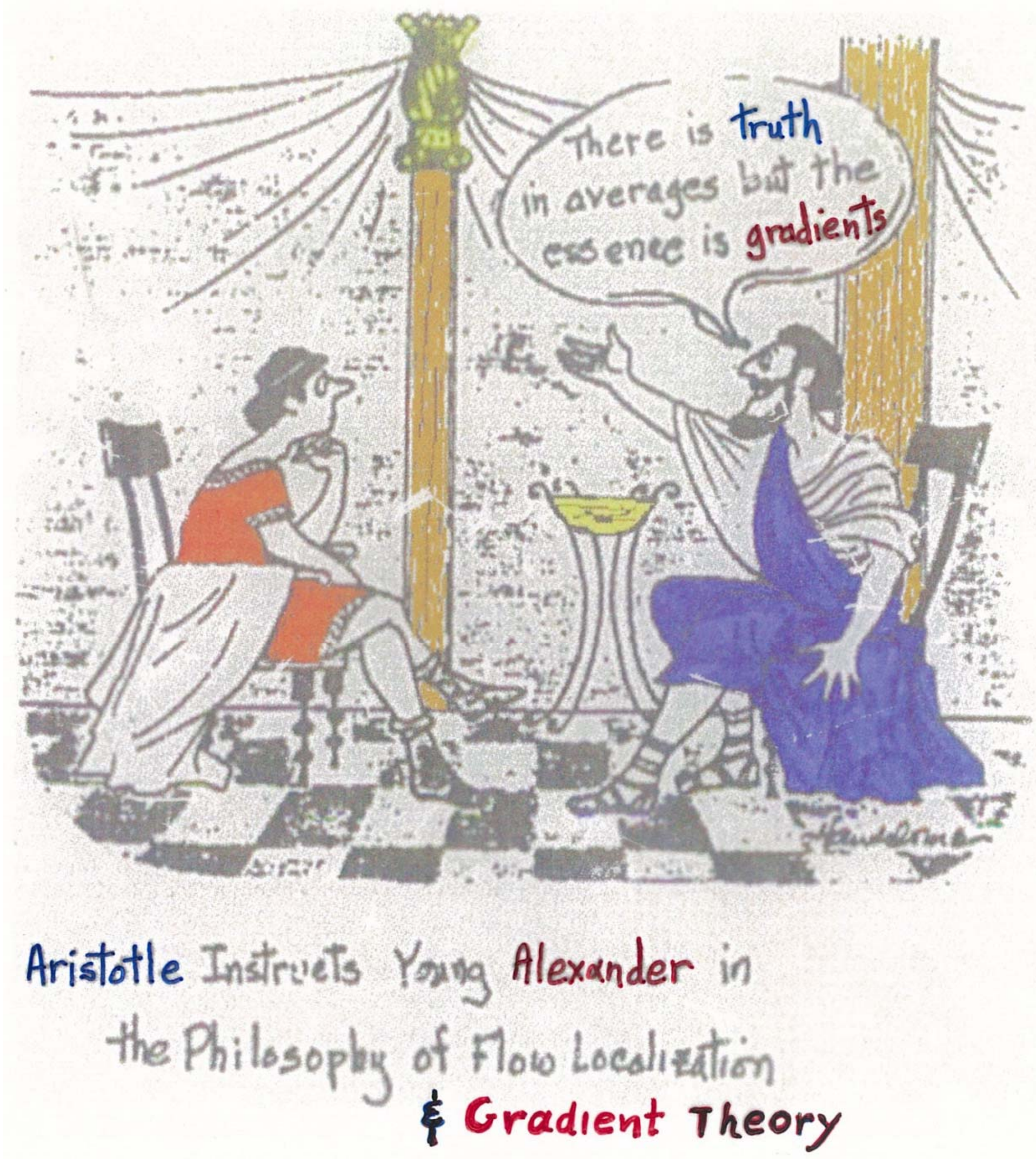
MULTIDISCIPLINARY GRADIENT MATERIAL MECHANICS IMPLICATIONS TO INTERNATIONAL RESEARCH AND EDUCATION

- ***Senior Collaborators*** →
  - Serrin / Minnesota
  - Walgraef / ULB
  - Romanov / Ioffe
- ***Senior PhD Students / Post Docs*** →
  - Bammann / Sandia – Mississippi State
  - Zbib / Washington State
  - Zaiser / U Edinburgh
  - Askes / U Sheffield
  - Konstantinidis / AUT
- ***Other Students*** →
  - R. Wilson - P. Taylor - D. Unger / US
  - M. Seefeldt - M. Gutkin - P. Cornetti - M. Lazar / EU
  - I. Tsagrakis - G. Efremidis - M. Avlonitis - D. Tragoudaras / GR
- ***Current PhD's*** →
  - O. Akintayo - Th. Byros - I. Konstantopoulos - N. Moschakis - A. Louizos
- ***Children*** →
  - Katerina / Nanotechnology
  - Elias / Music

1990 Int. Conf. on Aristotle's 2300th Birthday
[50 USSR Participants at Philippion]



A PHD *at* TWENTY-ONE, *the* WORLD *at* TWENTY-FIVE?

By Marcia Goodrich

Katerina Aifantis '01 is accustomed to being the youngest in the room.

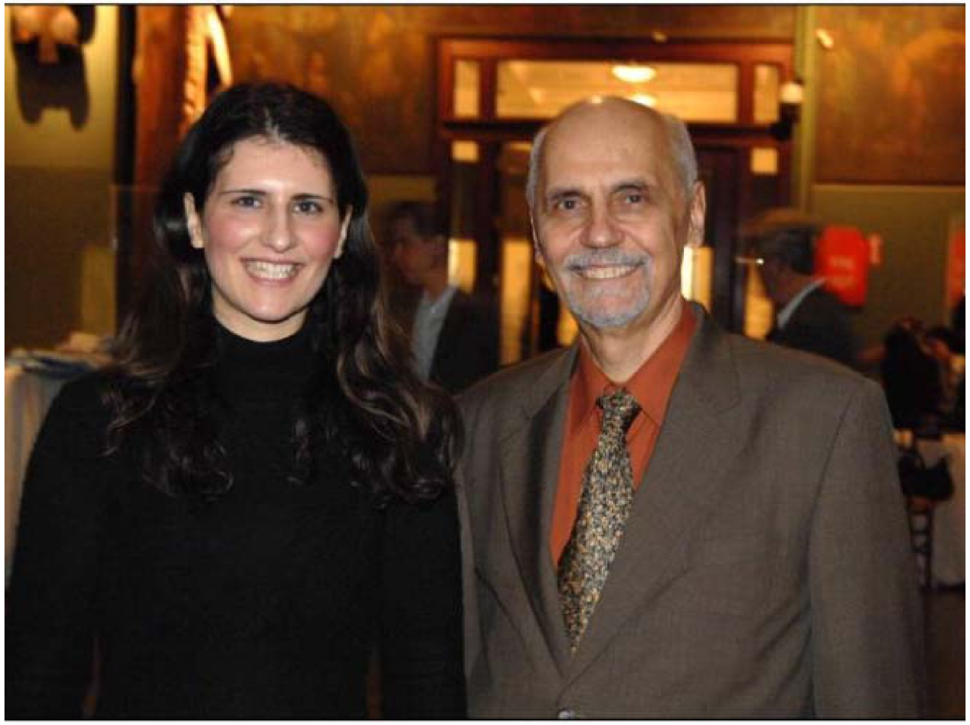
At the age of sixteen, the Houghton High School student sweet-talked her principal into letting her take courses at Michigan Tech, where she promptly aced calculus and chemistry.

"She just beat everyone in the class," remembers Associate Professor Paul Charlesworth. "She's one of the finest students to ever take my general chemistry course."

ERC STARTING GRANT

Probing the Micro-Nano Transition (MINATRAN): Theoretical and Experimental Foundations, Simulations and -Applications [1.3 Million Euros]

2008-2013

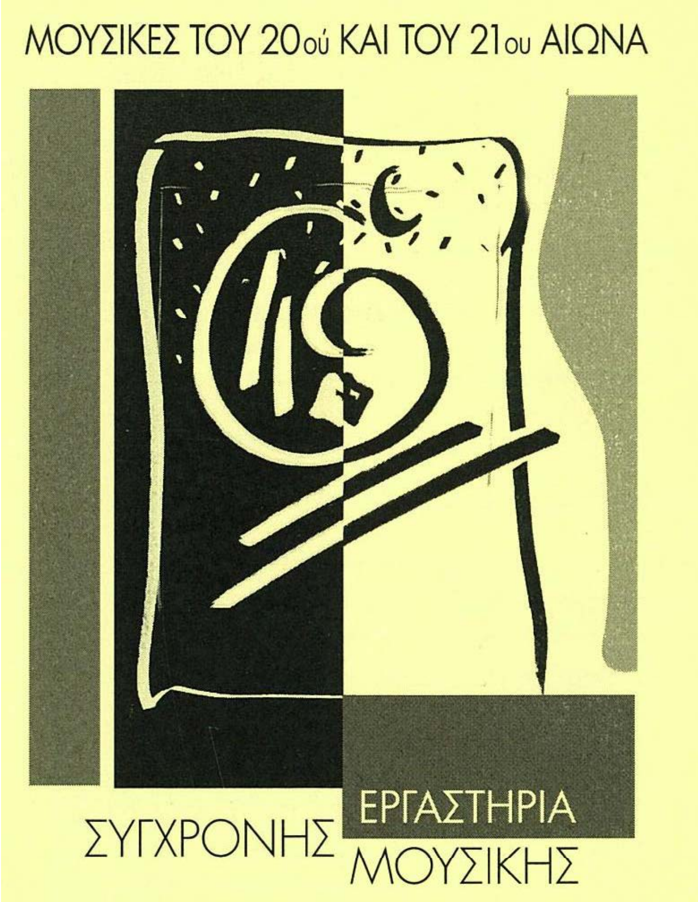


Dr. Potocnik

European Commissioner for Research

Professor Kafatos

President of ERC



μέγαρο μουσικής αθηνών
2008-2009

ΜΕ ΤΗΝ ΥΠΟΣΤΗΡΙΞΗ ΤΟΥ ΥΠΟΥΡΓΕΙΟΥ ΠΟΛΙΤΙΣΜΟΥ

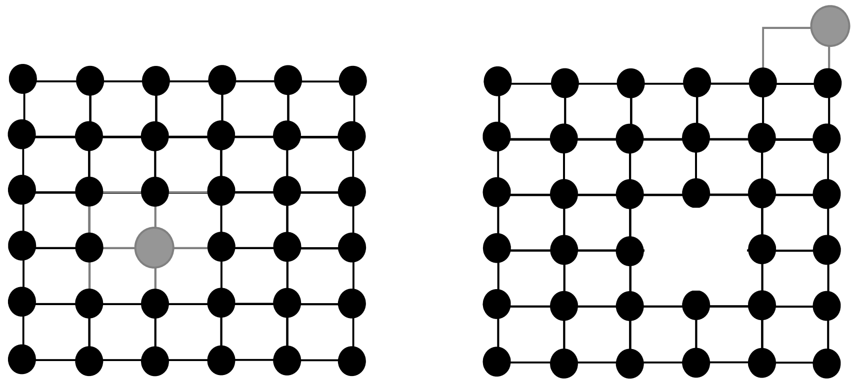
Sounds Like Music (2008)

Μουσικά αποσπάσματα που γράφτηκαν για «πιάνο», εμπλουτισμένα με «ηλεκτρονικούς ήχους». Έμφαση δίνεται στην εκτέλεση, για να μεταδοθεί μια συναισθηματική ηρεμία με τόνους βασισμένους στην απλότητα και τη λιτότητα νεανικών βιωματικών εμπειριών στα μοναχικά τοπία του Βόρειου Μίτσιγκαν και των Μεγάλων Λιμνών.

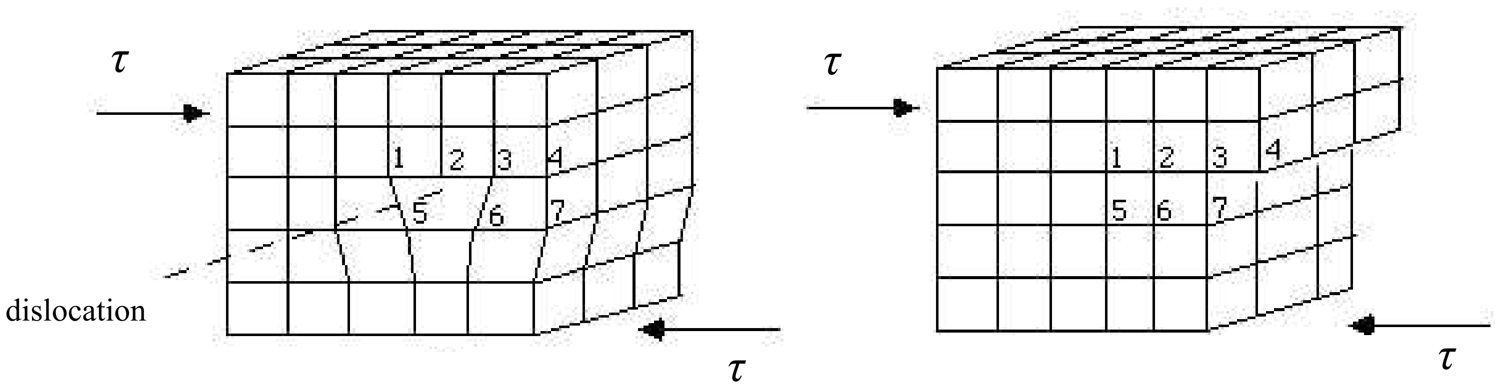
MOTIVATION FOR GRADIENT THEORIES

■ Self-Diffusion in Solids

- ***Vacancies***

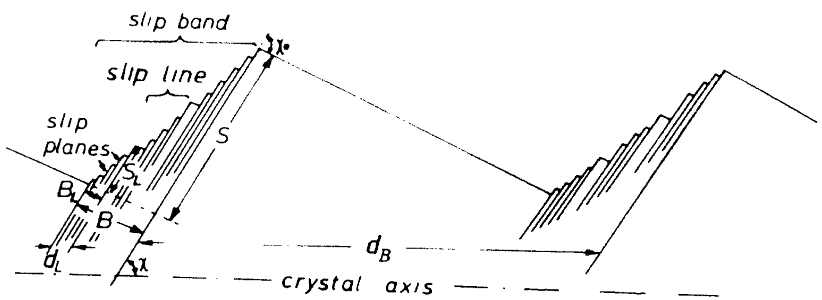


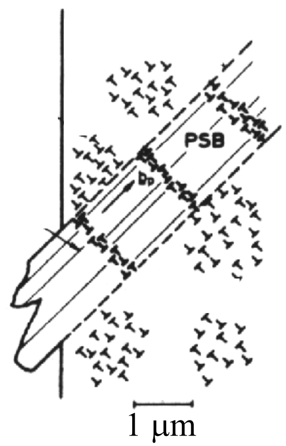
- ***Dislocations***

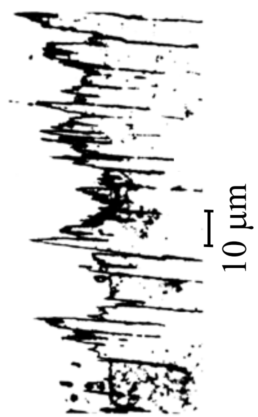


– A continuum with micro(nano)structure is viewed as a classical continuum which, in addition, can interchange mass, momentum, energy and entropy with its bounding surface. As a result, a surface region is excluded from the local (bulk) description; however, changes in the surface region are considered by means of the boundary conditions which are always given to us in a manner inherently coupled with the surface conditions

(*ECA: Mech. Res. Comm.* **5**, *139-145, 1978*)







- ***Balance Laws***

$$\rho = \rho^* \rho_s \qquad \text{. . . . .} \qquad \text{vacancy concentration}$$

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho v) = \hat{c} \qquad \text{. . . . .} \qquad \text{mass balance}$$

$$\frac{\partial T}{\partial x} = \hat{f} \qquad \text{. . . . .} \qquad \text{momentum balance}$$

- ***Constitutive Eqs***

$$T = -\alpha \rho, \quad \hat{f} = \beta j + \gamma \frac{\partial \rho}{\partial x}$$

$$\therefore \quad j = -D_s \frac{\partial \rho_s}{\partial x} \quad ; \quad j = \rho_s v, \quad D_s = \frac{\alpha + \gamma}{\beta}$$

i.e. 1st Fick's Law of Self-diffusion

\- Let $\hat{c} \equiv 0 \quad \rightarrow \quad \frac{\partial \rho_s}{\partial t} + \frac{\partial j}{\partial x} = 0$

$$\therefore \quad \frac{\partial \rho_s}{\partial t} = D_s \frac{\partial^2 \rho_s}{\partial x^2}$$

i.e. 2nd Fick's Law of Self-diffusion

■ Continuum Nano-Elasticity

- ***Balance Law (momentum)***

$$\mathrm{div}\boldsymbol{T} = \boldsymbol{f}$$

$$\boldsymbol{f} = \mathrm{div}(\mathrm{div}\underset{\sim}{\boldsymbol{M}}) \quad ; \qquad \underset{\sim}{\boldsymbol{M}}: \text{ 3rd order tensor}$$

$$\underset{\sim}{\boldsymbol{M}} = \nabla \boldsymbol{S} \quad ; \qquad \boldsymbol{S}: \text{ 2nd order tensor}$$

- ***Constitutive Eq.***

- The Simplest Model

$$\boldsymbol{S} \equiv c\boldsymbol{T}$$

$$\mathrm{div}(\boldsymbol{T} - \nabla^2 \boldsymbol{T}) = 0$$

- Elasticity:

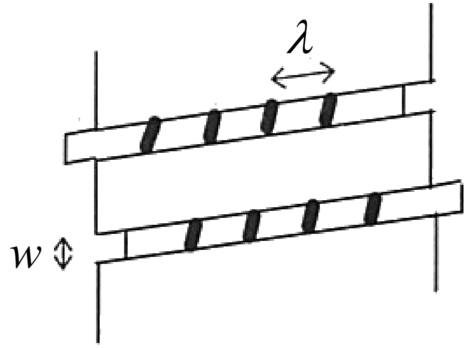
$$\boldsymbol{T} = \lambda\left(\mathrm{tr}\boldsymbol{\varepsilon}\right)\mathbf{1} + 2\mu\boldsymbol{\varepsilon}, \qquad \mathrm{div}\boldsymbol{T}^{nano} = 0$$

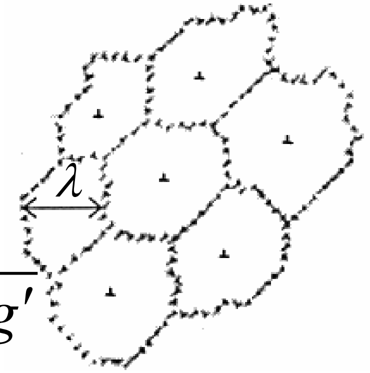
$$\boldsymbol{T}^{nano} = \lambda\left(\mathrm{tr}\boldsymbol{\varepsilon}\right)\mathbf{1} + 2\mu\boldsymbol{\varepsilon} - c\nabla^2\left[\lambda\left(\mathrm{tr}\boldsymbol{\varepsilon}\right)\mathbf{1} + 2\mu\boldsymbol{\varepsilon}\right]$$

i.e. Gradient Elasticity

■ More on Gradient Benchmark Problems

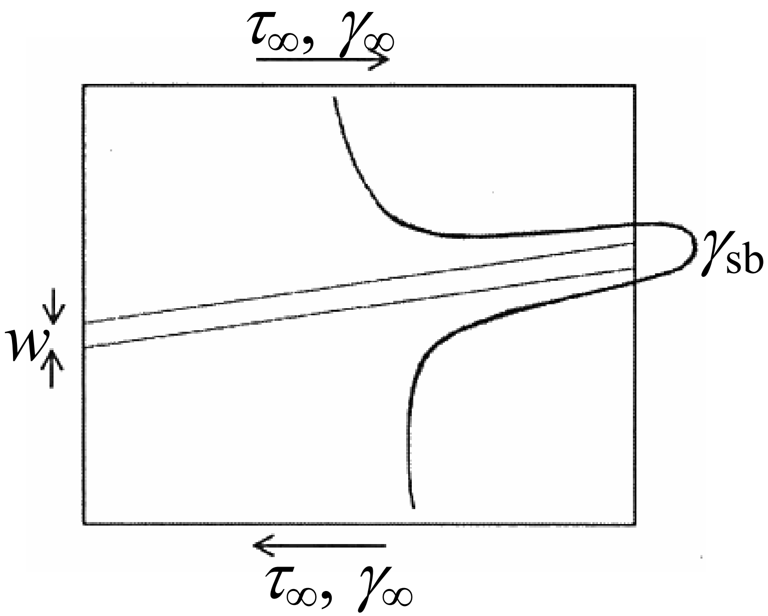
- $\dot{\rho} = g(\rho) + D\nabla^2 \rho$ … Gradient Dislocation Dynamics

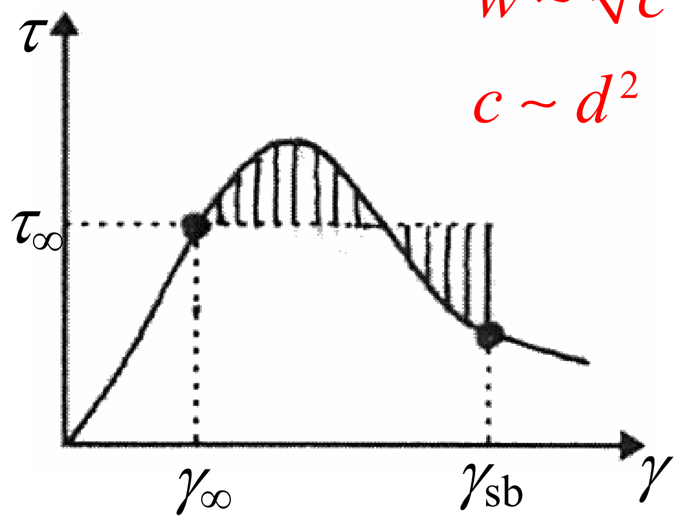




$\lambda \sim \sqrt{D / g'}$

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



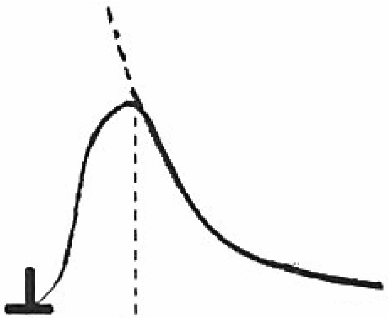


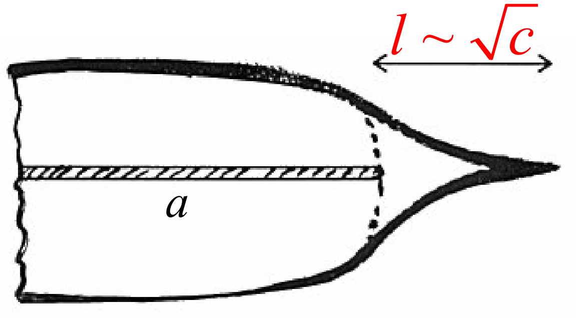
$w \sim \sqrt{c}$

$c \sim d^2$

10

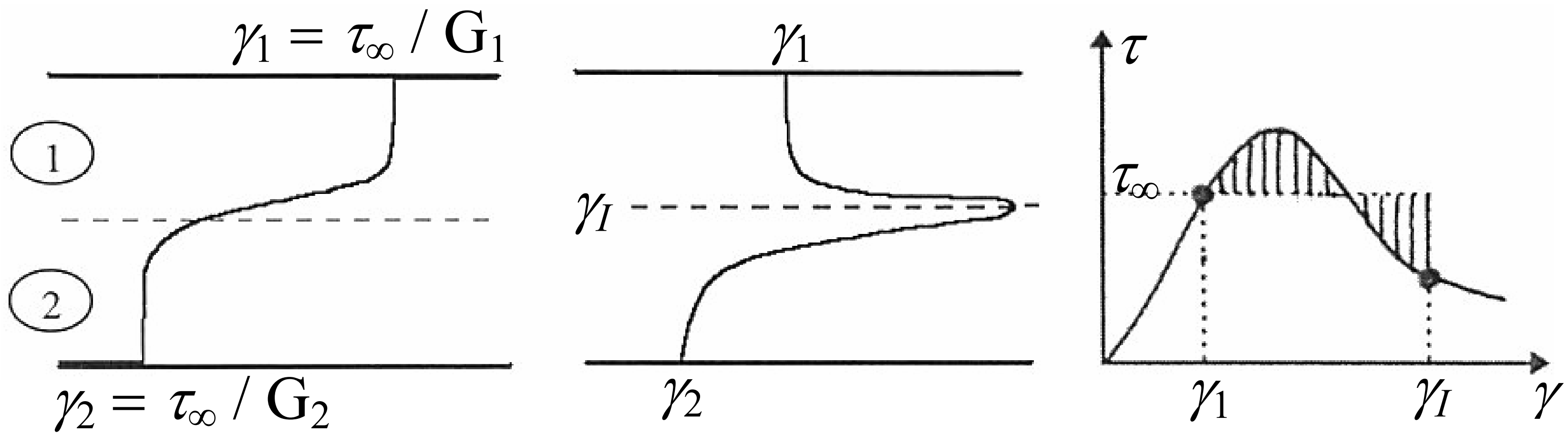
- $\boldsymbol{\sigma} = \lambda(\mathrm{tr}\,\boldsymbol{\varepsilon})\mathbf{1} + 2G\boldsymbol{\varepsilon} - c\nabla^2\left[\lambda(\mathrm{tr}\,\boldsymbol{\varepsilon})\mathbf{1} + 2G\boldsymbol{\varepsilon}\right]$ ... Gradient Elasticity





$r_o \sim \sqrt{c} \quad W_s \sim \ln\left(R/\sqrt{c}\right)$

- $\tau_\alpha = \kappa_\alpha(\gamma_\alpha) - c_\alpha \nabla^2 \gamma_\alpha \quad ; \quad \alpha = 1,2$ ... Solid Interfaces



■ Post-Newtonian (Euler Cauchy Continuum) Mechanics

- ***Basic Laws (mass & momentum)***

$$\partial_t \rho + \mathrm{div}(\rho \boldsymbol{\upsilon}) = 0\,, \quad \mathrm{div}\mathbf{T} = \rho \dot{\boldsymbol{\upsilon}}$$

- ***Constitutive Eqs (closure)***
  - *Elasticity* $\boldsymbol{T} = \lambda(tr\boldsymbol{\varepsilon})\mathbf{1} + 2\mu\boldsymbol{\varepsilon}$; $\boldsymbol{\varepsilon} = \tfrac{1}{2}(\nabla\boldsymbol{u} + \nabla\boldsymbol{u}^T)$

  ∴ Lamé Eqs : $\mu\nabla^2\boldsymbol{u} + (\lambda + \mu)\nabla\, div\boldsymbol{u} = \rho\ddot{\boldsymbol{u}}$

  - *Hydrodynamics* $\boldsymbol{T} = -p(\rho)\mathbf{1} + \lambda(tr\boldsymbol{d})\mathbf{1} + 2\mu\boldsymbol{d}$; $\boldsymbol{d} = \tfrac{1}{2}(\nabla\boldsymbol{\upsilon} + \nabla\boldsymbol{\upsilon}^T)$

  ∴ Navier-Stokes : $-\nabla p + \mu\nabla^2\boldsymbol{\upsilon} + (\lambda + \mu)\nabla\, div\boldsymbol{\upsilon} = \rho\left(\frac{\partial\boldsymbol{\upsilon}}{\partial t} + \boldsymbol{\upsilon}\, grad\boldsymbol{\upsilon}\right)$

- ***Plastic Flow / Fracture***

- *Complex Microstructures/Defects:* vacancies, voids, dislocations, polymer chains
- *Feynmann/Physics Texts:* Plasticity – Too difficult and complex to address
- *Prigogine/Self-organization – ECA/Gradients:* Internal length scales, plastic instabilities, dislocation patterning

■ A Note on Electromagnetism

- ***MacCullagh's (~1850) Eqs of the Rotationally Elastic Aether***

$$\boldsymbol{T} = k\boldsymbol{\omega} \quad ; \quad \boldsymbol{\omega} = 1/2\left(\nabla\boldsymbol{u} - \nabla\boldsymbol{u}^T\right)$$

$$\mathrm{div}\boldsymbol{T} = \rho\frac{\partial^2\boldsymbol{u}}{\partial t^2} \quad \Rightarrow \quad k\,\mathrm{curl}\,\mathrm{curl}\boldsymbol{u} + \rho\frac{\partial^2\boldsymbol{u}}{\partial t^2} = 0$$

Letting $\quad k\,\mathrm{curl}\boldsymbol{u} \quad \Rightarrow \quad a\boldsymbol{E} \quad \& \quad \rho\frac{\partial\boldsymbol{u}}{\partial t} \quad \Rightarrow \quad a\boldsymbol{B}$

$$\therefore \quad \mathrm{curl}\boldsymbol{E} + \frac{\partial\boldsymbol{B}}{\partial t} = 0 \quad ; \quad \mathrm{div}\boldsymbol{B} = 0$$

$\boldsymbol{E}$ ... electric field ; $\boldsymbol{B}$ ... magnetic flux

- ***By also noting the identities***

$$\operatorname{div}\operatorname{curl}\boldsymbol{u}=0 \qquad \& \qquad \operatorname{curl}\frac{\partial \boldsymbol{u}}{\partial t}-\frac{\partial}{\partial t}\operatorname{curl}\boldsymbol{u}=0$$

$$\therefore \quad \operatorname{div}\boldsymbol{E}=0 \qquad \& \qquad \frac{1}{\mu_0}\operatorname{curl}\boldsymbol{B}-\varepsilon\frac{\partial \boldsymbol{E}}{\partial t}=0$$

$$\text{where} \quad k \Rightarrow \frac{\beta}{\varepsilon} \quad , \quad \rho \Rightarrow \beta\mu_0$$

i.e.

$$\frac{\partial \boldsymbol{B}}{\partial t}+\operatorname{curl}\boldsymbol{E}=0 \quad ; \quad \operatorname{div}\boldsymbol{B}=0$$

$$\frac{\partial \boldsymbol{E}}{\partial t}-\frac{1}{\mu_0\varepsilon}\operatorname{curl}\boldsymbol{B}=0 \quad ; \quad \operatorname{div}\boldsymbol{E}=0$$

DIFFUSION
MECHANICAL BASIS FOR TRANSPORT IN SOLIDS

- **Fick 1855 / Fourier 1822:** $\mathbf{j} = -D\nabla\rho$
- **ECA 1980: Mechanics / Diffusive Force**

- ***Balance Laws:*** $\partial_t \rho + \mathrm{div}\mathbf{j} = 0 \quad , \quad \mathrm{div}\mathbf{T} = \mathbf{f}$

- ***Constitutive Equations:*** $\{\mathbf{T}, \mathbf{f}\} \longrightarrow \{\rho, \mathbf{j}, \ldots\}$

- ***Diffusion Classes***

  - *Fick 1855*

$$\left.\begin{aligned} \mathbf{T} &= -\pi\rho\mathbf{1} \\ \mathbf{f} &= \alpha\mathbf{j} \end{aligned}\right\} \Rightarrow \quad \frac{\partial\rho}{\partial t} = \mathrm{D}\nabla^2\rho \qquad (\mathrm{D} \equiv \pi/\alpha)$$

  - *Barenblatt 1963*

$$\left.\begin{aligned} \mathbf{T} &= (-\pi\rho + \bar{\pi}\,\mathrm{tr}\nabla\mathbf{j})\mathbf{1} \\ \mathbf{f} &= \alpha\mathbf{j} \end{aligned}\right\} \Rightarrow \quad \frac{\partial\rho}{\partial t} = \mathrm{D}\nabla^2\rho + \bar{\mathrm{D}}\frac{\partial}{\partial t}\nabla^2\rho \qquad (\bar{\mathrm{D}} \equiv \bar{\pi}/\alpha)$$

- *Cahn 1961*

$$\left.\begin{aligned}\mathbf{T} &= (-\pi\rho + \varepsilon\nabla^2\rho)\mathbf{1} \\ \mathbf{f} &= \alpha\mathbf{j}\end{aligned}\right\} \Rightarrow \quad \frac{\partial\rho}{\partial t} = \mathrm{D}\nabla^2\rho - \mathrm{E}\nabla^4\rho \qquad (\mathrm{E} \equiv \varepsilon/\alpha)$$

- *Cottrell 1948*

$$\left.\begin{aligned}\mathbf{T} &= -\pi\rho\mathbf{1} \\ \mathbf{f} &= \alpha\mathbf{j} + \beta\boldsymbol{\sigma}\nabla\rho - \gamma\rho\nabla\boldsymbol{\sigma}\end{aligned}\right\} \Rightarrow \quad \frac{\partial\rho}{\partial t} = \mathrm{D}^*\nabla^2\rho - \mathrm{M}^*\nabla\sigma\cdot\nabla\rho$$

$$(\mathrm{D}^* = \mathrm{D} + \mathrm{N}\sigma, \quad \mathrm{M}^* = \mathrm{M} - \mathrm{N})$$

- ***Note:*** Kinetic Theory of Gases (Maxwell 1860/67)
  Thermomechanics of Mixtures (Truesdell 1957)

■ Double Diffusivity / Diffusion in Nanocrystals

$$\frac{\partial \rho_\alpha}{\partial t} + \mathrm{div}\mathbf{j}_\alpha = \mathrm{c}_\alpha \qquad \mathrm{div}\mathbf{T}_\alpha + \mathbf{f}_\alpha = 0$$

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

- ***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 Eq.***

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

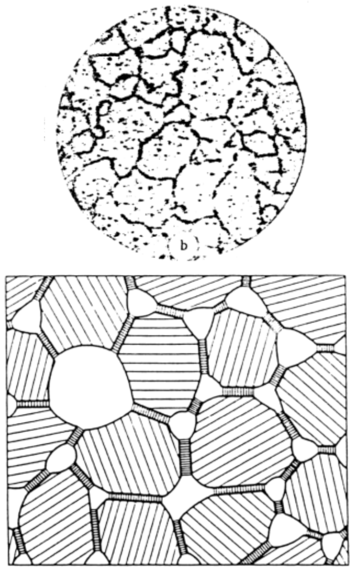
$$\tau = (\kappa_1 + \kappa_2)^{-1} \ , \ D = \tau(\kappa_1 D_2 + \kappa_2 D_1) \ , \ \bar{D} = \tau(D_1 + D_2) \ , \ \mathrm{E} = \tau D_1 D_2$$

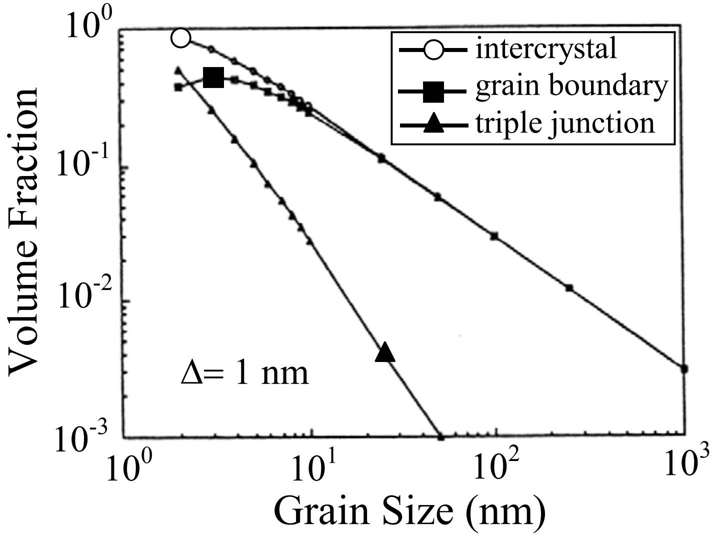
$$t \to \infty \Rightarrow \frac{\partial \rho}{\partial t} = D\nabla^2 \rho \quad ; \quad D = D_{eff} = \frac{\kappa_2}{\kappa_1 + \kappa_2} D_1 + \frac{\kappa_1}{\kappa_1 + \kappa_2} D_2$$

