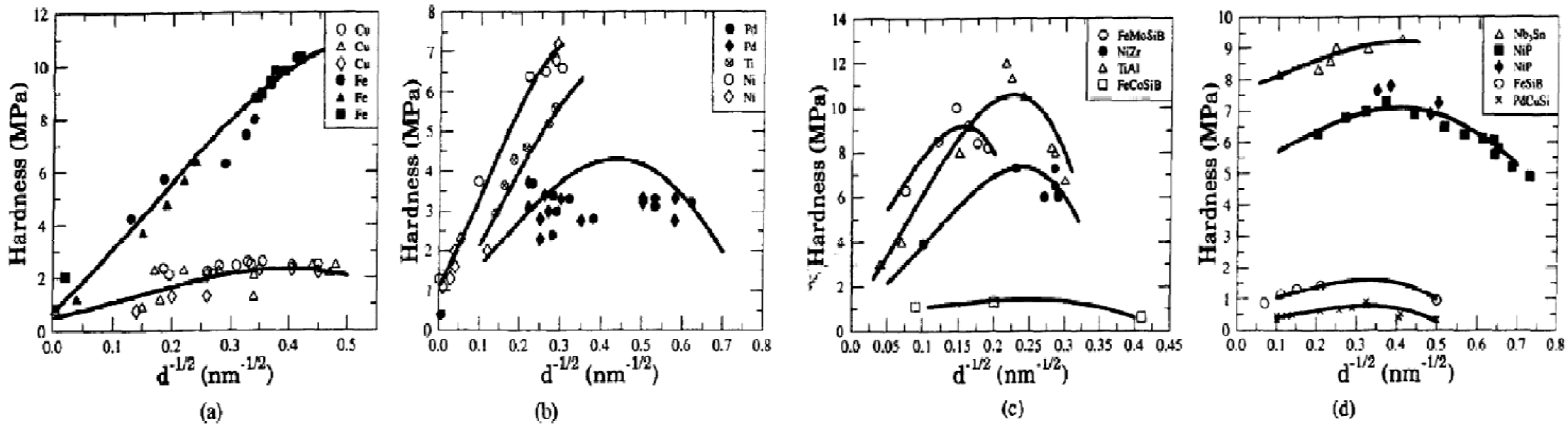
•Continuum elasticity Model has also been developed, which shows the importance of gradients in elasticity of nanophase materials

• *Improved Hall-Petch Relation*

$$H = H_G\left(1-f\right)+H_{GB}\ f \quad \Rightarrow \quad H=\left[\left(d-\delta\right)^3/d^3\right]H_G+\left[d^3-\left(d-\delta\right)^3/d^3\right]H_{GB}$$

$$H_G = H_{0G}+k_G d^{-1/2}\ , \qquad H_{GB}=H_{0GB}+k_{GB}d^{-1/2}\ , \quad k_{GB}=k_G\left(\frac{\ln\left(\vartheta d/r_0\right)}{\ln\left(\vartheta d_c/r_0\right)}\right)$$

$$\therefore \quad H = H_{0G}+k_G\left(\frac{\left(d-\delta\right)^3}{d^3}+\frac{d^3-\left(d-\delta\right)^3}{d^3}\frac{\ln\left(\vartheta\ \ d/r_0\right)}{\ln\left(\vartheta\ \ d_c/r_0\right)}\right)\ d^{-1/2}$$

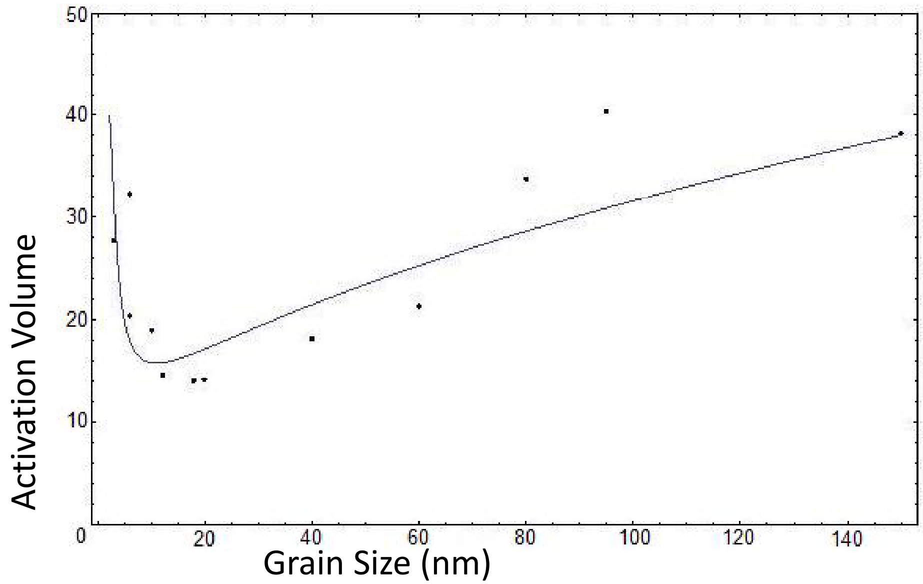


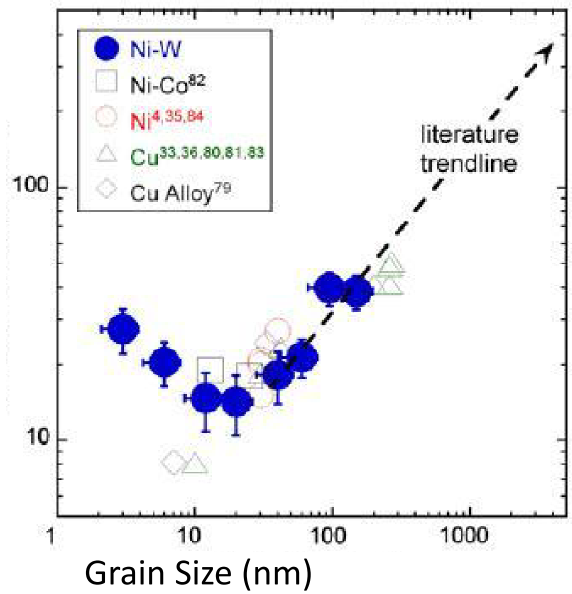
(a) & (b): nanocrystalline metals; (c) & (d): intermetallics

■ Activation Volume (υ)

- $$\upsilon = \sqrt{3}\, kT \frac{\partial \ln \dot{\varepsilon}}{\partial \sigma}$$
- ***Rule of Mixtures*** $$\frac{1}{\upsilon} = f \frac{1}{\upsilon_g} + (1-f)\frac{1}{\upsilon_{gb}}$$

$$f = (d-\delta)^3 / d^3 \quad ; \quad (1/\upsilon_g) = (1/\upsilon_g^0) + k_g d^{-1/2}$$





$$\upsilon_g^0 = 1000\, b^3, \quad \upsilon_{gb} = 30\, b^3, \quad \delta = 2\, nm, \quad k_g = 0.3\sqrt{nm}/b^3$$

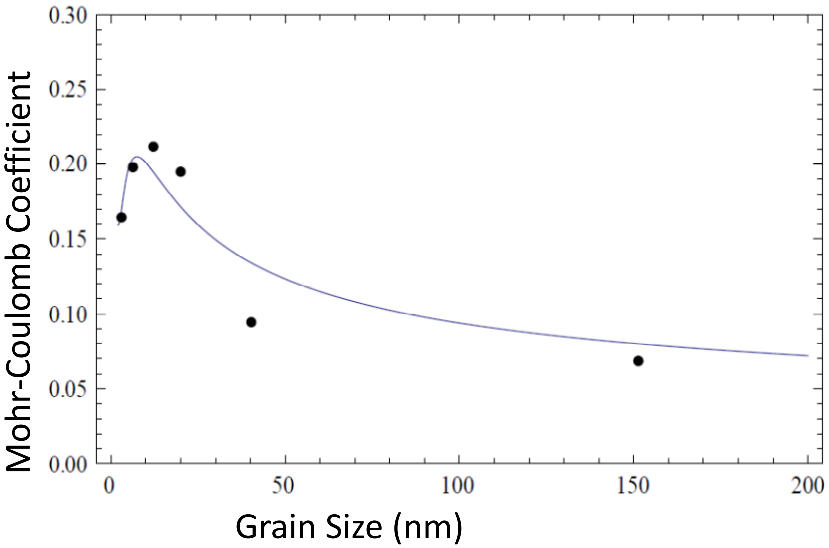
■ Pressure – Sensitivity Parameter (α)

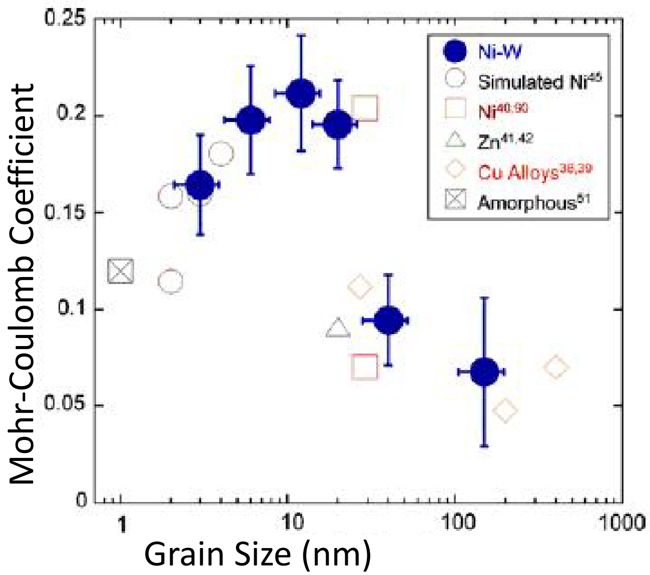
- $\sqrt{J} + \alpha p - \kappa = 0$

  Mohr-Coulomb Yield Condition used for the prediction of shear band Angle in Fe-10%Cu Nanopolycrystals

- ***Rule of Mixtures*** $\alpha = f\alpha_g + (1-f)\alpha_{gb}$

$$\alpha = \left[(d-\delta)^3 / d^3\right]\left(\alpha_g^0 + k_g d^{-1/2}\right) + \left\{1 - \left[(d-\delta)^3 / d^3\right]\right\}\alpha_{gb}$$





$$\alpha_g^0 = 0.02, \quad \alpha_{gb} = 0.16, \quad \delta = 2\,nm, \quad k_g = 0.7\sqrt{nm}$$

I. NANODIFFUSION

[Gradient Diffusion at the Nanoscale]

■ Double Diffusivity / Diffusion in Nanopolycrystals

$$\frac{\partial \rho_\alpha}{\partial t} + \mathrm{div}\mathbf{j}_\alpha = \mathrm{c}_\alpha \qquad \mathrm{div}\mathbf{T}_\alpha = \mathbf{f}_\alpha$$

$$\{\mathbf{T}_\alpha,\ \mathbf{f}_\alpha,\ \mathrm{c}_\alpha\} \longrightarrow \{\rho_\alpha, \mathbf{j}_\alpha, \ldots\};\ \ \alpha = 1,2$$

- ***Simplest Model***

$$\mathbf{T}_\alpha = -\pi_\alpha \rho_\alpha \mathbf{1} \quad ; \quad \mathbf{f}_\alpha = \alpha_\alpha \mathbf{j}_\alpha \quad ; \quad \mathrm{c}_\alpha = (-1)^\alpha [\kappa_1 \rho_1 - \kappa_2 \rho_2]$$

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

- ***Solution***

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

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

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

- ***Uncoupling / Higher-order Diffusion Equation***

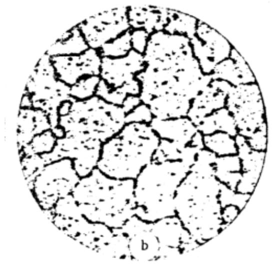
$$\frac{\partial\rho}{\partial t}+\tau\frac{\partial^2\rho}{\partial t^2}=D\nabla^2\rho+\bar{D}\frac{\partial}{\partial t}\nabla^2\rho-\mathrm{E}\nabla^4\rho$$

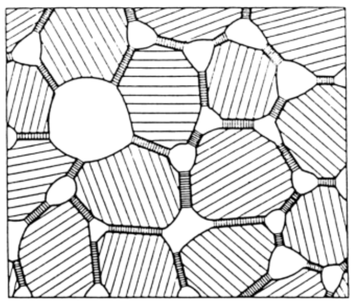
$$\tau=(\kappa_1+\kappa_2)^{-1}\ ,\ D=\tau(\kappa_1 D_2+\kappa_2 D_1)\ ,\ \bar{D}=\tau(D_1+D_2)\ ,\ \mathrm{E}=\tau D_1 D_2$$

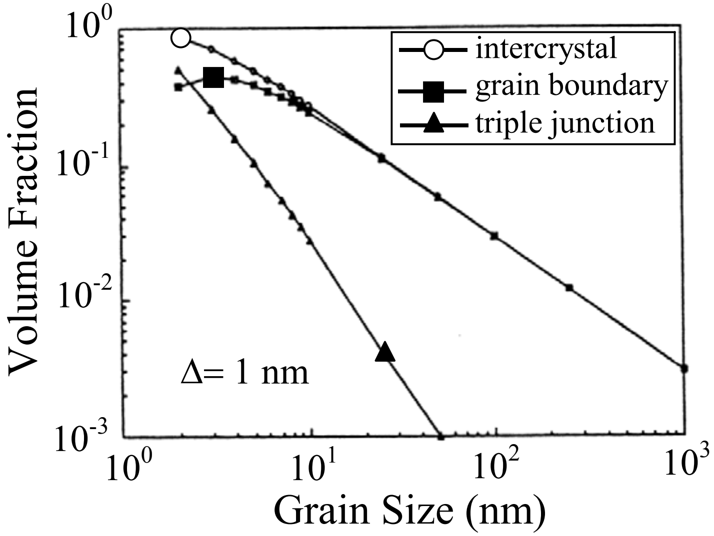
$$t\to\infty\Rightarrow\frac{\partial\rho}{\partial t}=D\nabla^2\rho\quad ;\quad D=D_{eff}=\frac{\kappa_2}{\kappa_1+\kappa_2}D_1+\frac{\kappa_1}{\kappa_1+\kappa_2}D_2$$
$$=f\,D_1+(1-f)D_2$$

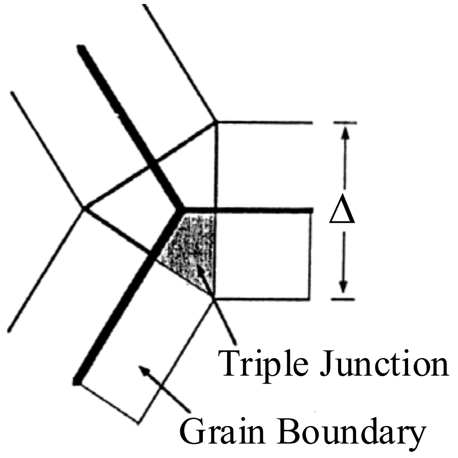
- ***Observations / Experiments***

- *Grain boundary space*



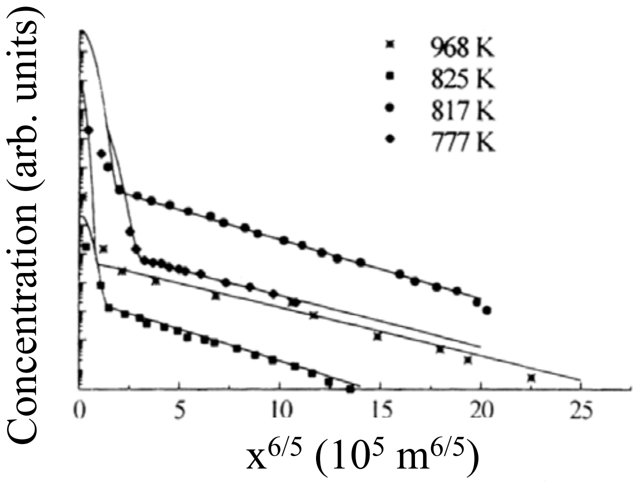




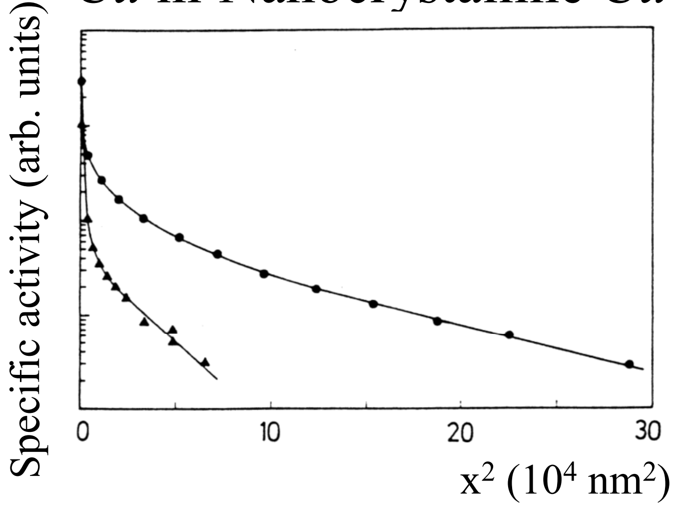


- *Diffusion Penetration Profiles*

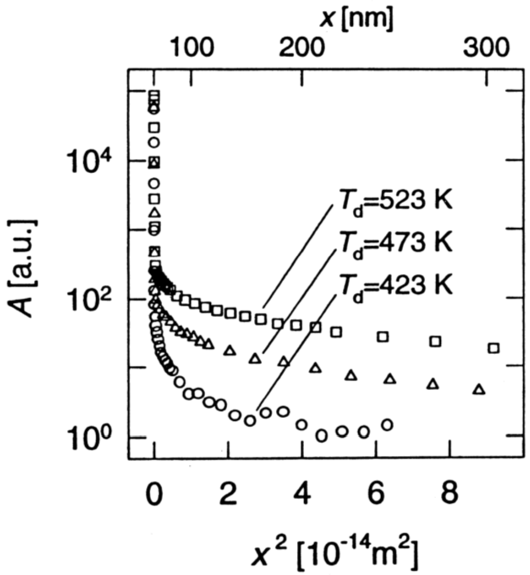
^{64}Cu in Polycrystalline Cu



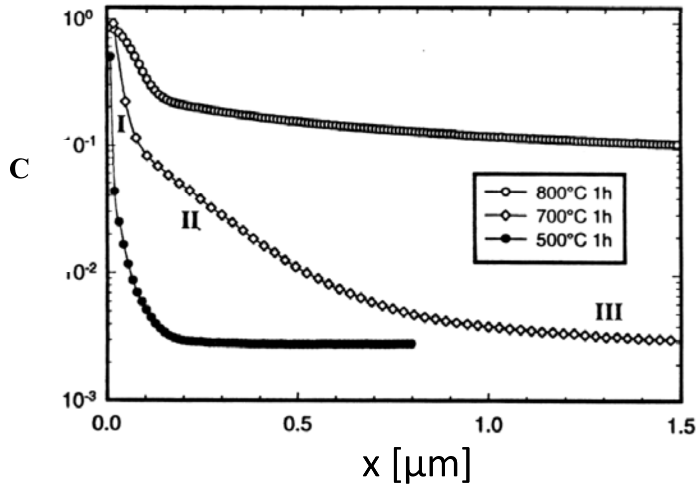
^{67}Cu in Nanocrystalline Cu



^{59}Fe in compacted $n-Pd$

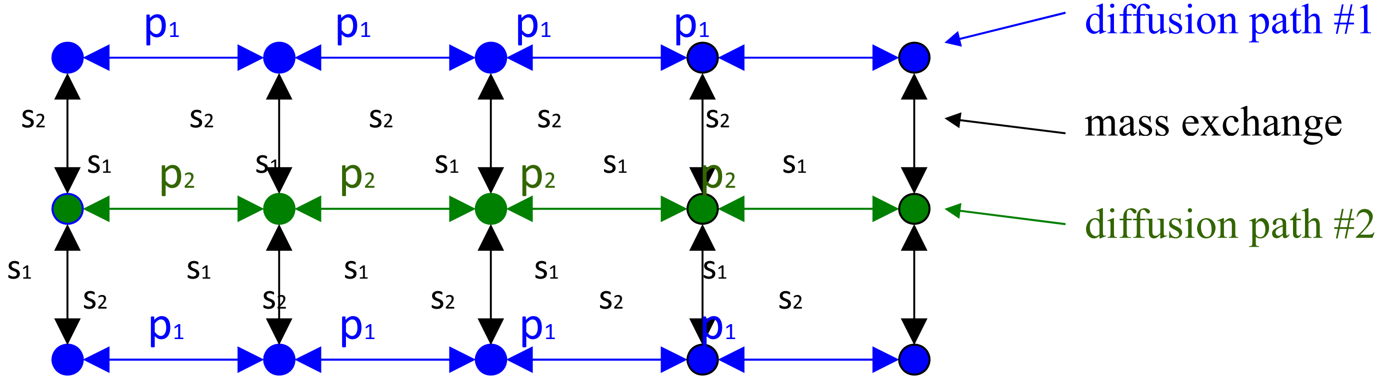


^{18}O in nano ZrO_2



▪ Random Walk Model

• *Random Walk on Graphs*



Graph: Two dimensional infinite grid

• Probabilities for jumps:

p_1 - diffusion path #1
p_2 - diffusion path #2
r_i - remain in position
s_2 - exchange #2 to #1
s_1 - exchange #1 to #2

$$\left.\right\} \begin{aligned} 2p_1 + 2s_1 + r_1 &= 1 \\ 2p_2 + 2s_2 + r_2 &= 1 \end{aligned}$$

• Assumptions:

Free particle (p_i=q_i);
Volume of fraction of paths #1 and #2 the same

- ***Discrete Version***

$$\left.\begin{array}{l}\#1:\ f(x,y,t+1)=p_1 f(x-1,y,t)+p_1 f(x+1,y,t)+s_2 f(x,y-1,t)+s_2 f(x,y+1,t)+r_1 f(x,y,t)\\ \#2:\ f(x,y,t+1)=p_2 f(x-1,y,t)+p_2 f(x+1,y,t)+s_1 f(x,y-1,t)+s_1 f(x,y+1,t)+r_2 f(x,y,t)\end{array}\right\}$$

- ***Continuous Version***

$$\frac{\partial\rho_1}{\partial t} = D_{11}\partial_{xx}\rho_1 + D_{12}\partial_{yy}\rho_2 - (\kappa_1\rho_1 - \kappa_2\rho_2), \quad \frac{\partial\rho_2}{\partial t} = D_{21}\partial_{yy}\rho_1 + D_{22}\partial_{xx}\rho_2 + (\kappa_1\rho_1 - \kappa_2\rho_2)$$

$$\left.\begin{array}{l} D_{11}=\dfrac{p_1}{\lambda_1}\ ,\ D_{12}=\dfrac{s_2}{\lambda_2}\ ,\ D_{21}=\dfrac{s_1}{\lambda_2}\ ,\ D_{22}=\dfrac{p_2}{\lambda_1} \\ \kappa_1=\dfrac{2s_1}{\Delta t}\ ,\ \kappa_2=\dfrac{2s_2}{\Delta t}\ ,\ \lim\limits_{\substack{\Delta x\to 0\\ \Delta t\to 0}}\dfrac{\Delta t}{(\Delta x)^2}=\lambda_1,\ \lim\limits_{\substack{\Delta y\to 0\\ \Delta t\to 0}}\dfrac{\Delta t}{(\Delta y)^2}=\lambda_2 \end{array}\right\}\Rightarrow$$

$$\begin{vmatrix}\kappa_1 & \kappa_2\\ D_{21} & D_{12}\end{vmatrix}=0\Rightarrow\kappa_1 D_{12}-\kappa_2 D_{21}=0$$

- When mass exchange much slower than diffusion i.e. $\lambda_2 >> \lambda_1 \rightarrow D_{12}=D_{21}=0$ i.e. cross effects negligible

- ***Special Case***
  - $\lambda_2 >> \lambda_1$; $s_1 = p_1$, $s_2 = p_2$
  - Discrete equations and continuous version in a similar way

$$\frac{\partial \rho_1}{\partial t} = \mathrm{D}_1 \partial_{xx} \rho_1 - (\kappa_1 \rho_1 - \kappa_2 \rho_2) \quad , \quad \frac{\partial \rho_2}{\partial t} = \mathrm{D}_2 \partial_{xx} \rho_2 + (\kappa_1 \rho_1 - \kappa_2 \rho_2)$$

  - Extra condition $\begin{vmatrix} D_1 & D_2 \\ \kappa_1 & \kappa_2 \end{vmatrix} = 0 \Rightarrow \kappa_2 D_1 - \kappa_1 D_2 = 0$

  - Diffusion of Co^{60} in polycrystal γ-Fe

$$D_1 \approx 4.34 \times 10^{-9}, D_2 \approx 1.36 \times 10^{-11}, \kappa_1 \approx 4 \times 10^{-4}, \kappa_2 \approx 4 \times 10^{-7}$$

$$\Rightarrow \kappa_2 D_1 - \kappa_1 D_2 \approx 10^{-15}$$

  - Diffusion of Ca^{2+} in MgO single crystal

$$D_1 \approx 7.64 \times 10^{-17}, D_2 \approx 6.65 \times 10^{-20}, \kappa_1 \approx 5 \times 10^{-3}, \kappa_2 \approx 1.5 \times 10^{-6}$$

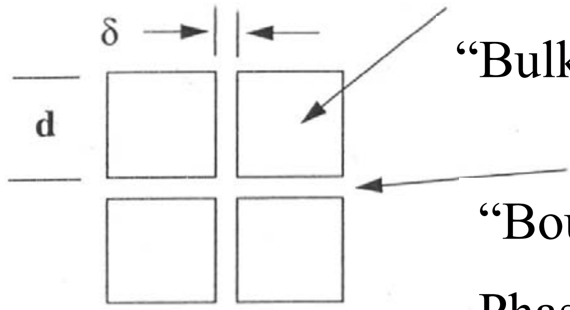
$$\Rightarrow \kappa_2 D_1 - \kappa_1 D_2 \approx 10^{-23}$$

II. NANOELASTICITY

[Gradient Elasticity at the Nanoscale]

■ Gradela: Gradient Elasticity for Nanopolycrystals

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



- ***Equilibrium***

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

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

- ***Elasticity for each phase***

Assume that each phase obeys Hooke's Law and that the interaction force is proportional to the difference of the individual displacements

$$\boldsymbol{\sigma}_k = \mathbf{L}_k \mathbf{u}_k, \quad k = 1,2; \quad \mathbf{f} = \alpha(\mathbf{u}_1 - \mathbf{u}_2)$$

$$\mathbf{L}_k = \lambda_k \mathbf{G} + \mu_k \hat{\nabla}; \quad \mathbf{G} = \mathbf{I}\, div \;; \quad \hat{\nabla} = \nabla + \nabla^T$$

Uncoupling $\Rightarrow$

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

- ***Gradela***

The above implies the following gradient-elasticity relation

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

i.e.

elasticity of nanopolycrystals depends on higher – order gradients in strain

- ***Ru-Aifantis Theorem***

$$u-c\nabla^2u=u_0$$

u … *Gradela Solution*

u_0 … *Classical Elasticity Solution*

■ Gradela Dislocation Nanomechanics

- ***Gradela:*** $$(1-c\nabla^2)\begin{bmatrix}\sigma_{ij}\\ \varepsilon_{ij}\end{bmatrix}=\begin{bmatrix}\sigma^0_{ij}\\ \varepsilon^0_{ij}\end{bmatrix}$$

- ***Screw Dislocation :***

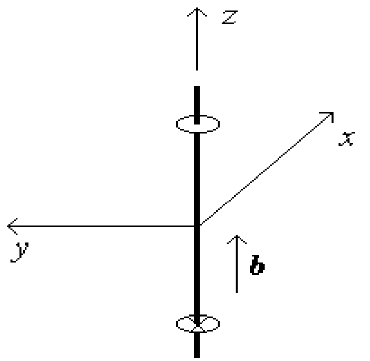
- Stress / Strain :

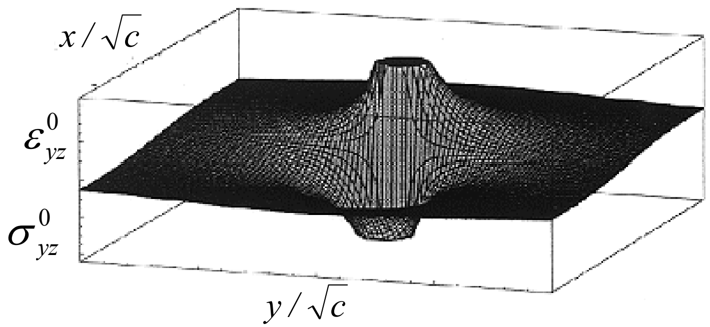
$$\begin{cases}\sigma_{xz}=\dfrac{\mu b_z}{4\pi}\left[-\dfrac{y}{r^2}+\dfrac{y}{r\sqrt{c}}K_1\left(r/\sqrt{c}\right)\right]; \qquad \sigma_{yz}=\ldots\\[2ex] \varepsilon_{xz}=\dfrac{b_z}{4\pi}\left[-\dfrac{y}{r^2}+\dfrac{y}{r\sqrt{c}}K_1\left(r/\sqrt{c}\right)\right]\ ; \qquad \varepsilon_{yz}=\ldots\end{cases}$$

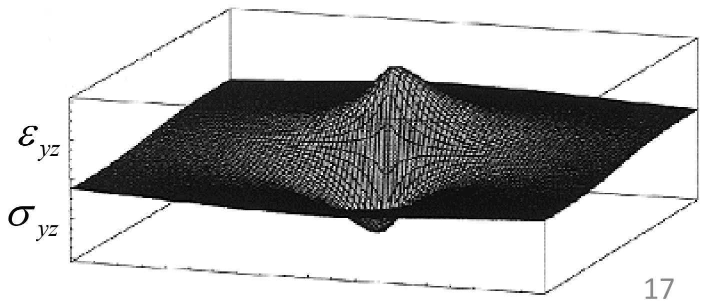
$$\therefore\quad \mathbf{r}\to 0 \quad\Rightarrow\quad \mathbf{K_1}\left(\mathbf{r}/\sqrt{\mathbf{c}}\right)\to\frac{\sqrt{\mathbf{c}}}{\mathbf{r}}\quad\Rightarrow\quad\left(\boldsymbol{\sigma}_{\mathbf{xz}},\boldsymbol{\varepsilon}_{\mathbf{yz}}\right)\to\mathbf{0}$$

- Self – energy : $$W_s=\frac{\mu b_z^2}{4\pi}\left\{\gamma^E+\ln\frac{R}{2\sqrt{c}}\right\}\quad\ldots\quad \gamma^E=0.577;\ \text{Euler constant}$$

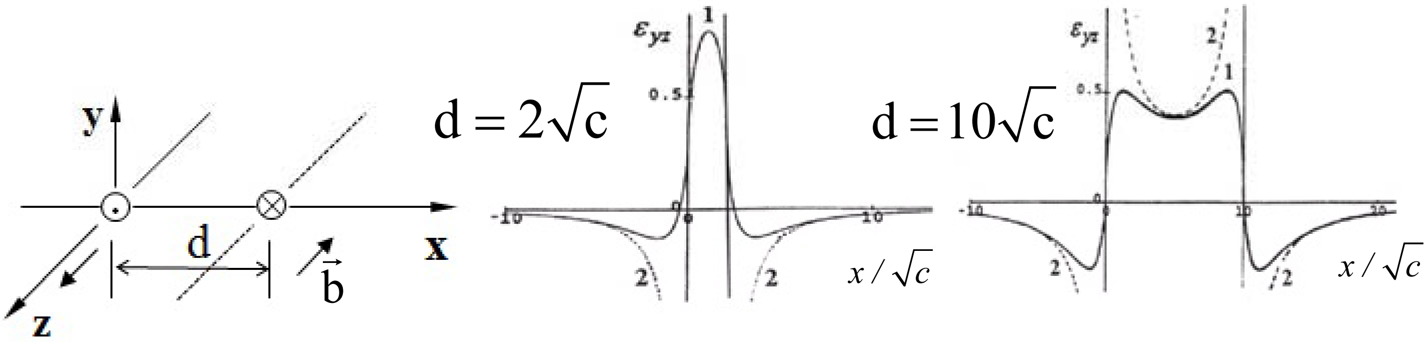
$$\therefore\quad \mathbf{r}\to 0\quad\Rightarrow\quad \textbf{no need for ad hoc dislocation core } \mathbf{r_0}$$





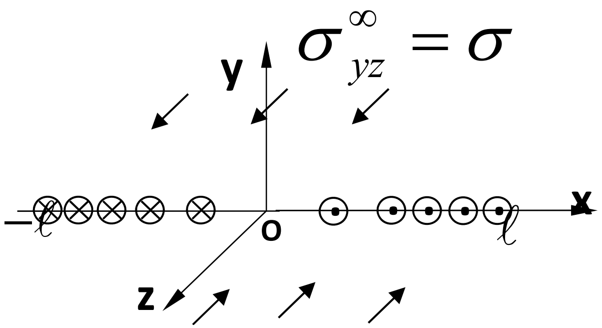


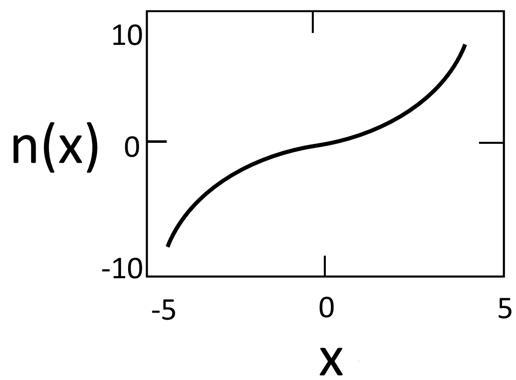
- ***Dislocation Dipoles [insight to nucleation / annihilation]***

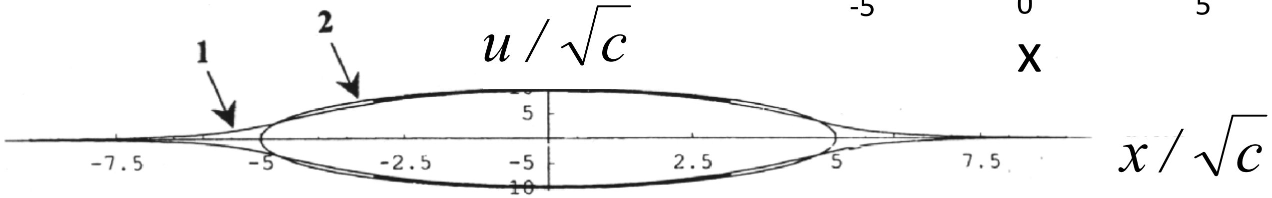


$\therefore \quad d \approx 10\sqrt{c}$.. *characteristic distance of "strong" interaction*

- ***Mode III Crack [continuous distribution of dislocations n(x)]***





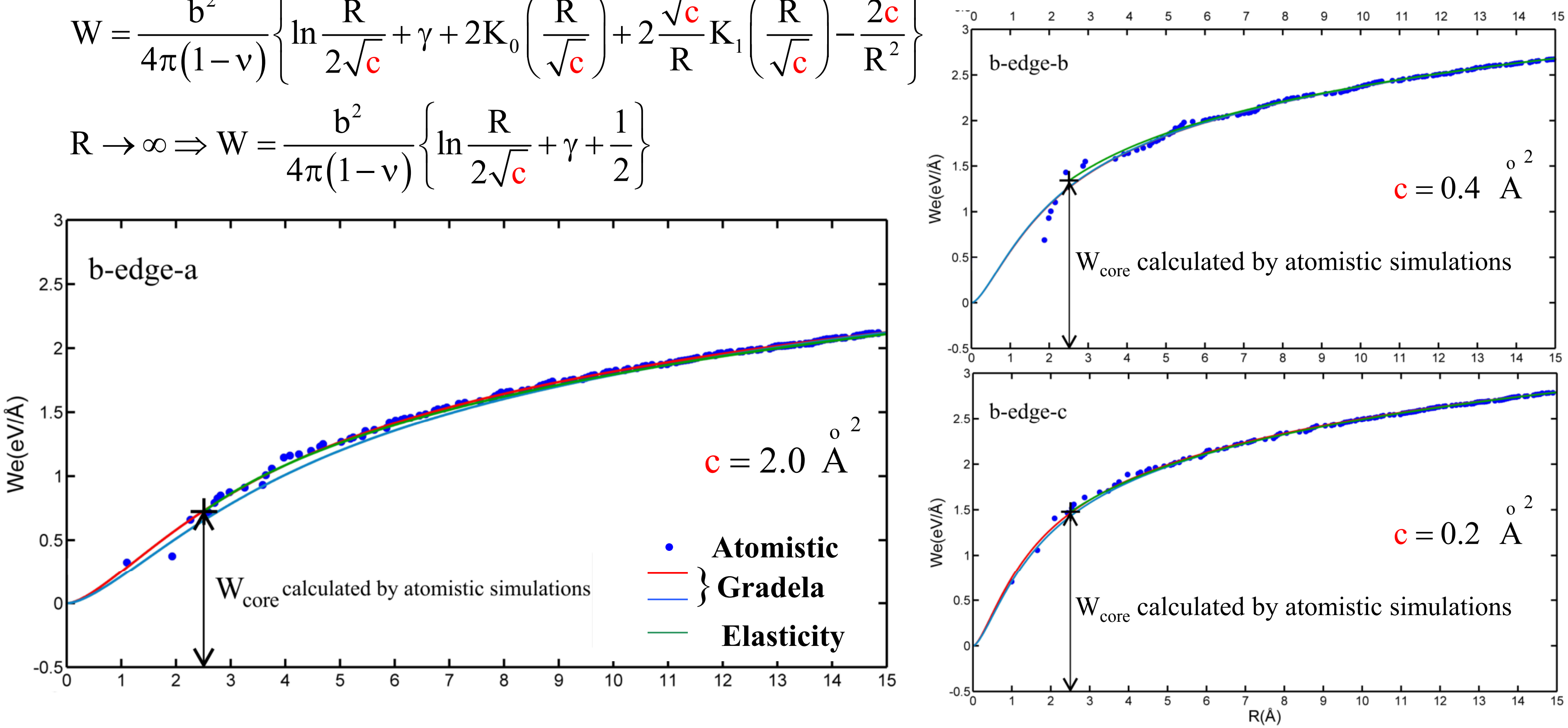


$\therefore$ *Barenblatt's "smooth closure" condition*

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

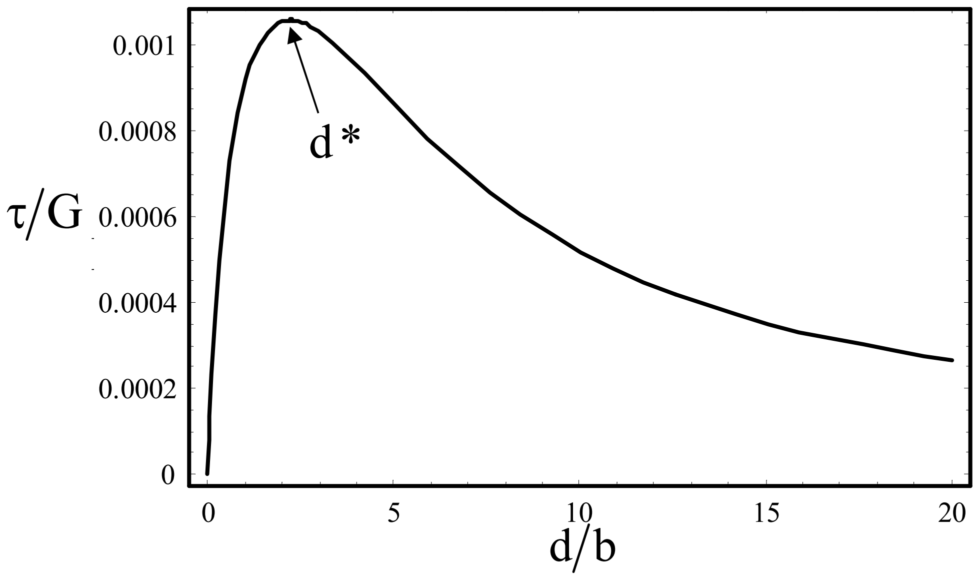
- *Image Force – Inverse Hall Petch Behavior*