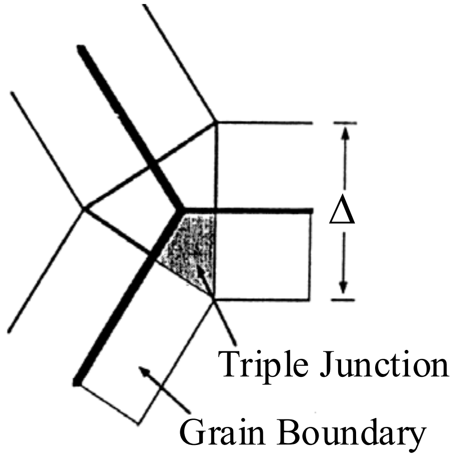
$$= f\, D_1 + (1 - f) D_2$$

- ***Observations / Experiments***

- *Grain boundary space*

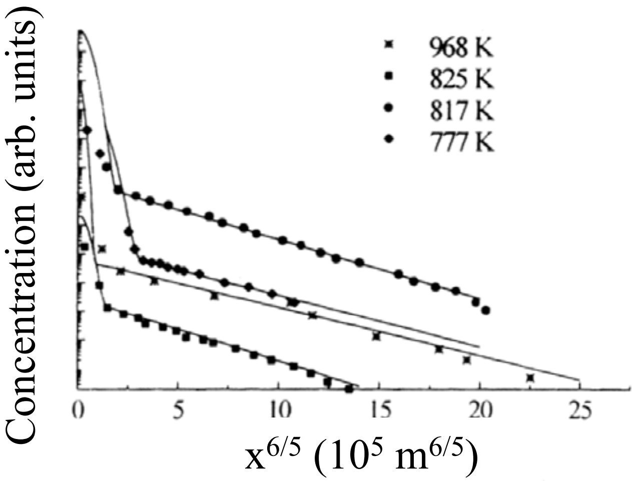




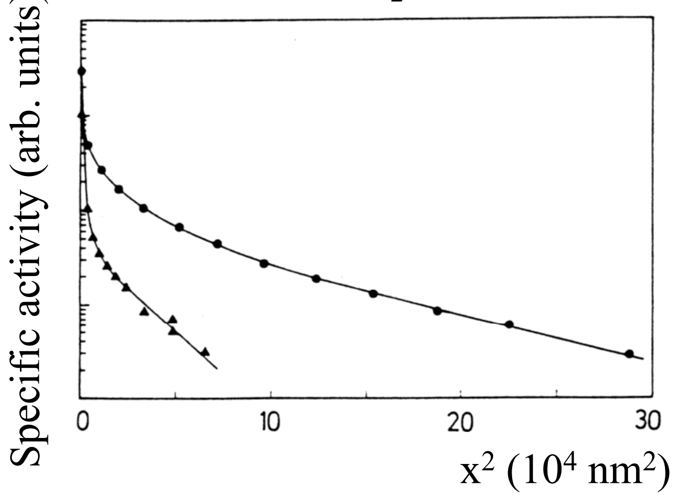


- *Diffusion Penetration Profiles*

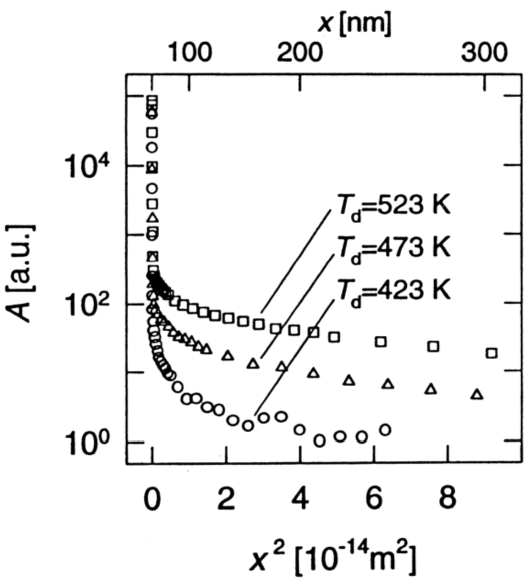
^{64}Cu in Polycrystalline Cu



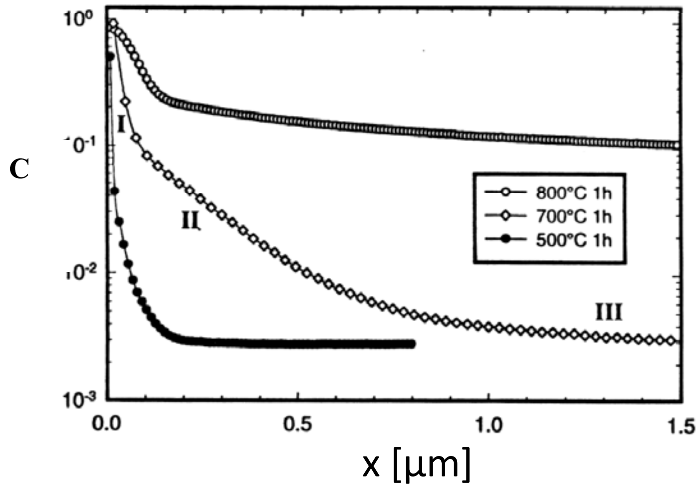
^{67}Cu in Nanocrystalline Cu



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



^{18}O in nano ZrO_2



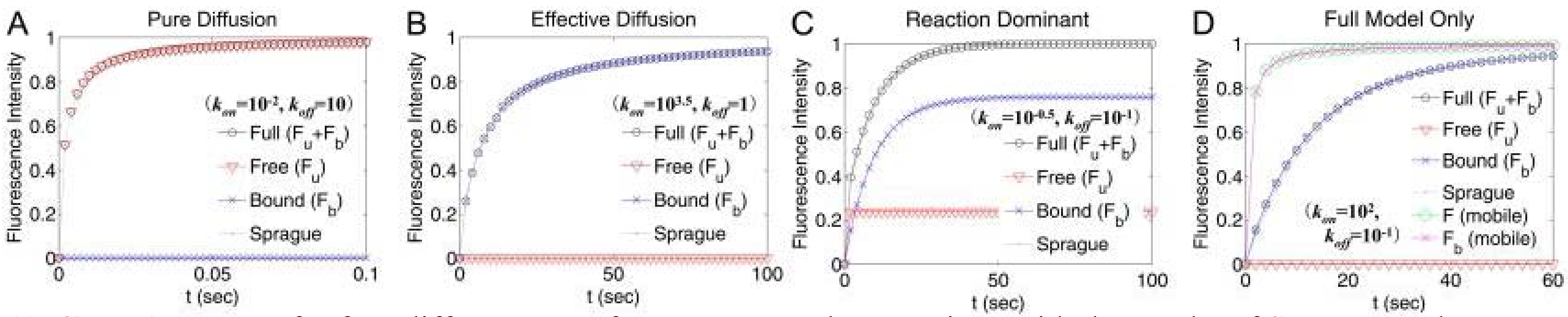
- **Rutherford Aris:** On the Permeability of Membranes with Parallel but Interconnected Pathways [*Math. Biosci.* **77**, 5-16 (1985)]

*This paper is dedicated to the memory of R. Bellman

$$A_1D_1\frac{d^2c_1}{dx^2} = k_1pc_1 - k_2pc_2 \quad ; \qquad A_2D_2\frac{d^2c_2}{dx^2} = -k_1pc_1 + k_2pc_2$$

- **M. Kang and A.K. Kenworthy:** A Closed-Form Analytic Expression for the Binding Diffusion Model [*Biophys. J.* **95**, L13-L15 (2008)]

$$U + R \underset{k_{off}}{\overset{k_{on}}{\rightleftarrows}} B \quad ; \qquad \begin{aligned}\dot{u} &= D_1\nabla^2 u - k_{on}u + k_{off}b \\ \dot{b} &= D_2\nabla^2 bu - k_{on}u - k_{off}b\end{aligned}$$



(A-C) FRAP curves for four different sets of parameters and comparison with the results of Sprague et al.

Refs

E.C. Aifantis, *Acta Mech.* **37**, 265-296 (1980).

E.C. Aifantis and J. Hill, *Q. J. Appl. Math.* **33**, 1-21 & 23-41 (1980)

- **F. Xu, K.A. Seffen and T.J. Lu:** Non-Fourier analysis of skin biothermomechanics [*Int. J. Heat Mass Transfer* **51**, 2237-2259 (2008)]

  – DPL (dual phase lag) model of bioheat transfer

$$\mathbf{q}(\mathbf{r},t)+\tau_q\frac{\partial \mathbf{q}(\mathbf{r},t)}{\partial t}=-k\left[\nabla T(\mathbf{r},t)+\tau_T\frac{\partial \nabla T(\mathbf{r},t)}{\partial t}\right]$$

- **S. Valette et al:** Heat affected zone in aluminum single crystals submitted to femtosecond laser irradiations [*Appl. Surf. Sci.* **239**, 381-386 (2005)]

  – 2-temperature model for metals irradiated by ultrasoft laser pulses

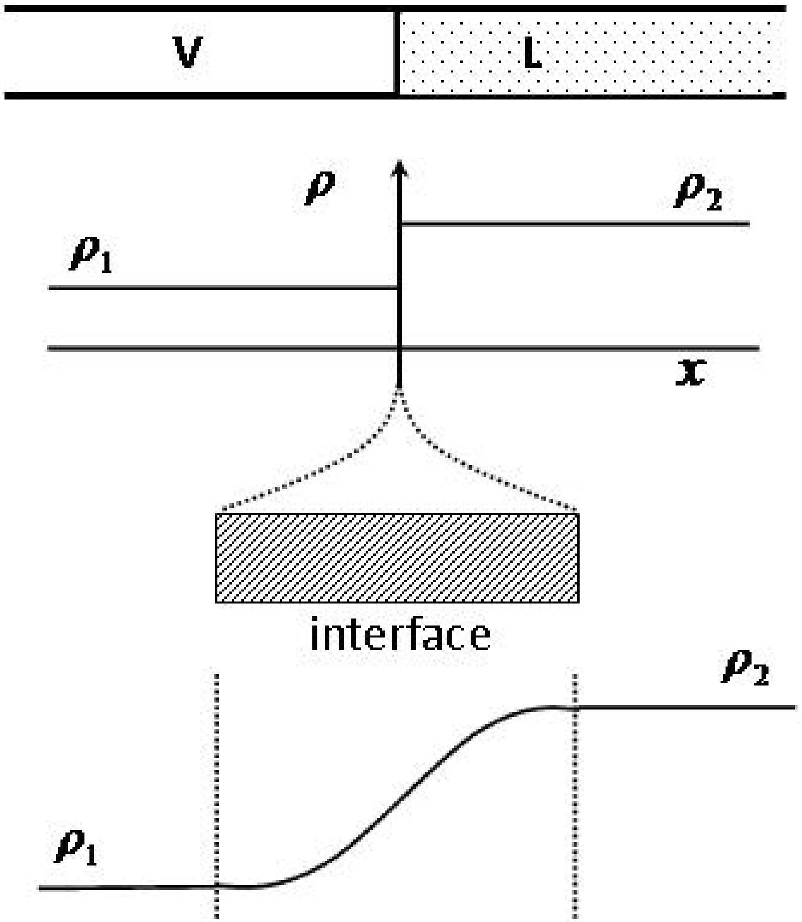
$$C_e\frac{\partial T_e}{\partial t}=\nabla(K_e\nabla T_e)-g(T_e-T_i)+S(r,z,t)$$

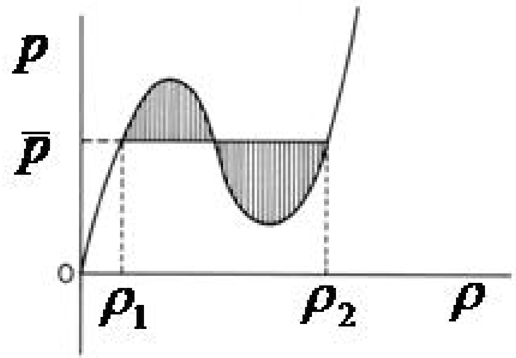
$$C_i\frac{\partial T_i}{\partial t}=\nabla(K_i\nabla T_i)+g(T_e-T_i)$$

T_e ... temperature of electron gas; T_i ... temperature of ions/phonon bath

INTERFACES
THE VdW/MAXWELL GRADIENT L-V INTERFACE

■Van der Waals 1873 / Maxwell 1875: Thermodynamics





$$p = p(\rho) = \frac{RT\rho}{1 - \mathrm{B}\rho} - \mathrm{A}\rho^2$$

$$p(\rho_1) = p(\rho_2) = \bar{p}$$

$$\int_{\rho_1}^{\rho_2} [p(\rho) - \bar{p}] \frac{d\rho}{\rho^2} = 0$$

■ Aifantis / Serrin 1983: Mechanics

- ***Equilibrium:*** $div\,\mathbf{T}=0$

- ***Constitutive Eq:*** $\mathbf{T}=\mathbf{f}(\rho,\nabla\rho,\nabla\nabla\rho)$

$$=\left[-p(\rho)+\alpha\nabla^2\rho+\beta\left|\nabla\rho\right|^2\right]\mathbf{1}+\gamma\nabla\nabla\rho+\delta\nabla\rho\otimes\nabla\rho$$

- ***Solution:*** $\mathrm{MR}\Rightarrow\dfrac{1}{\rho^2}\to E(\rho)=\dfrac{1}{a}\exp\left(2\int\dfrac{b}{a}d\rho\right);\quad a\equiv\alpha+\gamma,\ b\equiv\beta+\delta$

- ***Note:*** Maxwell (1876) ; Korteweg (1901) ; Truesdell (1949)

■ Solution Details – Remarks

- ***Planar Interfaces***

  - $\rho = \rho(x) \quad \Rightarrow \quad \begin{cases} T_{xx} = T = -p(\rho) + a\rho_{xx} + b\rho_x^2 \\ T_{yy} = T_{zz} = -p(\rho) + \alpha\rho_{xx} + \beta\rho_x^2 \end{cases}$

$$\partial \mathrm{T}/\partial x = 0 \;\Rightarrow\; a\rho_{xx} + b\rho_x^2 = p(\rho) - \overline{p}\,; \qquad \begin{cases} a \equiv \alpha + \gamma \\ b \equiv \beta + \delta \end{cases}$$

- Analytical Solutions / Conditions for Existence

$$p(\rho_1) = p(\rho_2) = \overline{p}\,, \quad \int_{\rho_1}^{\rho_2} [p(\rho) - \overline{p}]\mathrm{E}(\rho)\,d\rho = 0\,; \;\; \mathrm{E}(\rho) \equiv \frac{1}{a}\exp(2\int \frac{b}{a}\,d\rho)$$

$$x = x_0 + \int_{\rho(x_0)}^{\rho(x)} \frac{d\rho}{\sqrt{2F(\rho)/G(\rho)}}\,; \quad F \equiv \int_{\rho_1}^{\rho} (p - \overline{p})\mathrm{E}(\rho)\,d\rho\,; \quad G \equiv \alpha\,\mathrm{E}(\rho)$$

- *Surface Tension:* $\sigma = \int_{-\infty}^{\infty} \left\{ \frac{1}{2}\left(T_{yy} + T_{zz}\right) - T_{xx} \right\} dx = \int_{-\infty}^{\infty} c\,\rho_x^2\, dx\,; \quad c = \gamma' - \delta$

- *Statistical Models (D–S 1982):* $\gamma = 2\alpha\,, \quad \delta = 2\beta \quad \Rightarrow \quad c = \frac{2}{3}(a' - b)$

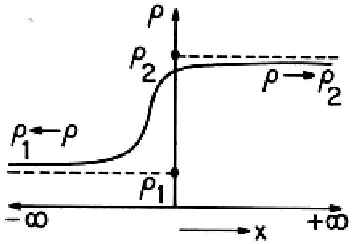
$$a = \frac{1}{16}\rho^2 u' + \frac{1}{2}\rho u\,, \quad b = \frac{1}{16}\rho^2 u'' + \frac{1}{4}\rho u' - \frac{1}{4}u\,, \quad c = \frac{1}{2}u + \frac{1}{4}\rho u'$$

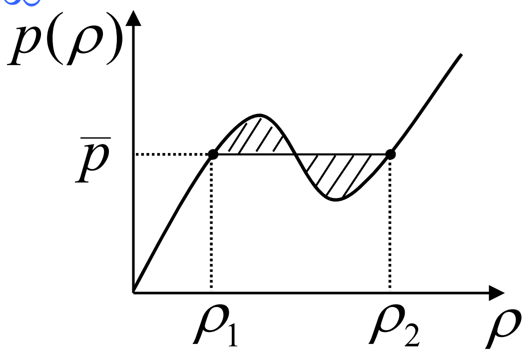
- *Validity of MR:* $\left(\frac{a}{\rho^2}\right)' = 2\left(\frac{b}{\rho^2}\right)$

$$\textit{Exps:}\ \mathrm{H_2O}\ \textbf{at}\ 100^0\ C\ \ldots \quad \frac{\rho_2}{\rho_1} \rightarrow \begin{cases} \sim 1603.\,.\,.\ \text{Steam Tables} \\ \sim 16.\,.\,.\,.\,.\ MR \\ \sim 1660.\,.\,.\ \text{Mechanics} \end{cases}$$

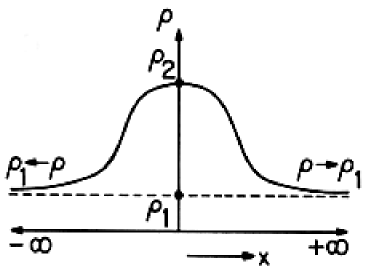
- ***Planar Interfaces / 1D Profiles***

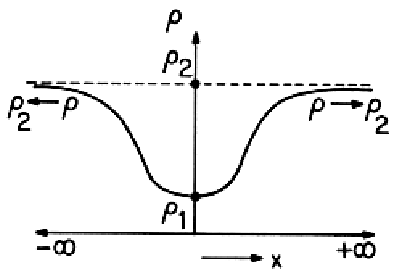
  - *Transitions (interfaces)* $\rho \rightarrow \rho_{1,2}$ *as* $x \rightarrow \mp\infty$

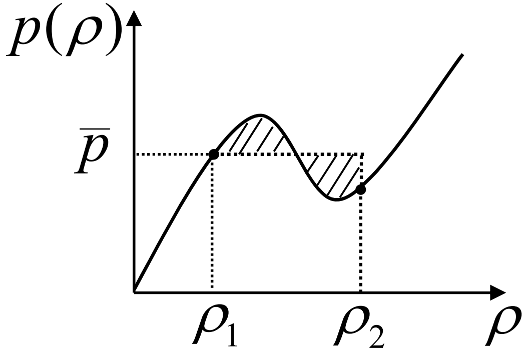




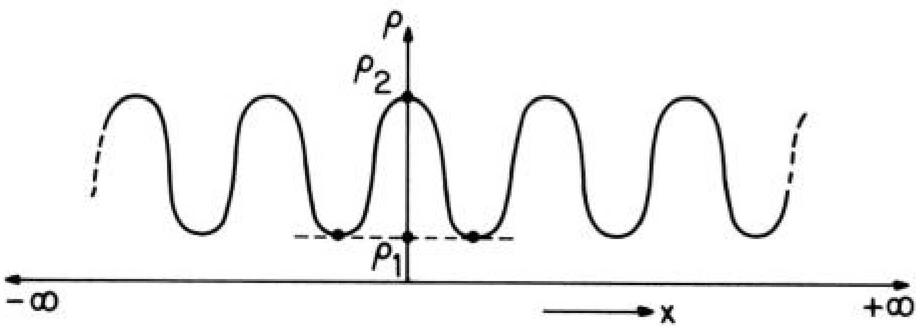
  - *Reversals (films)* $\rho \rightarrow \rho_1$ as $x \rightarrow \mp\infty$

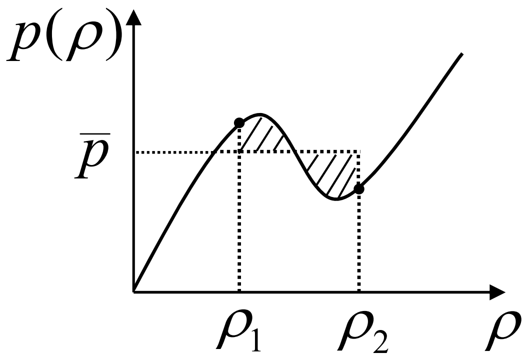






  - *Oscillations (layers)*

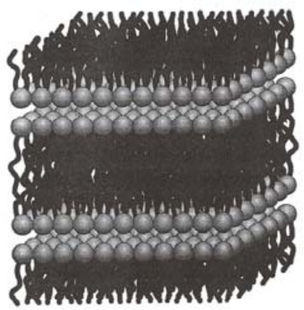




- ***General Interfaces / 3D Structures***

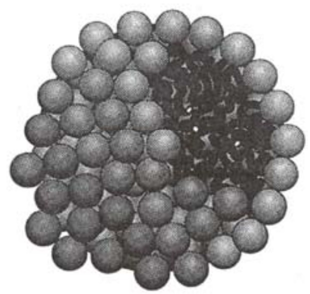
$$\nabla(-p + a\Box\rho + \tilde{b}|\nabla\rho|^2) = (c\Box\rho)\nabla\rho\,; \qquad \begin{cases} \tilde{b} = b + \dfrac{1}{2}\left(c - a\dfrac{c'}{c}\right) \\ \Box\rho \equiv \nabla^2\rho + \dfrac{1}{2}\dfrac{c'}{c}|\nabla\rho|^2 \end{cases}$$

$$\tilde{b} \not\equiv 0 \;\Rightarrow\; \rho = \rho(x)\,; \qquad \rho = \rho(r)\,; \qquad \rho = \rho(R)$$



layers

cylinders



spheres

Micelle Structures

■ VdW Variational Thermodynamics

- $F = \min \int_{-\infty}^{\infty} \left[f(\rho) + \frac{1}{2} c(\rho) \rho_x^2 \right] dx \,; \qquad \int_{-\infty}^{\infty} (\rho - \rho_o)\, dx = 0$

$$\Rightarrow \begin{cases} c\,\rho_{xx} + \frac{1}{2} c' \rho_x^2 = g - \bar{g}; \quad g = f'(\rho), \;\; \sigma = \int_{-\infty}^{\infty} c \rho_x^2 dx \\ g(\rho_1) = g(\rho_2) = \bar{g}; \qquad a = \rho c, \quad b = (\rho c' - c)/2 \end{cases}$$

$$p \equiv \rho g - f \quad \Rightarrow \quad p(\rho_1) = p(\rho_2) = \bar{p}\,; \qquad \int_{\rho_1}^{\rho_2} (p - \bar{p}) \frac{d\rho}{\rho^2} = 0$$

- *Molecular Models:* $\gamma = 2\alpha, \quad \delta = 2\beta \Rightarrow c = u/2 = \text{const}.$

- *3D Interfaces:* $\tilde{b} \equiv 0 \quad \Rightarrow \quad c\nabla^2 \rho + \frac{1}{2} c' |\nabla \rho|^2 = g(\rho) - \bar{g}$

■ Continuum Thermodynamics

- *Energy Balance (1st law):* $\rho\dot{\varepsilon} = \mathbf{T}\bullet\nabla\mathbf{v} - \operatorname{div}\boldsymbol{q} + \rho r + \hat{\varepsilon}$

- *2nd law:* $\rho\dot{\eta} + \operatorname{div}\dfrac{\boldsymbol{q}}{\theta} - \dfrac{\rho r}{\theta} \geq 0\,; \quad \psi = \varepsilon - \theta\eta = \hat{\psi}(\rho, \theta, \nabla\rho, \nabla\nabla\rho)$

- *Interstitial working:* $\hat{\varepsilon}$

(i) $\hat{\varepsilon} \equiv 0 \quad \Rightarrow \quad \psi_{\nabla\rho} = \psi_{\nabla\nabla\rho} = 0$

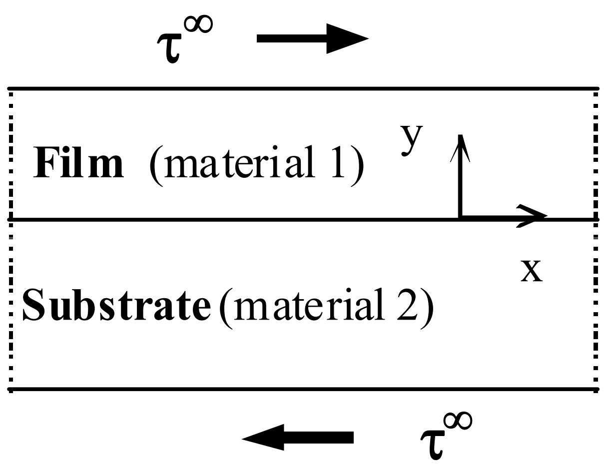
(ii) $\hat{\varepsilon} = \operatorname{div}\boldsymbol{h} \quad \Rightarrow \quad \boldsymbol{h} = \rho\,\dot{\rho}\,\psi_{\nabla\rho} \quad \Rightarrow \quad \{MR\ ,\ \gamma = 0\}$

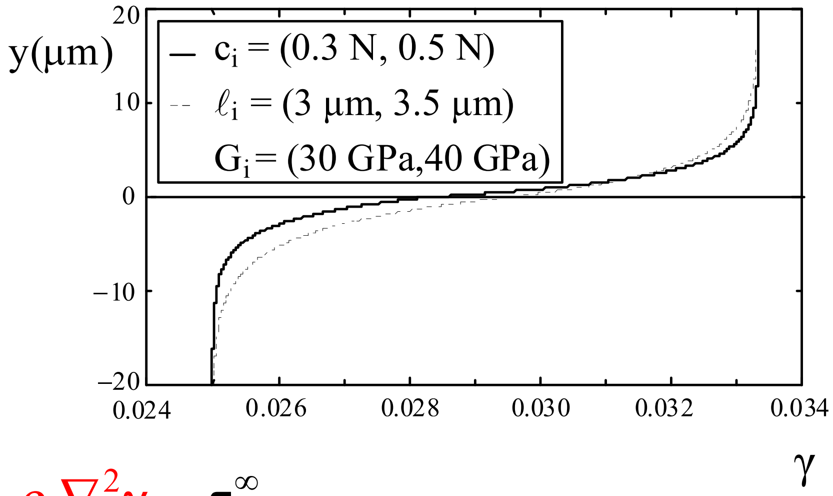
(iii) $\hat{\varepsilon} = \operatorname{div}\boldsymbol{h} + \hat{\mathbf{T}}\bullet\nabla\mathbf{v}\,; \quad \operatorname{div}\hat{\mathbf{T}} = 0 \quad \Rightarrow \quad \{MR\ ,\ \gamma \neq 0\}$

(iv) $\hat{\varepsilon} = \phi\dot{\rho} + \boldsymbol{\omega}\bullet\nabla\dot{\rho} + \hat{\mathbf{T}}\bullet\nabla\mathbf{v} \quad \Rightarrow \quad \{\neq MR\ ,\ \gamma \neq 0\}$

RECENT EXAMPLES
BENCHMARK PROBLEMS FROM SOLID MECHANICS

■ Gradient Solid / Solid Interface





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

- ***Elastic Bimaterial / Elastic Interface:*** $\kappa_i = G_i\gamma$; $\tau_I = G_I\gamma_I$

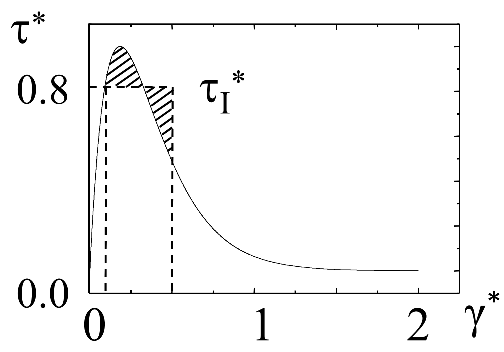
- Aifantis (1984) $\begin{cases} \gamma_1 = \gamma_2 \\ \partial\gamma_1 = \partial\gamma_2 \big|_{y=0} \end{cases} \Rightarrow \quad G_I = \dfrac{G_1 G_2\left(\sqrt{G_1/c_1} + \sqrt{G_2/c_2}\right)}{G_1\sqrt{G_2/c_2} + G_2\sqrt{G_1/c_1}}$

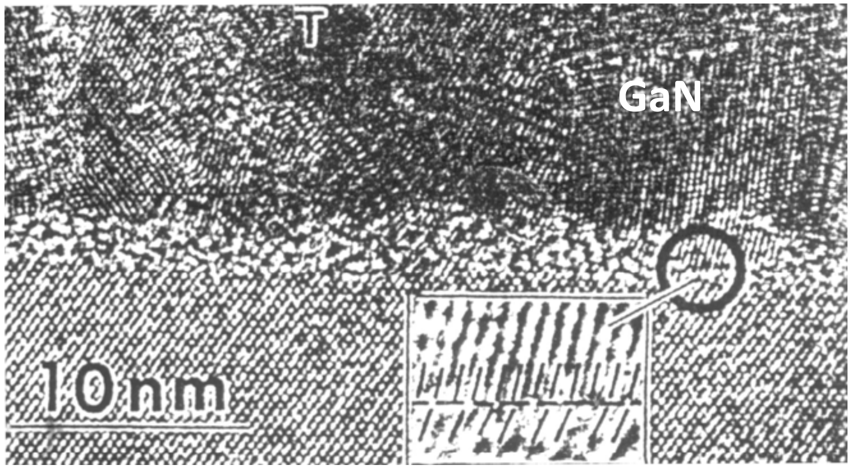
- Fleck-H (1994) $\begin{cases} \gamma_1 = \gamma_2 \\ \ell_1\partial\gamma_1 = \ell_2\partial\gamma_2 \big|_{y=0} \end{cases} \Rightarrow \quad G_I = \dfrac{G_1 G_2\left(\sqrt{G_1 c_1} + \sqrt{G_2 c_2}\right)}{G_1\sqrt{G_2 c_2} + G_2\sqrt{G_1 c_1}}$

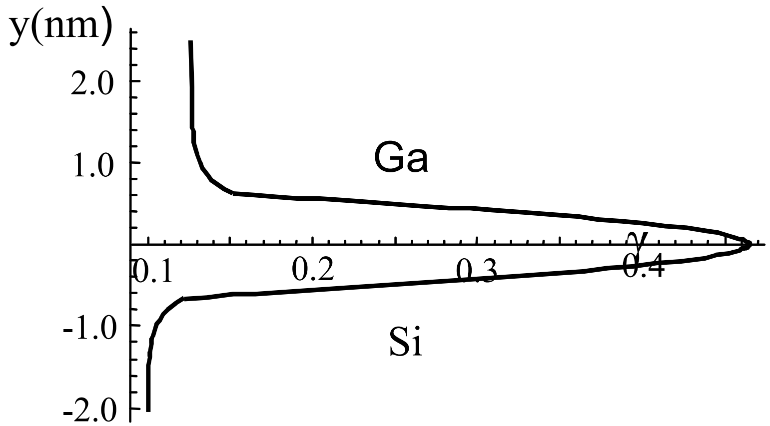
- ***Elastic Bimaterial / Inelastic Interface:*** $\boldsymbol{\kappa_i = G_i \gamma}$ **;** $\boldsymbol{\tau_I = G_I \gamma_I}$

  - *Scaled adhesive energy (Rose et al.):* $E^* = E/E_0 = -(1+\beta\gamma^*)\exp\left(-\beta\gamma^*\right)$

  - *Maxwell Rule:* $\int_{\gamma^*_\infty}^{\gamma^*_I} \left[\tau^*(\gamma^*) - \tau^*_I\right] d\gamma^* = 0$



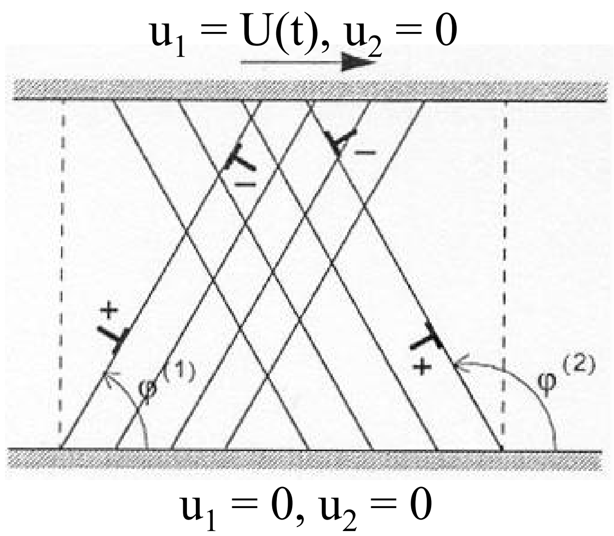




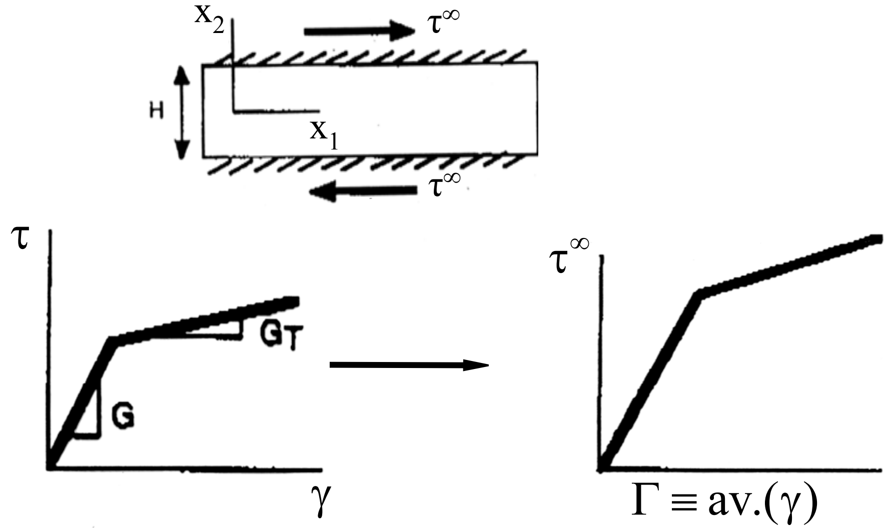
■ Plastic Boundary Layers

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

Discrete Dislocations (DD)



Fleck-Hutchinson (F-H)