  - *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

■ Gradela Crack Nanomechanics (Mode III)

• *Gradela: Mode III Cracking*

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

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

- ***Boundary Conditions***

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

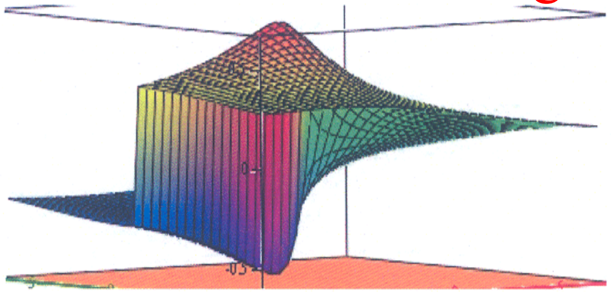
Vanishing of stresses at the origin: $\lim_{\mathbf{r}\to 0} \boldsymbol{\sigma}_{ij} = 0$

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

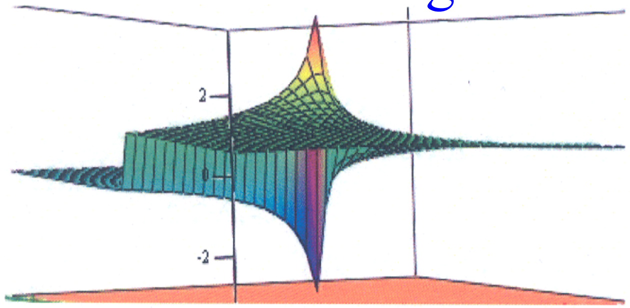
- ***Nonsingular stress distribution in Mode III***

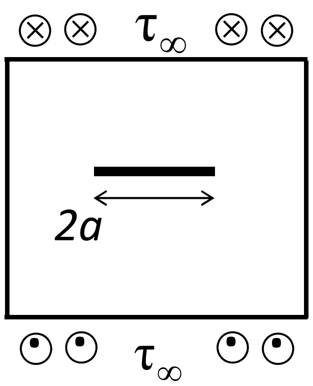
$$\sigma_{xz} = -\frac{K_{III}}{\sqrt{2\pi r}}\left[\sin\frac{\theta}{2}\left(1-\exp\left[-r/\sqrt{c}\right]\right)\right] \qquad \sigma_{yz} = \frac{K_{III}}{\sqrt{2\pi r}}\left[\cos\frac{\theta}{2}\left(1-\exp\left[-r/\sqrt{c}\right]\right)\right]$$

Gradient Stress non-singular

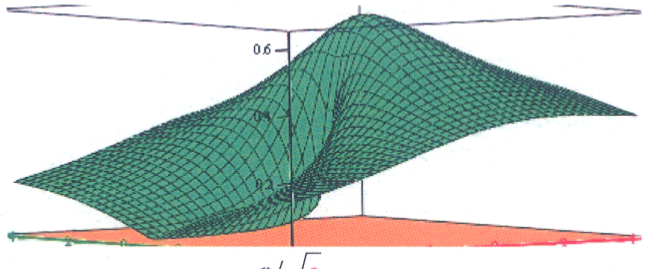


Classical Stress singular

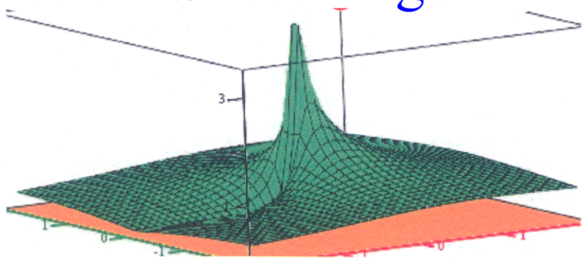




Gradient Stress non-singular



Classical Stress singular

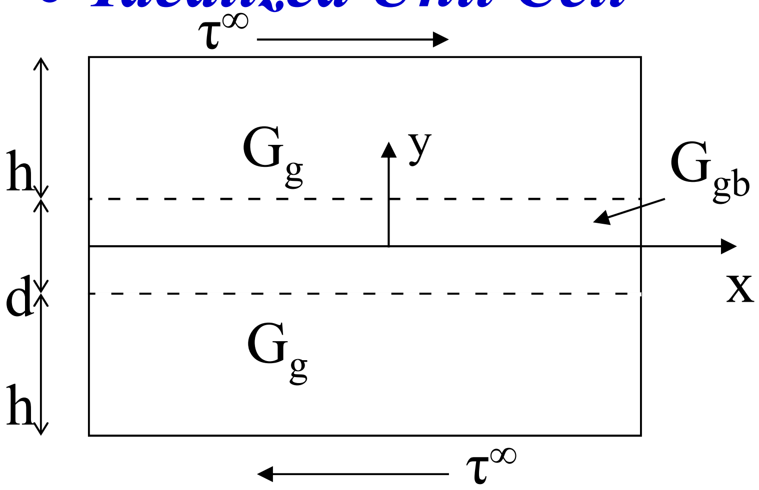


Note: $\left(1-e^{-r/\sqrt{c}}\right)\Big/\sqrt{r}$ max at $r \cong 1.25\sqrt{c}$

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

■ Effective Moduli of Nanopolycrystals

- ***Idealized Unit Cell***

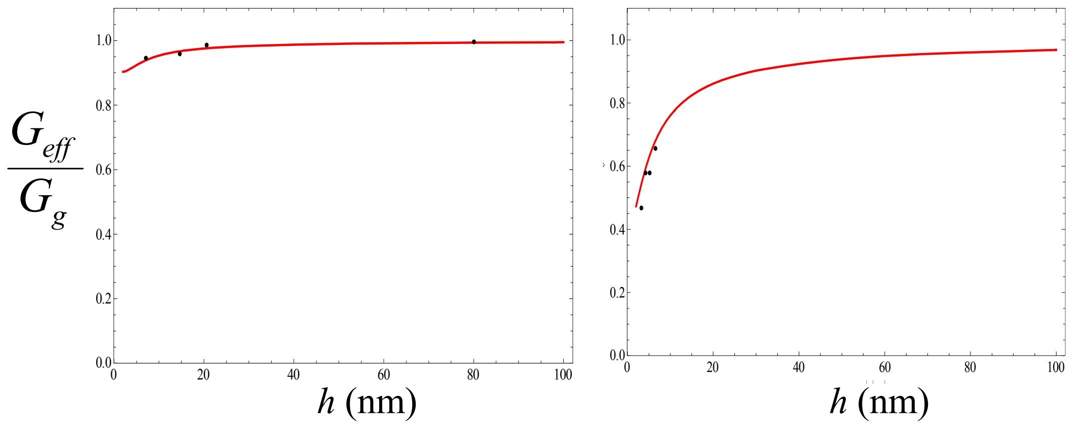


$$\tau = \kappa_i(\gamma) - c_i \nabla^2 \gamma = \tau^\infty$$

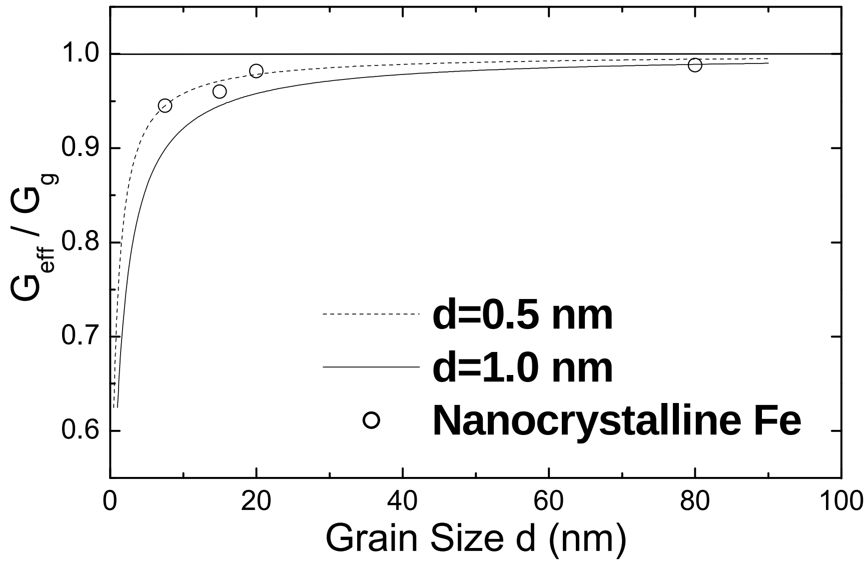
$$\text{Bc's}\ \begin{cases} \partial_y \gamma_{gb} = 0 & , \quad y=0 \\ \left.\begin{array}{l} \gamma_g = \gamma_{gb} \\ \partial_y \gamma_g = \partial_y \gamma_{gb} \end{array}\right\} & , \quad |y| = d/2 \\ \gamma_g = \tau^\infty / G & , \quad |y| = h + d/2 \end{cases}$$

- ***Average Strain/Effective Modulus***

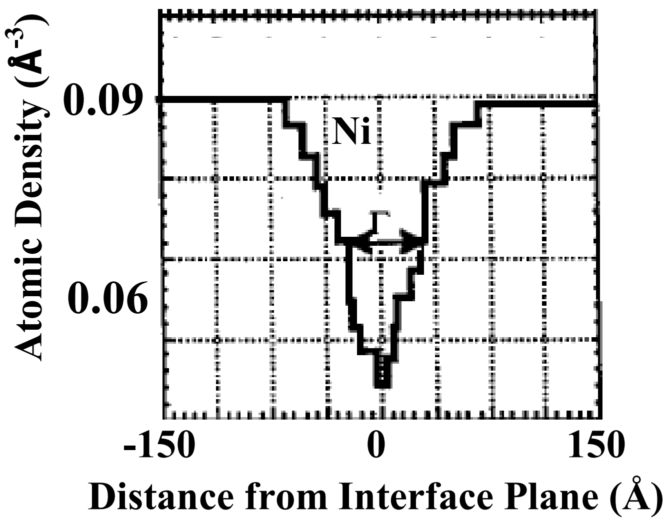
$$\bar{\gamma} = \frac{1}{(h+d/2)} \left(\int_0^{d/2} \gamma_{gb} dy + \int_0^{h+d/2} \gamma_g dy \right), \quad G_{eff} = \tau^\infty / \bar{\gamma}$$

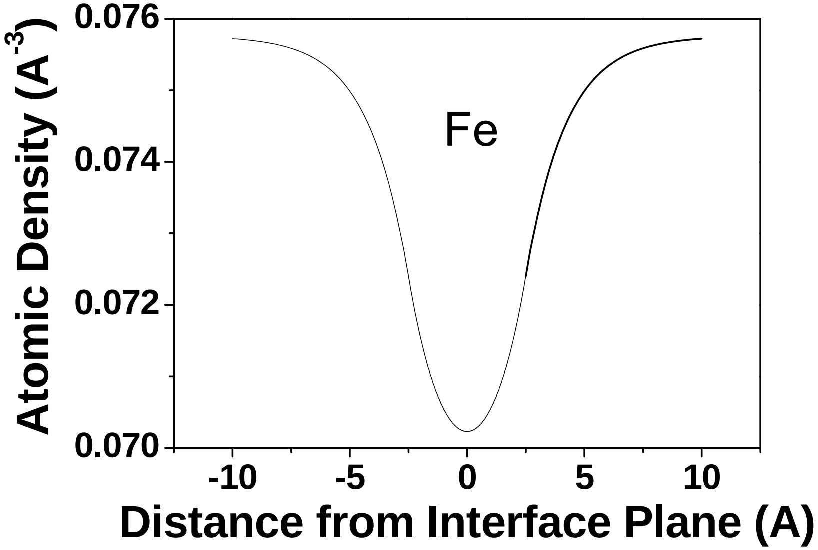


- ***Size Dependence / Experiments***



- ***Observations***





■ Gradela Dynamics:Euler–Bernoulli Beam(EBB)

- ***Standard Relations***

$$M = \int_A y\sigma dA$$

$A = 2\pi Rt$ ... area $\begin{bmatrix} R \ldots \text{radius} \\ h \ldots \text{thickness} \end{bmatrix}$

$I = \pi R^3 t$ ... moment of inertia

$c_e = \sqrt{E/\rho}$ ... elastic bar velocity

- ***Stress - strain relations - Internal Inertia***

$$\sigma = E\left(\varepsilon - l_s^2 \varepsilon_{,xx}\right) + \rho l_d^2 \ddot{\varepsilon}$$

l_s^2 ... static internal length

l_d^2 ... dynamic internal length

$$\Rightarrow M = -EI\left(u_{,xx} - l_s^2 u_{,xxxx}\right) - \rho I l_d^2 \ddot{u}_{,xx}$$

$$\therefore \rho A\ddot{u} = M_{,xx} = -EI(u_{,4x} - l_s^2 u_{,6x}) - \rho I l_d^2 \ddot{u}_{,4x}$$

- ***Wave Solution***

$$u(x,t) = \hat{u}\exp\left[2k(x - ct)\right]$$

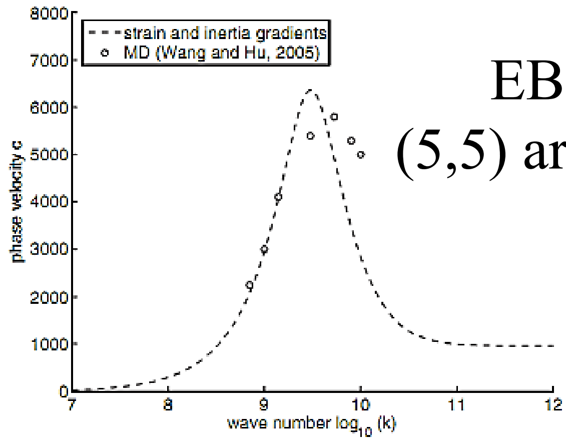
- ***Comparison with MD***

$\hat{u}$ amplitude

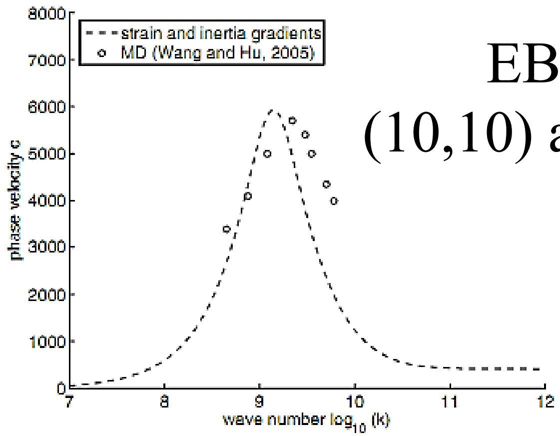
k wave number

c phase velocity

$$\frac{c}{c_e} = \frac{Ik^2}{A}\frac{1 + l_s^2 k^2}{1 + \frac{Ik^2}{A} l_d^2 k^2}$$



EBB theory
(5,5) armchair CNT



EBB theory
(10,10) armchair CNT

III. NANOPLASTICITY
[Gradient Plasticity at the Nanoscale]

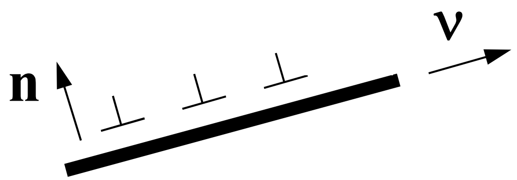
■ Motivation from Dislocation Slip

- ***Momentum Balance for Dislocated State***

$$\mathrm{div}\mathbf{T}^{\mathbf{D}} = \hat{\mathbf{f}}\ ; \quad \mathbf{T}^{\mathbf{D}} = \mathbf{S} - \mathbf{T}^{\mathrm{L}}\ ; \quad \mathrm{div}\mathbf{S} = 0$$

$\mathbf{T}^{\mathbf{D}}$...dislocation stress; $\hat{\mathbf{f}}$...dislocation-lattice interaction force

- ***Yield Condition:*** $f = \hat{\mathbf{f}} \cdot \boldsymbol{\nu} = 0; \quad \hat{\mathbf{f}} = \left(\hat{\alpha} + \hat{\beta} j - \hat{\gamma}\tau^{\mathrm{L}}\right)\boldsymbol{\nu}, \quad \tau^{\mathrm{L}} = \mathbf{T}^{\mathrm{L}} \cdot \mathbf{M}$



$$\mathbf{M} = \left(\boldsymbol{\nu} \otimes \mathbf{n}\right)_s, \quad \mathbf{D}^{\mathrm{p}} = \dot{\gamma}^{\mathrm{p}}\mathbf{M}; \quad \mathbf{T}^{\mathrm{D}} = t_m\mathbf{M} + t_n\mathbf{N}$$

$$\max\left\{\mathrm{tr}\mathbf{T}^{\mathrm{L}}\mathbf{D}^{\mathbf{p}}\right\};\ \mathrm{tr}\mathbf{M} = 0,\ \mathrm{tr}\mathbf{M}^2 = 1/2 \quad \Rightarrow \quad \mathbf{D}^{\mathbf{p}} = \frac{\dot{\gamma}^{\mathrm{p}}}{2\sqrt{J}}\mathbf{T}^{\mathrm{L}'}; \quad J = \frac{1}{2}\mathrm{tr}\left(\mathbf{T}^{\mathrm{L}'}\mathbf{T}^{\mathrm{L}'}\right)$$

$$\therefore \quad \tau = \sqrt{J} = \kappa\left(\gamma^{\mathrm{p}}\right)$$

- ***Inhomogeneous Back Stress:*** $\boldsymbol{T}^{D} = \boldsymbol{\alpha} + \boldsymbol{T}^{inh}$
  - $\boldsymbol{\alpha}$ *= homogeneous back stress … as before*

$$\mathbf{T}^{\mathbf{inh}} = \hat{\mathbf{g}}\left(\mathbf{n}, \boldsymbol{\nu}, \nabla\gamma^{p}\right)$$

$$\approx \left[\mathbf{n} \otimes \nabla\gamma^{p} + \left(\nabla\gamma^{p}\right) \otimes \mathbf{n}\right] + \left[\boldsymbol{\nu} \otimes \nabla\gamma^{p} + \left(\nabla\gamma^{p}\right) \otimes \boldsymbol{\nu}\right]$$

$$\mathrm{div}\mathbf{T}^{\mathbf{inh}} \approx \left(\mathbf{n} + \boldsymbol{\nu}\right)\nabla^{2}\gamma^{p} + \left(\mathbf{grad}^{2}\gamma^{p}\right)\left(\mathbf{n} + \boldsymbol{\nu}\right)$$

$$\left(\mathrm{div}\mathbf{T}^{\mathbf{inh}}\right) \cdot \boldsymbol{\nu} \approx \nabla^{2}\gamma^{p} + \gamma^{p}_{,ij}\left(\nu_{i}\nu_{j} + \nu_{i}n_{j}\right)$$

  - *Integrate over all possible orientations of* $(\boldsymbol{n}, \boldsymbol{\nu})$

$$\left(\mathrm{div}\mathbf{T}^{\mathbf{inh}}\right) \cdot \boldsymbol{\nu} \rightarrow \nabla^{2}\gamma^{p}$$

$$\therefore \quad \tau = \kappa\left(\gamma^{p}\right) - c\nabla^{2}\gamma^{p}$$

- ***Same Procedure for Nanopolycrystals***
  - *Representative slip plane → Representative planar GB*

■ Motivation from Averaging

- ***Self - Consistent Approximation***

- Simple Shear

$$\tau = \bar{\tau} - \beta \Delta \gamma$$

$$\bar{\tau} = \kappa(\bar{\gamma}) \, , \, \beta = \alpha\mu\{1 - 2S_{1212}\} \quad , \quad \Delta\gamma = \gamma - \bar{\gamma}$$

$$\bar{\gamma} = \frac{1}{V}\int_V \gamma(\boldsymbol{x}+\boldsymbol{r})dV \quad , \qquad V = \frac{4}{3}\pi R^3 \qquad \Rightarrow$$

$$\gamma(\boldsymbol{x}+\boldsymbol{r}) = \gamma(\boldsymbol{x}) + \nabla\gamma\cdot\boldsymbol{r} + \frac{1}{2!}\nabla^{(2)}\gamma\cdot\boldsymbol{r}\otimes\boldsymbol{r} + \ldots; \int_V \nabla^{2n+1}\gamma\cdot\boldsymbol{r}^{2n+1}dV = 0$$

$$\bar{\gamma} \approx \gamma + \frac{R^2}{10}\nabla^2\gamma \quad , \qquad R = d/2$$

$$\tau = \kappa(\gamma) - \frac{R^2}{10}(\beta + h)\nabla^2\gamma \quad ; \qquad \left\{ \beta = \alpha\mu\frac{7-5\nu}{15(1-\nu)} \right.$$

$$h = d\bar{\tau}/d\bar{\gamma}$$

$$\therefore \quad c = \frac{R^2}{10}(\beta + h) \qquad \Rightarrow \qquad c = Cd^2$$

- *Various Models for α*

- Lin 1954 $$\alpha = 1/(1 - S_{1212})$$

- Kroner (1958) / Budiansky – Wu (1962) $$\alpha = 1$$

- Berveiller – Zaoui 1979
  (Secant Model) $$\alpha = \frac{1}{1 + (\mu / 2H)}, \; H = \frac{\bar{\tau}}{\bar{\gamma}}$$

- Hill (1965) / Hutchinson (1970)
  (Tangent Model) $$\alpha = \frac{h(7 - 5\nu')}{\{6\mu(4 - 5\nu') + 15h(1 - \nu')\}(1 - 2S_{1212})}$$

$$\nu' = \frac{\nu h + \mu(1 + \nu)}{h + 2\mu(1 + \nu)}; \; h = \frac{d\bar{\tau}}{d\bar{\gamma}}$$

■ Motivation from Internal Variable Theory

- ***Adiabatic Approximation (Defect Kinetics)***

$$\tau = \hat{\kappa}(\gamma, \alpha) \quad ; \quad \dot{\alpha} = D\partial_{xx}^2\alpha + \hat{g}(\gamma, \alpha)$$

$$\begin{cases} \tau = \hat{\kappa}(\gamma) - \lambda\alpha \\ \dot{\alpha} = D\alpha_{xx} + \Lambda\gamma - M\alpha \end{cases} ; \quad \{\lambda, \Lambda, M\} = \text{constants}$$

$$\dot{\alpha}_q = -Dq^2\alpha_q + \Lambda\gamma_q - M\alpha_q \;\; ; \;\; \dot{\alpha}_q \approx 0 \, , \;\; \frac{Dq^2}{M} << 1 \;\; \Rightarrow \;\; \alpha \approx \frac{\Lambda}{M}\gamma - \frac{\Lambda D}{M^2}\gamma_{xx}$$

$$\therefore \quad \tau = \kappa(\gamma) - c\gamma_{xx} \quad ; \quad \begin{cases} \kappa(\gamma) \equiv \hat{\kappa}(\gamma) - \dfrac{\lambda\Lambda}{M}\gamma \\ c \equiv \lambda\dfrac{\Lambda D}{M^2} \end{cases}$$

- ***Note:*** $\tau = \kappa(\gamma) - \mu(\gamma)\alpha \; ; \; \dot{\alpha} + D\alpha_{xx} = \lambda(\gamma)\alpha$

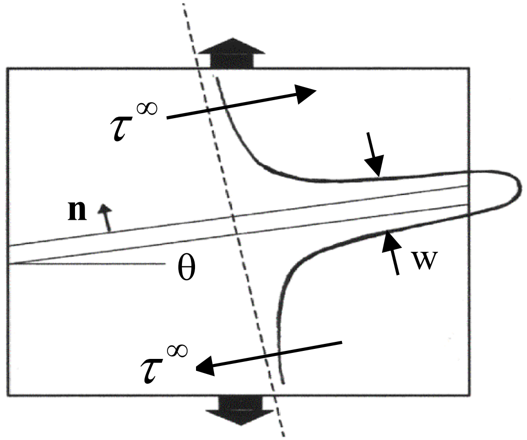
$$\therefore \quad \tau = \kappa(\gamma) - c(\gamma)\gamma_{xx} - c^*(\gamma)\gamma_x^2$$

■ Implications to Localization of Plastic Flow
[Shear Bands & Necks]

- ***Constitutive Equation***

$$\mathbf{S}' = -p\mathbf{1} + 2\mu\mathbf{D} \quad ;$$

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

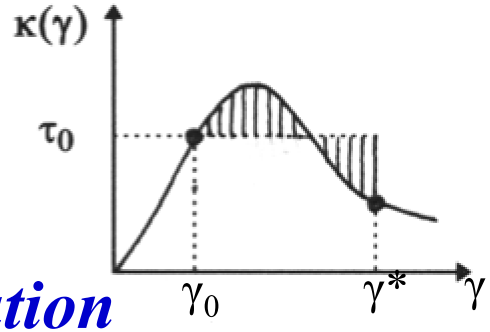


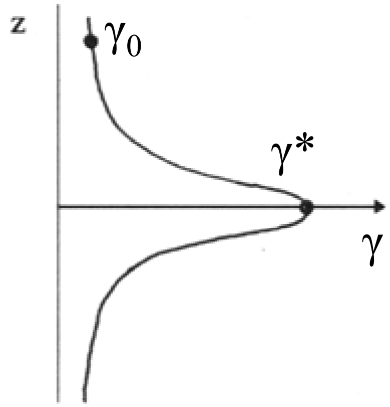
- ***Linear Stability / SB Orientation***

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

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

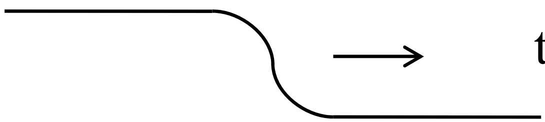
$$c\gamma_{zz} = \kappa(\gamma) - \tau_0$$





- ***Necks/Front Propagation***

Same Procedure

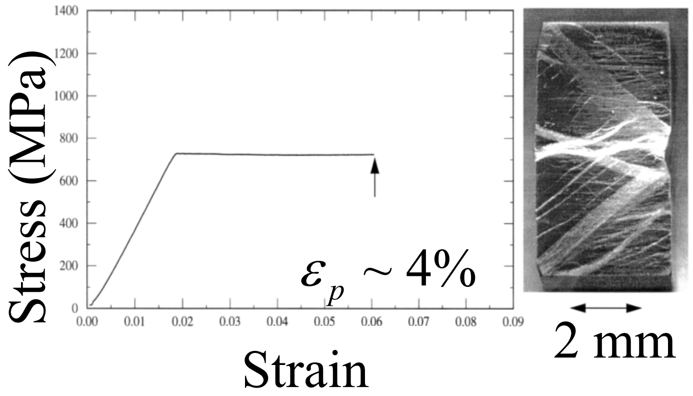


$\longrightarrow$ transitions

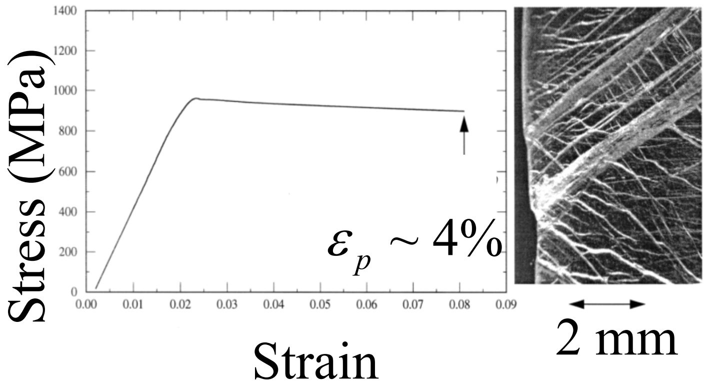
■ Multiple Shear Banding

- Compression of Bulk Nanostructured Fe – 10% Cu Polycrystals

d ~1370 nm, σ_y ~750 MPa
angle ~ 49^0



d ~540 nm, σ_y ~960 MPa
angle ~ 49^0



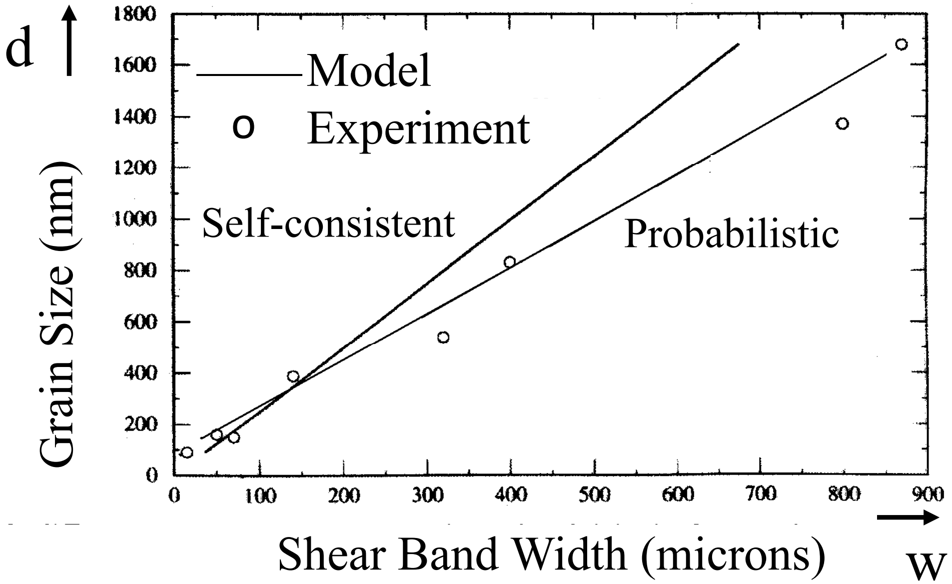
- Shear band width analysis

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

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

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

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



■ Front Propagation in a Disordered Field

- ***1-D Gradient Model***

$$\sigma = \kappa(\varepsilon) - c\frac{\partial^2 \varepsilon}{\partial x^2} \qquad \partial\sigma/\partial x = 0 \Rightarrow \sigma = \sigma_0$$

$$\therefore \quad \sigma_0 = \kappa(\varepsilon) - c\frac{\partial^2 \varepsilon}{\partial x^2}$$

- ***Front Propagation***
  - Transition-type solution
  - Fronts propagate only when $\sigma_0 = \sigma_p$ (Maxwell stress)

- ***Introduction of Disorder/Perturbations***

$$\varepsilon \to \varepsilon + \delta\,\varepsilon_1; \qquad \sigma_0 \to \sigma_0 + \delta\,\sigma_1$$

Fluctuating strength: $\kappa(\varepsilon) \to \kappa(\varepsilon) + \delta f(\varepsilon, x)$; δ "small" random parameter

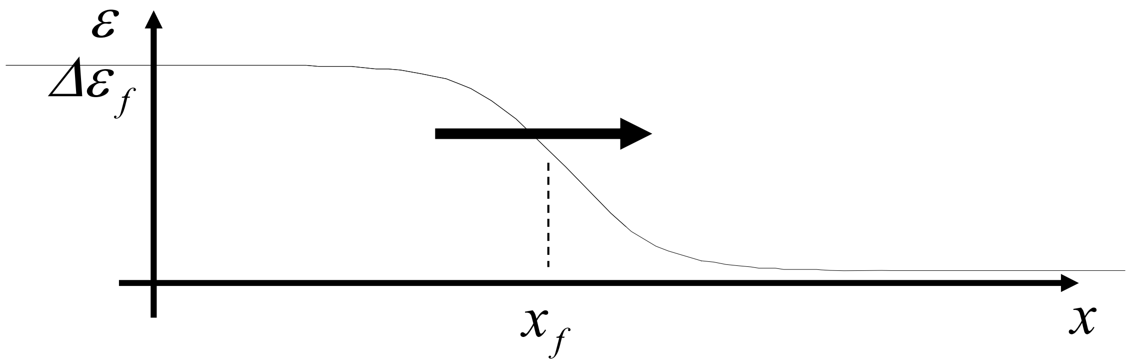
$$\therefore \quad \sigma_0 = \kappa(\varepsilon) + \delta f(\varepsilon, x) - c\frac{\partial^2 \varepsilon}{\partial x^2} \qquad (c \sim 1)$$

BC's: $\varepsilon_{,x}(\pm\infty)=0, \quad \varepsilon(\infty)=\varepsilon_{\infty}=0, \quad \varepsilon(-\infty)=\varepsilon_{-\infty}=\Delta\varepsilon_f>0$

$$\frac{\varepsilon_{,x}^2}{2}+\sigma_0\,\varepsilon-V(\varepsilon)-\delta\int_{-\infty}^{\infty} f(\varepsilon,x')\,\varepsilon_{,x'}dx'=0 \Rightarrow \left(\sigma_0\to\sigma_0+\delta\,\sigma_1\right)\Rightarrow$$

$$\Rightarrow\begin{cases}\dfrac{\varepsilon_{,x}^2}{2}+\sigma_0\,\varepsilon-V(\varepsilon)=0; \qquad V(\varepsilon)=\displaystyle\int_{-\infty}^{\infty}\kappa(\varepsilon)\varepsilon_{,x}dx \\[2ex] \delta\,\sigma_1=\dfrac{\delta}{\Delta\varepsilon_f}\displaystyle\int_{-\infty}^{\infty} f(\varepsilon,x)\,\varepsilon_{,x'}dx'\end{cases}$$

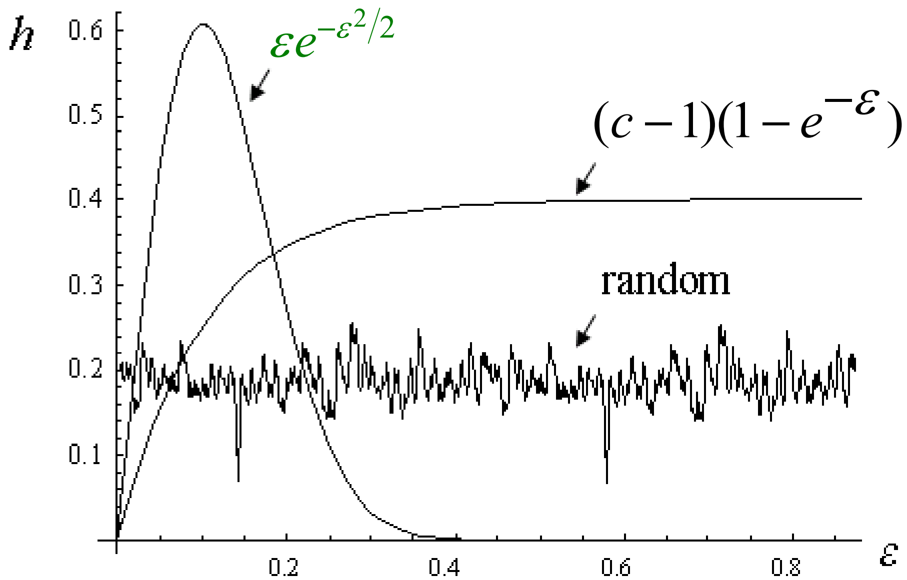
– *Front "locus" shifts along specimen* $\varepsilon=\varepsilon(x-x_f)$