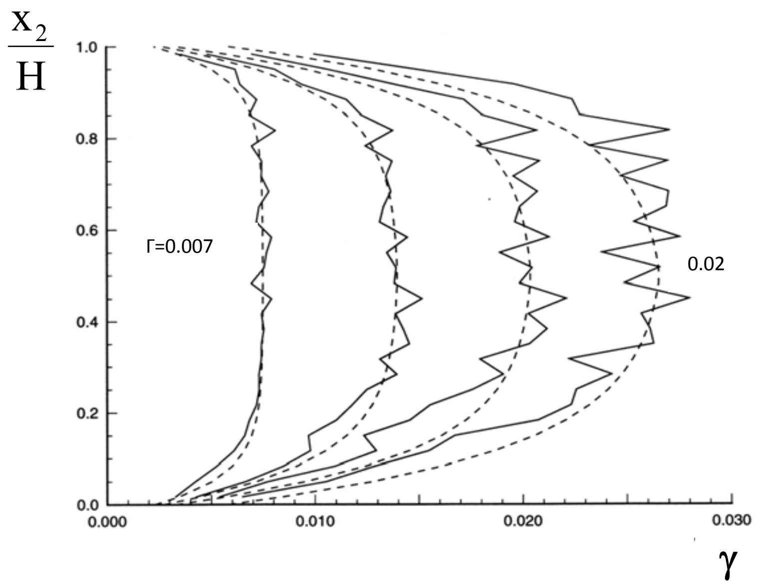


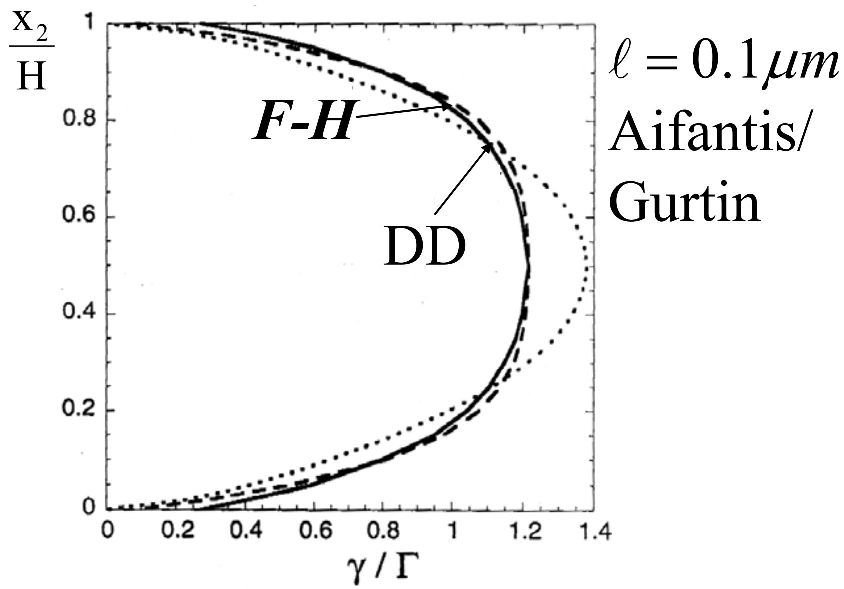
- ***Aifantis (1984) / Gurtin (2000)***

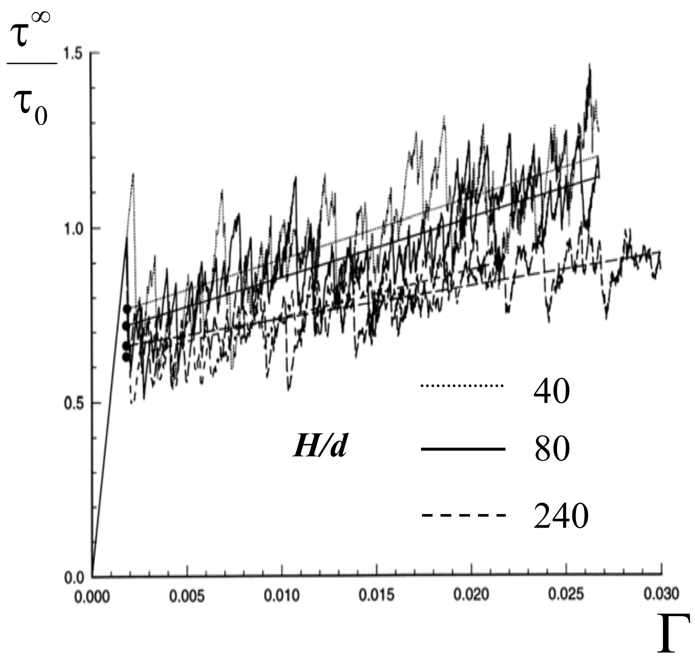
$$\tau = \tau_0 + G_T\gamma - G_T\ell^2\nabla^2\gamma = \tau^\infty \ \Rightarrow \ \gamma = \frac{\tau^\infty}{G} + \frac{\tau^\infty - \tau_0}{G_T}\left[1 - \frac{\cosh(x_2/\ell)}{\cosh(H/\ell)}\right]$$

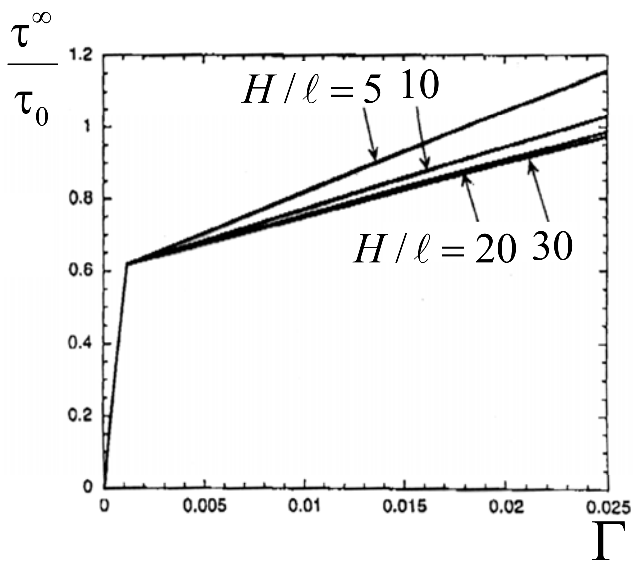
$$\Gamma = \frac{1}{H}\int_{-H/2}^{H/2} \gamma(x_2)dx_2 = \frac{\tau^\infty}{G} + \frac{\tau^\infty - \tau_0}{G_T}\left(1 - \frac{2\ell}{H}\tanh\frac{H}{2\ell}\right)$$

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



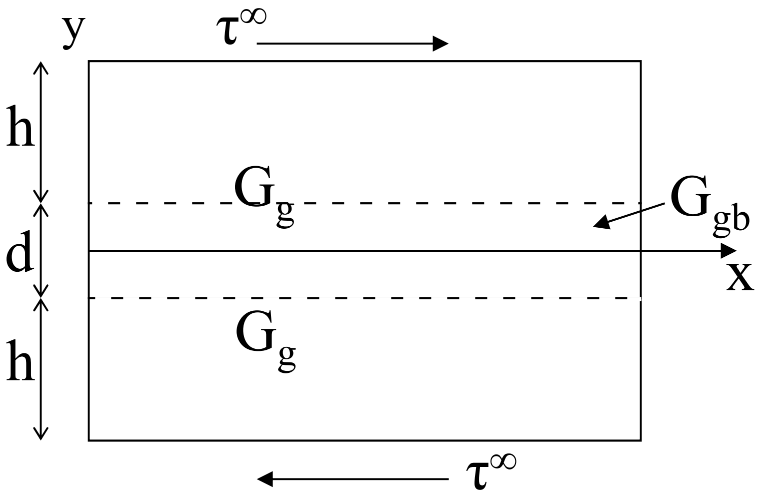






■ Effective Moduli of Nanopolycrystals

- ***Idealized Unit Cell***



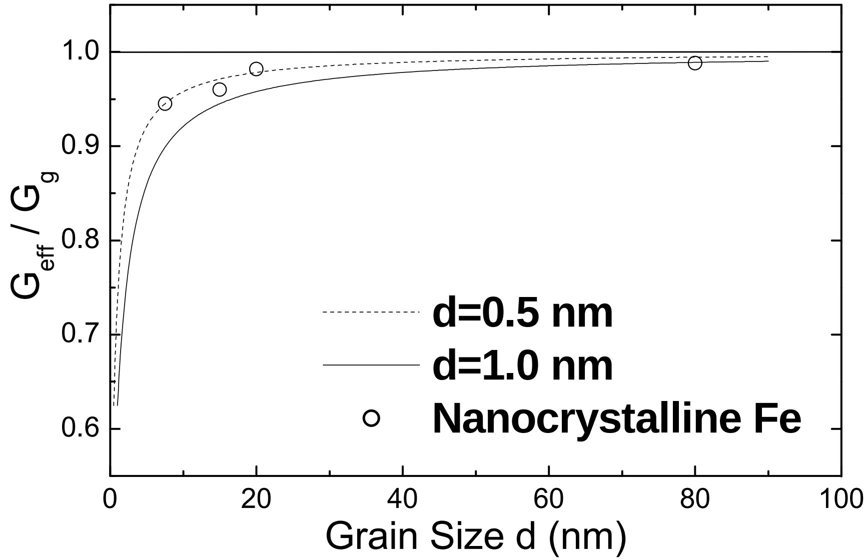
$$
\text{Bc's}\quad \begin{cases} \partial_y \gamma_{gb} = 0 & , \ y=0 \\ \left.\begin{array}{l} \gamma_g = \gamma_{gb} \\ \partial_y \gamma_g = \partial_y \gamma_{gb} \end{array}\right\} & , \ |y| = d/2 \\ \gamma_g = \tau^\infty / G & , \ |y| = h + d/2 \end{cases}
$$

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

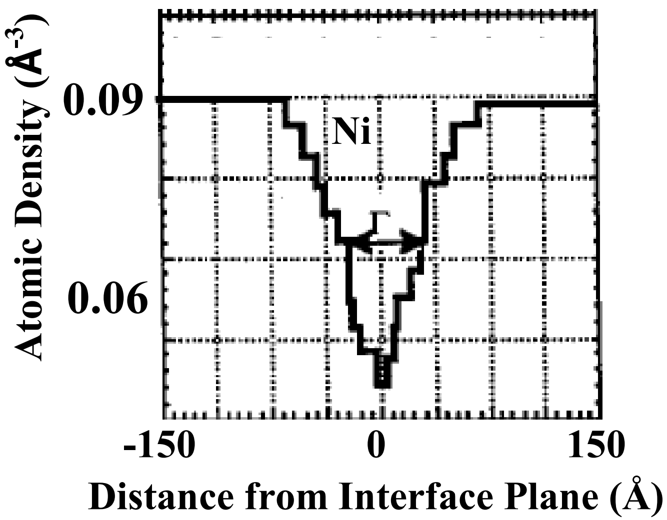
- ***Average Strain/Effective Modulus***

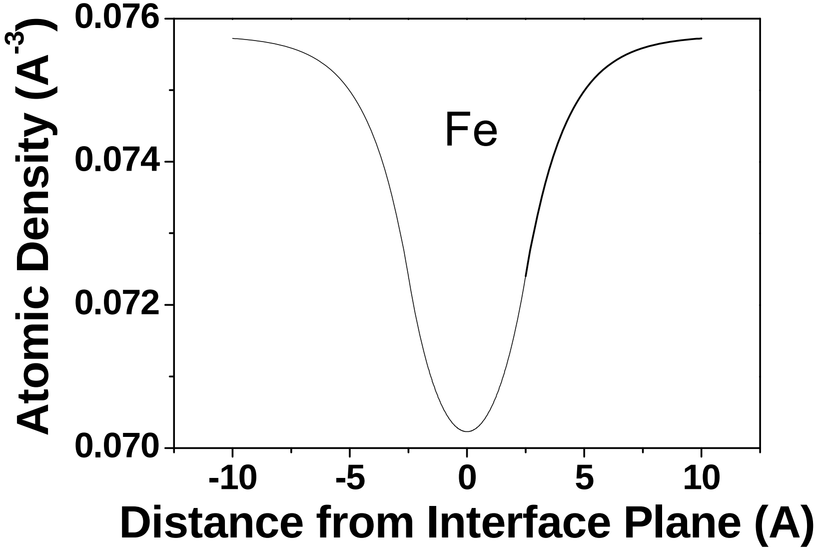
$$
\Gamma = \frac{1}{(h + d/2)} \left(\int_0^{d/2} \gamma_{gb} dy + \int_0^{h+d/2} \gamma_g dy \right), \quad G_{eff} = \tau^\infty / \Gamma
$$

- ***Size Dependence / Experiments***



- ***Observations***





■ A Note on the Origin of Gradients

- ***Self - Consistent Approximation***

- Simple Shear

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

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

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

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

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

$$\tau = \kappa(\gamma) - \frac{R^2}{10}(\beta + h)\nabla^2\gamma \quad ; \qquad \begin{cases} \beta = \alpha\mu\dfrac{7-5\nu}{15(1-\nu)} \\ h = d\bar{\tau}/d\bar{\gamma} \end{cases}$$

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

- *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)
  $$\alpha = \frac{h(7 - 5\nu')}{\{6\mu(4 - 5\nu') + 15h(1 - \nu')\}(1 - 2S_{1212})}$$
  $$\nu' = \frac{\nu h + \mu(1 + \nu)}{h + 2\mu(1 + \nu)}; \; h = \frac{d\bar{\tau}}{d\bar{\gamma}}$$

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

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

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

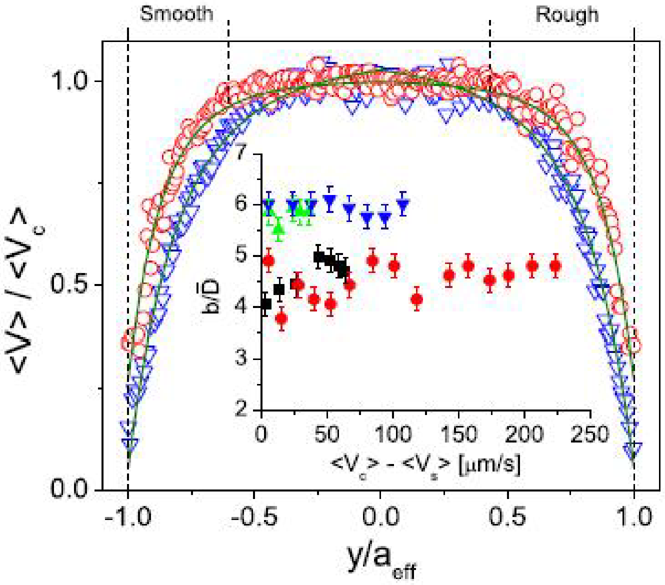
$$\dot{\alpha}_q = -Dq^2\alpha_q + \Lambda\gamma_q - M\alpha_q \;\; ; \;\; \dot{\alpha}_q \approx 0 \, , \;\; \frac{Dq^2}{M} << 1 \quad \Rightarrow \quad \alpha \approx \frac{\Lambda}{M}\gamma - \frac{\Lambda D}{M^2}\gamma_{xx}$$

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

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

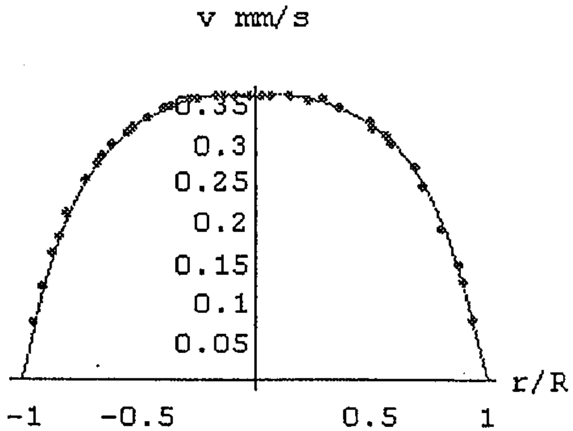
$$\therefore \quad \tau = \kappa(\gamma) - c(\gamma)\gamma_{xx} - c^*(\gamma)\gamma_x^2$$

- **L. Isa, R. Besseling & W.C.K. Poon**, Shear Zones in the Capillary Flow of Colloidal Suspensions [*Phys. Rev. Lett.* **98**, 198305 (2007)]



Averaged velocity profile as a function of y/a_{eff} for smooth (red, O) and rough (blue, ∇) walls

- **Silber et al / Goldsmith & Turitto Experiments**



Poiseuille flow of a transparent suspension through circular glass capillaries of R = 51.8 μm Ghost cells and tracer red cells; Hematocrit H = 52%

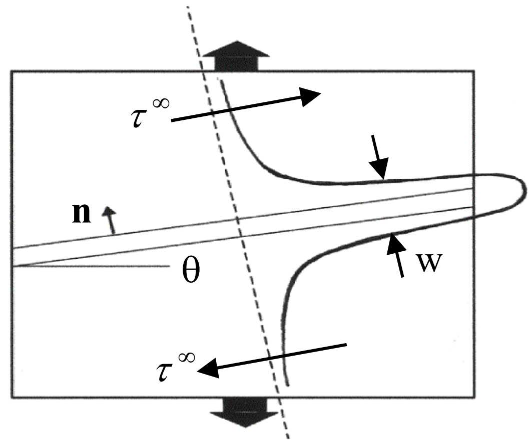
LOCALIZATION
SHEAR BANDS AND NECKS

■ Gradient Plasticity: ECA 1984 / 87, Zbib's Thesis '88

- ***Constitutive Eq.***

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

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

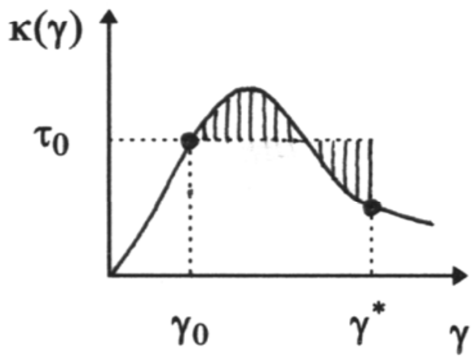


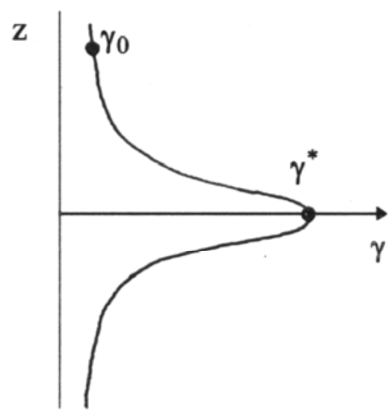
- ***Linear Stability / SB Orientation***

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

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

$$c\gamma_{zz} = \kappa(\gamma) - \tau^\infty$$

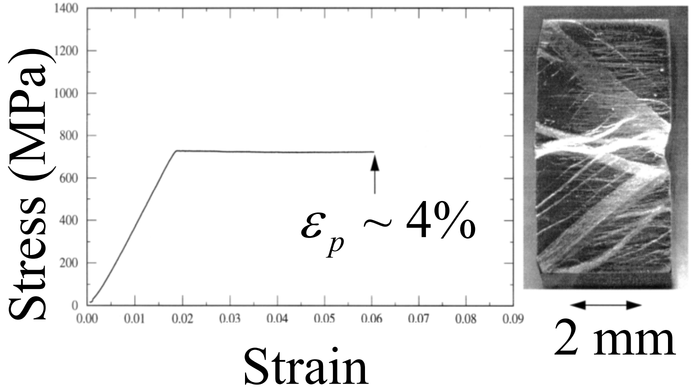




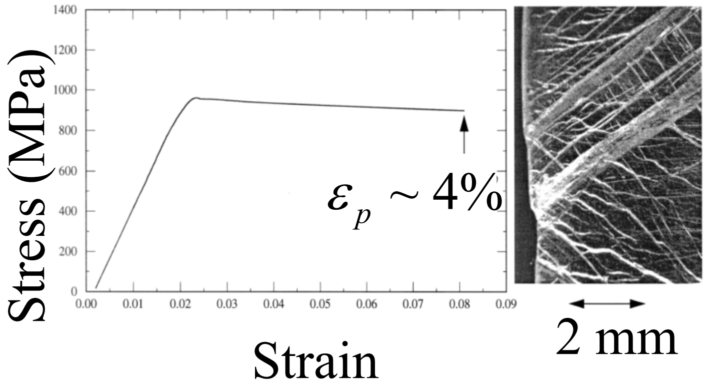
■ Bulk Nanostructured Fe – 10% Cu Polycrystals

- Compression tests

d ~1370 nm, σ_y ~750 Mpa
angle ~ 49^0



d ~540 nm, σ_y ~960 MPa
angle ~ 49^0



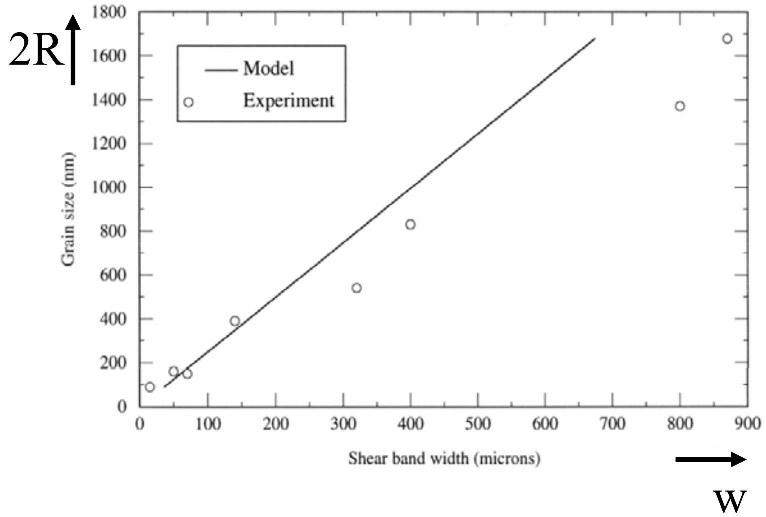
- Shear band width analysis

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

$$w \sim 0.4\sqrt{c}$$

$$c \sim \frac{R^2}{10}(\beta + h)$$

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



■ Gradient Hyperelasticity: Triantafyllidis/ECA '86

- ***Strain Energy***

$$W = W(\mathbf{F}) + c\,h(\mathbf{F}, \nabla\mathbf{F}) \quad \text{.......} h \text{ quadratic in } \mathbf{G} = \nabla\mathbf{F}$$

- $c = 0$: Equilibrium / Loss of Ellipticity

$$\text{Div}\left[W_{\mathbf{F}}\right] = 0 \quad , \quad \text{Det}\left[W_{\mathbf{FF}}\mathbf{n} \otimes \mathbf{n}\right] \leq 0$$

n unit vector perpendicular to localized zone

- $c \neq 0$: Equilibrium / Ellipticity

$$\text{Div}\left[W_{\mathbf{F}} + c\left(h_{\mathbf{F}} - \text{Div}h_{\nabla\mathbf{F}}\right)\right] = 0$$

$$cB_{ijklmn}\alpha_i\alpha_l n_j n_k n_m n_n > 0 \quad \begin{cases} B_{ijklm} \equiv \dfrac{\partial^2 h}{\partial G_{ijk}\partial G_{lmn}} \\ h = \dfrac{1}{2}G_{ijk}G_{lmn}B_{ijklmn} \end{cases}$$

- ***3-D Localized Deformation Solution***

$$\mathbf{x} = \overset{\circ}{\mathbf{F}}\,\mathbf{X} + \mathbf{a}\,f\left(y\right) \;;\; y = \mathbf{n}\cdot\mathbf{X} \;;\; \mathbf{F} = \overset{\circ}{\mathbf{F}} + \gamma\,\mathbf{a}\otimes\mathbf{n} \;;\; \gamma = f'$$

$$c\,h\,\gamma_{yy} + \frac{1}{2}c\,h'\,\gamma_y^2 = \frac{\mathrm{d}W}{\mathrm{d}\gamma} - \tau_\infty \;;\; \gamma\left(y \to \pm\infty\right) = \gamma_\infty \;;\; \gamma_{max} = \gamma_*$$

(f …shape ; $\mathbf{n}$ … $\perp$ band direction , $\mathbf{a}$ …amplitude)

- ***Conditions of Existence of Solutions***

(i) $\dfrac{\mathrm{d}W}{\mathrm{d}\gamma_\infty} > \dfrac{\mathrm{d}W}{\mathrm{d}\gamma_*} \Rightarrow \dfrac{\mathrm{d}^2W}{\mathrm{d}\gamma^2} \le 0 \Rightarrow \left[\dfrac{\partial^2 W}{\partial F_{\mathrm{ij}}\partial F_{kl}}\right] a_i a_k n_j n_l \le 0$

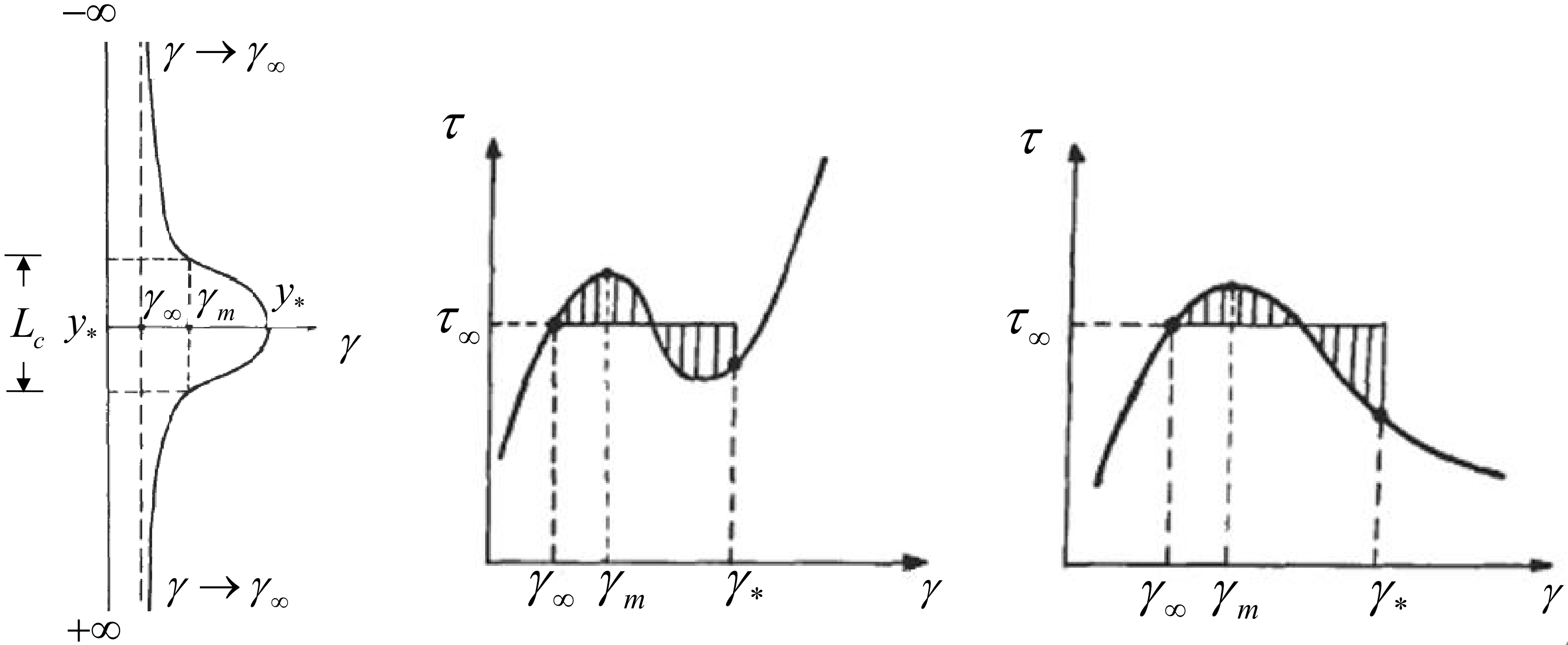
Classical ellipticity condition: determines band direction

(ii) $W\left(\gamma_*\right) - W\left(\gamma_\infty\right) = \dfrac{\mathrm{d}W}{\mathrm{d}\gamma_\infty}\left(\gamma_* - \gamma_\infty\right)$ **,** i.e. Maxwell's line

- ***Solution***

$$y = y_0 - \sqrt{c} \int_{\gamma(y_0)}^{\gamma(y)} \frac{h(\gamma)\mathrm{d}\gamma}{2\left[W(\gamma) - W(\gamma_\infty) - \mathrm{d}W/\mathrm{d}\gamma_\infty(\gamma - \gamma_\infty)\right]^{1/2}}$$

$$L_c = \Delta y = \sqrt{c} \int_{\gamma_m}^{\gamma_*} \frac{h(\gamma)\mathrm{d}\gamma}{2\left[W(\gamma) - W(\gamma_\infty) - \mathrm{d}W/\mathrm{d}\gamma_\infty(\gamma - \gamma_\infty)\right]^{1/2}}$$



- ***Blatz – Ko Material***

- $$W_{BK} = \frac{\mu}{2}\left[\frac{\mathrm{II}_C}{\mathrm{III}_C} + 2\sqrt{\mathrm{III}_C} - 5 \right]$$

$$W_1 = W_{BK} + \frac{c}{2}\frac{\partial F_{ij}}{\partial X_k}\frac{\partial F_{ij}}{\partial X_k} \quad \left(W_2 = W_{BK} + \frac{c}{2}\frac{\partial C_{ij}}{\partial X_k}\frac{\partial C_{ij}}{\partial X_k} \right)$$

- For $\quad \mathring{\mathbf{F}} = \mathbf{1}\ \ \&\ \ \mathbf{a}\cdot\mathbf{n} \equiv \phi\,;\ \ \mathrm{II}_C = 3 + 4\phi\gamma + \left(1+\phi^2\right)\gamma,\ \ \mathrm{III}_C = \left(1+\phi\gamma\right)^2$

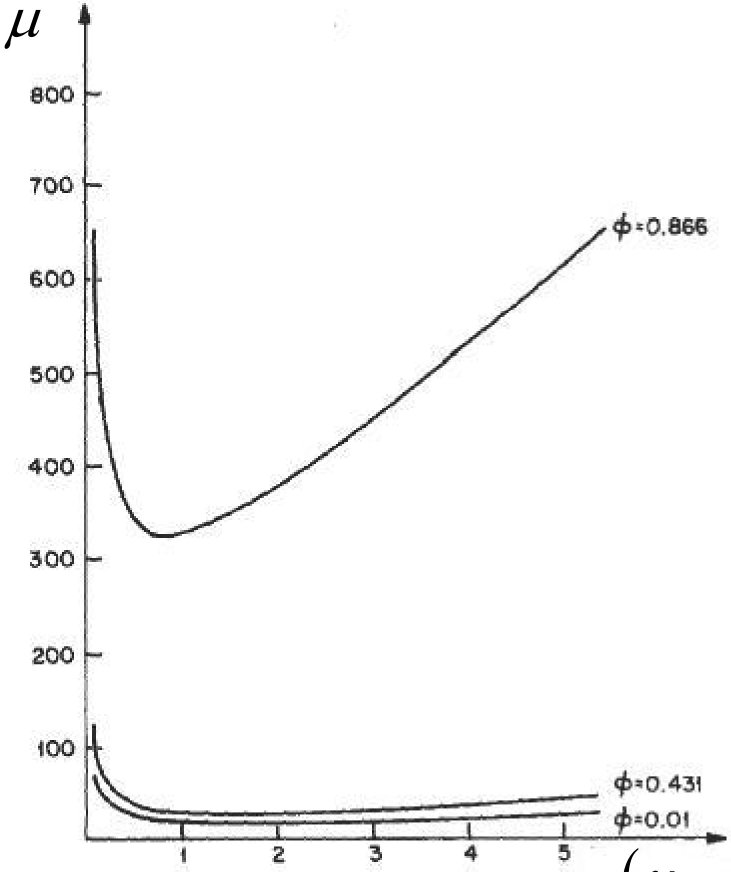
$$W_{BK} = \mu\left[\left(\frac{1}{2\phi^2} + \delta \right)\left(1 - \frac{1}{\delta} \right) \right] \quad , \quad \delta = 1 + \gamma\phi$$

- $$\gamma_m = \frac{1+2\phi^2}{2\phi\left(1-\phi^2\right)} \quad ; \quad \gamma_* = F\left(\gamma_\infty\right)$$

$$L_C = \frac{2}{\phi}\left(\frac{c}{\mu}\right)^{1/2} \int_{\gamma_m}^{\gamma_*} \left(\frac{0.5}{H}\right)^{1/2} \mathrm{d}\gamma$$

$$H=\left(\frac{1}{2\phi^2}+\delta\right)\left(1-\frac{1}{\delta}\right)^2-\left(\frac{1}{2\phi^2}+\delta_\infty\right)\left(1-\frac{1}{\delta_\infty}\right)^2-\left(\frac{1}{\phi^2\delta_\infty^2}+\frac{1}{\delta_\infty}+1\right)(\delta-\delta_\infty)$$

$L_C/\sqrt{c/\mu}$



$(\gamma_*-\gamma_\infty)/\gamma_m$

▪ Statistical / Random Aspects

- ***Microscopic vs. Macroscopic Constitutive Eq.***

$$\sigma = \kappa(\varepsilon) \qquad \text{vs.} \qquad \bar{\sigma} = \bar{\kappa}(\bar{\varepsilon})\,; \quad \bar{\varepsilon} = \langle \varepsilon \rangle, \quad \bar{\sigma} = \langle \sigma \rangle$$

(σ, ε) ... random microscopic fields

$(\bar{\sigma}, \bar{\varepsilon})$ ... average macroscopic fields

- ***Taylor expansion + Averaging***

$$\sigma = \kappa(\varepsilon) + (\varepsilon - \bar{\varepsilon})\frac{\partial \kappa}{\partial \varepsilon} \quad \Rightarrow \quad \bar{\sigma} + c_\sigma \frac{\partial^2 \bar{\sigma}}{\partial x^2} = \bar{\kappa}(\bar{\varepsilon}) + c_\varepsilon \frac{\partial^2 \bar{\varepsilon}}{\partial x^2}$$

$$c_\sigma \equiv \left(\left. \frac{\partial^2 \Lambda(r)}{\partial r^2} \right|_{r=0} \right)^{-1}; \quad c_\varepsilon \equiv h \left(\left. \frac{\partial^2 \Lambda(r)}{\partial r^2} \right|_{r=0} \right)^{-1}; \quad h \equiv \frac{\partial \bar{\kappa}}{\partial \bar{\varepsilon}}$$

$\Lambda(r)$ ... correlation function ; h ... hardening coefficient

▪Bulk Nanostructured Fe-10%Cu Polycrystals

- ***Compression Tests – Shear Band Patterns***

grain size: 150nm

$\ell_{cor} = 85\mu m$

grain size: 300nm

$\ell_{cor} = 386\mu m$

grain size: 830nm

$\ell_{cor} = 1143\mu m$

- ***Correlation Function and Corresponding Correlation Length***

  - *Moving Average Process*

$$\xi_L = \frac{1}{L}\int_{x-L/2}^{x+L/2} \xi(x)dx \, , \qquad \begin{cases} \xi(x): & \text{stationary random process} \\ L: & \text{window of observation} \end{cases}$$

  - *Variance/Correlation Function + Correlation Length*

$$f(L) = g_L^2 / g^2 \, , \quad f(L) = \frac{2}{L}\int_0^L (1-\frac{r}{L})\Lambda(r)dr \, ; \qquad g^2: \text{ variance}$$

$$\Lambda(r) = \left\{1 - \frac{m-1}{2}\left(\frac{|r|}{\ell_{cor}}\right)^m\right\}\left\{1+\left(\frac{|r|}{\ell_{cor}}\right)^m\right\}^{-2-\frac{1}{m}} , m = 2$$

$$\ell_{cor} = \lim_{L\to\infty} L\, f(L)$$

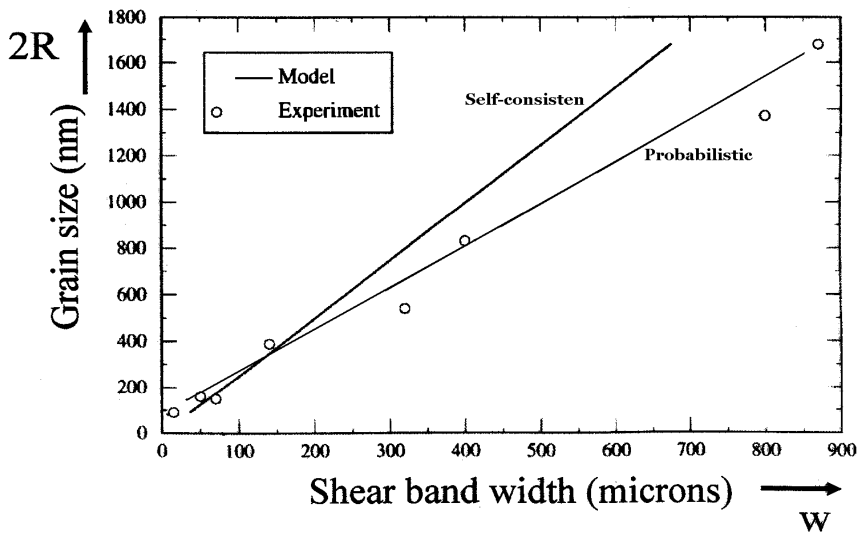
- *Shear band width analysis*

$$\tau = k(\gamma) - c\nabla^2\gamma, \qquad c = -h\left(\left.\frac{\partial^2 \Lambda(r)}{\partial r^2}\right|_{r=0}\right)^{-1} = -h\,\ell_{cor}^2, \qquad w = \alpha\sqrt{c}$$

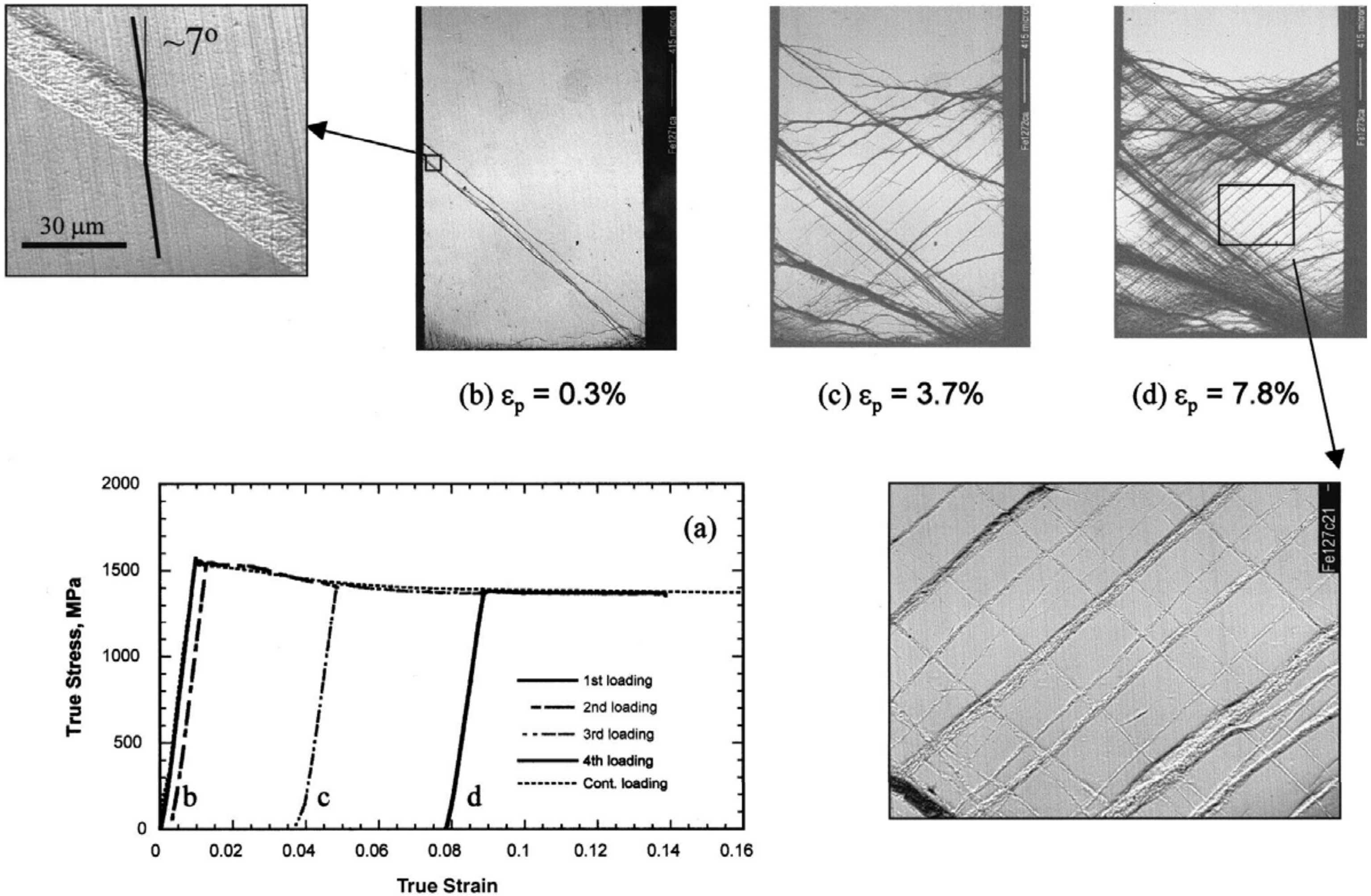
- *Calibration for 300nm grain size*

$$w = \alpha\sqrt{-h\left(\partial^2 \Lambda(r)/\partial r^2\big|_{r=0}\right)^{-1}} = \alpha\sqrt{-h}\,\ell_{cor} \rightarrow \alpha^2(-h) \approx 0.85$$

- *Modeling of experimental data*



■ More on Nano Shear Bands: n-Fe (Ma et al)



Stress-strain behavior and development of shear bands. Compression test of a Fe sample with an average grain size of 268 nm with loading, unloading, and reloading at various strain levels (~0.3%, 3.7%, and 7.8%).