- ***Statistical Properties of Stress Perturbations***
  - Assume short-range correlated:

$$f(\varepsilon,x) = h(\varepsilon)\,g(x); \quad \langle g(x)\,g(x')\rangle = \xi\delta(x-x')$$

$$\langle \delta\sigma_1^2 \rangle = \xi \frac{\delta^2}{(\Delta\varepsilon_f)^2} \int_{-\infty}^{\infty} h^2(\varepsilon)\,\varepsilon_{,x}\,dx \qquad \xi = \ell_{corr} \quad (\sim 1)$$



- ***Implementation***

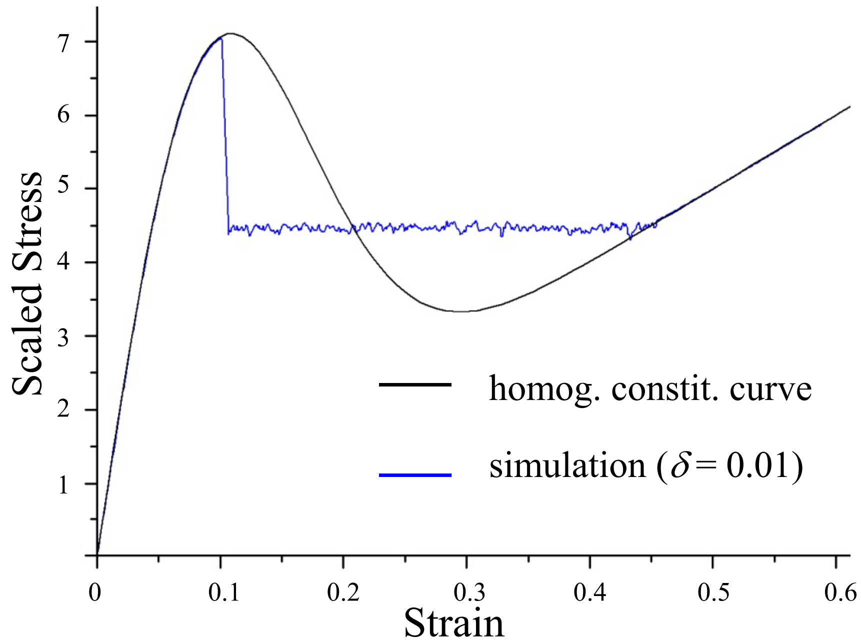
$$\kappa(\varepsilon) = \varepsilon\, e^{-\varepsilon^2/2} + k\varepsilon\,; \qquad\qquad k = \text{const.} \;\ldots\;\; \text{linear hardening}$$

$$V(\varepsilon) = e^{-\varepsilon^2/2} - \frac{k}{2}\varepsilon^2$$

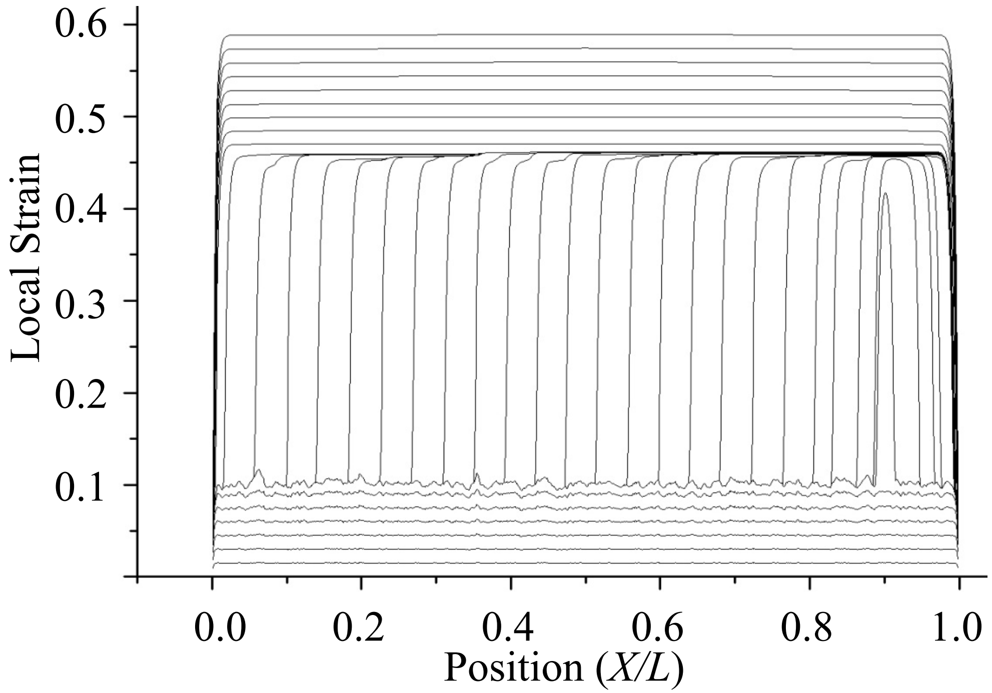
$$f(\varepsilon, x) = \varepsilon\, e^{-\varepsilon^2/2}\, g(x)$$

$$x - x_0 = \int_{\varepsilon_{-\infty}}^{\varepsilon} \frac{d\varepsilon}{\sqrt{-2\left[e^{-\varepsilon^2/2} - \frac{k}{2}\varepsilon^2 + \sigma_0\left(\varepsilon - \varepsilon_{-\infty}\right)\right] - V\left(\varepsilon - \varepsilon_{-\infty}\right)}}$$

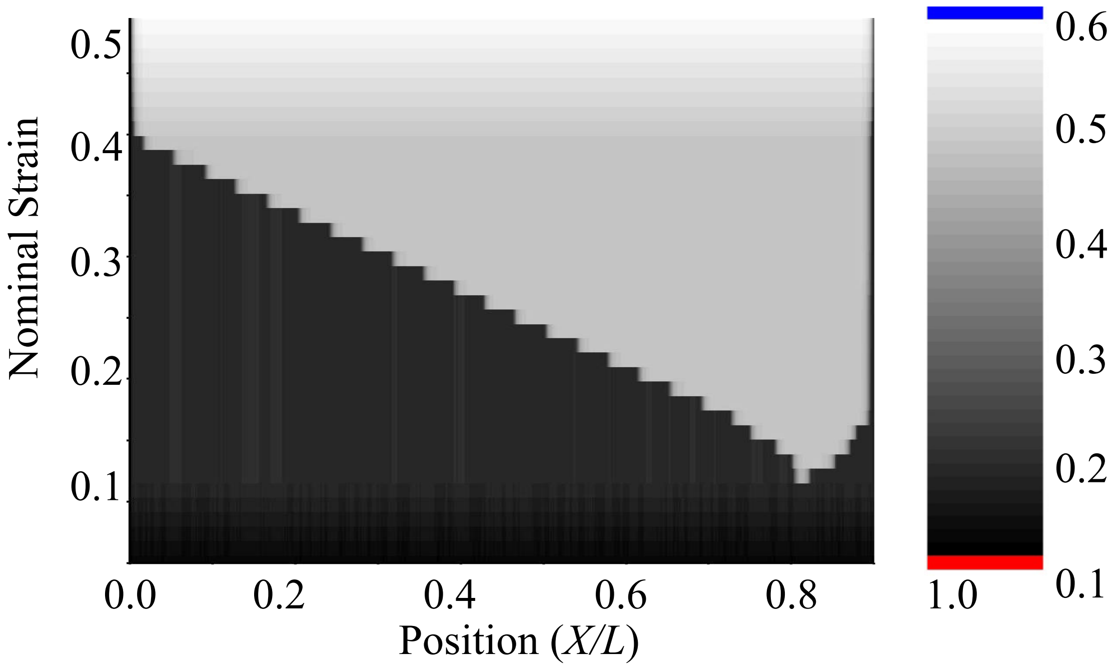
$$\left\langle \delta\sigma_1^2 \right\rangle = \xi \frac{\delta^2}{\left(\Delta\varepsilon_f\right)^2} \int_{\varepsilon_{-\infty}}^{\varepsilon_{\infty}} \left(-2\left[e^{-\varepsilon^2/2} - \frac{k}{2}\varepsilon^2 + \sigma_0\varepsilon - V\left(\varepsilon_\infty\right)\right]\right) \varepsilon^2\, e^{-\varepsilon^2}\, d\varepsilon$$



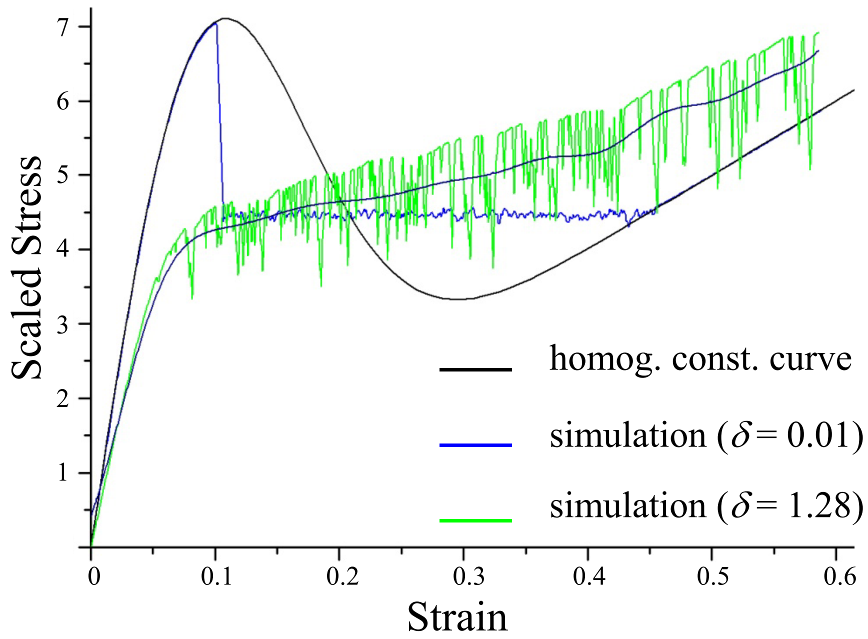
Scaled Stress
Strain
homog. constit. curve
simulation (δ = 0.01)

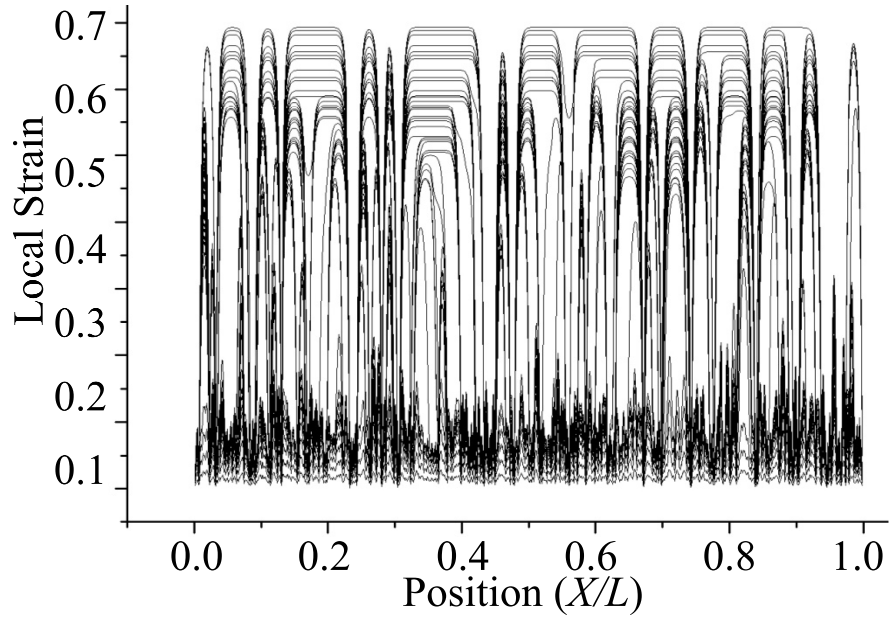


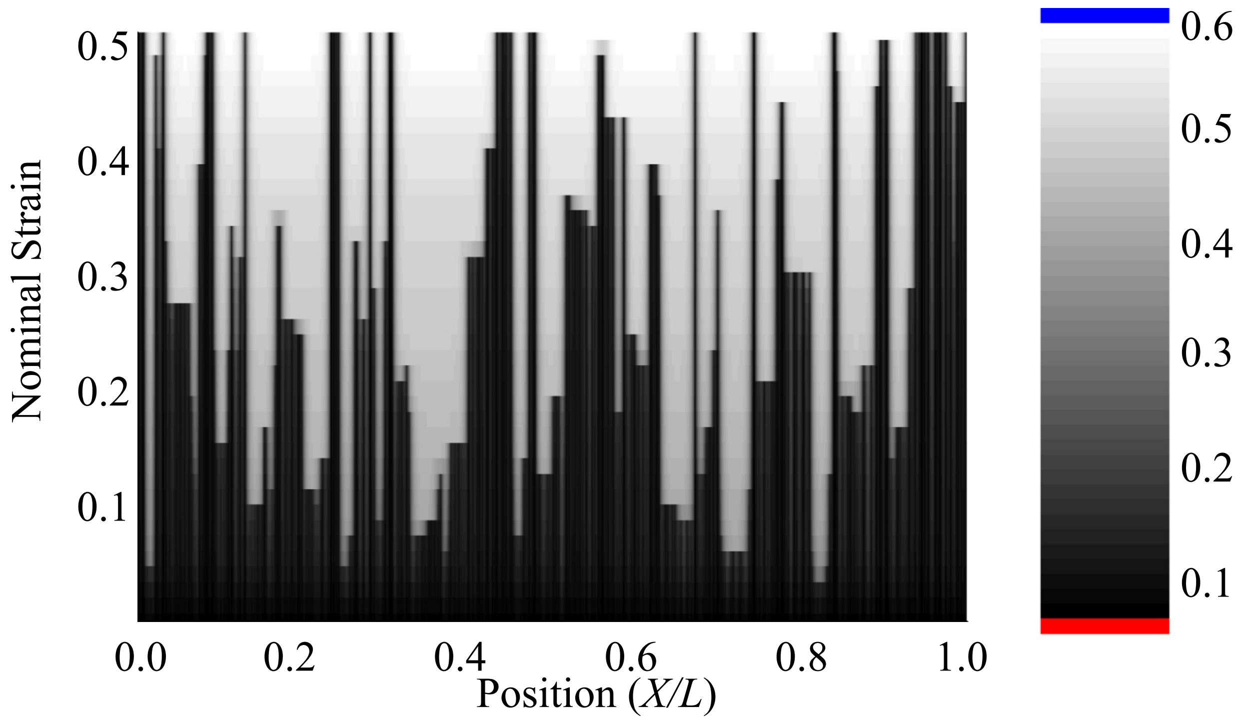
Local Strain
Position (X/L)



Nominal Strain
Position (X/L)
1.0


Scaled Stress
Strain
homog. const. curve
simulation (δ = 0.01)
simulation (δ = 1.28)


Local Strain
Position (X/L)


Nominal Strain
Position (X/L)

■ Multiple Shear Banding in UFG Polycrystals

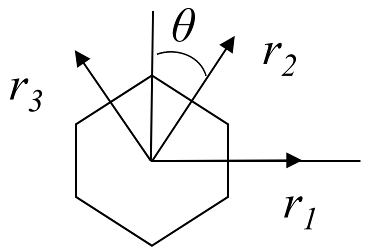
- Voronoi tessellation of 60×20 hexagonal regularly distributed cells

- 2-D Gradient model

$$\sigma_0 = \kappa(\varepsilon) - c\left[\frac{\partial^2 \varepsilon}{\partial x^2} + \frac{\partial^2 \varepsilon}{\partial y^2}\right] ; \qquad \kappa(\varepsilon) = E\,\varepsilon\, exp\left[-\varepsilon^2/\alpha\right] + k\varepsilon$$

- 2-D Stochasticity-enhanced Gradient model

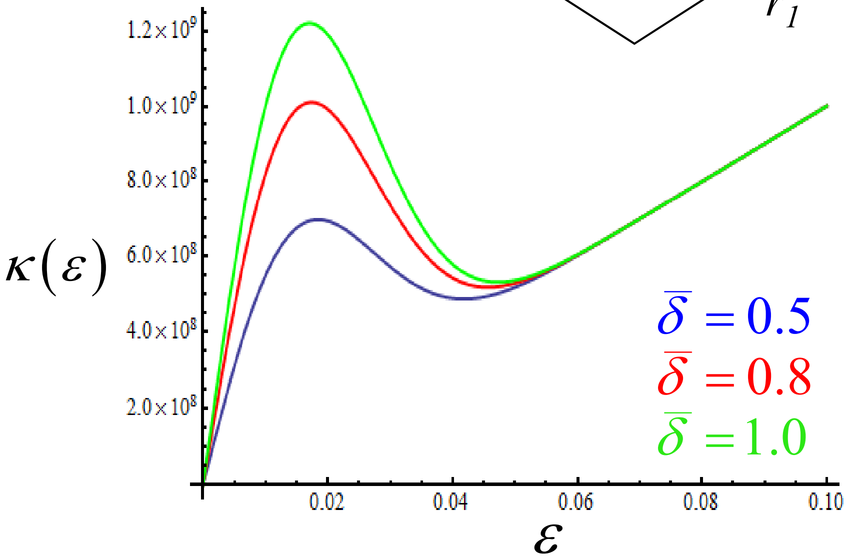
$$\sigma_0 = \kappa(\varepsilon) - c\left[\cos\theta_1 \frac{\partial^2 \varepsilon}{\partial r_1^2} + \cos\theta_2 \frac{\partial^2 \varepsilon}{\partial r_2^2} + \cos\theta_3 \frac{\partial^2 \varepsilon}{\partial r_3^2}\right]$$



Randomness in $\kappa(\varepsilon)$

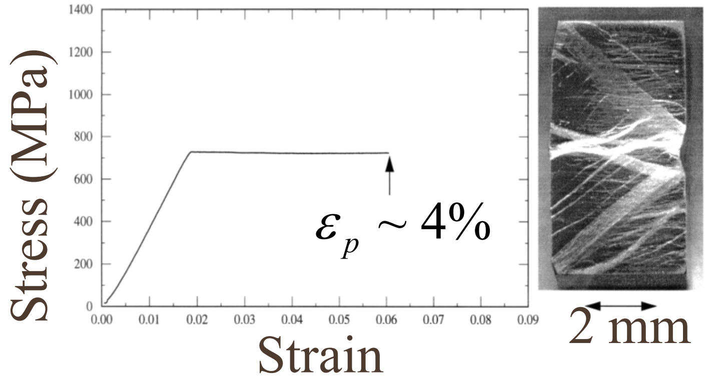
$$\kappa(\varepsilon) = \delta\left[E\,\varepsilon\, exp\left(-\frac{\varepsilon^2}{\alpha}\right)\right] + k\varepsilon$$