▪Neck Formation / Propagation

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

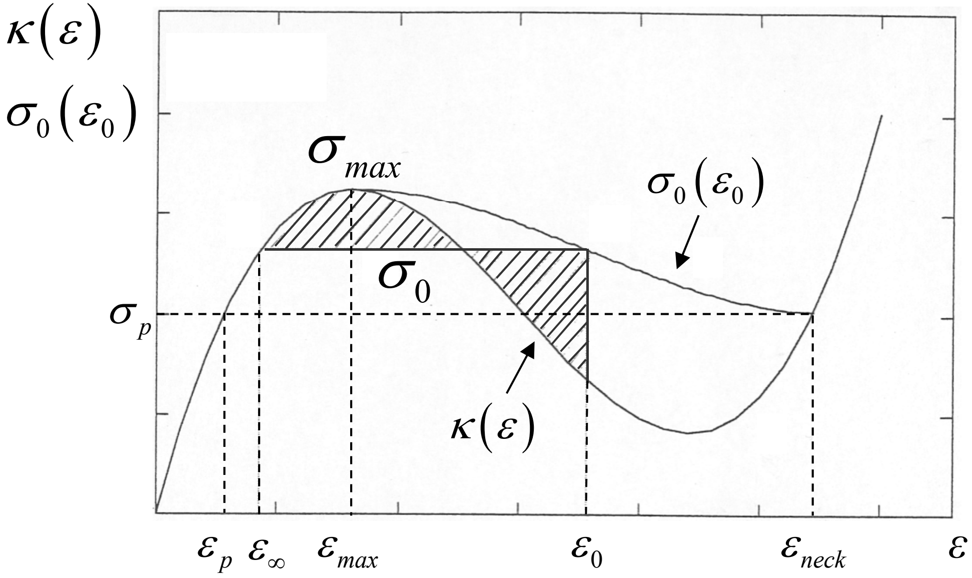
$$\sigma = \kappa(\varepsilon) - c\frac{\partial^2 \varepsilon}{\partial x^2} \qquad \partial\sigma/\partial x = 0 \Rightarrow \sigma = \sigma_0$$

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

- ***Neck Formation***

$$\kappa(\varepsilon) = A\varepsilon^3 + B\varepsilon^2 + C\varepsilon \qquad \text{bc's: } \partial_x \varepsilon_0 = 0, \quad \varepsilon(\infty) = \varepsilon_\infty$$

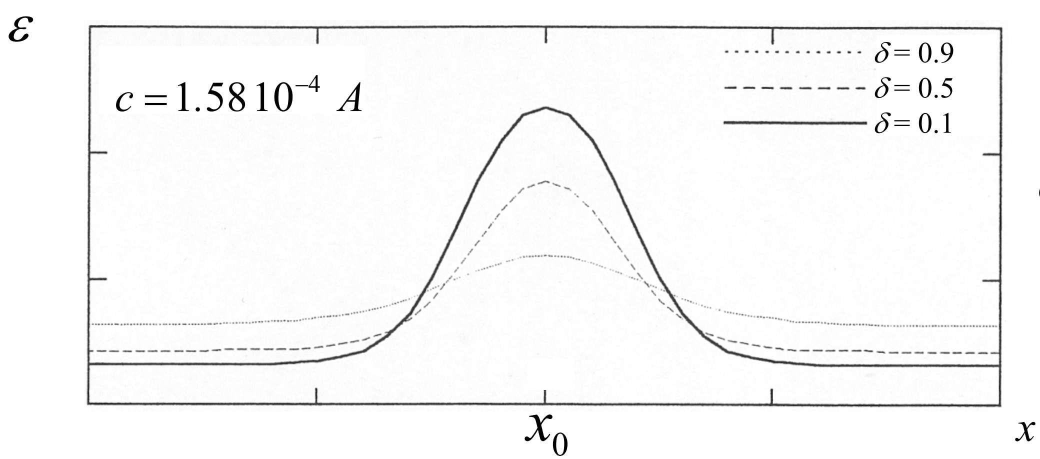
$$x - x_0 = \pm\int_{\varepsilon_0}^{\varepsilon}\left(\frac{2}{c}\int_{\varepsilon_\infty}^{\varepsilon}\left(A\varepsilon^3 + B\varepsilon^2 + C\varepsilon - \sigma_0\right)d\varepsilon\right)^{-1/2} d\varepsilon$$



$$\sigma_{max} \geq \sigma_0 \geq \sigma_p$$

$$\varepsilon_{max} \geq \varepsilon_\infty \geq \varepsilon_p$$

$$\varepsilon_{max} \leq \varepsilon_0 \leq \varepsilon_{neck}$$

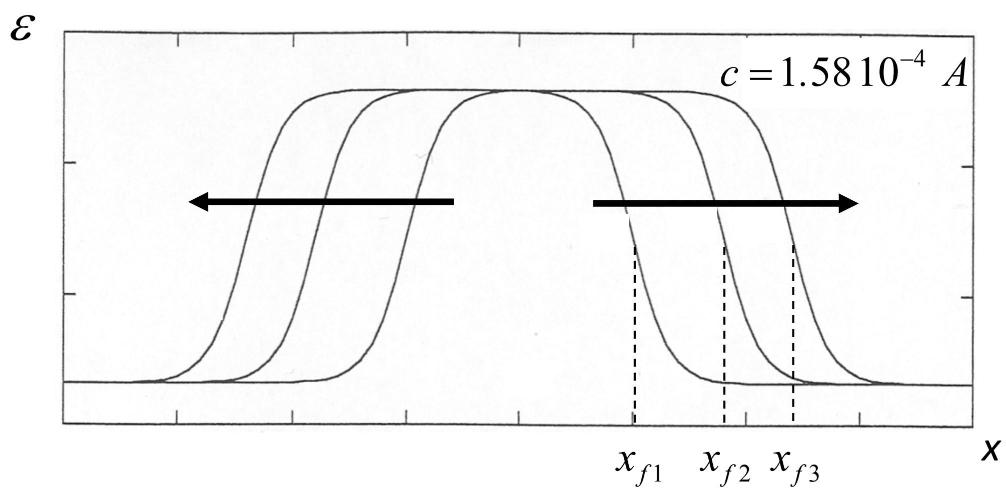


$$\delta = \frac{\sigma_0 - \sigma_p}{\sigma_{max} - \sigma_p}$$

- ***Neck Propagation***

$\sigma_0 = \sigma_p$ (Maxwell stress) bc's: $\varepsilon(\infty) = \varepsilon_p$, $\varepsilon(x_{ft}) = \varepsilon_{ft}$

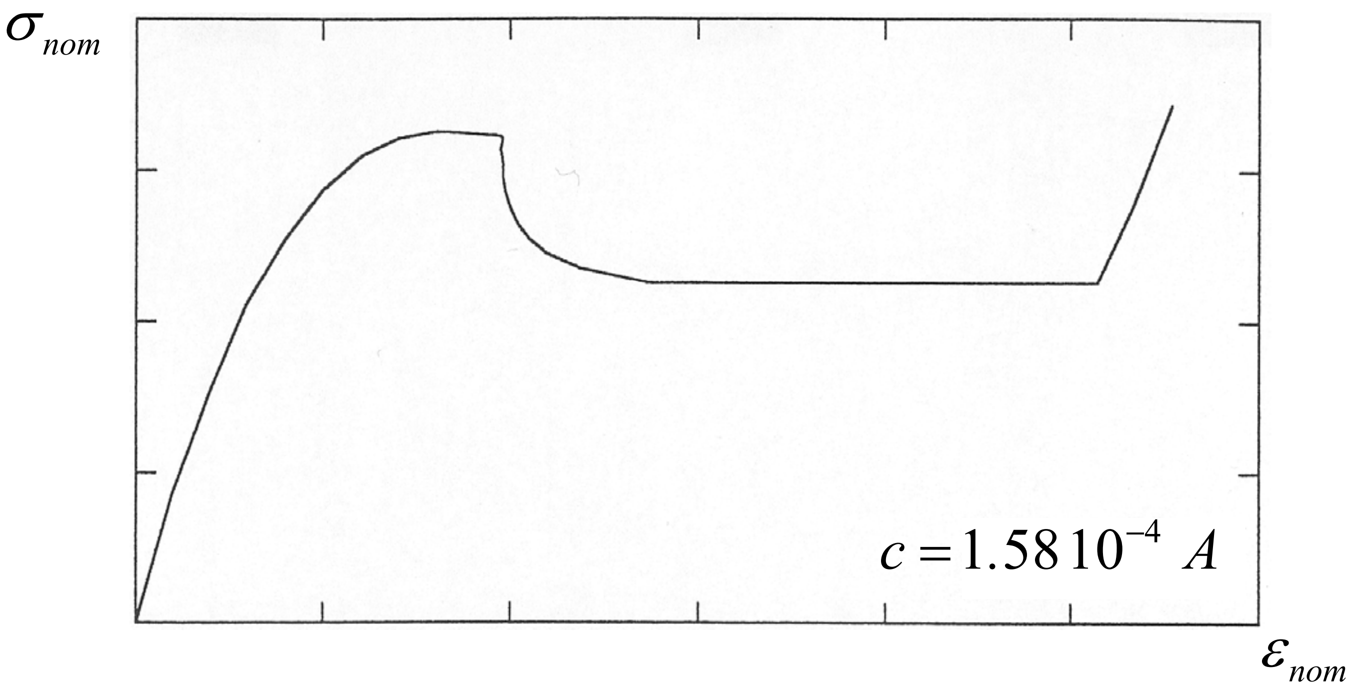
$$x - x_{fi} = \pm \int_{\varepsilon_{fi}}^{\varepsilon} \left(\frac{2}{c} \int_{\varepsilon_p}^{\varepsilon} \left(A\varepsilon^3 + B\varepsilon^2 + C\varepsilon - \sigma_p \right) d\varepsilon \right)^{-1/2} d\varepsilon$$



- ***Nominal Stress – Nominal Strain Curve***

$$\sigma_{nom} = \sigma_0$$

$$\varepsilon_{nom} = \frac{L - L_0}{L_0}; \qquad L_0 = \int_{-L/2}^{L/2} \left[1 + \varepsilon(x)\right]^{-1} dx$$



▪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” parameter

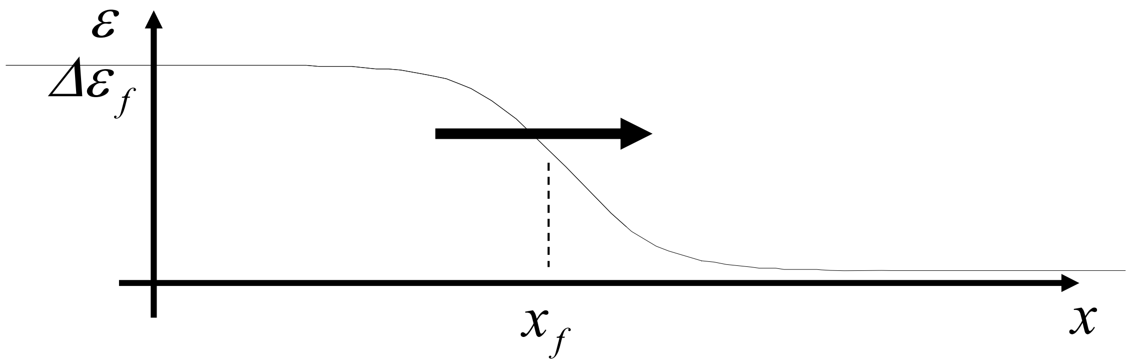
$$\therefore \quad \sigma_0 = \kappa(\varepsilon) + \delta f(\varepsilon, x) - c\frac{\partial^2 \varepsilon}{\partial x^2} \qquad (c = 1)$$

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

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

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

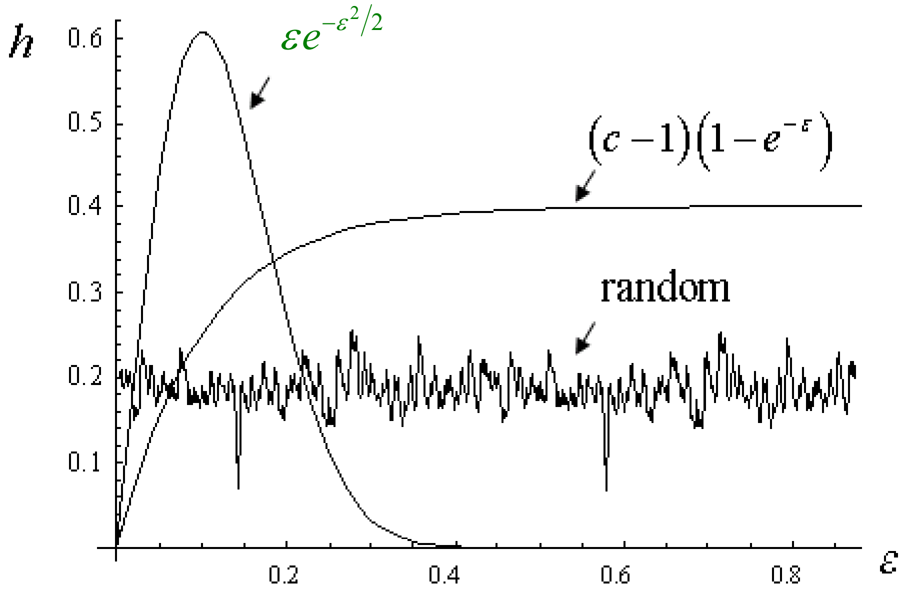
– *Front "locus" shifts along specimen* $\varepsilon=\varepsilon(x-x_f)$



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

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

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



- ***Implementation***

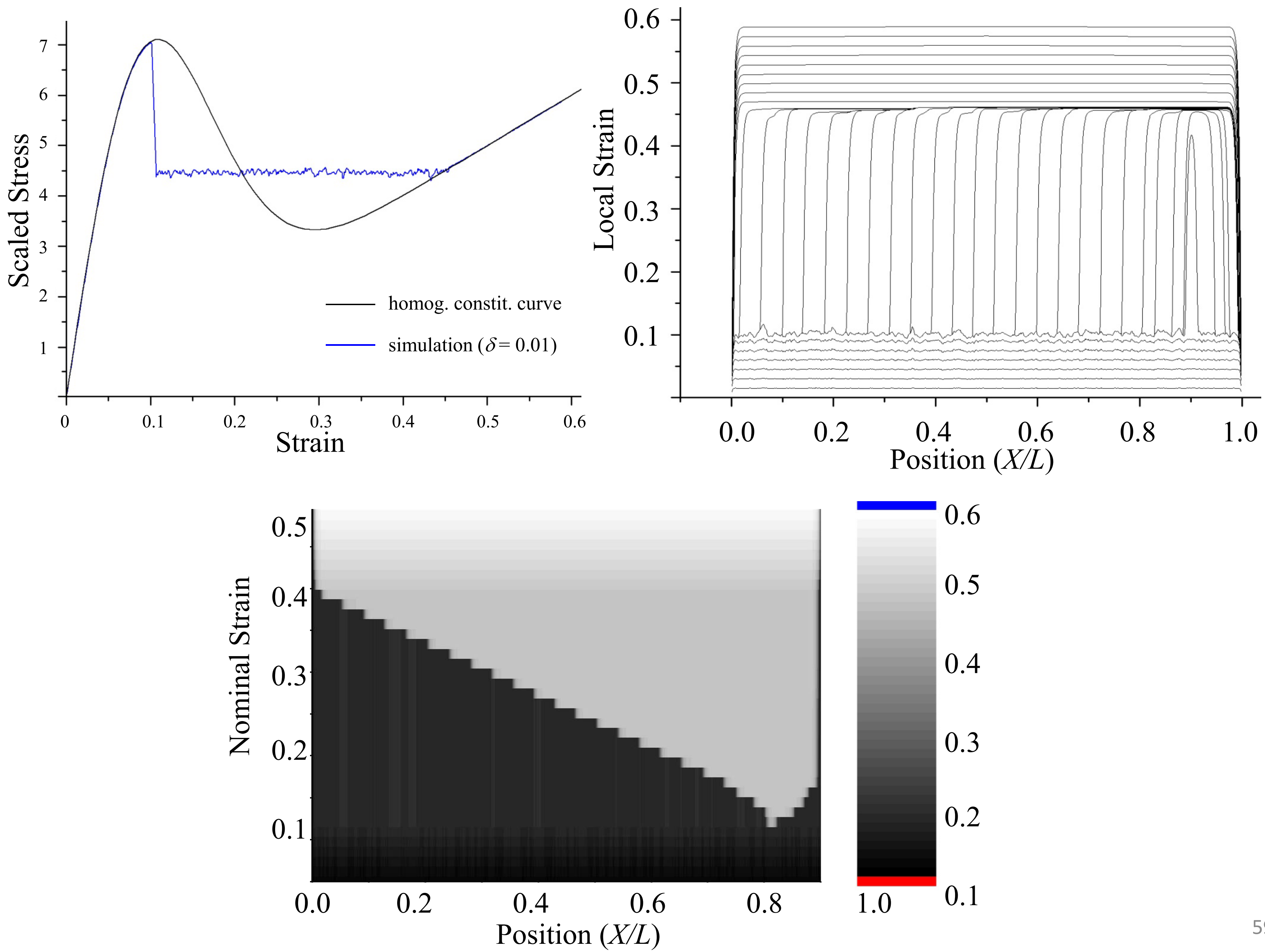
$$\kappa(\varepsilon) = \varepsilon\, e^{-\varepsilon^2/2} + \theta\varepsilon\ ; \qquad \theta = \text{const.}\ \ldots\ \text{linear hardening}$$

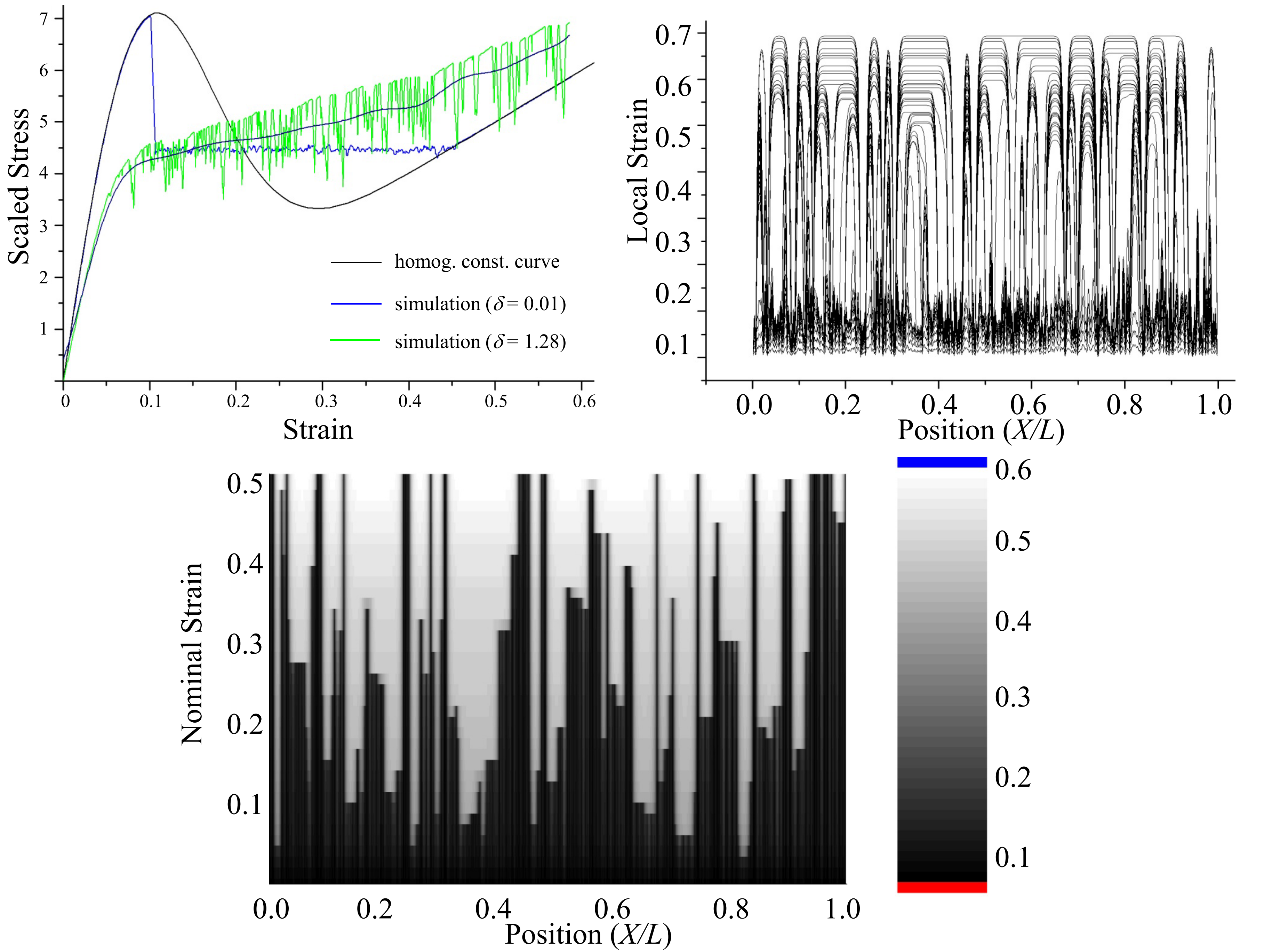
$$V(\varepsilon) = e^{-\varepsilon^2/2} - \frac{\theta}{2}\varepsilon^2$$

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

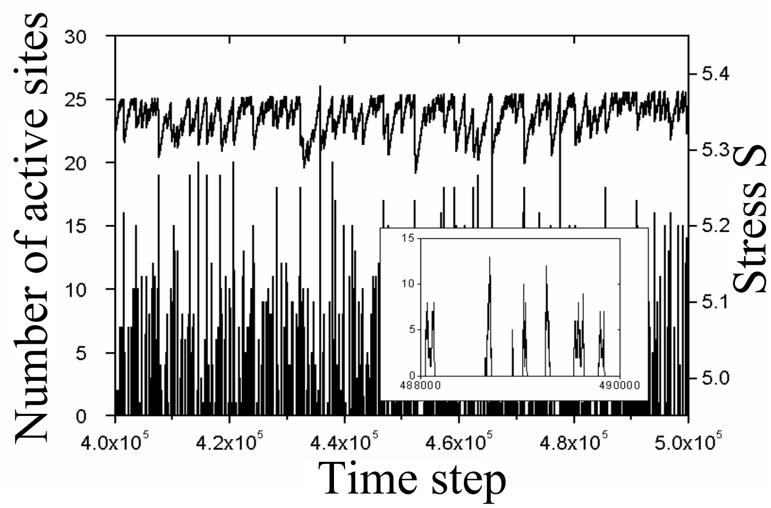
$$x - x_0 = \int_{\varepsilon_{-\infty}}^{\varepsilon} \frac{d\varepsilon}{\sqrt{-2\left[e^{-\varepsilon^2/2} - \frac{\theta}{2}\varepsilon^2 + \sigma_0(\varepsilon - \varepsilon_{-\infty})\right]} - V(\varepsilon - \varepsilon_{-\infty})}$$

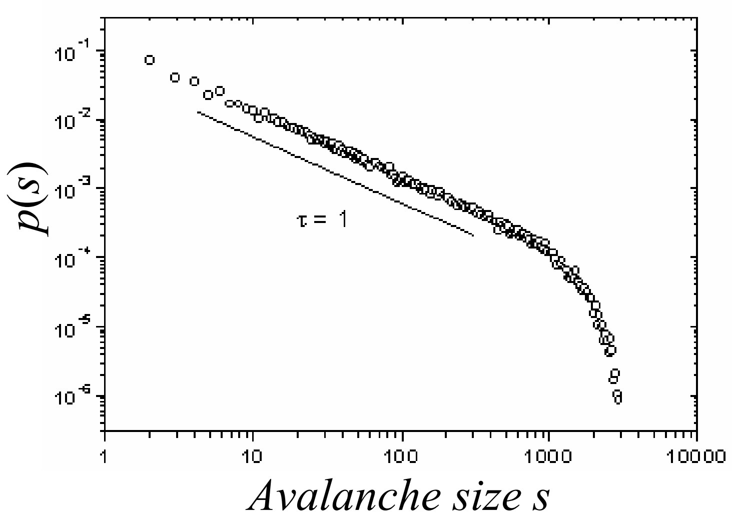
$$\left\langle \delta\sigma_1^2 \right\rangle = \xi \frac{\delta^2}{\left(\Delta\varepsilon_f\right)^2} \int_{\varepsilon_{-\infty}}^{\varepsilon_{\infty}} \left(-2\left[e^{-\varepsilon^2/2} - \frac{\theta}{2}\varepsilon^2 + \sigma_0\varepsilon - V(\varepsilon_\infty)\right]\right) \varepsilon^2 e^{-\varepsilon^2}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


Scaled Stress
Strain
homog. constit. curve
simulation (δ = 0.01)
Local Strain
Position (X/L)
Nominal Strain
Position (X/L)
0.6
0.5
0.4
0.3
0.2
0.1
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)

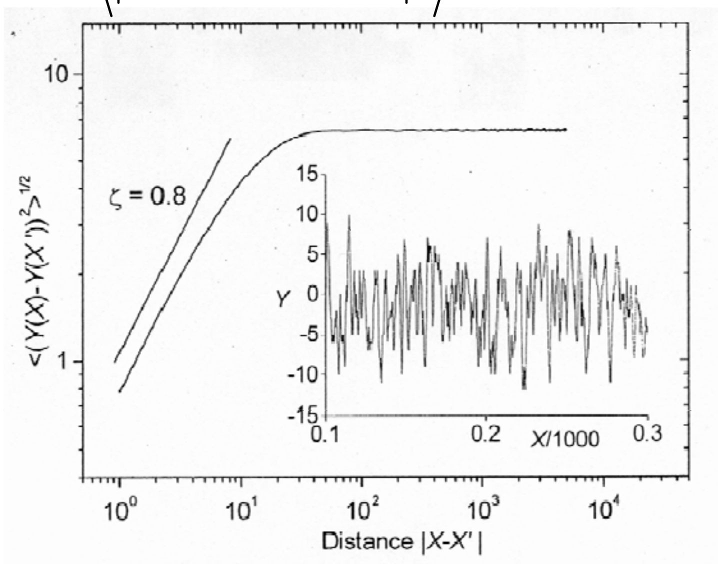
- ***Slip Patterning / Avalanches***

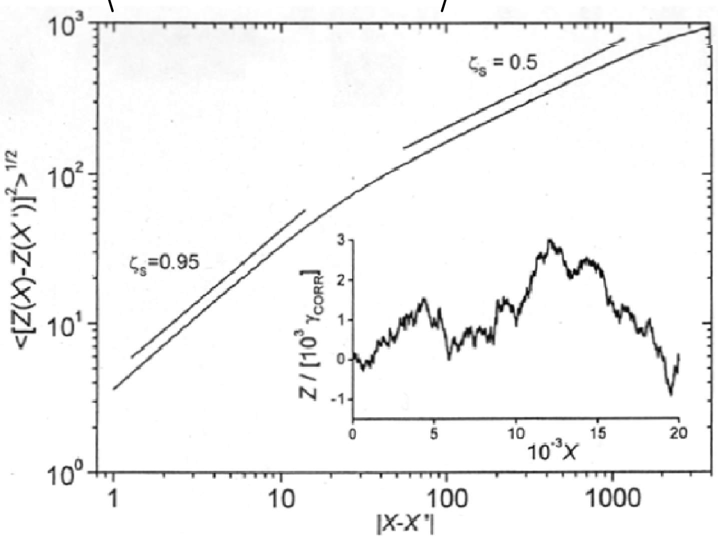




- ***Strain Distribution Y(X) / Surface Profile Z(X)***

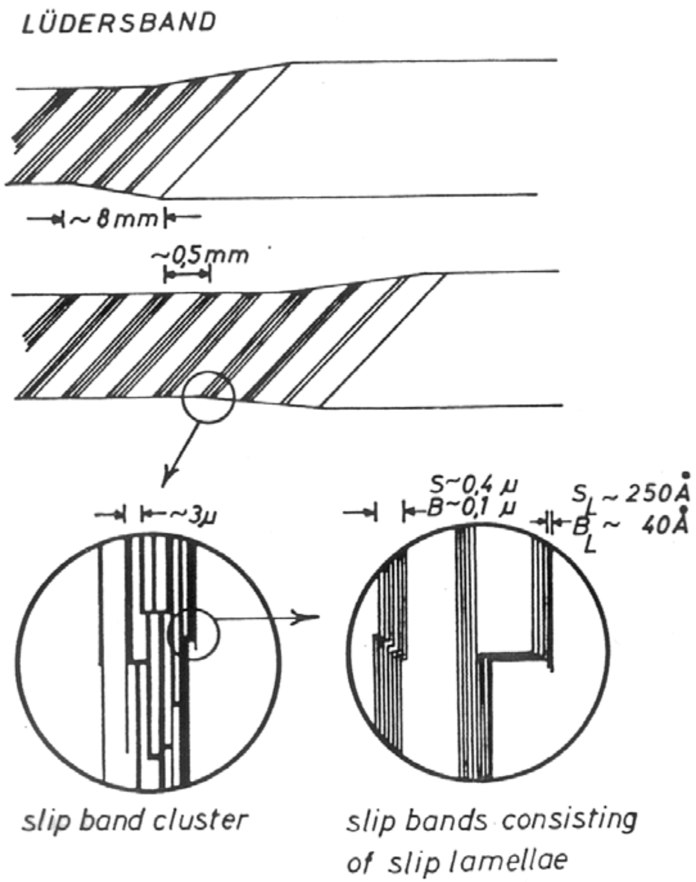
$$\left\langle \left| Y(X) - Y(X') \right|^2 \right\rangle^{1/2} \sim \left| X - X' \right|^{\zeta} \qquad \left\langle \left| Z(X) - Z(X') \right|^2 \right\rangle^{1/2} \sim \left| X - X' \right|^{\zeta}$$