δ : Weibull random variable

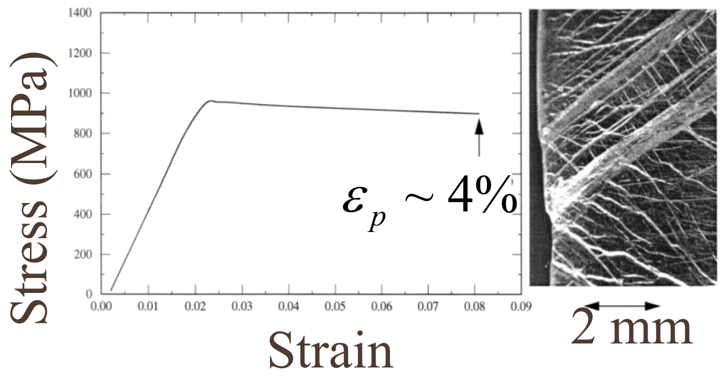


- *Compression Tests*

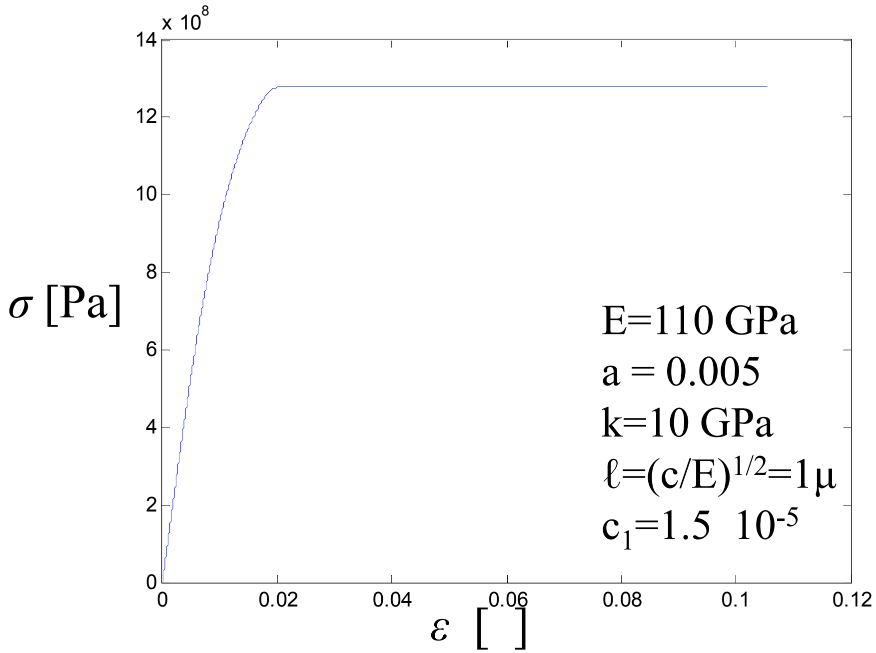
d ~1370 nm, σ_y ~750 MPa
angle ~ 49^0

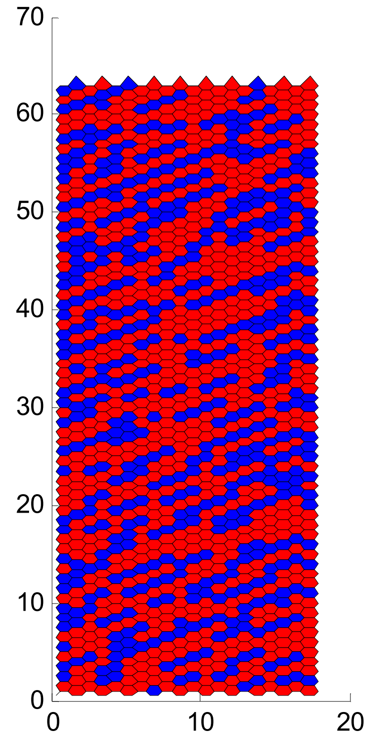


d ~540 nm, σ_y ~960 MPa
angle ~ 49^0



- *Simulation Results*





■ Size Effects in Tension/Compression

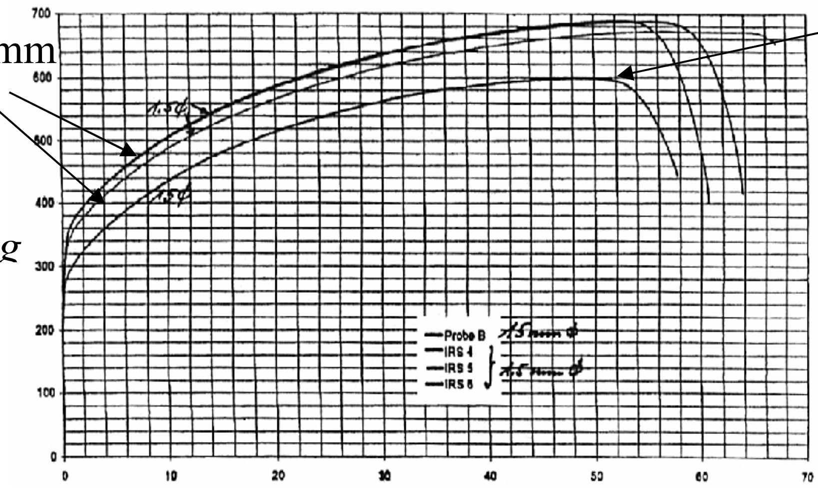
- ***Lack of Macroscopic Gradients in Tension***

a) Steel cylindrical macro-bars

D=15 mm

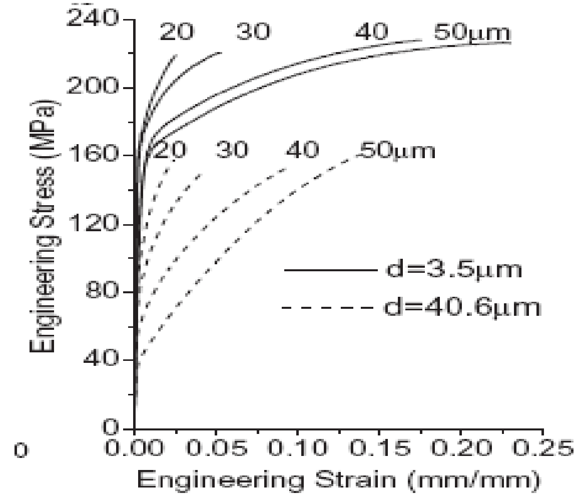
D=1.5 mm

σ_{eng}



Data from ECA et al 1998 ε_{eng}

b) Ag micro-wires



Data from Ngan 2011

Size effect modeling? → Gradient Internal Variable "α"

$$\sigma = \kappa(\varepsilon) + \lambda(\bar{\alpha}) \quad ; \quad \bar{\alpha} = \frac{1}{\upsilon}\int_{\upsilon} \alpha \, d\upsilon \ , \ \dot{\alpha} = D\nabla^2\alpha + \Lambda\varepsilon^q - M\alpha$$

i.e.

"σ" depends on ε and an averaged internal variable "$\bar{\alpha}$" whose microscopic counterpart "α" evolves inhomogeneously: ∇^2 transport term

- ***Adiabatic Elimination of "α"*** $(\dot{\alpha} \sim 0)$

- *Radial symmetry* $\alpha = \alpha(r)$

$$\Rightarrow \alpha(r) = AK_0\left(r/\sqrt{c}\right) + BI_0\left(r/\sqrt{c}\right) + \lambda\varepsilon^q \qquad \begin{cases} c \equiv D/M \\ \lambda \equiv \Lambda/M \end{cases}$$

BC's : $\alpha(r)$ finite $\forall\, r > 0 \Rightarrow A \equiv 0$

$$\left.\frac{\partial\alpha}{\partial r}\right|_{r=R} = \frac{\alpha_c}{\sqrt{c}} = \frac{\lambda\varepsilon^q}{\sqrt{c}}$$ … zero flux of α at $r = 0$

- *Assume* : $\kappa(\varepsilon) = Y + k_0\varepsilon^n$ (*); $\lambda(\bar{\alpha}) = k_0^*\bar{\alpha}^m$ … Ludwig type

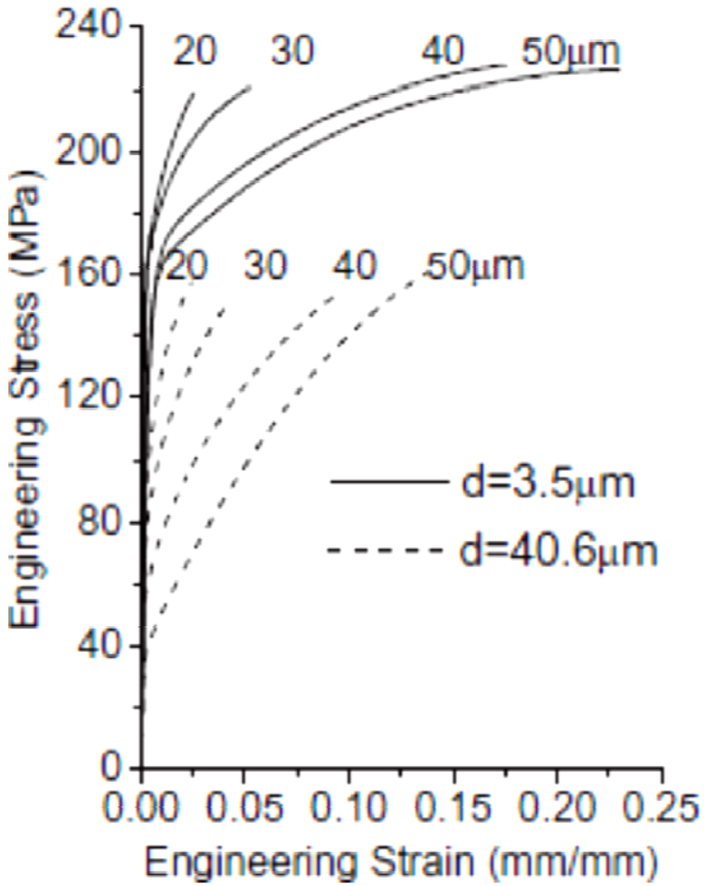
$$\therefore \quad \sigma = Y + k_0\varepsilon^n + k_0^*\left[\lambda\varepsilon\right]^{qm}\left[1 + 2\beta e^{\varepsilon/2}\right]^m \quad (**)$$

(**) Interprets the size effects in tension of previous slide

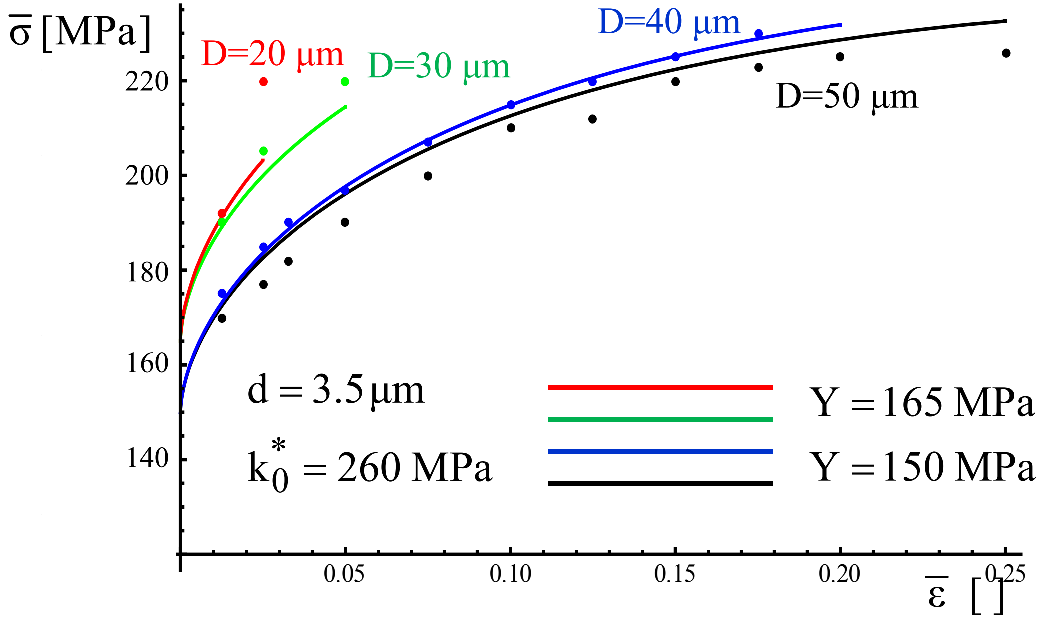
- *Note* : Grain size dependence can be introduced in (*), e.g. according to H-P relation, in order to capture intrinsic (d) and extrinsic (D) size effects simultaneously

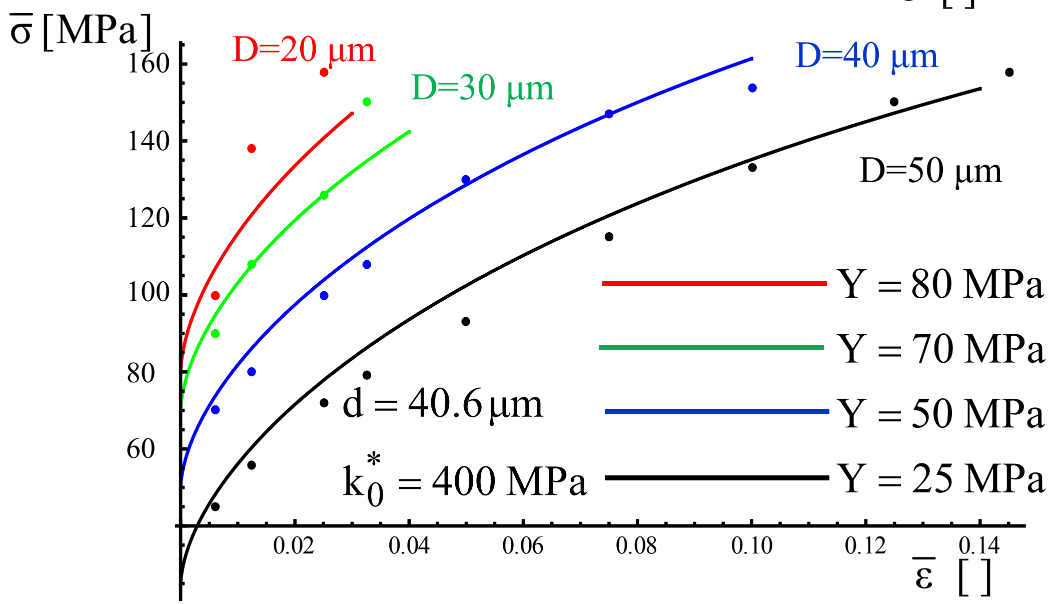
- ***Size Effects on Tensile Strength of Mg Microwires***

$$k_0 = 40\text{ MPa};\quad m = n = 0.6;\quad q = 1;\quad \ell = 3.5\ \mu\text{m}$$



(Chen & Ngan, 2011)



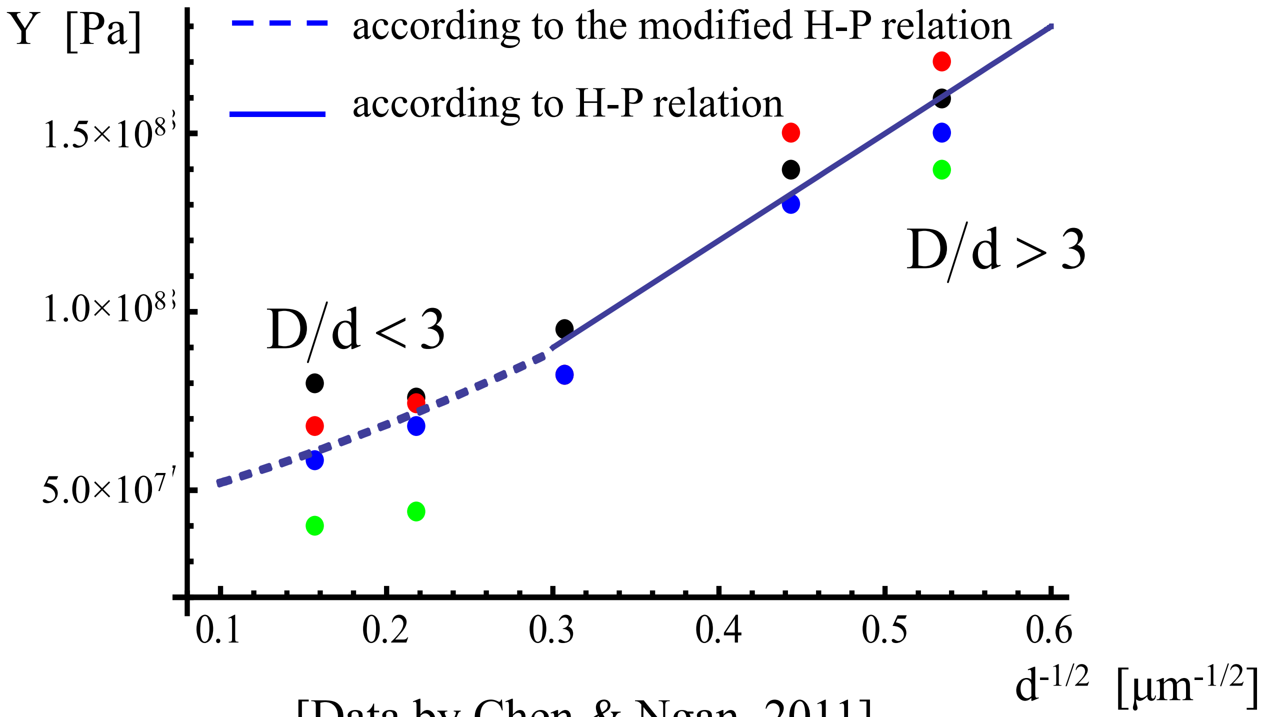


- ***Modified H-P Relation: Application to Ag Nanowires***

$$Y = Y_0 + \frac{k_Y}{\sqrt{d}} + \frac{k_Y^*}{d}$$

$$D/d > 3: \quad k_Y = 300\ \text{MPa}\sqrt{\mu\text{m}} \qquad \text{(H-P)}$$

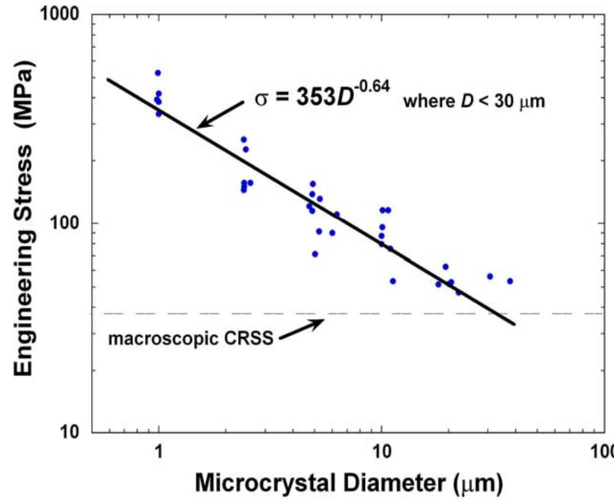
$$D/d < 3: \quad k_Y = 100\ \text{MPa}\sqrt{\mu\text{m}}; \quad k_Y^* = 210\ \text{N/m} \qquad \text{(Modified H-P)}$$