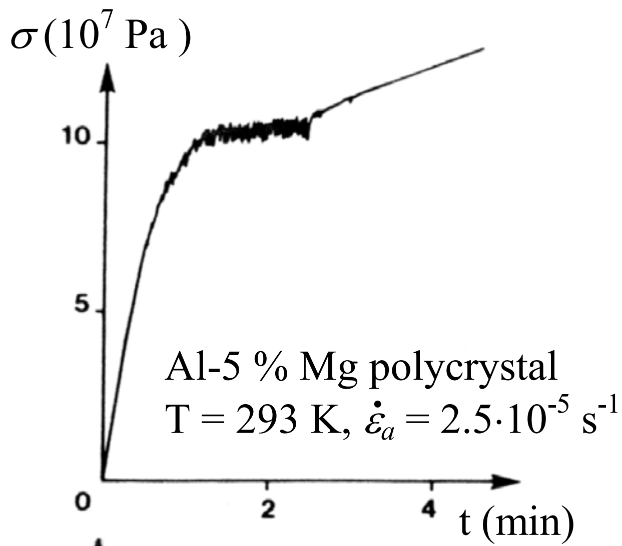


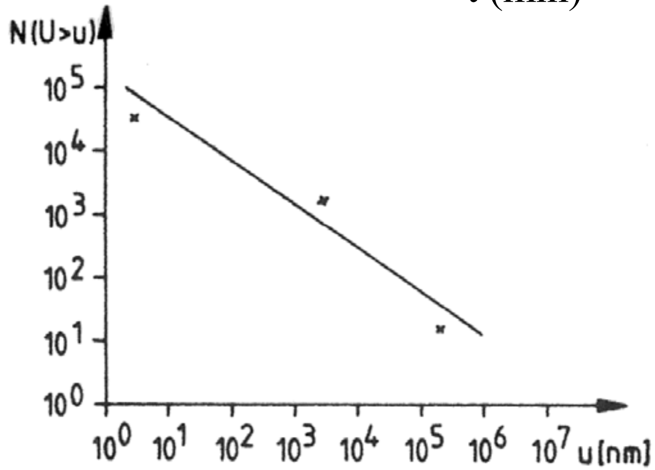


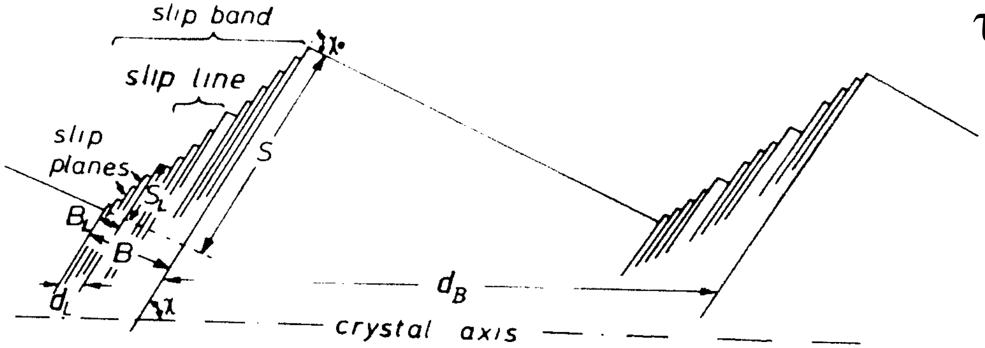
MORE ON TRAVELLING DEFORMATION BANDS

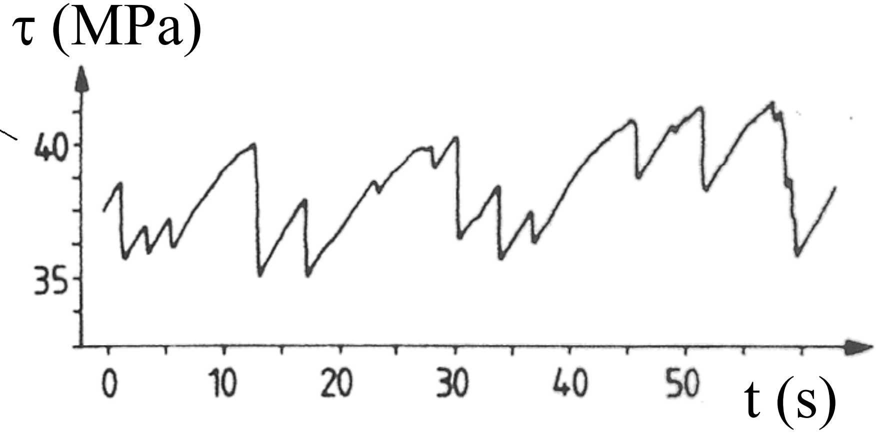
■ Lüders bands (LB)

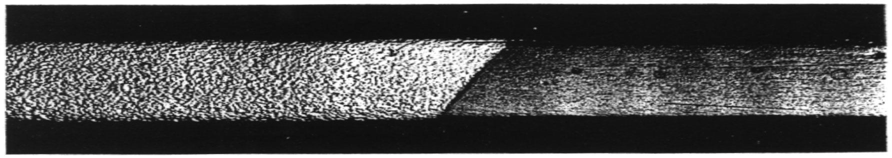


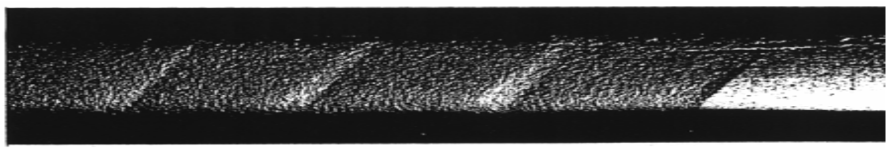


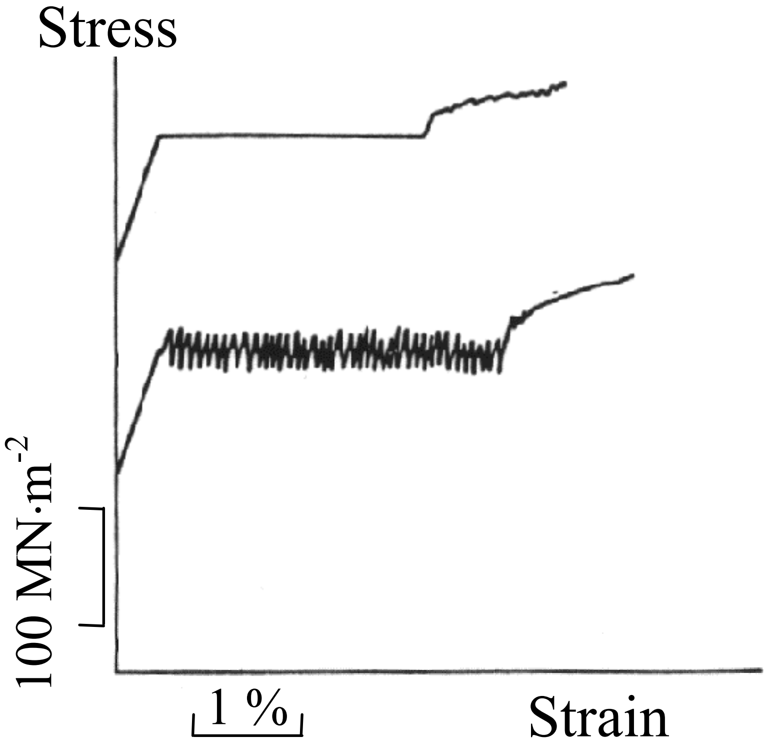



slip band
slip line
slip planes
S
S_L
B_L
B
d_L
d_B
χ
crystal axis


τ (MPa)
40
35
0
10
20
30
40
50
t (s)

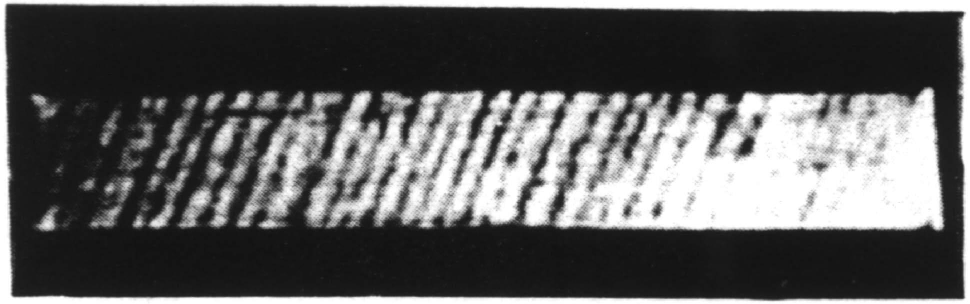


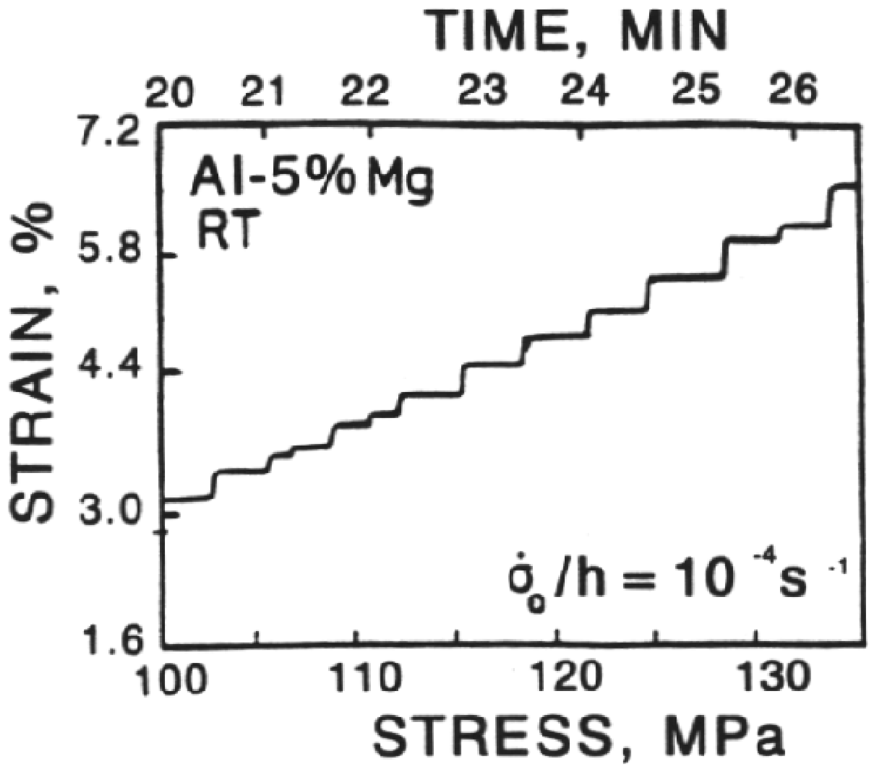


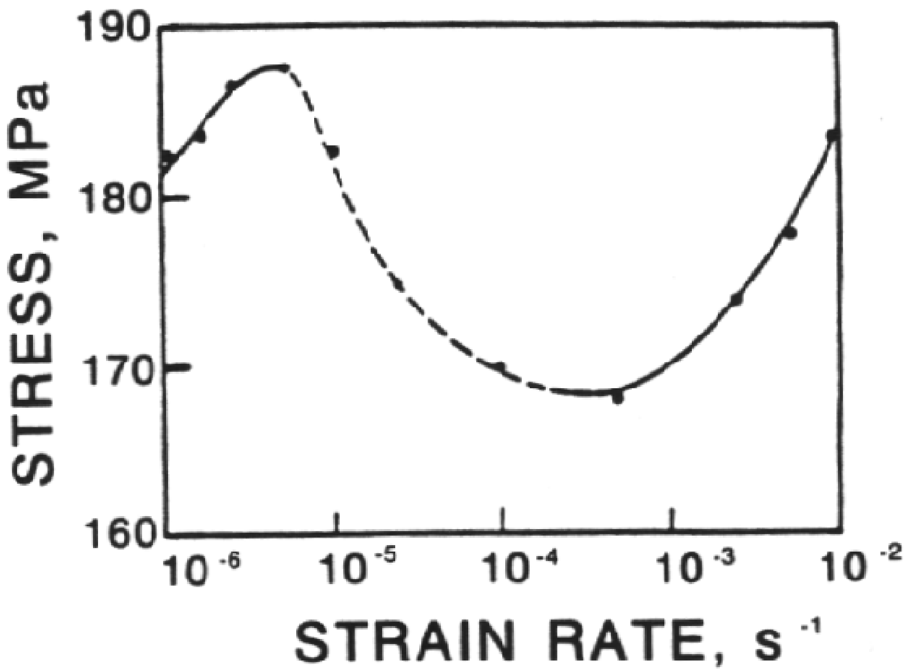

Stress
100 MN·m^{-2}
1 %
Strain

■ Portevin-Le Chatelier bands (PLC)

- $\dot{\sigma} = const.$ *(Al – 5% Mg)*







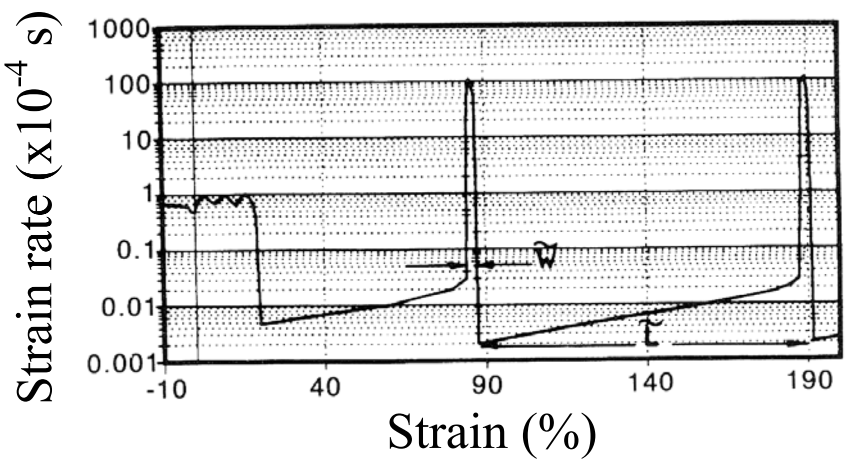
- ***PLC (Preliminary) Modeling***

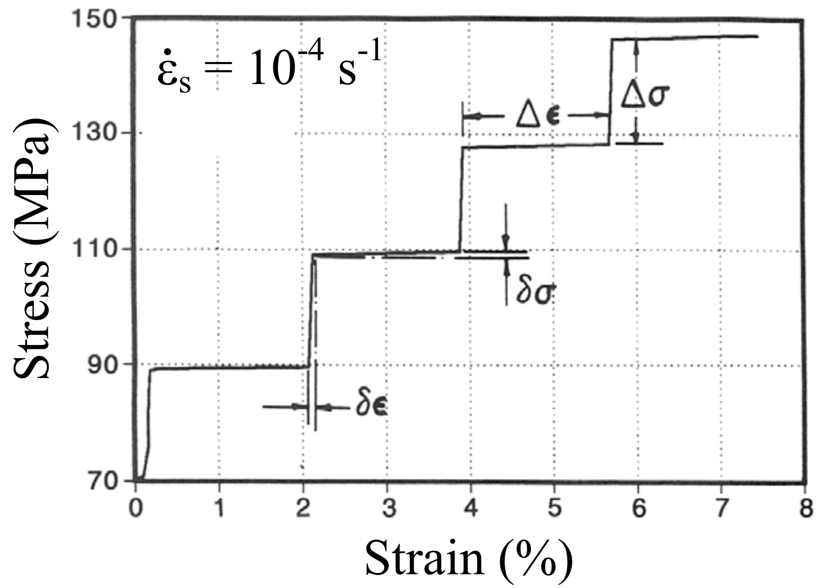
$$\sigma = h\varepsilon + f(\dot{\varepsilon}) + c\varepsilon_{xx}$$

$$\sigma = \dot{\sigma}_o t \quad ; \qquad \dot{\sigma}_o = h\dot{\varepsilon}_s$$

$$\dot{\varepsilon} = z(Vt - x) \quad ; \qquad \eta = \sqrt{\frac{h}{c}}(Vt - x)\,;$$

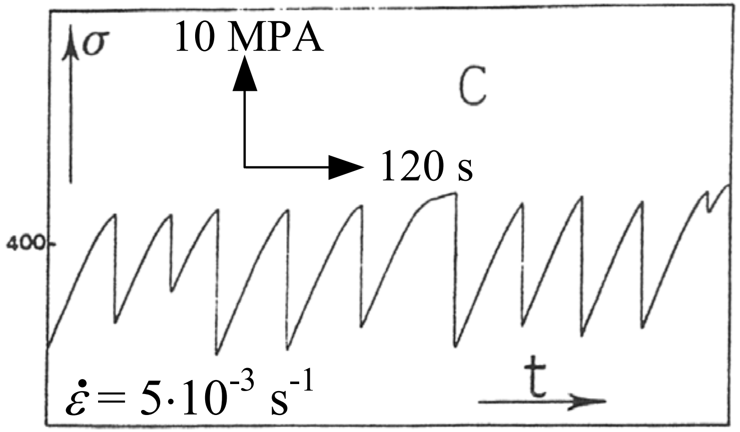
$$z_{\eta\eta} + \mu f'(z) z_\eta + (z - z_s) = 0 \quad \text{.......... Lienard's Eq.}$$

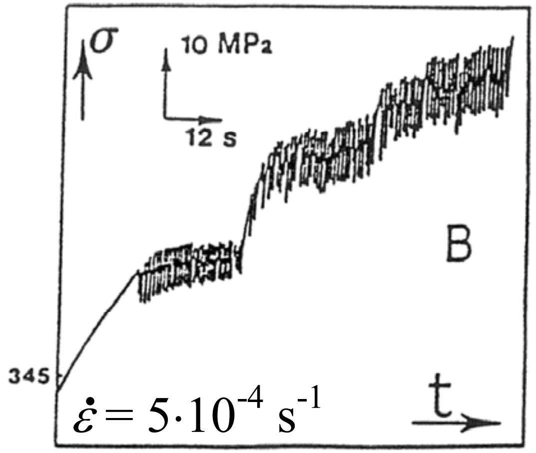


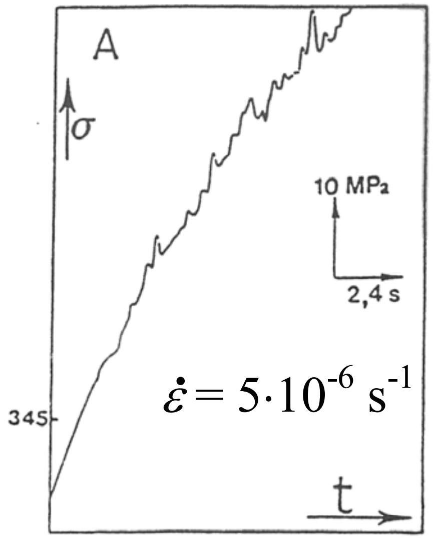


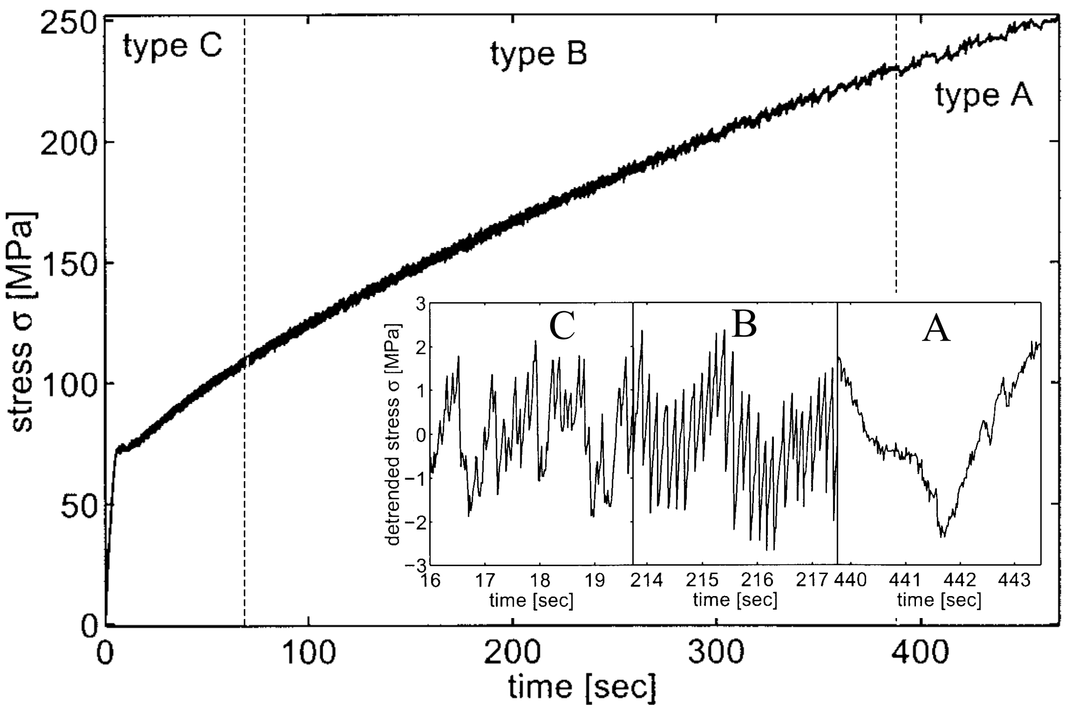
■ PLC Experimental Details

- $\dot{\varepsilon} = const.$ *(Al – 5% Mg)*







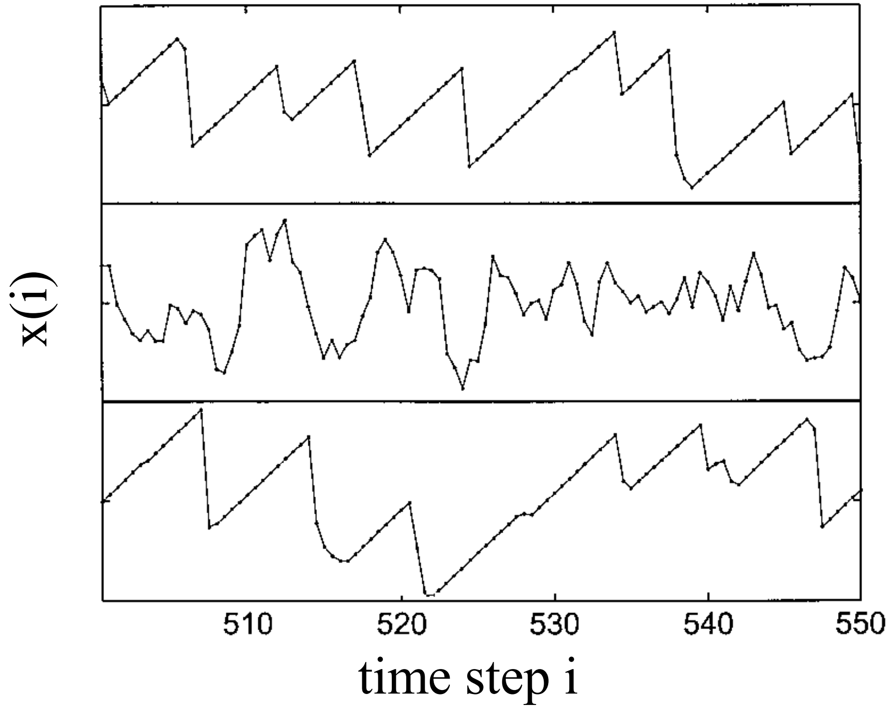


Cu - 15% Al polycrystal

C: stochastic nucleation
B: stop-and-go
A: solitary plastic waves

- ***PLC Time Series Analysis (with Kougioumtzis et al)***

Time series of PLC effect and surrogate time series



Original PLC time series

Stochastic time series with the same autocorrelation and amplitude distribution as PLC (algorithm STAP)

Stochastic time series with the same stick-slip patterns as PLC but in random order (algorithm SUDT)

- PLC has nonlinear dynamics

- PLC has no significant correlations between successive stick-slips

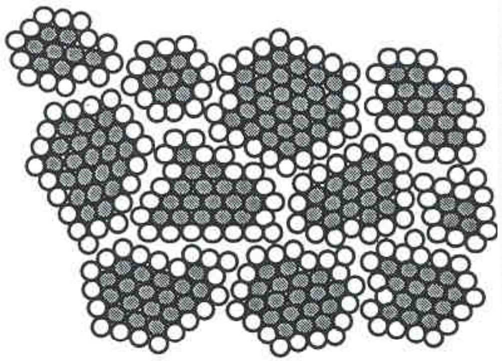
■ Grain Configuration at the Nanoscale

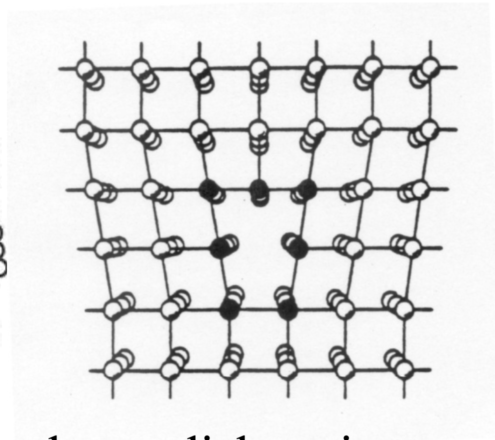
Traditional Polycrystals……. 10 – 100 μm

Nanopolycrystals……………5 – 100 nm

Grain D

1-50 nm





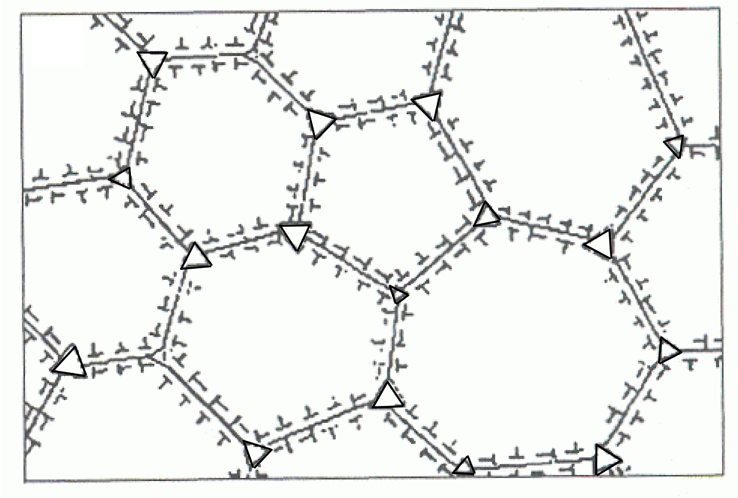
Core d

~1 nm

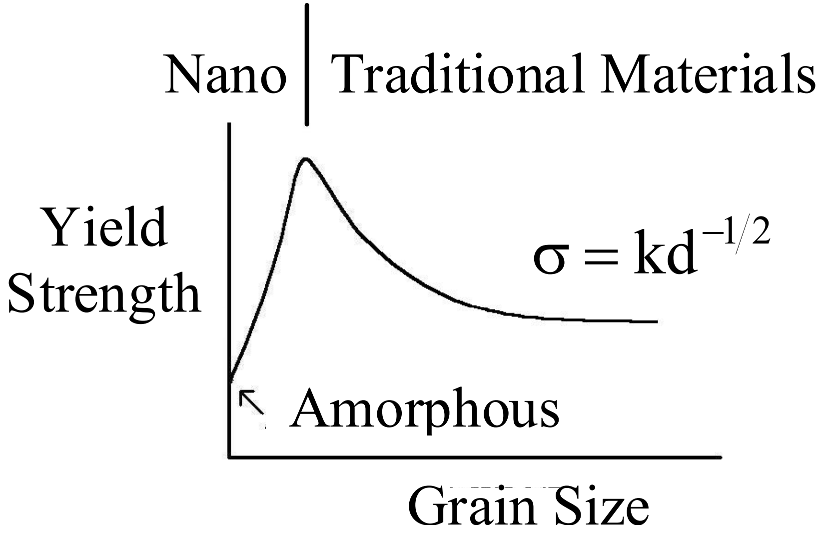
Grain size (D) of the same order as dislocation core (d)

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

■ Dislocations / Disclinations at the Nanoscale



Plasticity Mechanisms ?



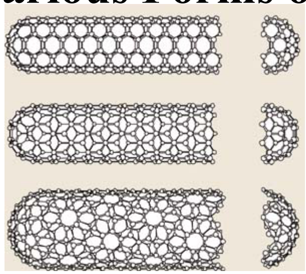
Inverse Hall-Petch Relation ?

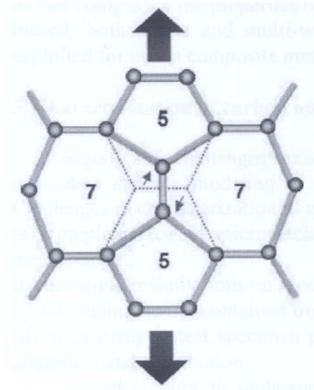
■ Improved/Engineered Properties

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

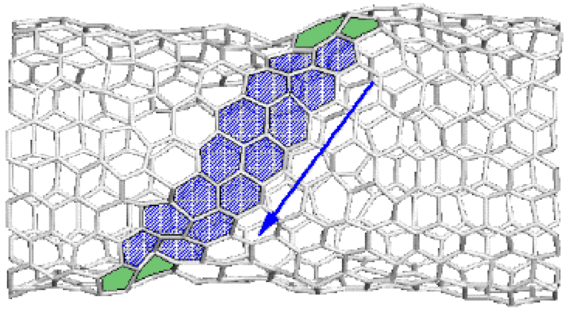
■ Nanotubes

Various Forms of CNTs

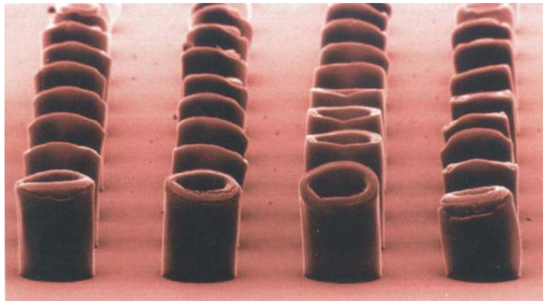




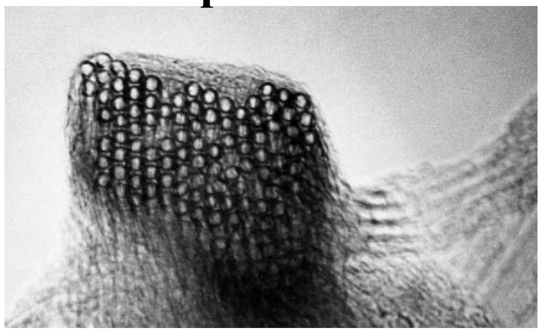
5/7 Dislocation-like Defects in CNTs



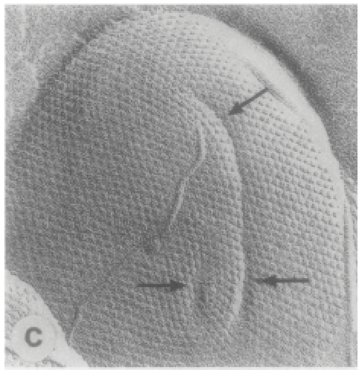
Multiwalled CNTs

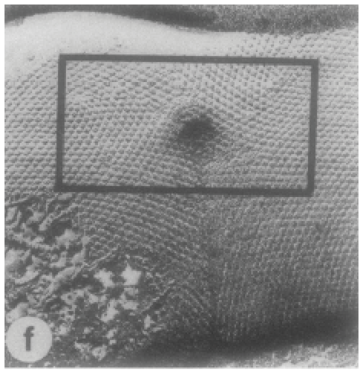


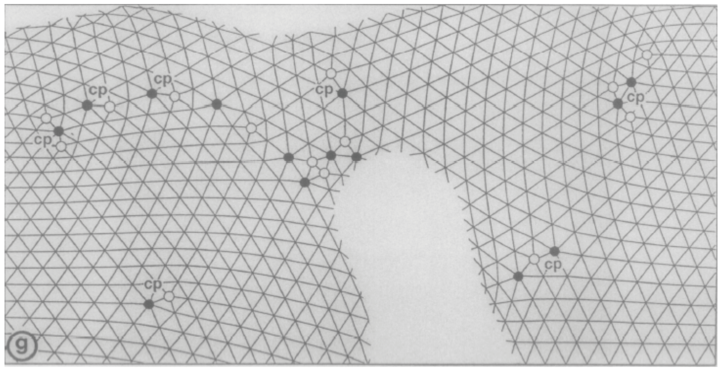
Ropes of CNTs



■ Nanobiomembranes/M. sinense Cells

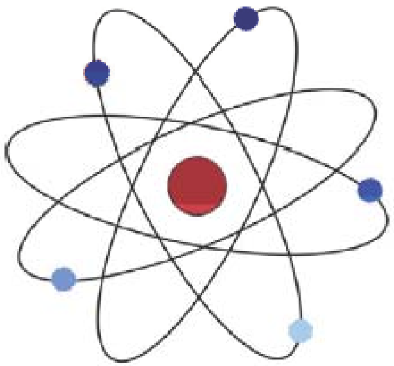






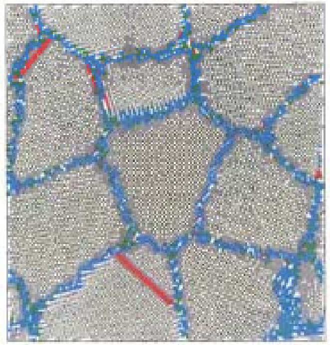
■ From Atomic/Nano to Micro/Macro

Quantum



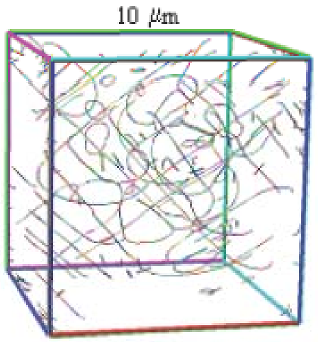
Quantum Mechanics
$10^{-11} – 10^{-10}$ m
$10^{-16} – 10^{-12}$ sec

Atomistic



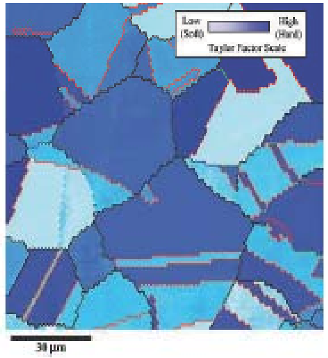
Molecular Dynamics
$10^{-9} – 10^{-6}$ m
$10^{-13} – 10^{-10}$ sec

Microscale



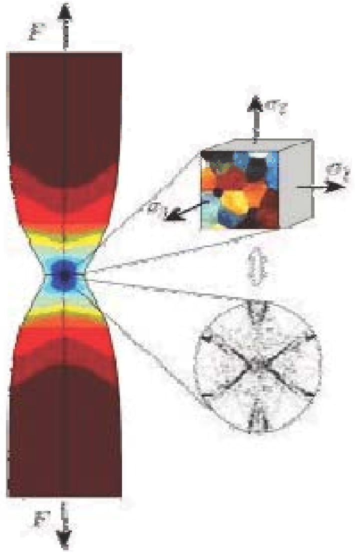
Dislocation Dynamics
$10^{-8} – 10^{-5}$ m
$10^{-12} – 10^{-8}$ sec

Mesoscale



Grain Boundary Mechanics
$10^{-6} – 10^{-3}$ m
$10^{-10} – 10^{-6}$ sec

Continuum



Continuum Mechanics
$> 10^{-3}$ m
$> 10^{-6}$ sec

Density Functional Theory

■ Hohenberg-Kohn theorem (exact)

The total energy of an interacting inhomogeneous electron gas in the presence of an external potential $V_{ext}(r)$ is a functional of the density ρ

$$E = \int V_{ext}(\vec{r})\rho(\vec{r})d\vec{r} + F[\rho]$$

Kohn-Sham: (still exact!)

$$E = T_o[\rho] + \int V_{ext}\rho(\vec{r})d\vec{r} + \frac{1}{2}\int \frac{\rho(\vec{r})\rho(\vec{r}\,')}{|\vec{r}\,' - \vec{r}|}d\vec{r}d\vec{r}\,' + E_{xc}[\rho]$$

$E_{kinetic}$ non interacting | E_{ne} | $E_{coulomb}$ E_{ee} | E_{xc} exchange-correlation

In KS the many body problem of interacting electrons and nuclei is mapped to a one-electron reference system that leads to the same density as the real system.