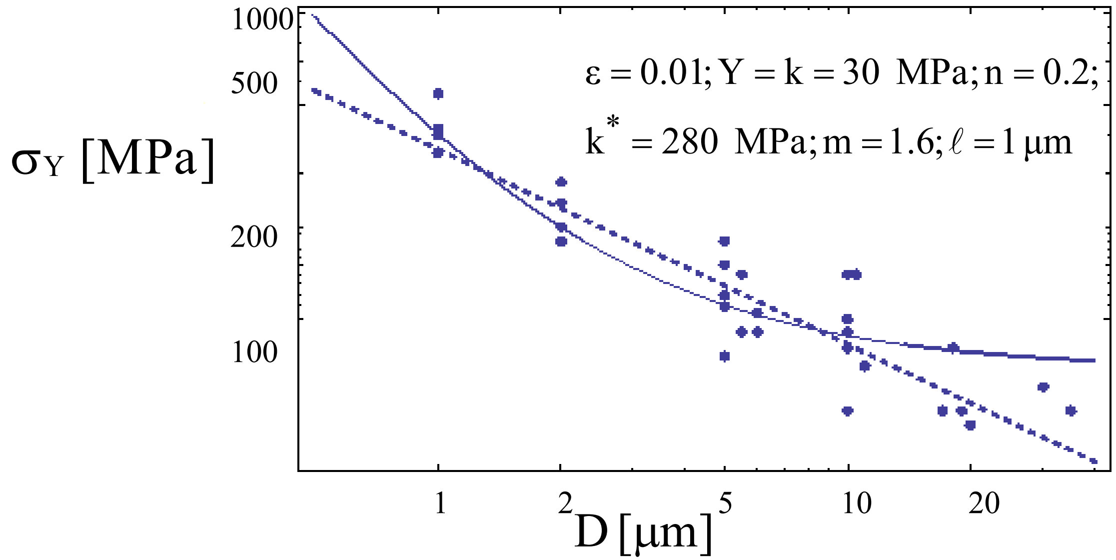
[Data by Chen & Ngan, 2011]

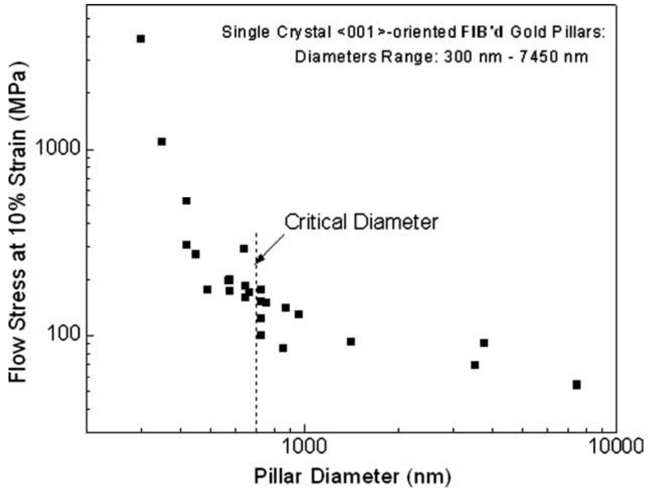
• *Size Effects in Yield of Micropillars*

$$\sigma = Y + k\varepsilon^{n} + k^{*}\varepsilon\left[1 + 2\beta e^{\varepsilon/2}\right]^{m};\ \beta = \frac{2\ell}{D} \rightarrow \sigma = \frac{Y + k\ln\left(1+\bar{\varepsilon}\right)^{n} + k^{*}\ln\left(1+\bar{\varepsilon}\right)\left(1 + 4\frac{\ell}{D}\left(1+\bar{\varepsilon}\right)\right)^{m}}{\left(1+\bar{\varepsilon}\right)}$$

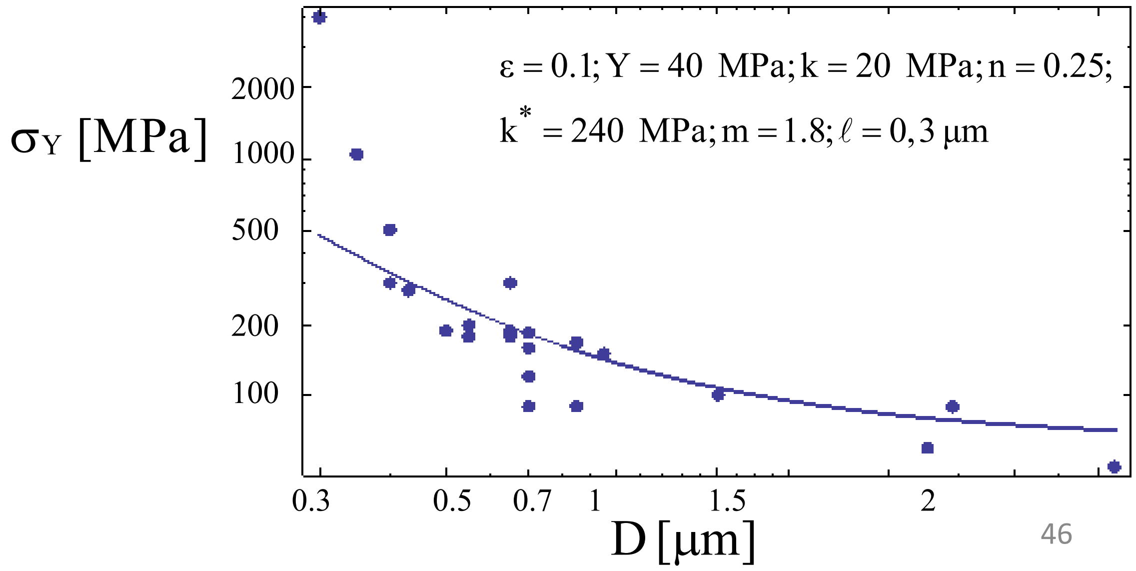


(Dimiduk et al, 2005)

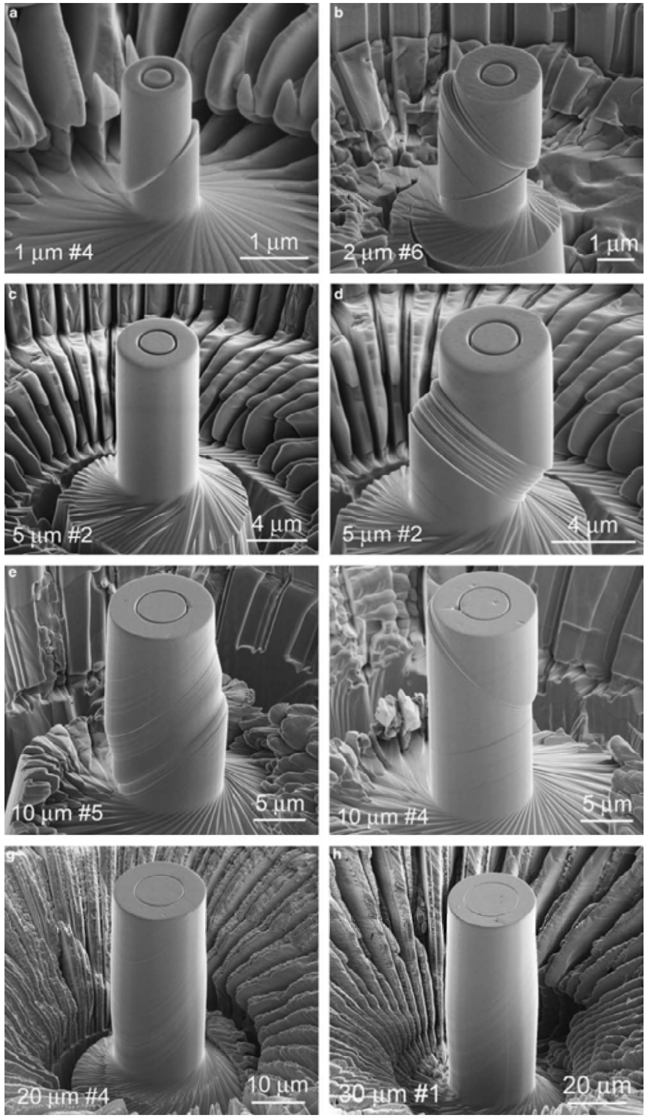


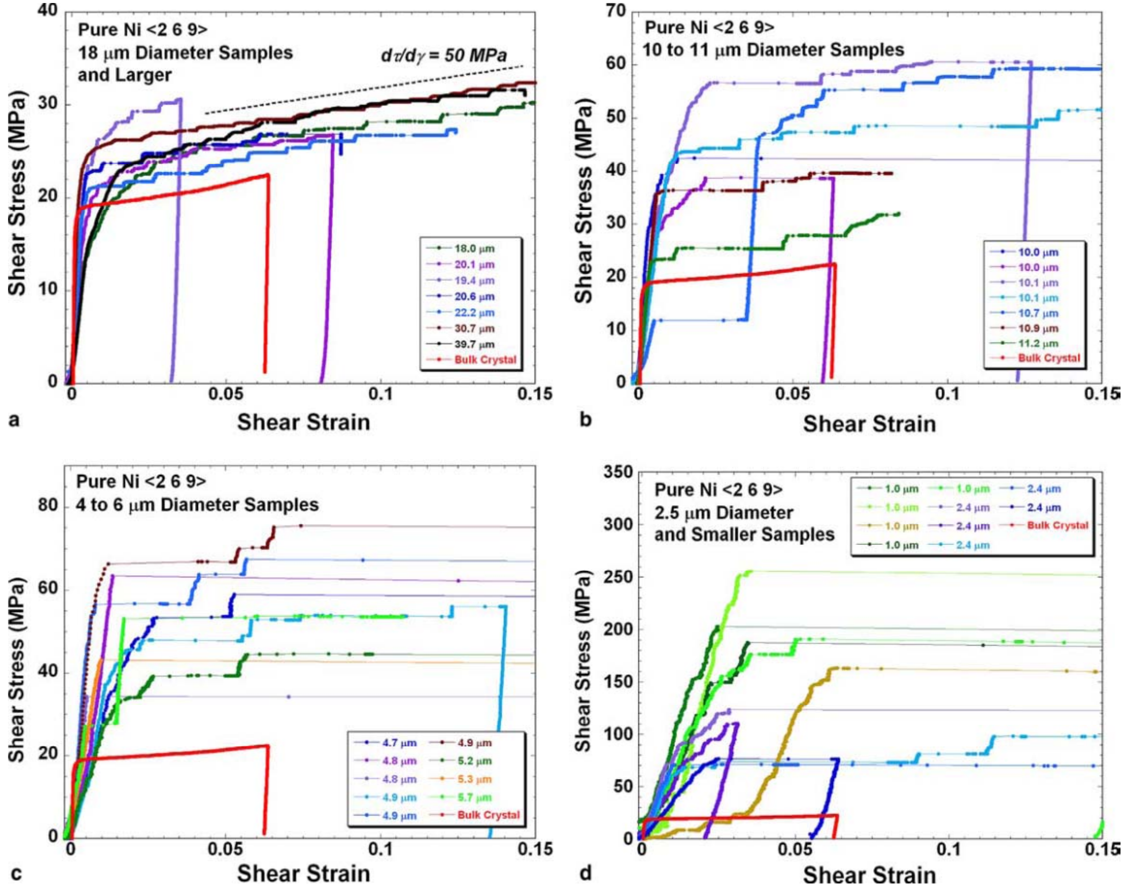


(Greer et al, 2005)



■ Stochasticity & Serrations in Compressed Micropillars





Dimiduk et al, 2005

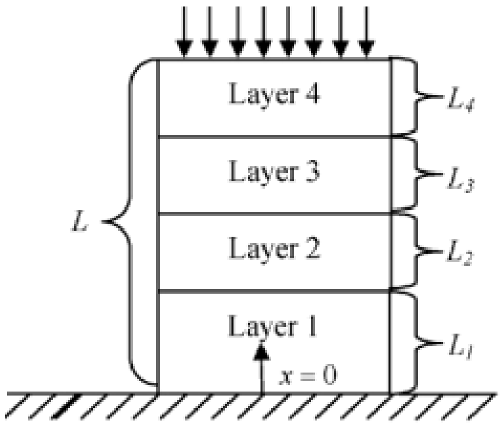
- ***Serrated Plastic Flow in Micropillars***

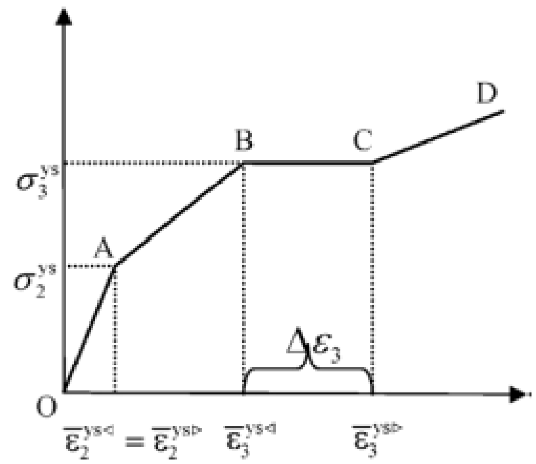
- *Governing Deterministic Equations*

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

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

(Zhang and K.E. Aifantis, 2011)





- *Serrations*

Strain bursts (Δε) 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*

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

$$\mathrm{PDF}(\delta) = \frac{\kappa}{\lambda}\left(\frac{\delta}{\lambda}\right)^{\kappa-1} e^{-(\delta/\lambda)^{\kappa}}; \quad \bar{\delta} = \lambda \Gamma\left[1+(1/\kappa)\right], \quad \left\langle \delta^2 \right\rangle = \lambda^2 \Gamma\left[1+(2/\kappa)\right] - \bar{\delta}^2$$

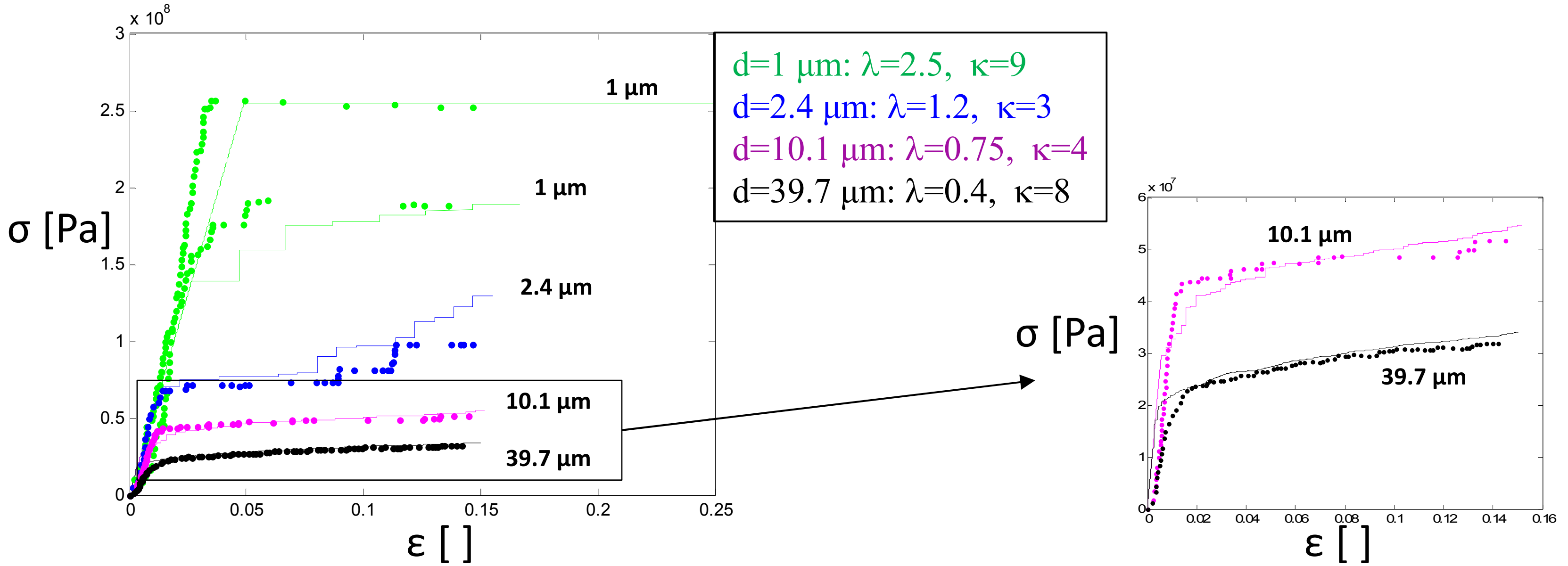
κ/λ : shape/scale parameters

- ***Cellular Automata Simulations***

  - Lattice of 6d×1 cells of size 0.5 μm× d μm (3:1 height to diameter ratio)
  - Force controlled simulation
  - Weibull distributed cell yield stress

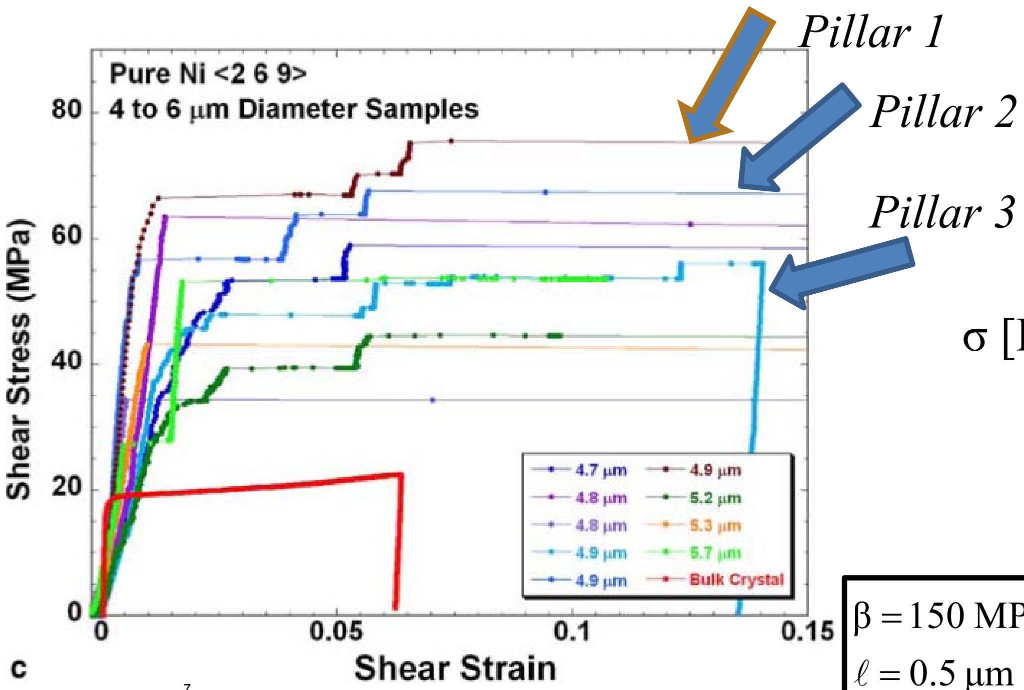
- ***Intermittent Size-dependent Micropillar Plasticity***