Kohn-Sham equations

LDA, GGA

$$E = T_o[\rho] + \int V_{ext}\,\rho(\vec{r})\,d\vec{r} + \frac{1}{2}\int \frac{\rho(\vec{r})\rho(\vec{r}\,')}{|\vec{r}\,' - \vec{r}|}d\vec{r}\,d\vec{r}\,' + E_{xc}[\rho]$$

E_{kin} (non interacting) E_{ne} E_{ee} E exchange correlation

vary ρ

1-electron equations (Kohn Sham)

$$\{-\frac{1}{2}\nabla^2 + V_{ext}(\vec{r}) + V_C(\rho(\vec{r})) + V_{xc}(\rho(\vec{r}))\}\Phi_i(\vec{r}) = \varepsilon_i \Phi_i(\vec{r})$$

-Z/r

$$\int \frac{\rho(\vec{r})}{|\vec{r}\,' - \vec{r}|}d\vec{r}$$

$$\frac{\partial E_{xc}(\rho)}{\partial \rho}$$

$$\rho(\vec{r}) = \sum_{\varepsilon_i \le E_F} |\Phi_i|^2$$

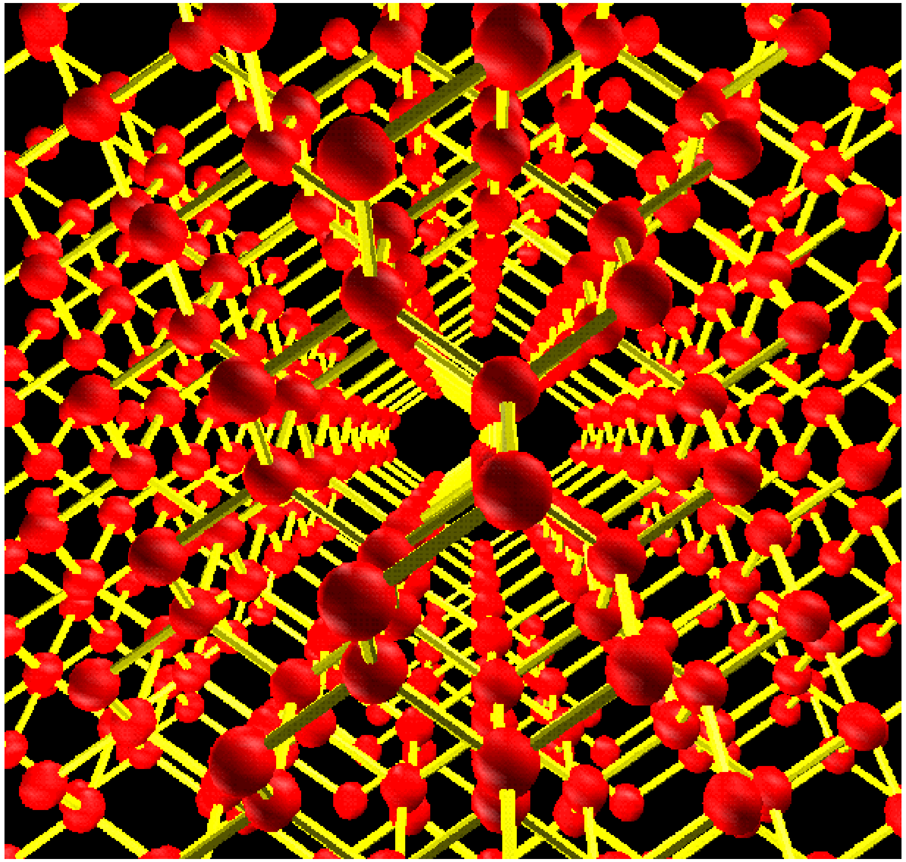
$$E_{xc}^{LDA} \propto \int \rho(r)\ \varepsilon_{xc}^{hom.}[\rho(r)]\ dr$$

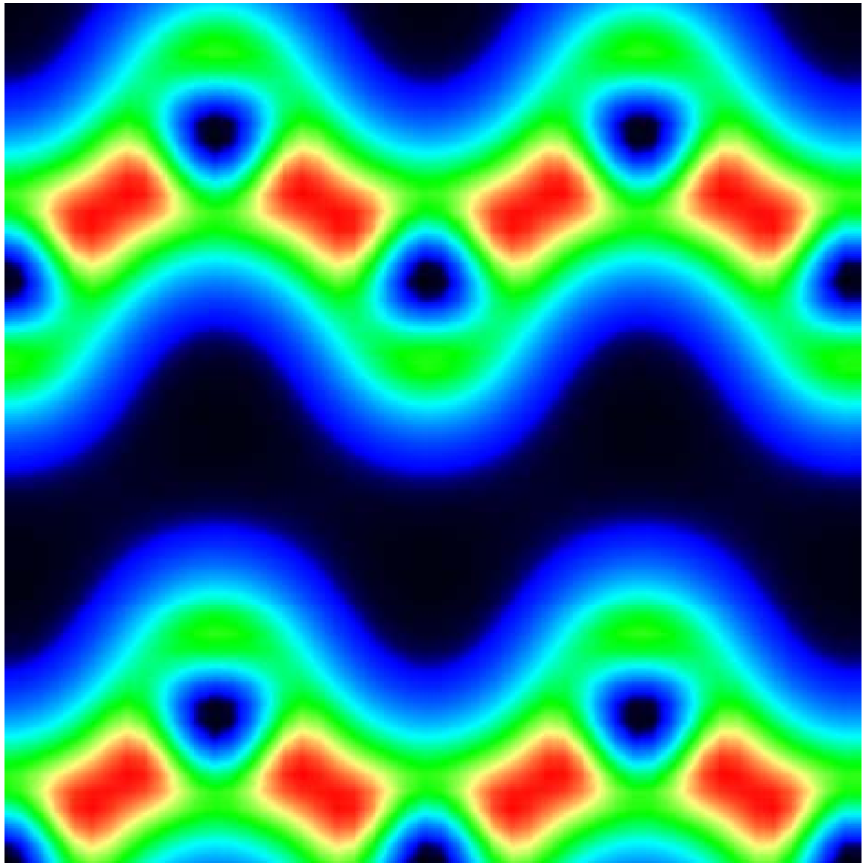
$$E_{xc}^{GGA} \propto \int \rho(r)\ F[\rho(r), \nabla\rho(r)]\ dr$$

LDA
GGA
treats both, exchange and correlation effects, but approximately

New (better ?) functionals are still an active field of research

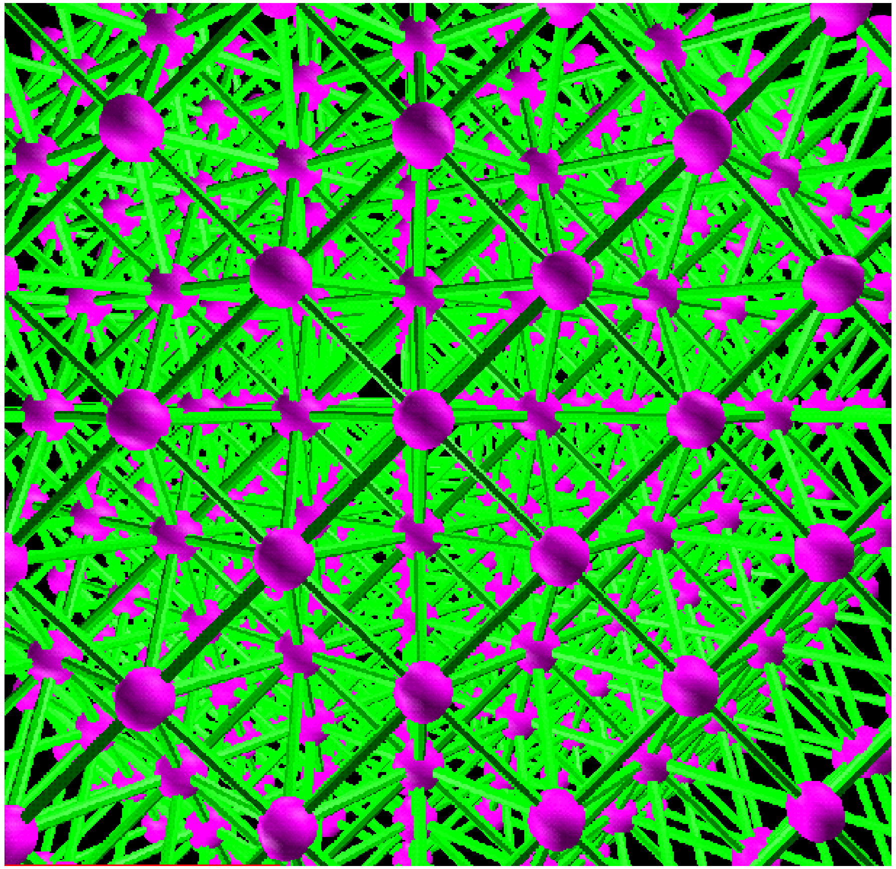
Applications of Density Functional Theory

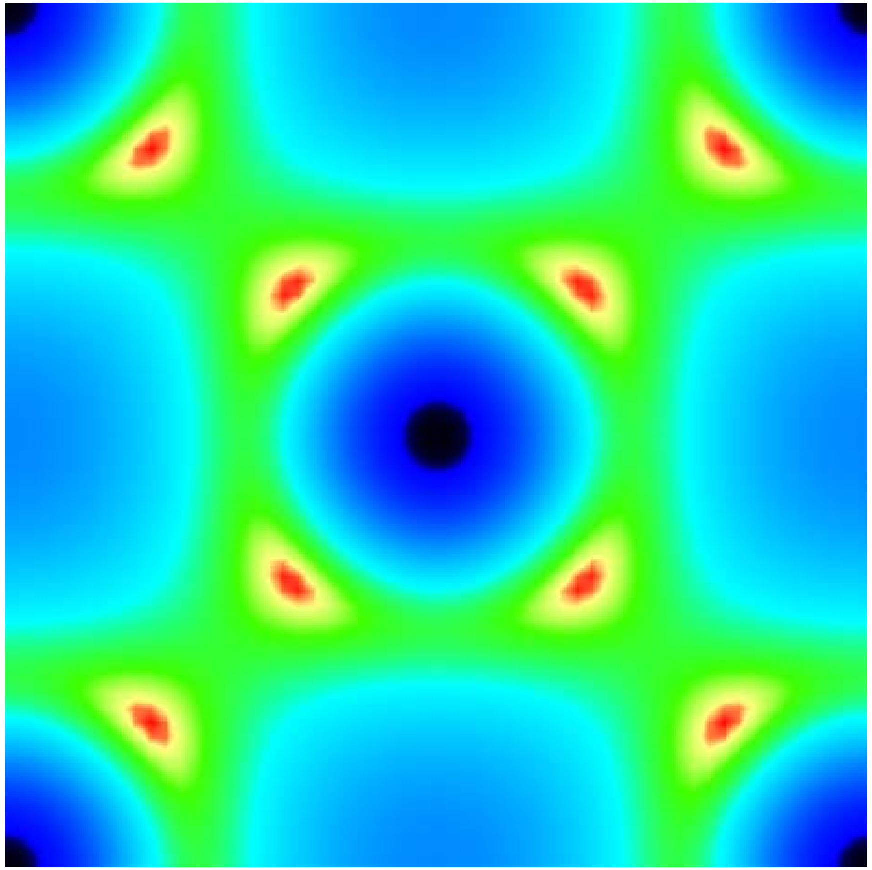




Crystal structure of Si:
diamond crystal and electronic charge density on (110) plane

Applications of Density Functional Theory

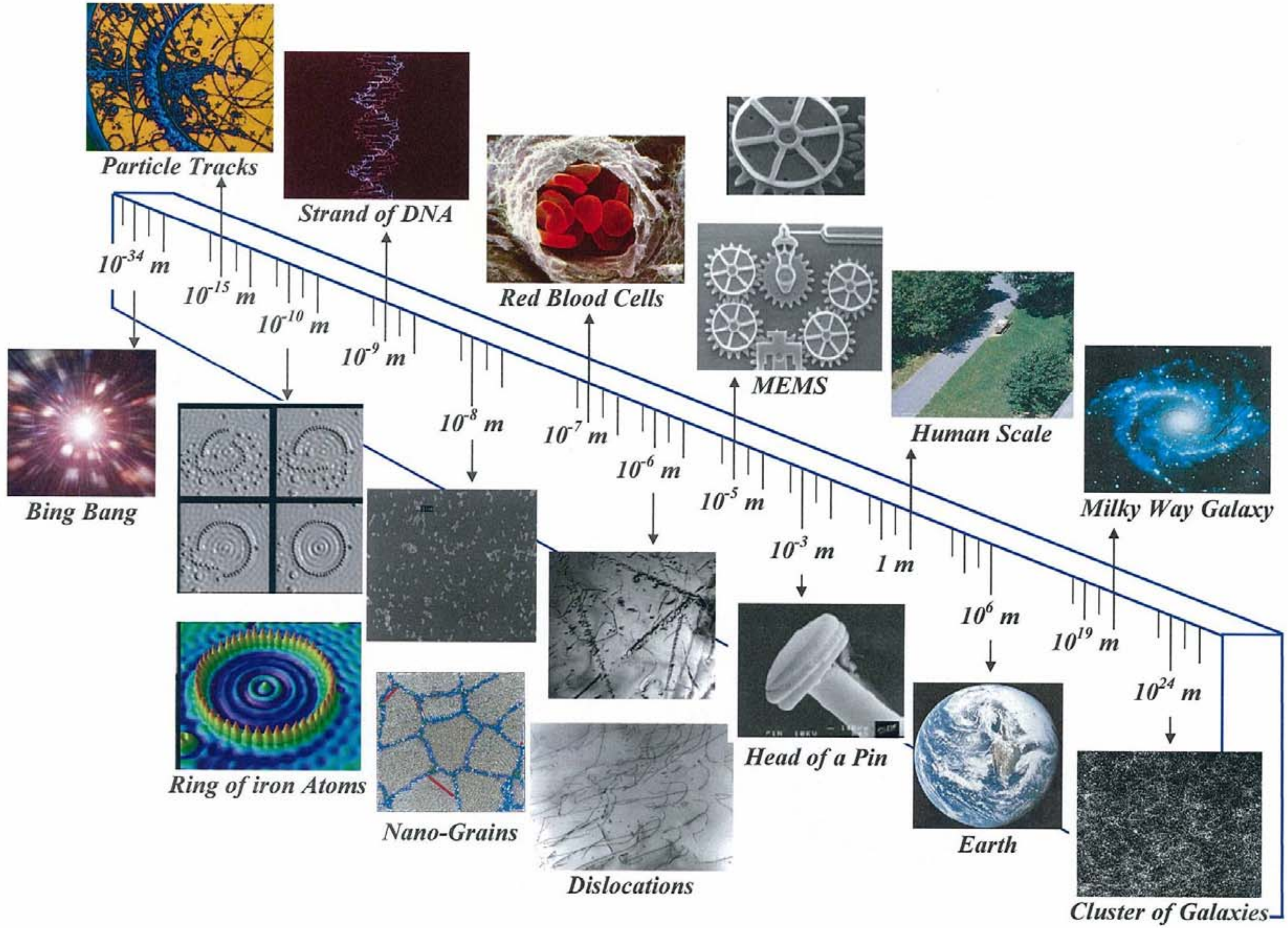




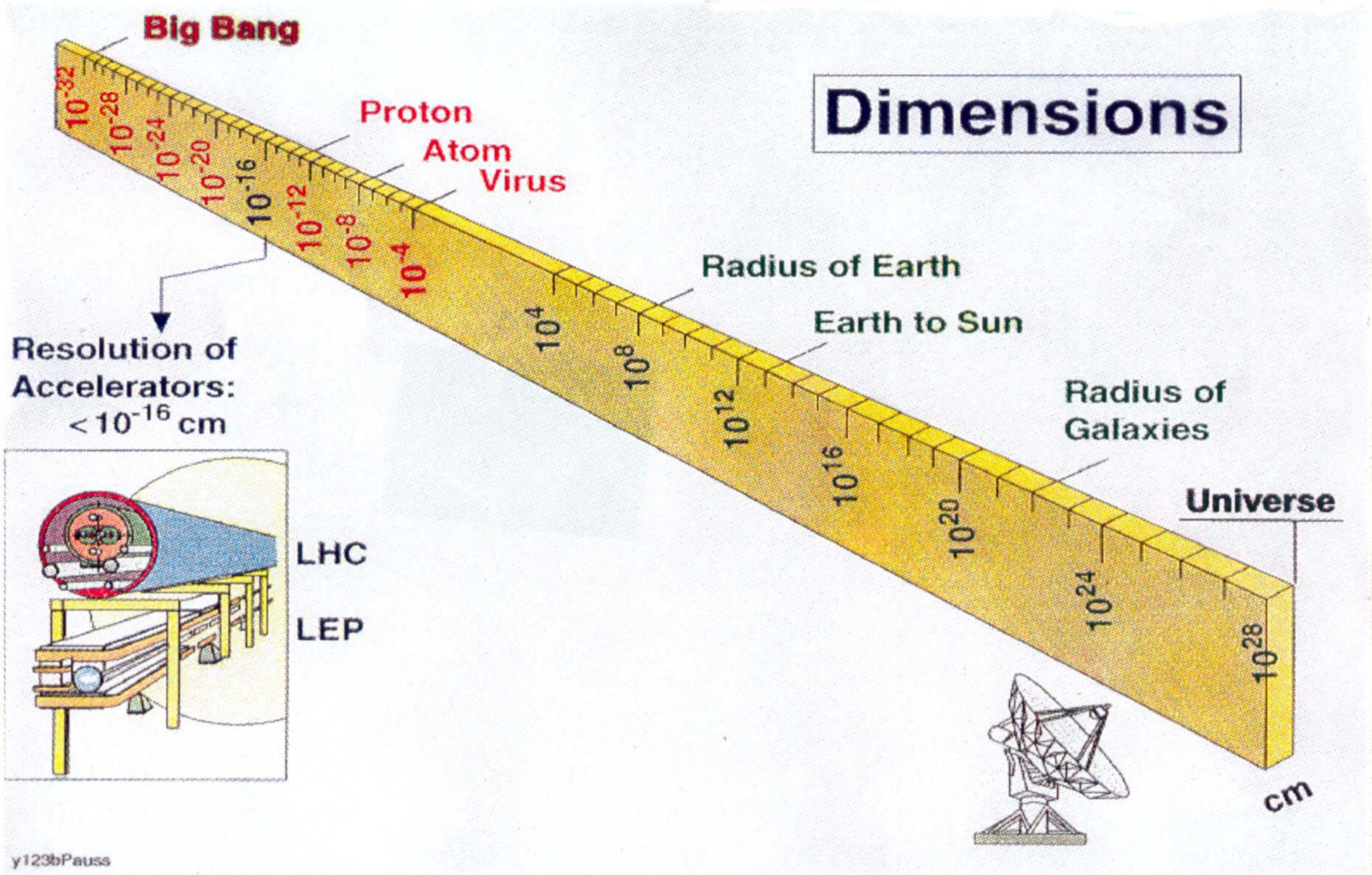
Crystal structure of Al:
FCC crystal and electronic charge density on (100) plane

A SENSE OF SCALE

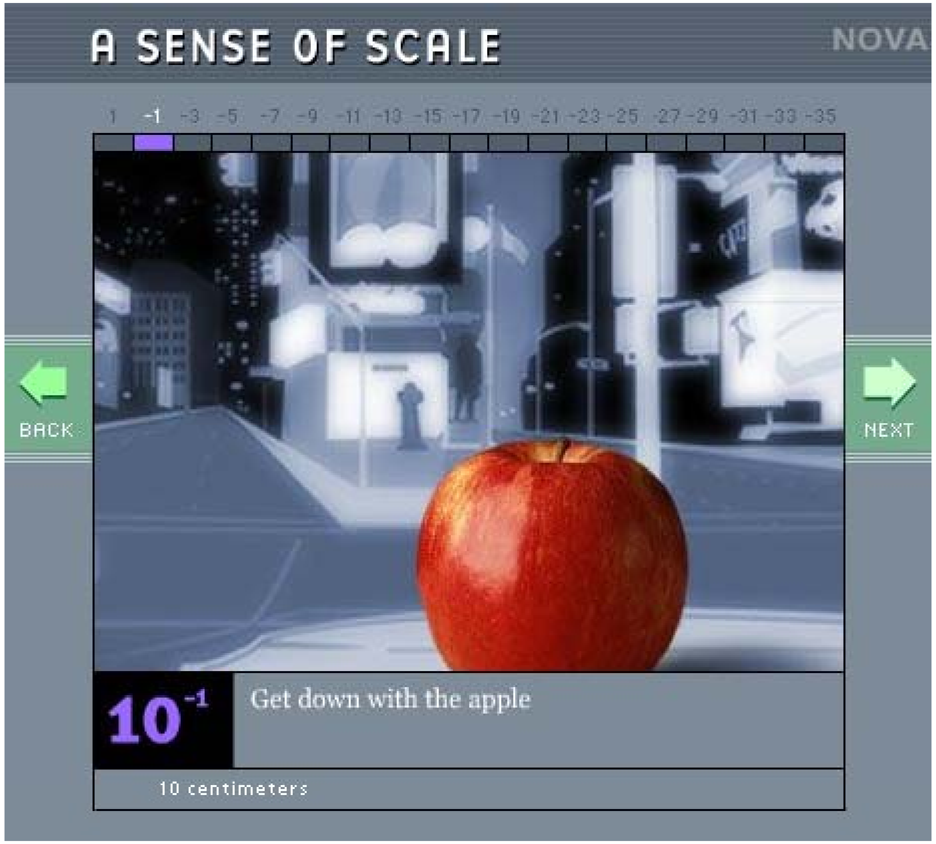
- **From: $10^{-34} – 10^{24}$ m**

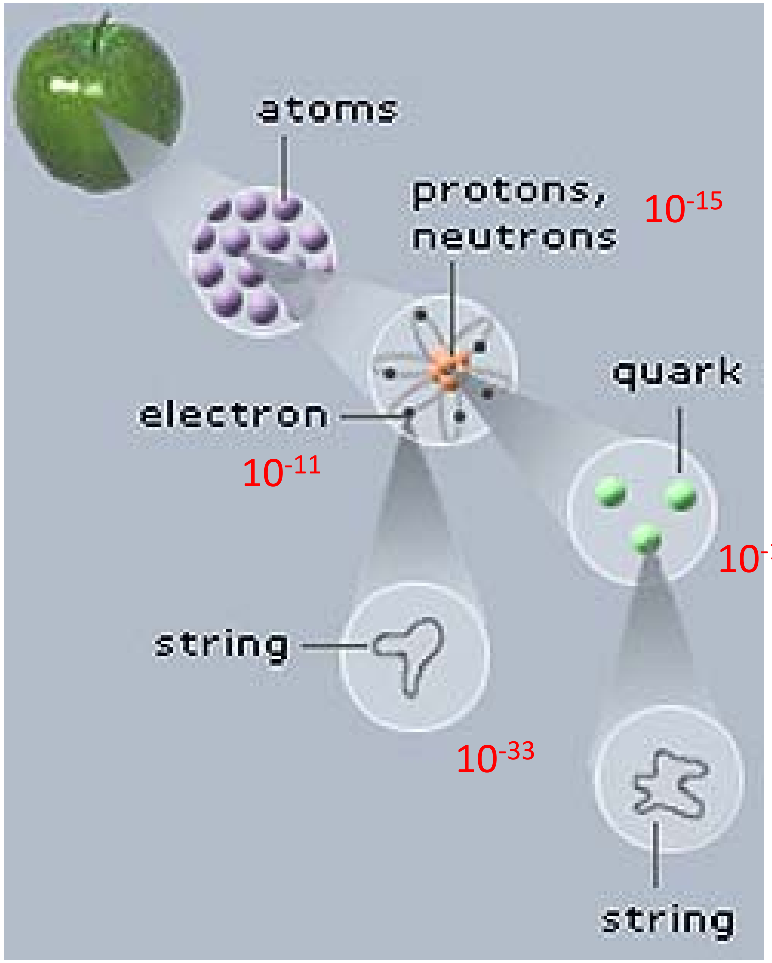


- **From: $10^{-32} – 10^{28}$ m**



■ Below Newton's Apple

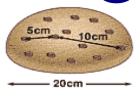


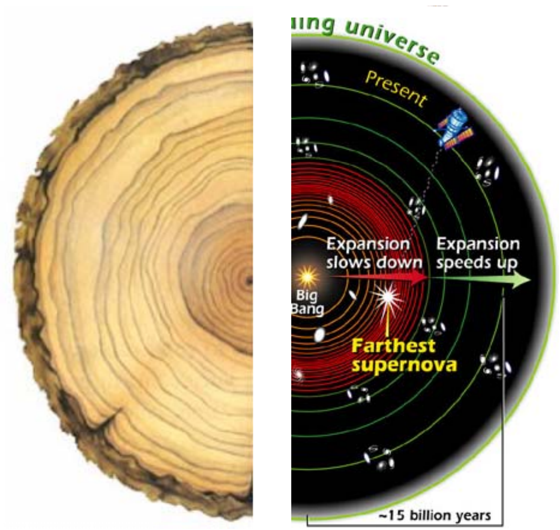


■ Interesting (?) Analogies

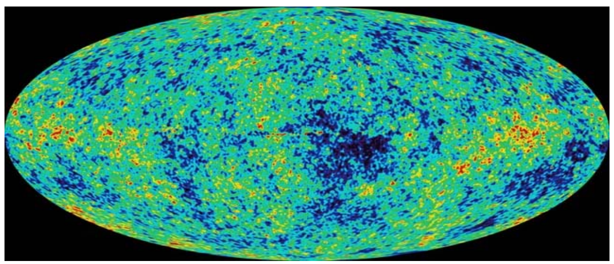
Hot Big Bang

Hubble : 1928



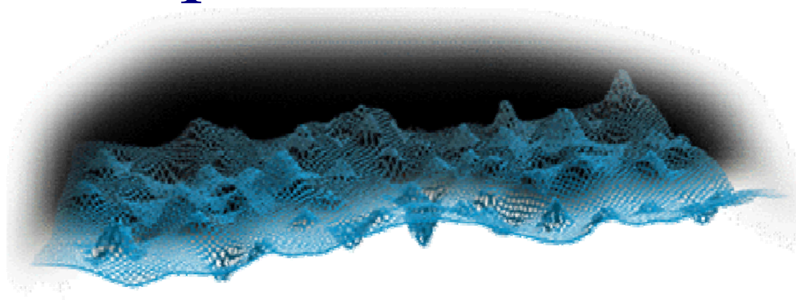


Penzias & Wilson : 1965



COBE : 1992 WMAP : 2003

Spacetime Foam



NANOMATERIALS & NANOMECHANICS

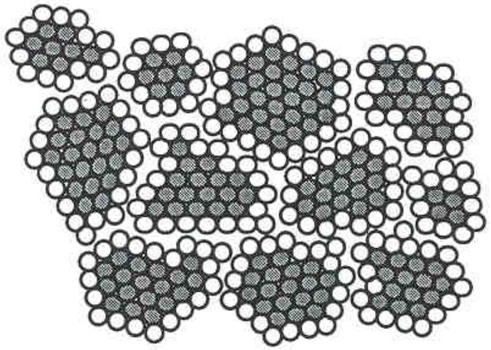
Nanopolycrystals: Observations/Metal Physics Aspects

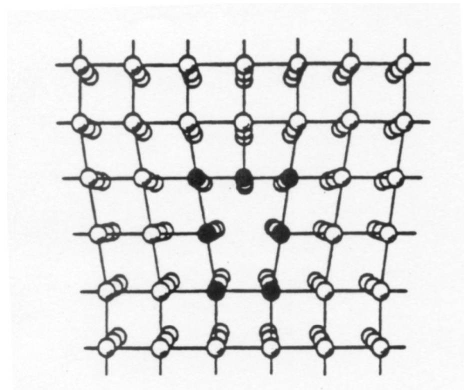
■ Grain Configuration at the Nanoscale

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

Grain d

1-50 nm



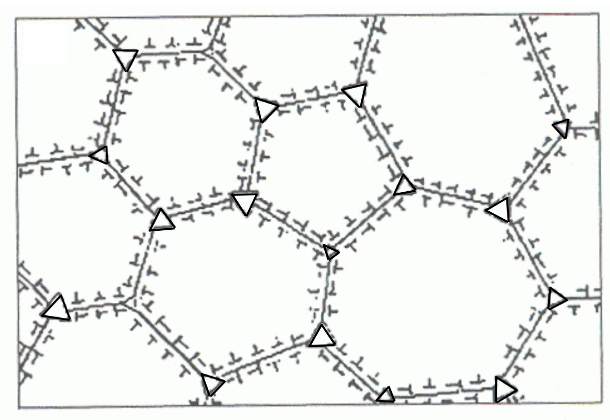


Core r_0

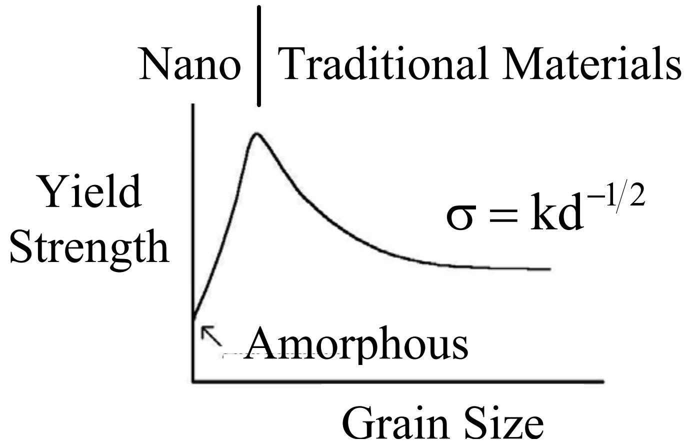
~1 nm

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

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



Plasticity Mechanisms ?

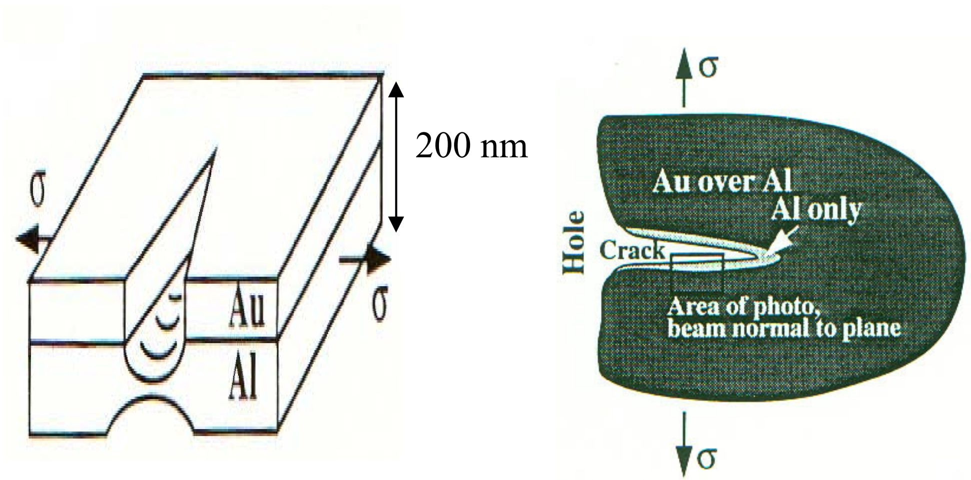


Inverse Hall-Petch Relation ?

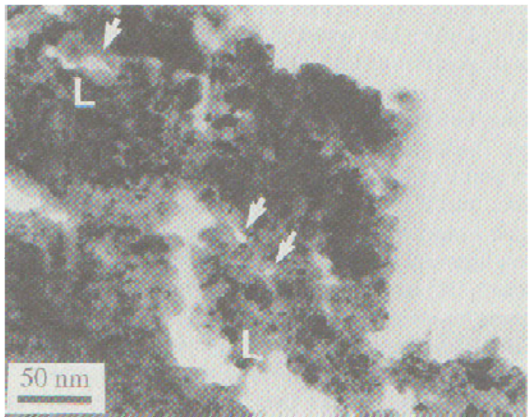
■ Improved/Engineered Properties: Examples

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 Deformation Testing/MTU Early Observ.

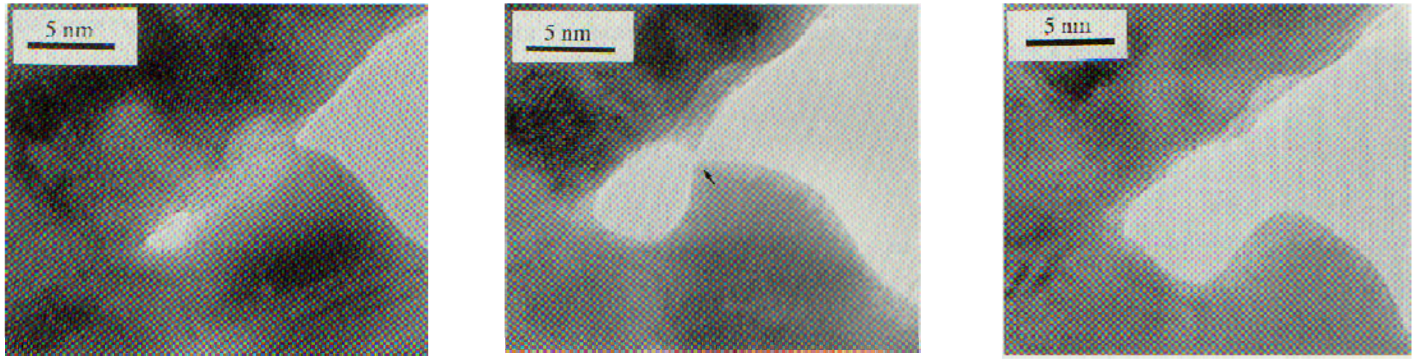


Schematics

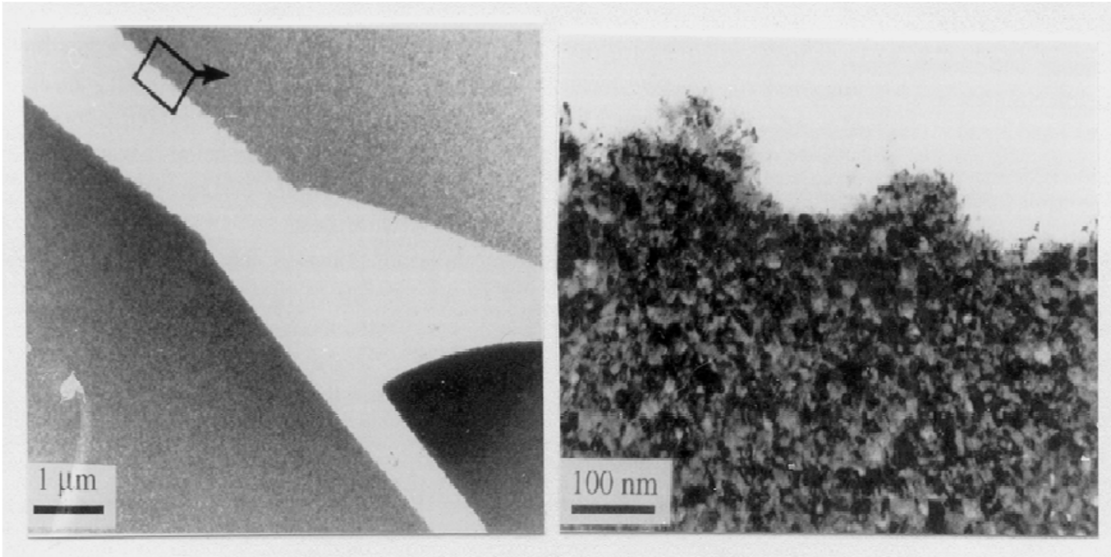


8 nm Au on Al: Nanovoid Coalescense

- ***Nanovoid Nucleation***

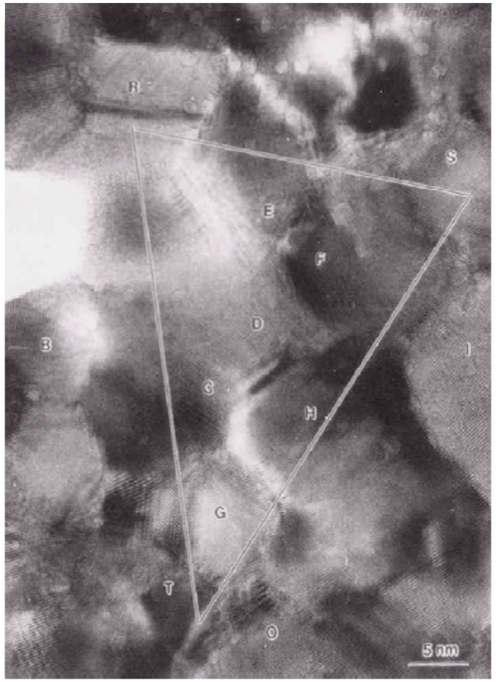


8 nm Au on C: Nanocrack growth via nanopore formation



25 nm Au on C: Periodic Crack profiles and bifurcation

• *Grain Rotation / Dislocation Emergence*

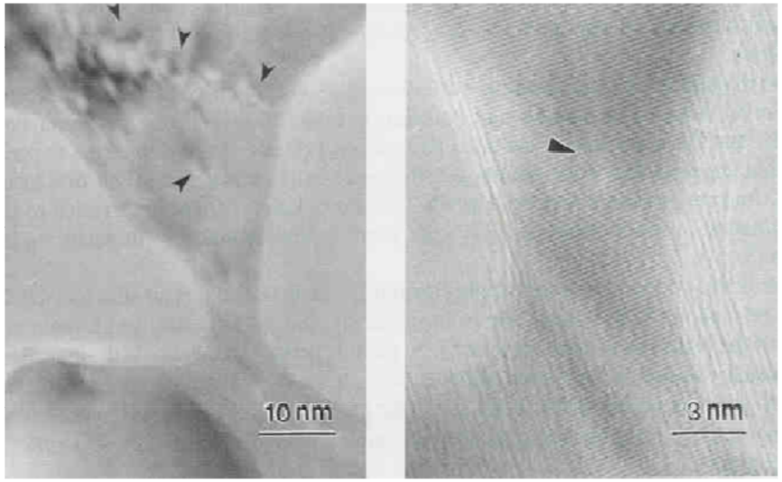


10 nm Au: 6-15 degrees relative grain rotation

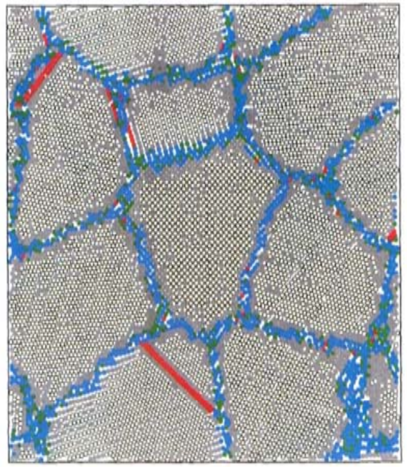
Elementary Rosette Analysis

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



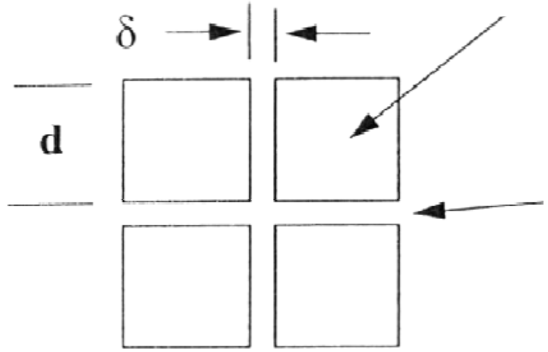
100 nm Au film



~12 nm Ni nanopolycrystals

Initial Simple – Minded Models

- ***Model: 2–Phase Material / Rule of Mixtures***



"Bulk" Phase, Hall – Petch relation

$$\sigma_G = \kappa_1 + \frac{\beta_1}{\sqrt{d}}$$

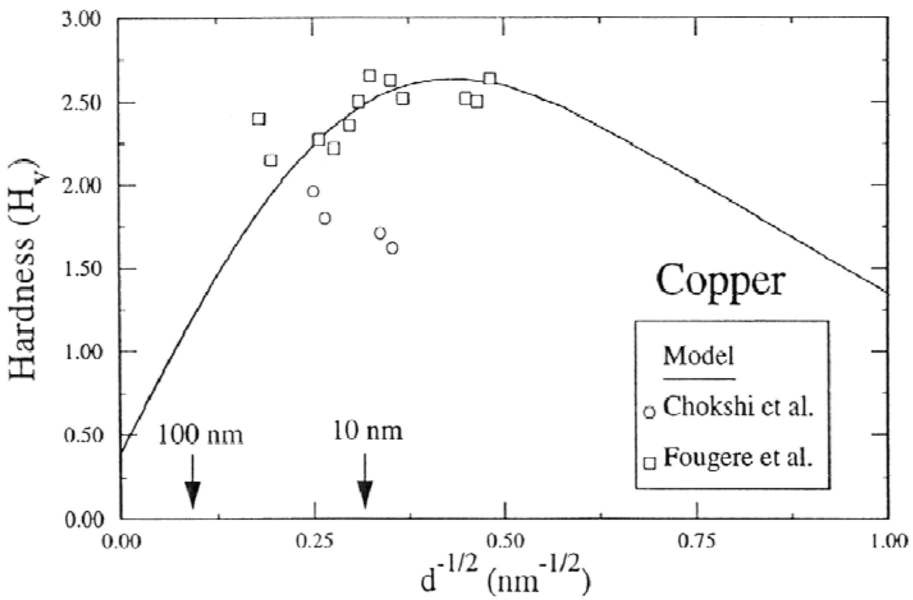
"Boundary" Phase, Constant strength related to amorphous material or grain boundary sliding (σ_{GB})

- Volume Fraction

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

- Rule of Mixtures

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



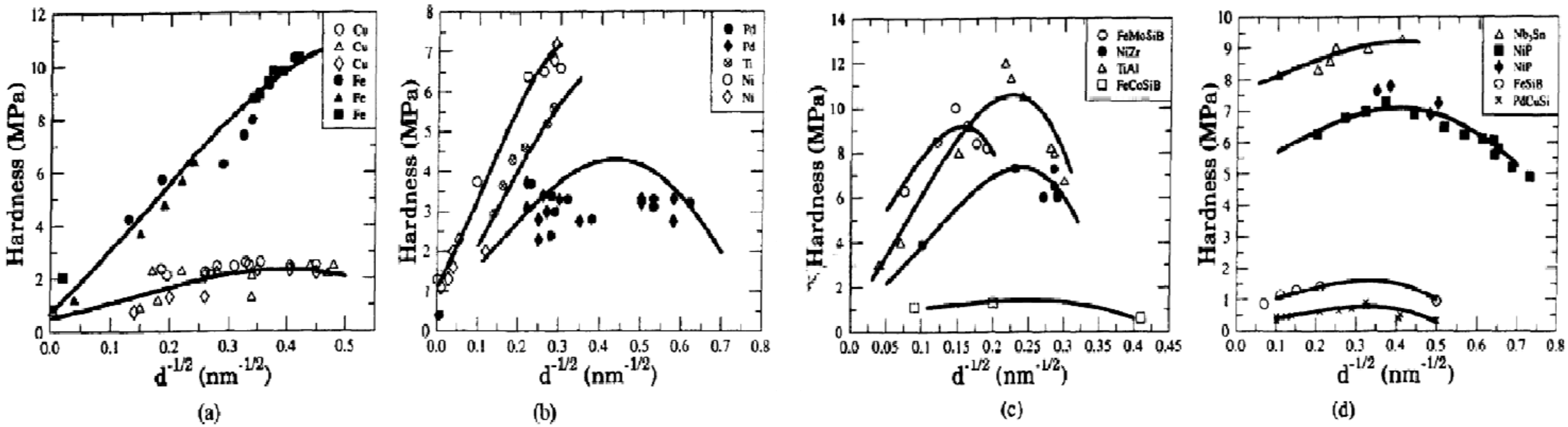
- *Continuum Model predicts behavior of NanoCrystalline Materials*
- *Continuum Model can sort out conflicting Materials Science data*
- *Continuum elasticity Model has also been developed, which shows the importance of gradients in elasticity of nanophase materials*

■ Improved Inverse Hall-Petch Relation

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

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

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

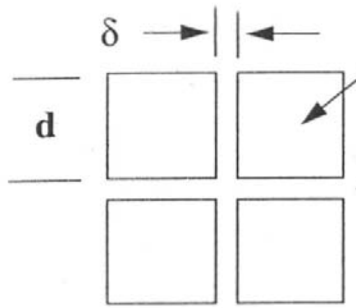


(a) & (b): nanocrystalline metals; (c) & (d): intermetallics

GRADIENT ELASTICITY (GRADELA)
[Elasticity Of Nanopolycrystals]

■ Gradela: Nanopolycrystalline Materials

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



- ***Equilibrium***

$$div\boldsymbol{\sigma}_{\mathbf{1}} = \mathbf{f}, \quad div\boldsymbol{\sigma}_{\mathbf{2}} = -\mathbf{f} \text{ ....} \textit{for each phase}$$

$$div\boldsymbol{\sigma} = 0, \quad \boldsymbol{\sigma} = \boldsymbol{\sigma}_{\mathbf{1}} + \boldsymbol{\sigma}_{\mathbf{2}} \text{ ....} \textit{total}$$

- ***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

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

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

Uncoupling $\Rightarrow$

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

- ***Gradient Elasticity***

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***

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

■ Gradela: A Scale Invariance Argument

- ***2D Atomic Lattice Configuration (n, ν)***

- Strain:

$$\varepsilon = \hat{\varepsilon}\left(\mathbf{n}, \nu;\ e\right) = \alpha_1\left(\mathbf{n} \otimes \mathbf{n}\right) + \alpha_2\left(\nu \otimes \nu\right) + \alpha_2\left(\mathbf{n} \otimes \nu + \nu \otimes \mathbf{n}\right)$$

$$\alpha_i = \hat{\alpha}_i\left(e\right); \quad \alpha_1 = \alpha_2 \quad \ldots \quad \text{isotropy}$$

$e \ldots$ atomic lattice chain strain

$$\therefore \quad \boldsymbol{\varepsilon} = \alpha e\mathbf{1} + \beta e\mathbf{M} \qquad (1)$$

$$\mathbf{n} \otimes \mathbf{n} + \nu \otimes \nu = \mathbf{1}\,; \quad \frac{1}{2}\left(\mathbf{n} \otimes \nu + \nu \otimes \mathbf{n}\right) = \mathbf{M}$$

$$\alpha_1 = \alpha_2 = \alpha e\,, \quad \alpha_3 = 1/2\beta e\,; \quad \left(\alpha, \beta\right)\ldots \text{constants}$$

- Stress:

$$\sigma = \hat{\sigma}\left(\mathbf{n}, \nu;\ s\right)$$

$$\therefore \quad \boldsymbol{\sigma} = as\mathbf{1} + \beta s\mathbf{M} \qquad (2)$$

$s \ldots$ atomic lattice chain stress ; $\left(a, b\right)\ldots$ constants

- ***Atomic Chain Stress – Strain Relation***

$$s = k\left(e - c\nabla^2 e\right) \tag{3}$$

k ... lattice atomic chain elastic modulus

c ... gradient coefficient

- ***Elimination of M from (1)-(3)***

$$\boldsymbol{\sigma} = \lambda\left(\mathrm{tr}\boldsymbol{\varepsilon}\right)\mathbf{1} + 2\mu\boldsymbol{\varepsilon} - c\nabla^2\left[\lambda\left(\mathrm{tr}\boldsymbol{\varepsilon}\right)\mathbf{1} + 2\mu\boldsymbol{\varepsilon}\right]$$

$$\lambda \equiv \frac{k}{3}\left(\frac{a}{\alpha} - \frac{b}{\beta}\right); \quad \mu \equiv \frac{k}{2}\frac{b}{\beta}$$

▪ A Note on Mindlin's Strain Gradient Theory

- ***Strain Energy Density***

$$w=\frac{1}{2}\lambda\varepsilon_{ii}\varepsilon_{jj}+\mu\varepsilon_{ij}\varepsilon_{ij}+\alpha_1\varepsilon_{ij,j}\varepsilon_{ik,k}+\alpha_2\varepsilon_{ii,k}\varepsilon_{jk,j}+\alpha_3\varepsilon_{ii,k}\varepsilon_{jj,k}+$$

$$+\alpha_4\varepsilon_{ij,k}\varepsilon_{ij,k}+\alpha_5\varepsilon_{ij,k}\varepsilon_{jk,i}$$

$$\therefore\quad \sigma_{ij}^E\equiv\frac{\partial w}{\partial\varepsilon_{ij}}=\lambda\varepsilon_{\ell\ell}\delta_{ij}+2\mu\varepsilon_{ij}\quad ;\quad \left(\varepsilon_{ij}\equiv\frac{\partial w}{\partial\sigma_{ij}^E}=\frac{1}{2\mu}\sigma_{ij}^E-\frac{\nu}{2\mu(1+\nu)}\sigma_{\ell\ell}^E\delta_{ij}\right)$$

$$\tau_{ijk}\equiv\frac{\partial w}{\partial\varepsilon_{ij,k}}=\alpha_1\left(\varepsilon_{i\ell,\ell}\delta_{jk}+\varepsilon_{j\ell,\ell}\delta_{ik}\right)+\frac{1}{2}\alpha_2\left(\varepsilon_{\ell\ell,i}\delta_{jk}+\varepsilon_{\ell\ell,j}\delta_{ik}+2\varepsilon_{k\ell,\ell}\delta_{ij}\right)+$$

$$+2\alpha_3\varepsilon_{\ell\ell,k}\delta_{ij}+2\alpha_4\varepsilon_{ij,k}+\alpha_5\left(\varepsilon_{ik,j}+\varepsilon_{jk,i}\right)$$

σ_{ij}^E ... elastic – like stress ; $\sigma_{ij}^E=\sigma_{ji}^E$ ... 6 components

$\tau_{ij\kappa}$ ... dipolar – like stress ; $\tau_{ijk}=\tau_{jik}$ ... 18 components

- ***Equilibrium***

$$\partial_j\left(\sigma^E_{ij} - \partial_k \tau_{ijk}\right) = 0$$

$$\therefore \quad \partial_j\Big[\lambda\varepsilon_{\ell\ell}\delta_{ij} + 2\mu\varepsilon_{ij} - (\alpha_1 + \alpha_5)\left(\varepsilon_{i\ell,\ell j} + \varepsilon_{j\ell,\ell j}\right) - \alpha_2\left(\varepsilon_{\ell\ell,ij} + \varepsilon_{k\ell,k\ell}\right) - $$

$$- 2\left(\alpha_3\nabla^2\varepsilon_{kk}\delta_{ij} + \alpha_4\nabla^2\varepsilon_{ij}\right)\Big] = 0$$

i.e. formidable to solve in general

- ***Special Solutions***

- (i) Feynman 1962 ... Linear Theory of Gravity

$$\left[\alpha_5 = 0\,; \quad \sigma^E_{ij,j} = 0\,; \quad \tau_{ijk,jk} = 0\right]$$

$$\text{4D} \quad \text{gradient theory} \begin{cases} \text{metric : strain tensor} \\ \text{gravitation : metrical elasticity of spacetime} \end{cases}$$

$$\alpha_1\left(\nabla^2\varepsilon_{i\ell,\ell}+\varepsilon_{j\ell,\ell ji}\right)+\alpha_2\left(\nabla^2\varepsilon_{\ell\ell,i}+\varepsilon_{j\ell,\ell ji}\right)+2\left(\alpha_3\nabla^2\varepsilon_{\ell\ell,i}+\alpha_4\nabla^2\varepsilon_{ij,j}\right)=0$$

$$\left(\alpha_1+\alpha_2\right)\varepsilon_{j\ell,j\ell i}+\nabla^2\left[\left(\alpha_1+2\alpha_4\right)\varepsilon_{i\ell,\ell}+\left(\alpha_2+2\alpha_3\right)\varepsilon_{\ell\ell,i}\right]=0 \quad (*)$$

$$\text{choose}\ \ \alpha_1=-\alpha_2=-2\mu c\,; \quad \alpha_3=-\alpha_4=-\mu c \quad \Rightarrow \quad (*)\ \text{is identity}$$

$$\Rightarrow \frac{1}{2\mu c}\tau_{ijk,k}=\left(\text{inc}\,\varepsilon\right)_{ij}=-\epsilon_{ik\ell}\epsilon_{jmn}\varepsilon_{\ell n,km}$$

$$=\nabla^2\varepsilon_{ij}+\varepsilon_{k\ell,\ell k}\delta_{ij}+\varepsilon_{kk,ij}-\varepsilon_{ik,kj}-\varepsilon_{jk,ki}-\nabla^2\varepsilon_{kk}\delta_{ij}$$

i.e.

3D linear Einstein tensor used in the gauge theory of dislocations (Malysev/Lazar)

- (ii) ECA 1992 ... Linear theory of Gradela

$$\left[\alpha_1 = \alpha_2 = \alpha_5 = 0\,; \quad \alpha_3 = \lambda c/2, \quad \alpha_4 = \mu c\right]$$

$$\therefore \quad W = \frac{1}{2}\sigma_{ij}^{E}\varepsilon_{ij} + \frac{c}{2}\sigma_{ij,k}^{E}\varepsilon_{ij,k} \quad ; \qquad \frac{\partial W}{\partial \varepsilon_{ij,k}} = c\sigma_{ij,k}^{E}\,, \quad \frac{\partial W}{\partial \sigma_{ij,k}^{E}} = c\varepsilon_{ij,k}$$

$$\tau_{ijk} = c\sigma_{ij,k}^{E} = c\left(\lambda\varepsilon_{\ell\ell,k}\delta_{ij} + 2\mu\varepsilon_{ij,k}\right)$$

$$\text{Let} \;\; \sigma_{ij} \equiv \sigma_{ij}^{E} - \tau_{ijk,k} \;; \quad \sigma_{ij,j} = 0$$

$$\boldsymbol{\sigma} = \lambda\left(\mathrm{tr}\boldsymbol{\varepsilon}\right)\mathbf{1} + 2\mu\boldsymbol{\varepsilon} - c\nabla^2\left[\lambda\left(\mathrm{tr}\boldsymbol{\varepsilon}\right)\mathbf{1} + 2\mu\boldsymbol{\varepsilon}\right]$$

- ***Remarks***
  - *Remark 1*

$$\left(1-c\nabla^2\right)\boldsymbol{\sigma}^E=\boldsymbol{\sigma}\ ;\quad \mathrm{div}\boldsymbol{\sigma}=0$$

$$\therefore\ \ 2D:\quad \boldsymbol{\sigma}^E(r)=\int_V\alpha\left(r-r'\right)\boldsymbol{\sigma}\left(r'\right)dv\ ;\quad \alpha\left(r-r'\right)=\frac{1}{2\pi c}K_0\left(\frac{r}{\sqrt{c}}\right)$$

  - *Remark 2*

$$\left(1-c\nabla^2\right)\boldsymbol{\varepsilon}=\boldsymbol{\varepsilon}^E\ ;\quad \boldsymbol{\varepsilon}^E\equiv\frac{1}{2\mu}\boldsymbol{\sigma}-\frac{\nu}{2\mu\left(1+\nu\right)}\left(\mathrm{tr}\boldsymbol{\sigma}\right)\mathbf{1}$$

i.e. Ru –Aifantis theorem for strains

  - *Remark 3*

$$\left(1-c\nabla^2\right)\boldsymbol{\sigma}^E=\left(1-c\nabla^2\right)\left[\lambda\left(\mathrm{tr}\boldsymbol{\varepsilon}\right)\mathbf{1}+2\mu\boldsymbol{\varepsilon}\right]$$

i.e. Ru –Aifantis stress/strains Gradela with $\boldsymbol{\sigma}^E$ *instead of* $\boldsymbol{\sigma}$

■ Gradela: Eshelby Stress / J–Integral / Peach-Koehler Force

- ***Basic Relations***

$$w = \frac{1}{2} C_{ijk\ell} \left(\beta_{ij} \beta_{k\ell} + \ell^2 \beta_{ij,m} \beta_{k\ell,m} \right)$$

$$C_{ijk\ell} \equiv \lambda \delta_{ij} \delta_{k\ell} + \mu \left(\delta_{ik} \delta_{j\ell} + \delta_{i\ell} \delta_{jk} \right)$$

$$\beta_{ij} \text{ ...elastic distortion ;} \quad \alpha_{ij} \equiv \varepsilon_{jk\ell} \beta_{i\ell,k} , \quad \alpha_{ij,j} = 0$$

$$\sigma_{ij,j} = 0 ; \quad \sigma_{ij} = \tau_{ij} - \tau_{ijk,k} ; \quad \begin{cases} \tau_{ij} \equiv \dfrac{\partial w}{\partial \beta_{ij}} \\ \tau_{ijk} \equiv \dfrac{\partial w}{\partial \beta_{ij,k}} \end{cases}$$

- ***Eshelby Stress***

$$P_{kj} = w \delta_{jk} - \sigma_{ij} \beta_{ik} - \tau_{ij\ell} \beta_{ik,\ell} = w \delta_{jk} - \left[\left(1 - \ell^2 \nabla^2 \right) \tau_{ij} \right] \beta_{ik} - \ell^2 \tau_{ij,\ell} \beta_{ik,\ell}$$

- ***J–Integral***

$$J_k = \int P_{kj} n_j \, dS$$

- ***Peach-Koehler / Configurational Force***

$$F_k^{PK} = \varepsilon_{kj\ell} \tau_{ij} b_i n_\ell$$

- ***Note / Compatible Case:*** $\beta_{ij} = u_{i,j}$

$$P_{kj} = w\delta_{jk} - \sigma_{ij} u_{i,k} - \tau_{ij\ell} u_{i,k\ell} \; ; \quad P_{kj,j} \equiv 0$$

$$= w\delta_{jk} - \left[\left(1 - \ell^2 \nabla^2 \right) \tau_{ij} \right] u_{i,k} - \ell^2 \tau_{ij,\ell} u_{i,k\ell}$$

■ 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 :***

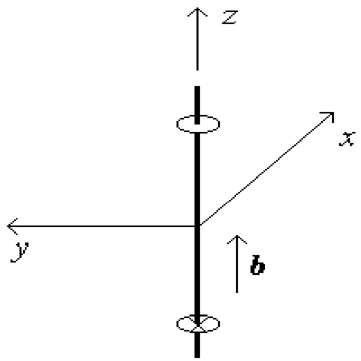
- Stress / Strain :

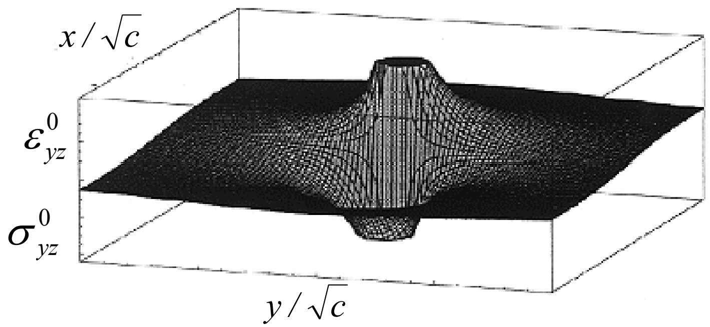
$$\begin{cases}\sigma_{xz}=\dfrac{\mu b_z}{4\pi}\left[-\dfrac{y}{r^2}+\dfrac{y}{r\sqrt{c}}K_1\left(r/\sqrt{c}\right)\right]; & \sigma_{yz}=\ldots\\[2ex] \varepsilon_{xz}=\dfrac{b_z}{4\pi}\left[-\dfrac{y}{r^2}+\dfrac{y}{r\sqrt{c}}K_1\left(r/\sqrt{c}\right)\right]; & \varepsilon_{yz}=\ldots\end{cases}$$

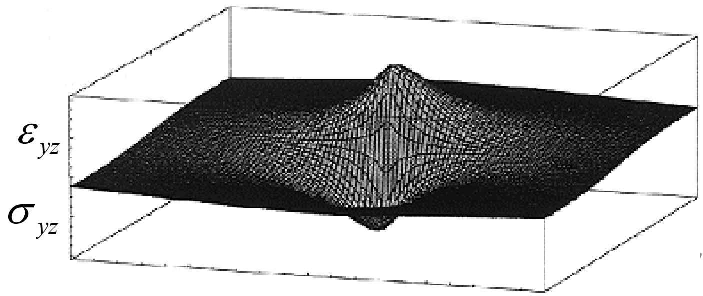
$$\therefore\quad \mathbf{r}\to\mathbf{0}\quad\Rightarrow\quad \mathbf{K_1}\left(\mathbf{r}/\sqrt{\mathbf{c}}\right)\to\frac{\sqrt{\mathbf{c}}}{\mathbf{r}}\quad\Rightarrow\quad\left(\boldsymbol{\sigma}_{\mathbf{xz}},\boldsymbol{\varepsilon}_{\mathbf{yz}}\right)\to\mathbf{0}$$

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

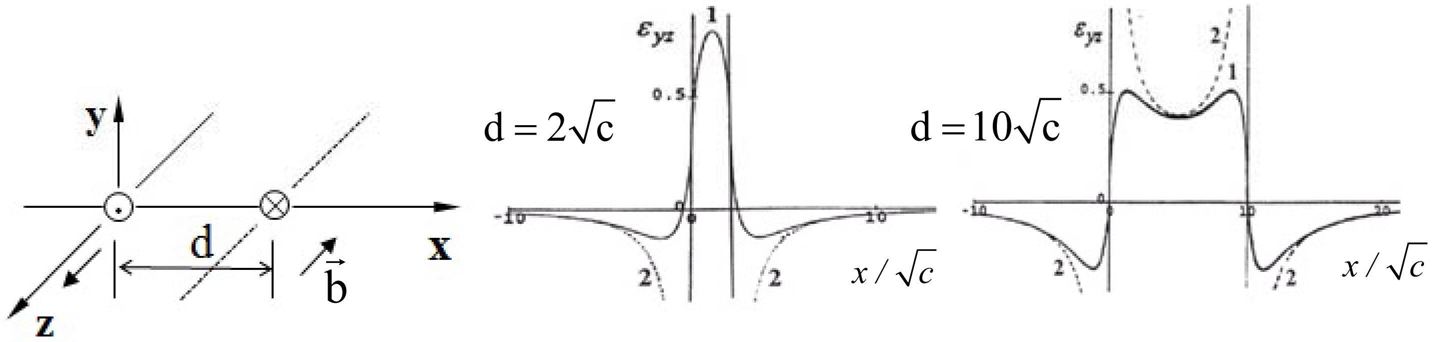
$$\therefore\quad \mathbf{r}\to\mathbf{0}\quad\Rightarrow\quad \textbf{no need for ad hoc dislocation core } \mathbf{r_0}$$





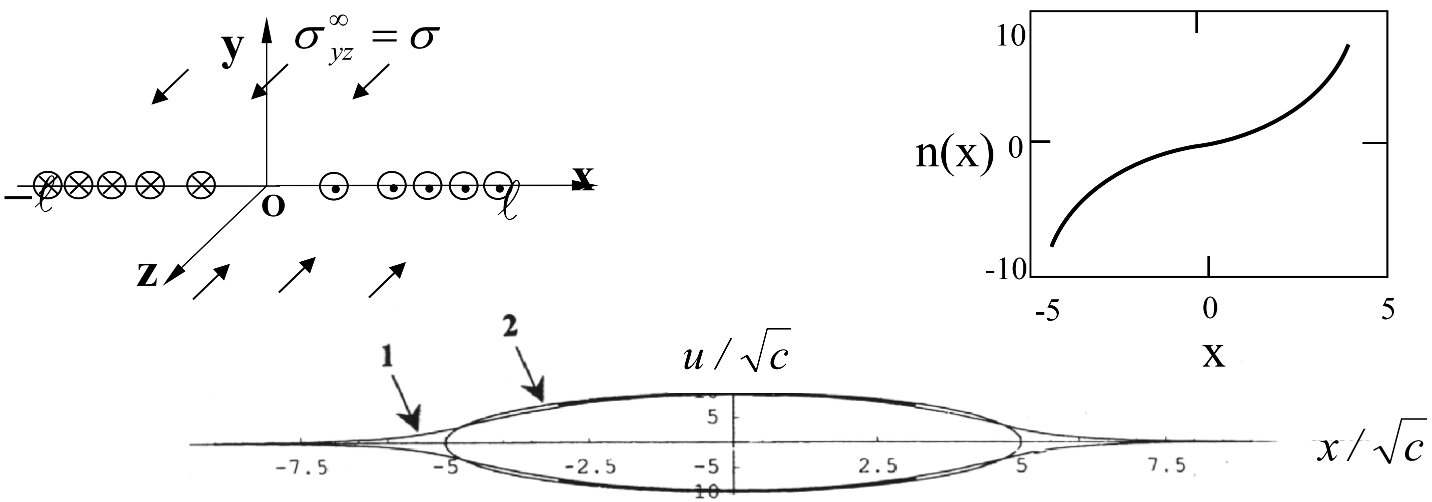


- ***Dislocation Dipoles [insight to nucleation / annihilation]***



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

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

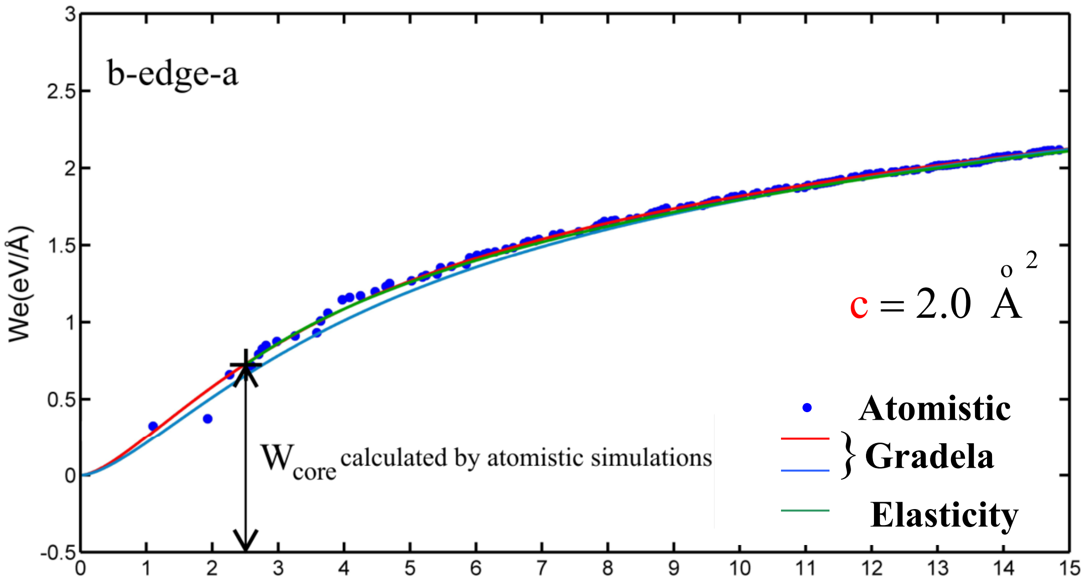


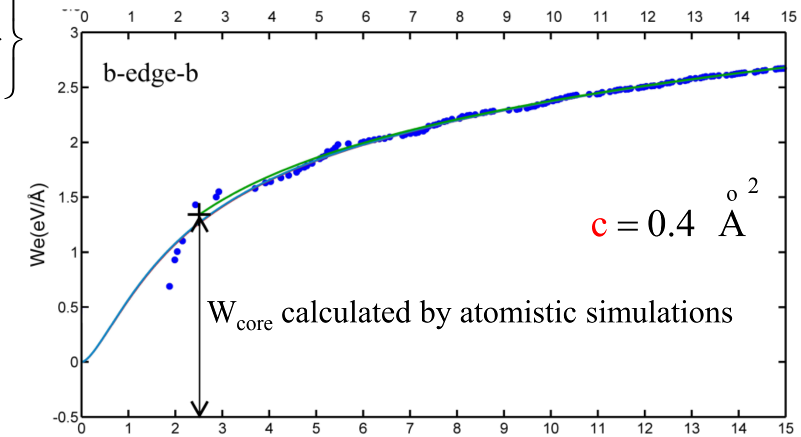
$\therefore$ *Barenblatt's "smooth closure" condition*

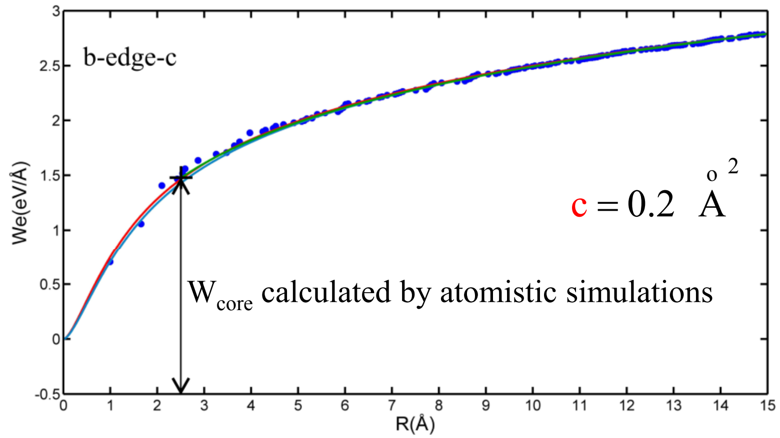
• *Comparison with MD Simulations (Stilliger – Weber Potential)*

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

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







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

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

- *X-ray Line Profile Analysis*

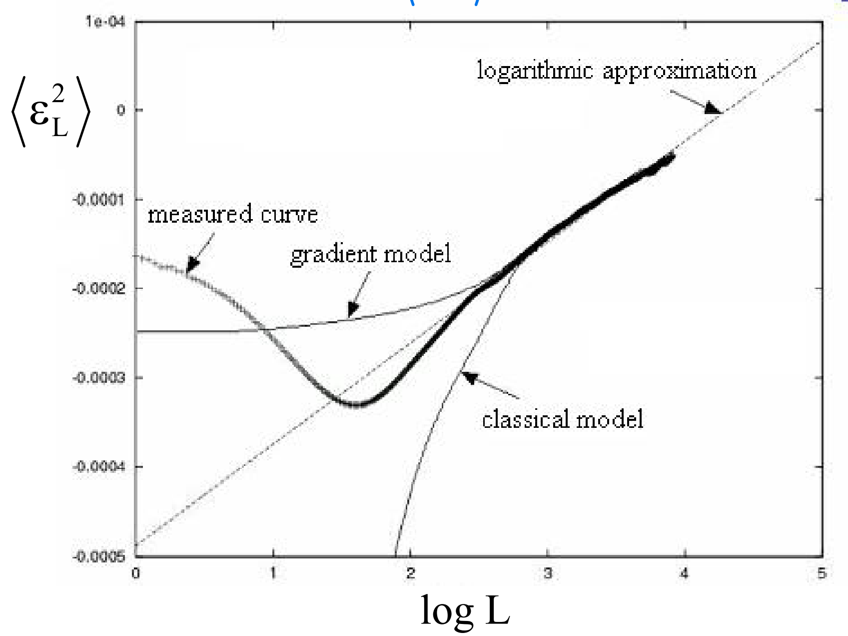
  - *Gradela Soltn for ε_{xx} of edge ⊥ $(\mathbf{b} = b\,\mathbf{e}_x)$*

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

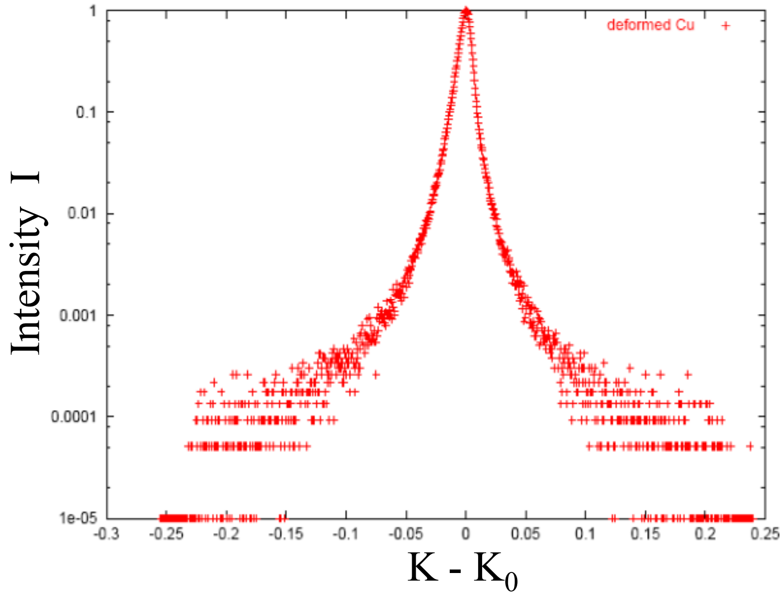
$$\varepsilon_{xx} = -\frac{b}{4\pi(1-\nu)}\frac{(1-2\nu)r^2 + 2x^2}{r^4} + \frac{b}{2\pi(1-\nu)}y\left[\left(y^2 - \nu r^2\right)\Phi_1 + \left(3x^2 - y^2\right)\Phi_2\right]$$