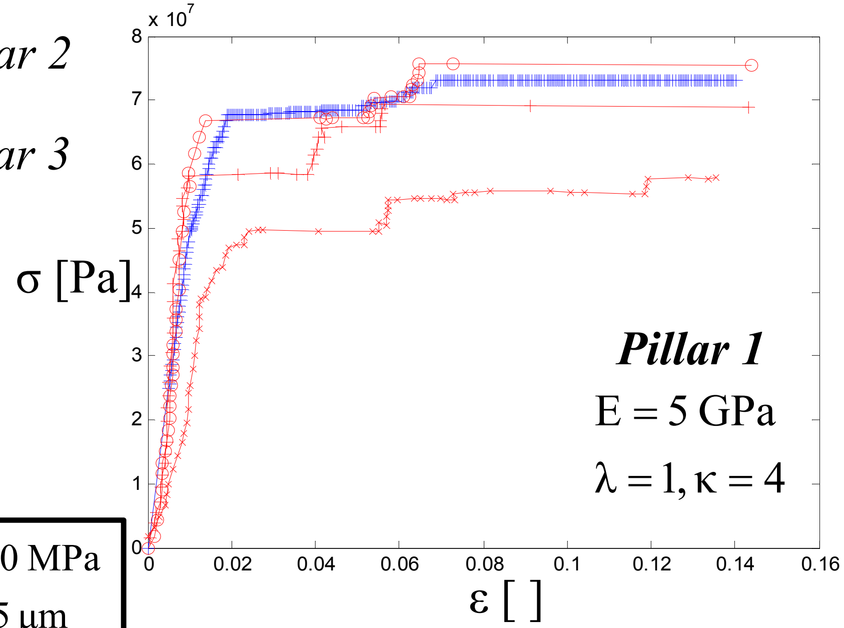
$$E = 5\text{ GPa};\quad \beta = 150\text{ MPa};\quad \ell = 0.5\ \mu\text{m};\quad Y^0 = 80\text{ MPa}$$



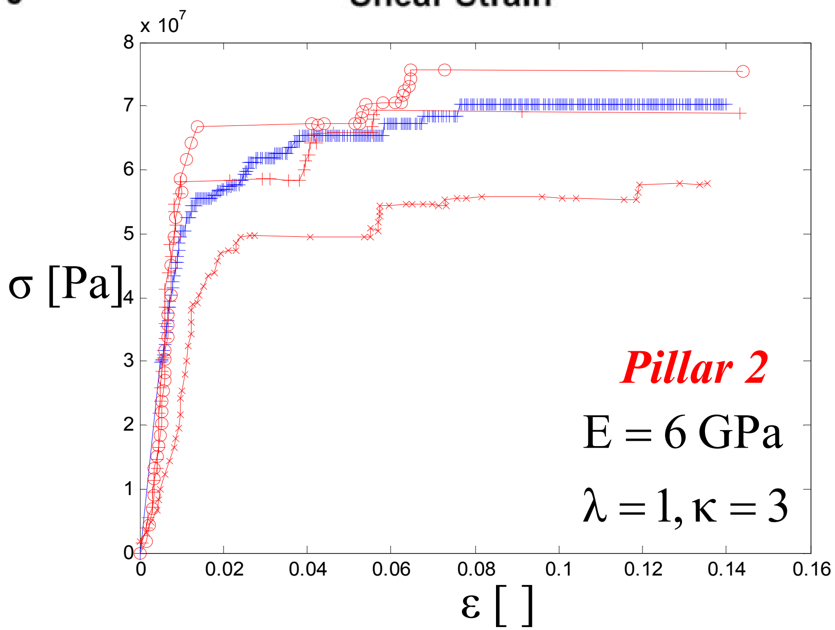
K.E. Aifantis & Konstantinidis, forthcoming

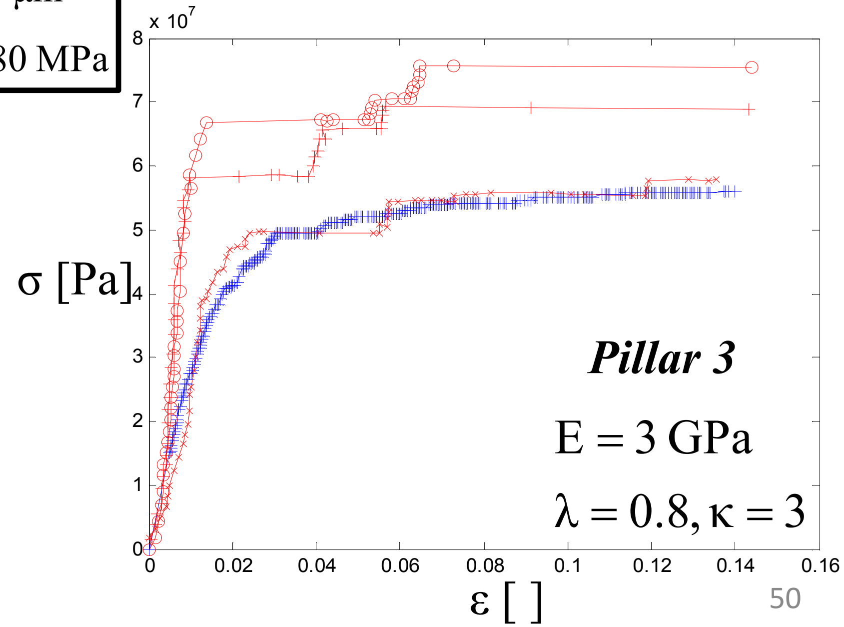
- ***Random Response of Same Diameter (4.9 mm) Micropillars***



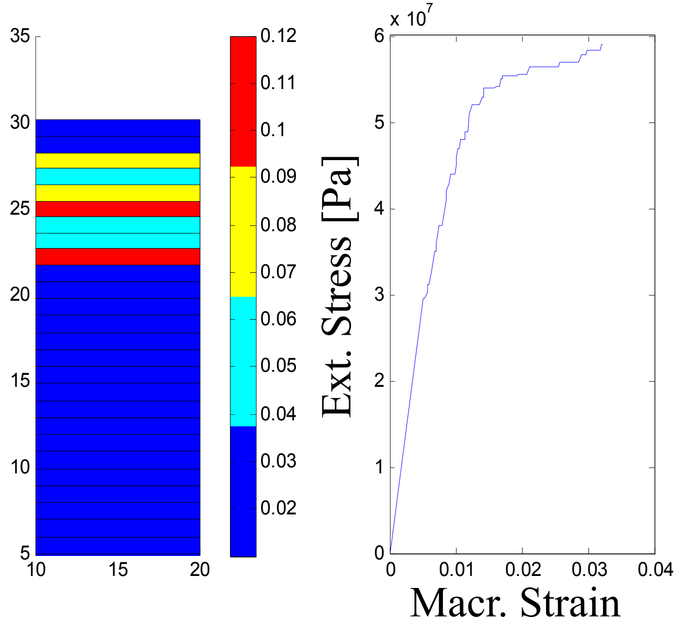


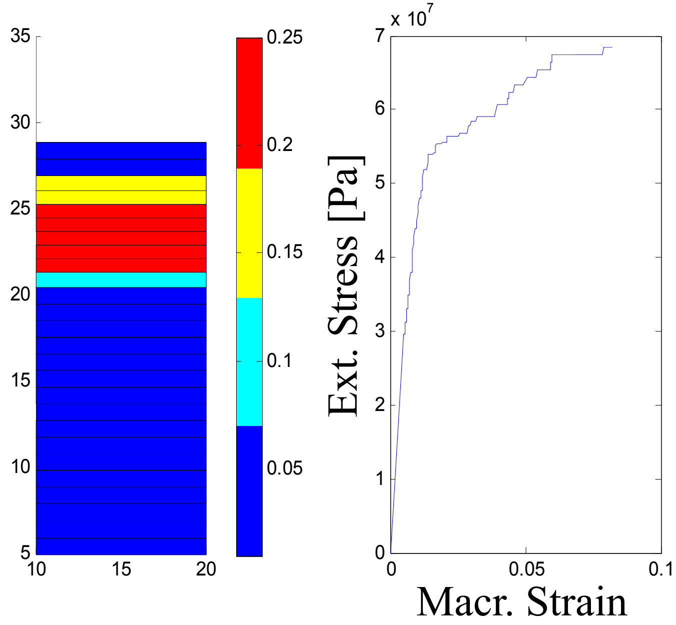
$\beta = 150$ MPa
$\ell = 0.5\ \mu m$
$Y_i^0 = 80$ MPa

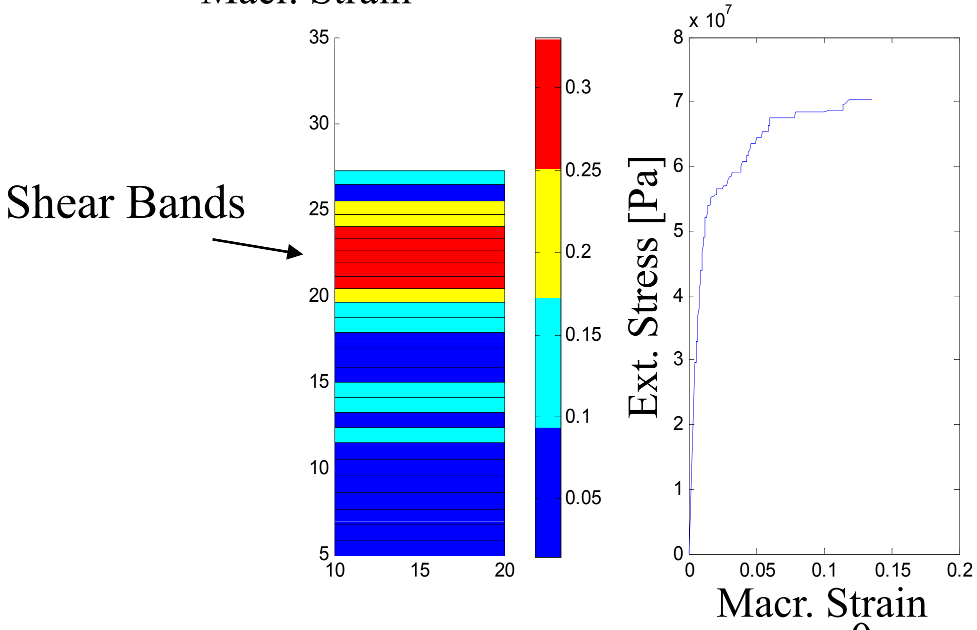




- Example: Simulation Details for Pillar 2







$$E = 6\text{ GPa};\quad \beta = 150\text{ MPa};\quad \ell = 0.5\ \mu\text{m};\quad Y_i^0 = 80\text{ MPa};\quad \lambda = 1, \kappa = 3$$

■ Input from Entropy Statistics

• Boltzmann-Gibbs Entropy

$$S = -k_B \sum_i P(I)\, ln\, P(I)\,; \quad k_B = 1.38065 \cdot 10^{-23} \;\; J/K$$

• Tsallis Entropy

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

- Maximum entropy principle leads to q-exponential distribution

$$P(I) = \left[1 + (q-1)I\right]^{1/(1-q)}$$

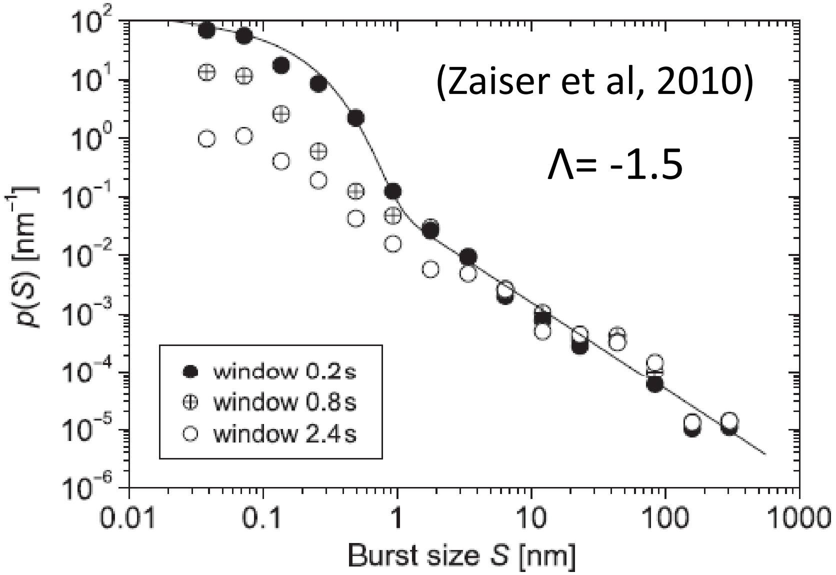
- Generalization

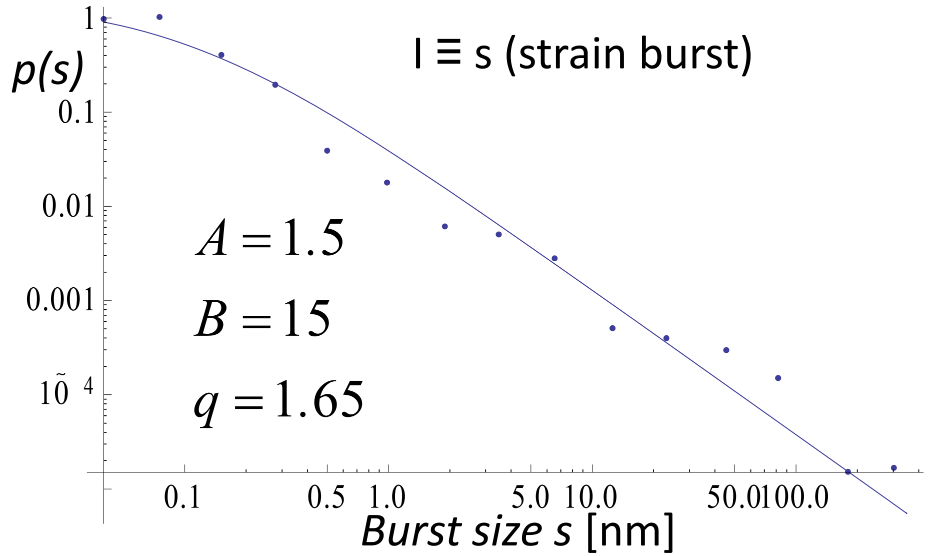
$$\therefore \quad p(I) = A\left[1 + B(q-1)I\right]^{1/(1-q)}$$

(instead of $p(I) \sim I^{\Lambda}$ as commonly done)

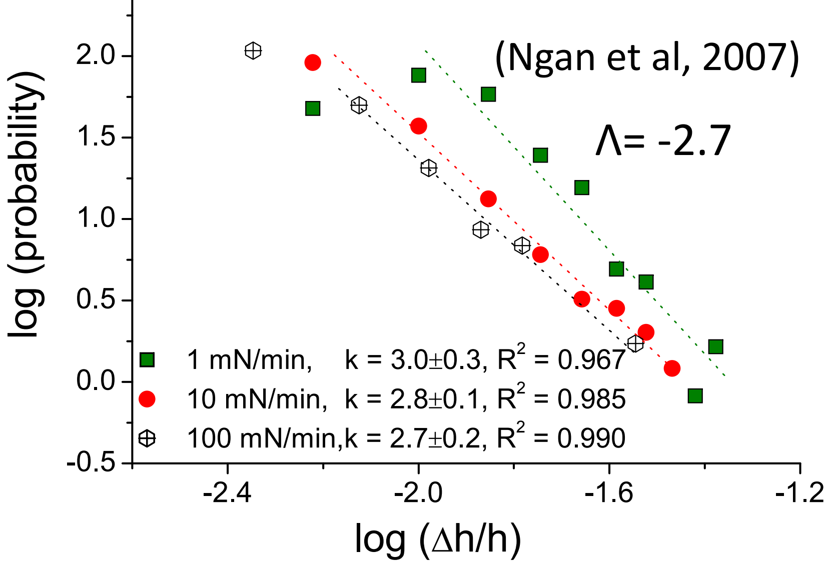
*Note: Using the Tsallis entropy formulation the "events" with high probability but low intensity are **not** ignored, as is the case with power-law formulations*

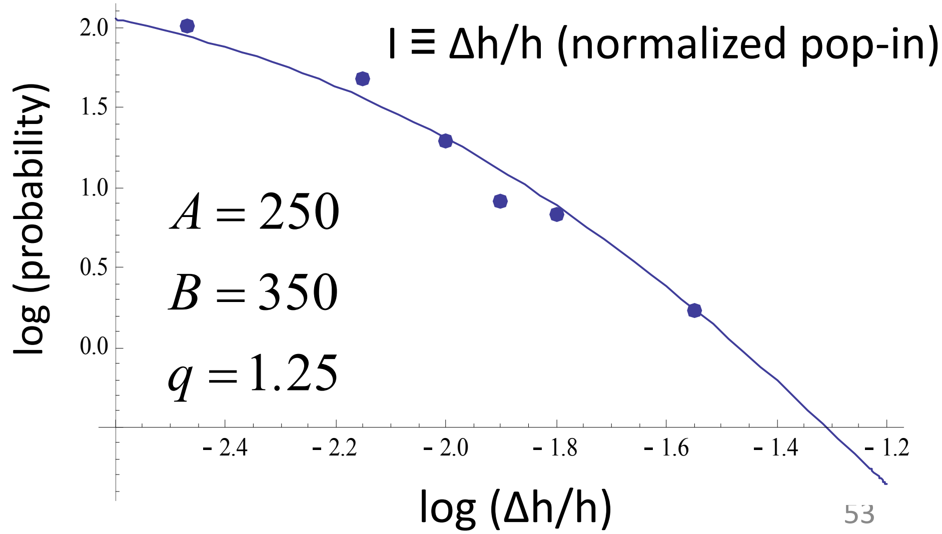
• Strain Bursts in Mo Micropillars under Compression





• Pop-ins in $Zr_{52.5}Al_{10}Ni_{10}Cu_{15}Be_{12.5}$ Glasses under Indentation





• Extracting Information on Randomness / PDF

Probability of bursts of size s

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

Burst size relation to local yield stress

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

(L: cell size)

Probability of strain bursts from n "sites"

$$P(s/L) = P\left(\varepsilon_y^{loc}\right)P\left(\varepsilon_y^{loc}\right)\ldots P\left(\varepsilon_y^{loc}\right) = P\left(\sigma_y^{loc}\right)^n$$

$$\therefore \qquad P\left(\sigma_y^{loc}\right) = A^{1/n}\left[1+(q-1)Bn\frac{\sigma_y^{loc}}{E}\right]^{1/(1-q)n}$$