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

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

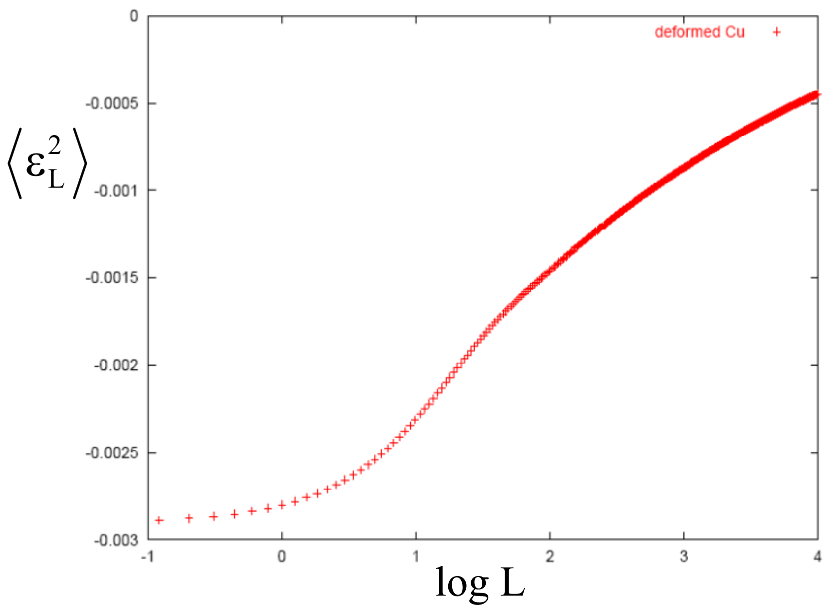


- *X-ray line profile for deformed Cu single crystal*



The measured (count intensity I) line profile of the (111) reflection of a deformed single crystal Cu sample: the intensity is plotted as a function of $K - K_0$, where $K = (2\sin\theta)/\lambda$ and K_0 is the K value at the exact Bragg position. The intensity scale is logarithmic

- $\langle \varepsilon_L^2 \rangle$ *for deformed Cu single crystal*



The mean square strain $\langle \varepsilon_L^2 \rangle$ as a function of log L, determined experimentally for deformed Cu single crystal by FT. It is noted that $\langle \varepsilon_L^2 \rangle$ obtained this way *is not singular*, but it tends to a finite value for $L \to 0$

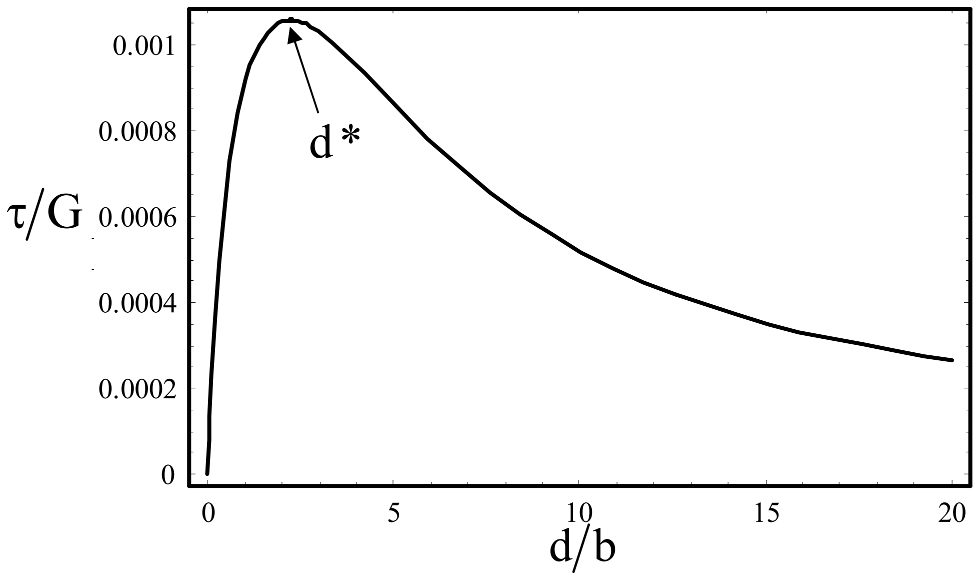
• *Image Force – Inverse Hall Petch Behavior*

- *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: $\lim_{\mathbf{r}\to\infty} \boldsymbol{\sigma}_{ij} = \boldsymbol{\sigma}_{ij}{}^{\mathbf{0}}$

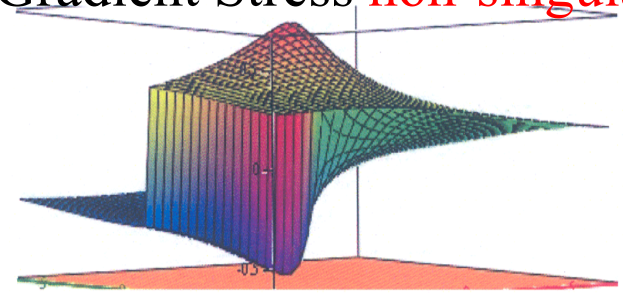
  Vanishing of stresses at the origin: $\lim_{\mathbf{r}\to 0} \boldsymbol{\sigma}_{ij} = 0$

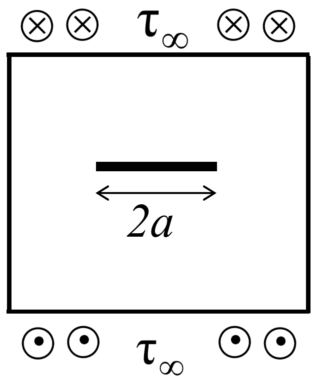
  Zero tractions on crack surfaces: $\sigma_{zy}(x, 0^{\pm}) = 0$; $|x| \le a$

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

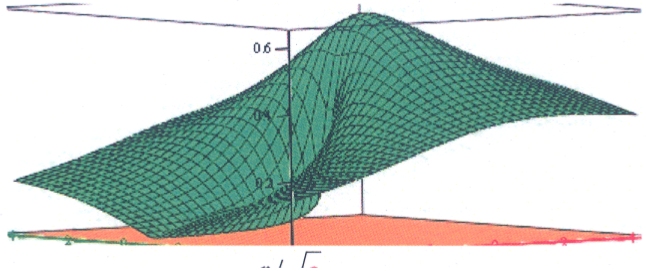
$$\sigma_{xz} = -\frac{K_{III}}{\sqrt{2\pi r}}\left[\sin\frac{\theta}{2}\left(1-\exp\left[-r/\sqrt{c}\right]\right)\right] \qquad \sigma_{yz} = \frac{K_{III}}{\sqrt{2\pi r}}\left[\cos\frac{\theta}{2}\left(1-\exp\left[-r/\sqrt{c}\right]\right)\right]$$

Gradient Stress non-singular

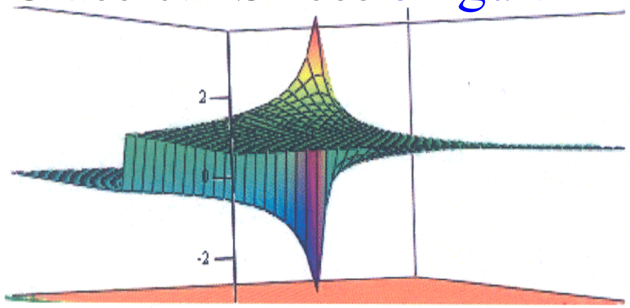




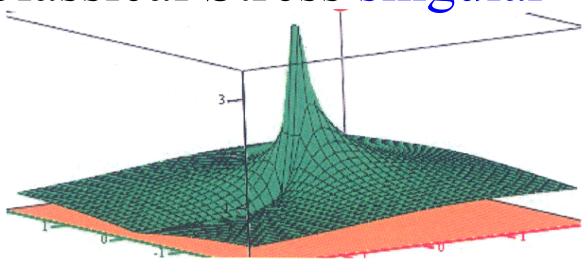
Gradient Stress non-singular



Classical Stress singular



Classical Stress singular



Note: $\dfrac{\left(1-e^{-r/\sqrt{c}}\right)}{\sqrt{r}}$ attains a maximum value at $r \cong 1.25\sqrt{c}$

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

■ Gradela Crack Nanomechanics (Mode I)

- ***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: $\lim\limits_{\mathbf{r}\to\infty}\boldsymbol{\sigma}_{ij}=\boldsymbol{\sigma}_{ij}^{\mathbf{0}}$

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

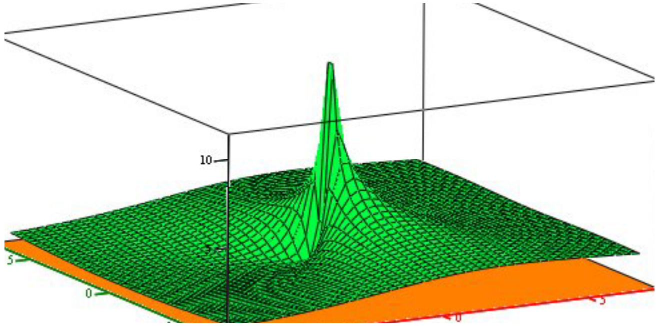
Zero tractions on crack surfaces

$$\sigma_{xy}(x,0^{\pm})=\sigma_{yy}(x,0^{\pm})=0 \;\; ; \quad |x|\le a$$

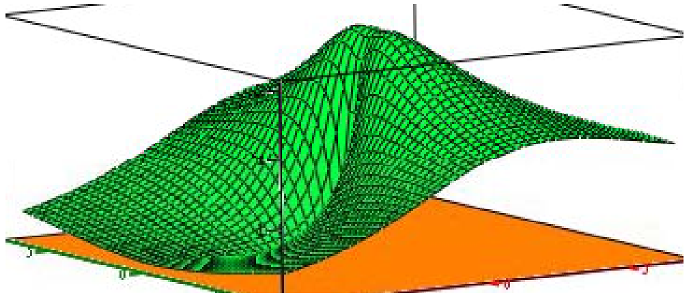
• *Nonsingular stress distribution in Mode I*

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

Classical Stress singular

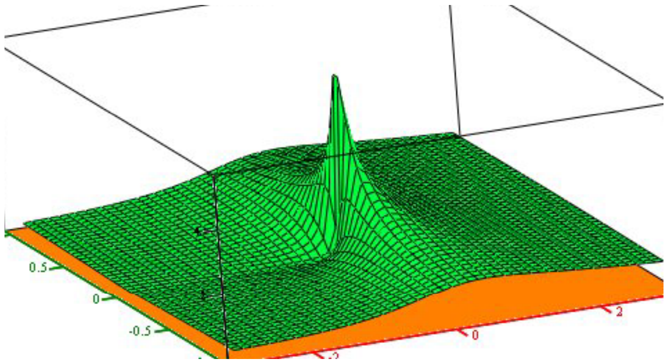


Gradient Stress non-singular

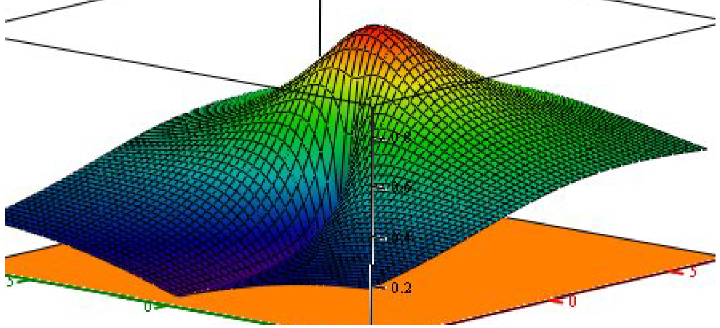


$$\sigma_{zz} = \frac{K_I \nu \sqrt{2}}{\sqrt{\pi r}}\cos\frac{\theta}{2}\left(1-e^{-r/\sqrt{c}}\right)$$

Classical Stress singular



Gradient Stress non-singular



$\sigma_{xx} = \ \ldots$; $\sigma_{xy} = \ \ldots$

- ***Details of Solution***
  - Note

$$\cos\frac{\theta}{2}\left(1+\sin\frac{\theta}{2}\sin\frac{3\theta}{2}\right)=\frac{5}{4}\cos\frac{\theta}{2}-\frac{1}{4}\cos\frac{5\theta}{2} \qquad (*)$$

  - Then

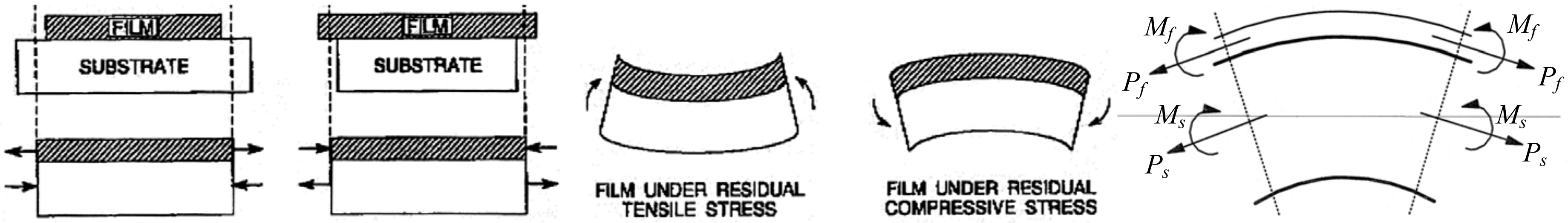
$$\sigma_{yy}-c\nabla^2\sigma_{yy}=\frac{K_I}{\sqrt{2\pi r}}\left[\frac{5}{4}\cos\frac{\theta}{2}-\frac{1}{4}\cos\frac{5\theta}{2}\right]$$

  - Solve 2 Inhomogeneous Helmholtz Eqs Separately
  - General + Particular Solution
  - Apply bc's & Conditions at ∞
  - Use again (*) to obtain

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

ADDITIONAL BENCHMARK PROBLEMS

■ Internal Stress in Thin Films



Axial Strain: $(\varepsilon_{xx})_i = \kappa(\bar{y}_i - y)$; ***Load Balance***: $P_s + P_f = 0$;

Moment Balance: $P_s(\bar{y} - \bar{y}_s) + P_f(\bar{y} - \bar{y}_f) + M_s + M_f = 0$

$$M_i = w\int_0^{h_i} \sigma_{xx}(\bar{y}_i - y)\,\mathrm{d}y\,; \quad (\mathrm{i} = s, f)\,;\ \bar{y}_s = h_s/2\,;\ \bar{y}_f = h_s + h_f/2$$

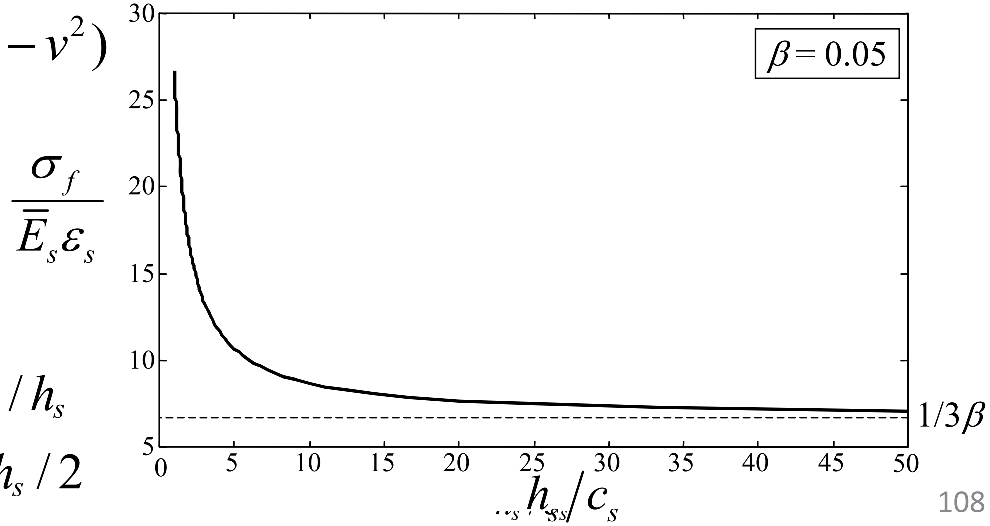
Gradient Elasticity:

$$\sigma_{xx} = \bar{E}\left(\varepsilon_{xx} + c\,\mathrm{sign}(\varepsilon_{xx})\left|\nabla\varepsilon_{xx}\right|\right) \quad ; \quad \bar{E} = E/(1-\nu^2)$$

Modified Stoney Formula:

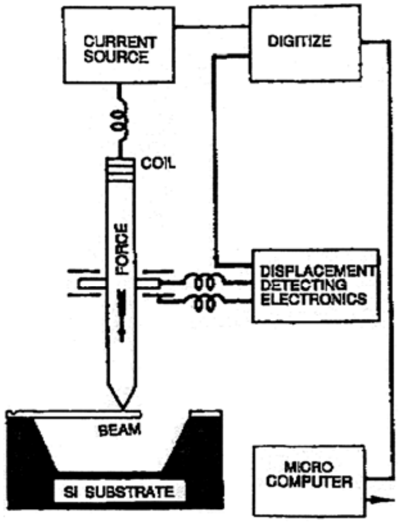
$$\therefore\ \sigma_f = \frac{P_f}{wh_f} = \kappa\frac{\bar{E}_s h_s^2}{6h_f}\left(1 + \frac{3c_s}{h_s}\right)$$

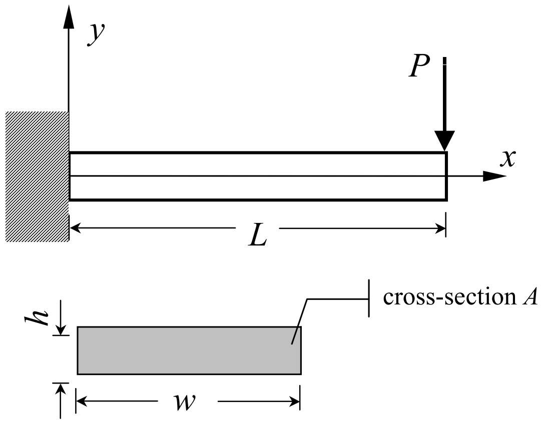
$$\Rightarrow\ \frac{\sigma_f}{\bar{E}_s\varepsilon_s} = \frac{1}{3\beta}\left[1 + 3\left(\frac{h_s}{c_s}\right)^{-1}\right] \quad ; \quad \begin{cases}\beta = h_f/h_s \\ \varepsilon_s = \kappa h_s/2\end{cases}$$



■ Bending of Cantilever Microbeams

Nanoindenter loading mechanism applied to a cantilever microbeam of a thin film material





Moment Equilibrium: $M = P(L-x) = \int_A \sigma_{xx} y \, dA$

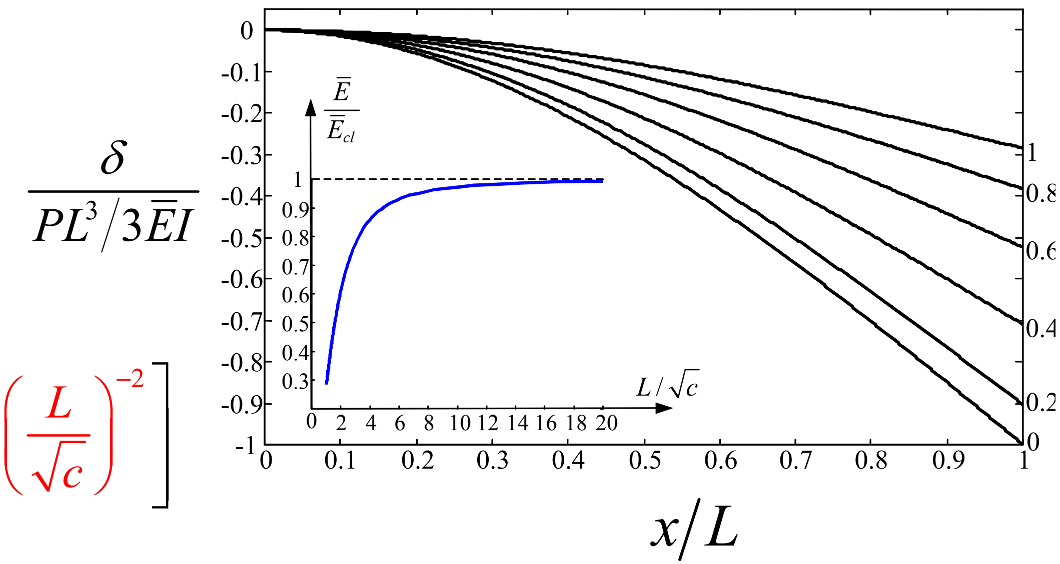
Axial Strain: $\varepsilon_{xx} = \kappa y; \; \kappa = \dfrac{\mathrm{d}^2\delta}{\mathrm{d}x^2}$

Gradient Elasticity: $\sigma_{xx} = \bar{E}(\varepsilon_{xx} - c\nabla^2\varepsilon_{xx})$

$$\bar{E} = E/(1-\nu^2)$$

$$\frac{\mathrm{d}^2\delta}{\mathrm{d}x^2} - c\frac{\mathrm{d}^4\delta}{\mathrm{d}x^4} = \frac{P}{\bar{E}I}(L-x)$$

$$\bar{E} = \frac{PL^3}{3\delta_{\max}I}\left[1 + 3\left(\frac{L}{\sqrt{c}}\right)^{-3}\tanh\left(\frac{L}{\sqrt{c}}\right) - 3\left(\frac{L}{\sqrt{c}}\right)^{-2}\right]$$

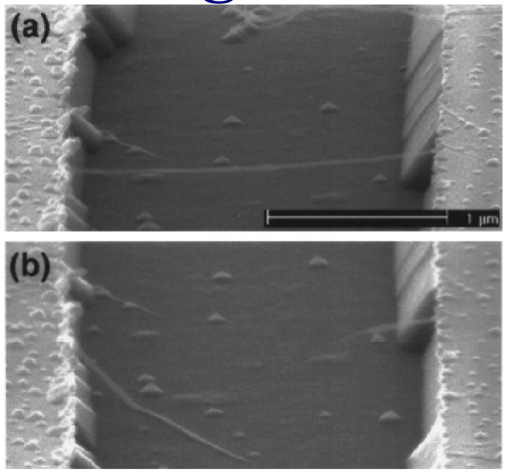


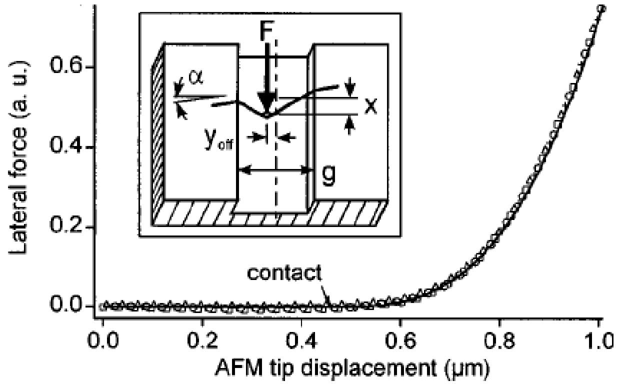
STRUCTURAL MECHANICS OF NANOTUBES

■Nanotubes as elastic strings

$$F = 2T\sin\theta = 2T\frac{2x}{L} \sim 8k \times \left(\frac{x^2}{g}\right)$$

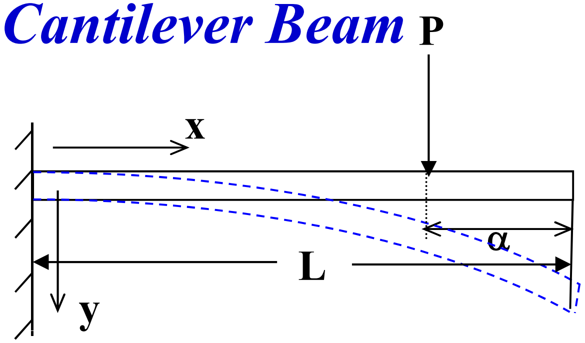
$$T = k(L - L_o); \quad L = \sqrt{g^2 + x^2}$$





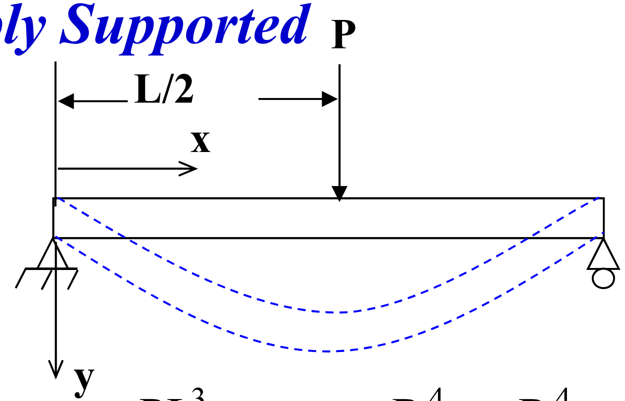
■Nanotubes as beams

•Cantilever Beam



$$y = \frac{P\alpha^2}{6EI}(3x - \alpha) \qquad \frac{P}{y} \sim \frac{1}{\alpha^3}$$

•Simply Supported

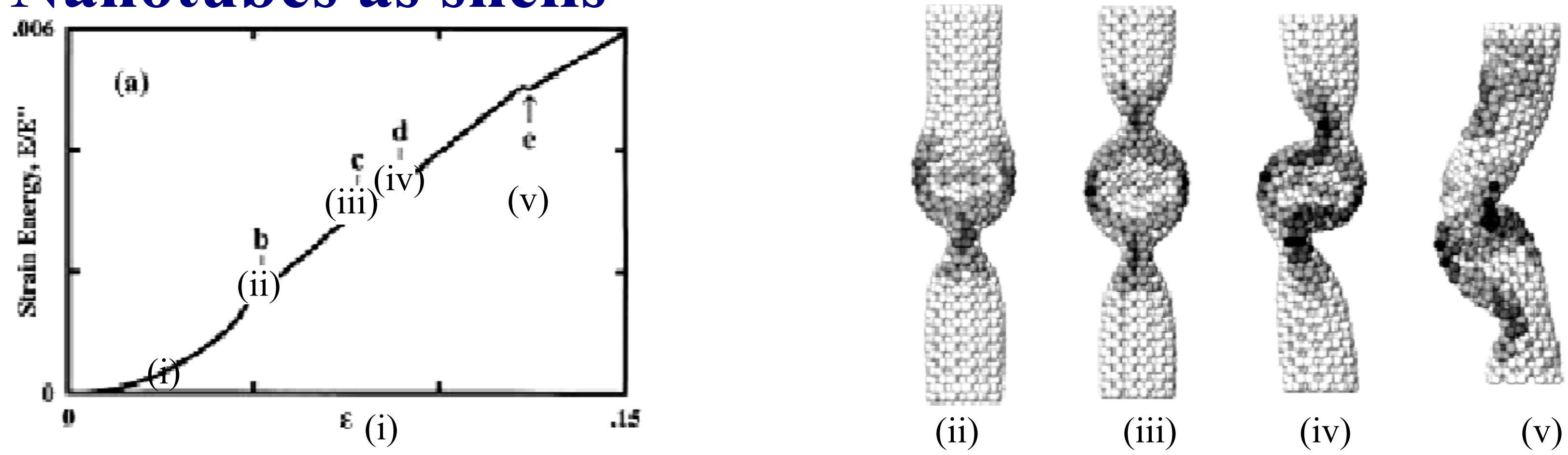


$$y = \frac{PL^3}{48EI} \qquad I = \pi\frac{R_{out}^4 - R_{in}^4}{4}$$

•Euler Buckling

$$P = \frac{\pi^2 EI}{L^2} \qquad (E = 1\,TPa, \quad L = 250\,nm, \quad d = 5\,nm) \qquad \therefore P \simeq 5\,nN$$

■ Nanotubes as shells



MD-simulated nanotube of length L = 6 nm, diameter d = 1 nm, and armchair helicity (7,7) under axial compression. The strain energy displays four singularities corresponding to shape changes. At ε_1 = 0.05 the cylinder buckles into the pattern (ii), displaying two identical flattenings—"fins" perpendicular to each other. Further increase of ´ enhances this pattern gradually until at ε_2 = 0.076 the tube switches to a three-fin pattern (iii), which still possesses a straight axis. In a buckling sideways at ε_3 = 0.09 the flattenings serve as hinges, and only a plane of symmetry is preserved (iv). At ε_4 = 0.13 an entirely squashed asymmetric configuration forms.

$$E = \frac{1}{2}\iint \{D\ [(\kappa_x + \kappa_y)^2 - 2(1-\nu)(\kappa_x\kappa_y - \kappa_{xy}^2)]$$

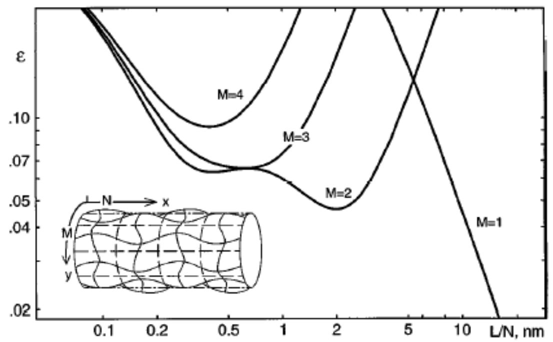
$$+ \frac{C}{1-\nu^2}\ [(\varepsilon_x + \varepsilon_y)^2 - 2(1-\nu)(\varepsilon_x\varepsilon_y - \varepsilon_{xy}^2)]\}$$

$$C = E\,h \quad D = \frac{E\ \ h^3}{12(1-\nu^2)}$$

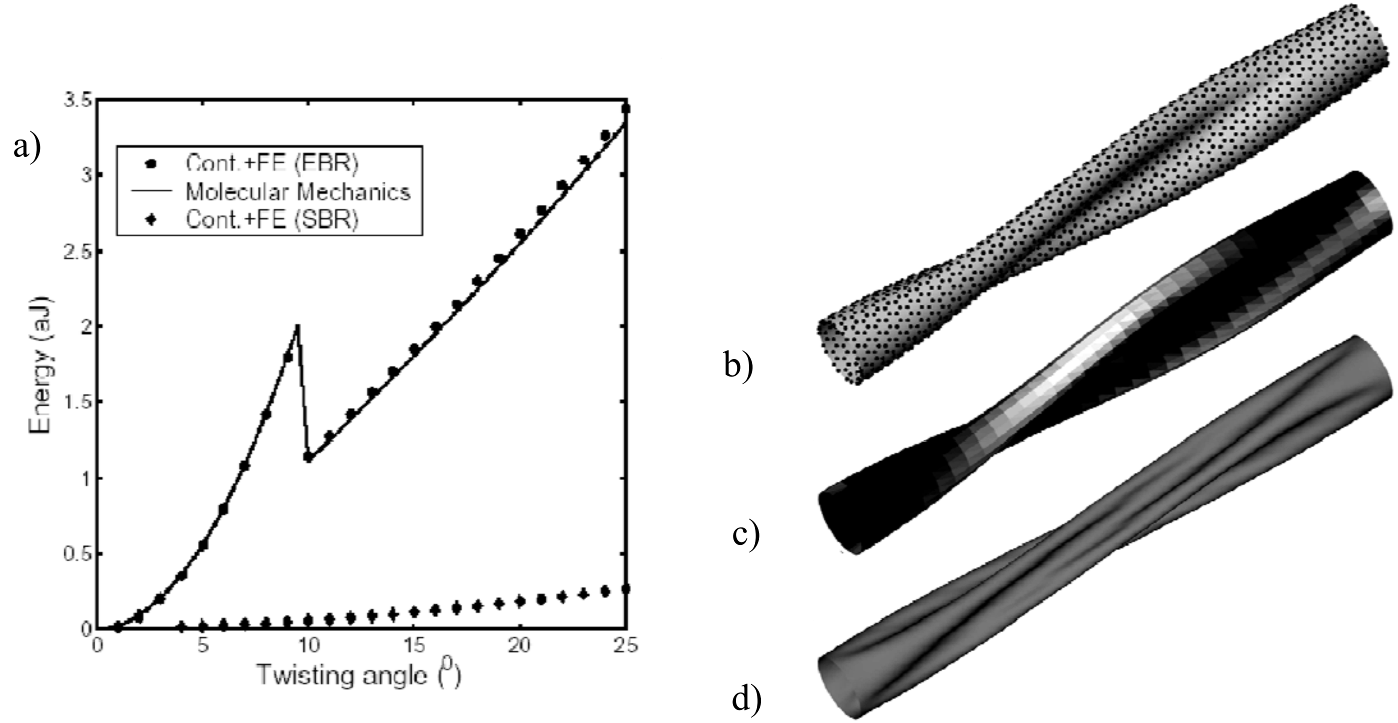
(flexural rigidity)

h = thickness of walls

$$E = 5\,\mathrm{TPa} \quad h = 0.06\ \ nm \quad \varepsilon_c = (0.077)d^{-1}$$



The critical strain levels for a continuous, 1 nm wide tube as a function of its scaled length L/N. A buckling pattern (M,N) is defined by the number of half waves $2M$ and N in the y and x directions, respectively; e.g. a (4,4) pattern is shown in the inset.

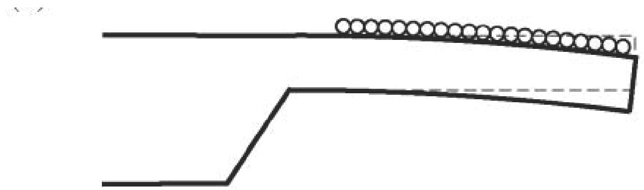


a) Twisted [10-10] nanotube: comparison of the strain energy relative to the relaxed nanotube as a function of the twisting angle for Molecular Mechanics (line), the continuum membrane based on the exponential Born rule (circles) and a continuum membranes based on the standard Born rule (diamonds). Set of 3 nanotube simulations: b) Comparison of new exponential Born theory as compared to MD simulations, c) exponential Born theory, d) standard Born theory applied to membranes; it differs markedly from the exponential Born approach.

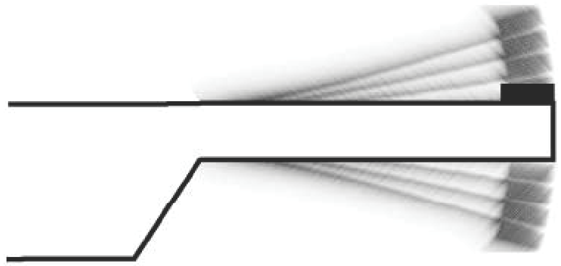
■ Micro/Nano Cantilevers as Biological Sensors

- Upper side of the cantilever covered with a coating (sensor layer)
- Sensor layer binds specific molecules

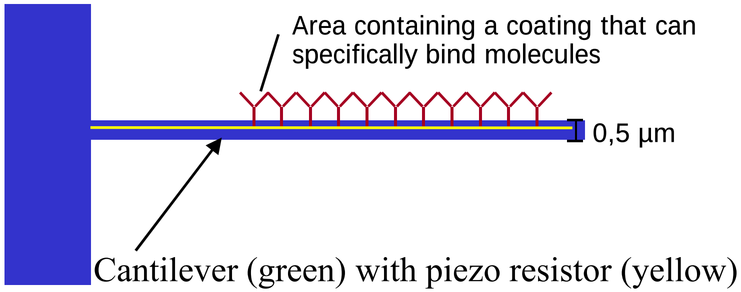
  - Surface stress variation: cantilever bending



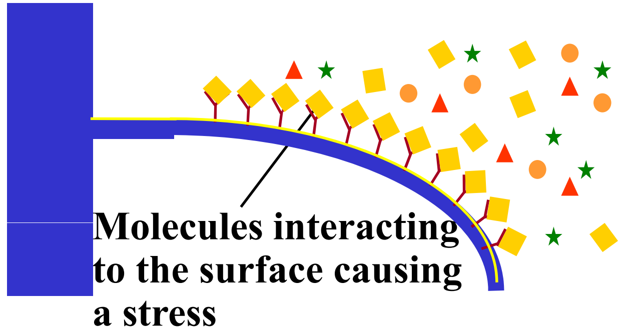
  - Resonance frequency variation

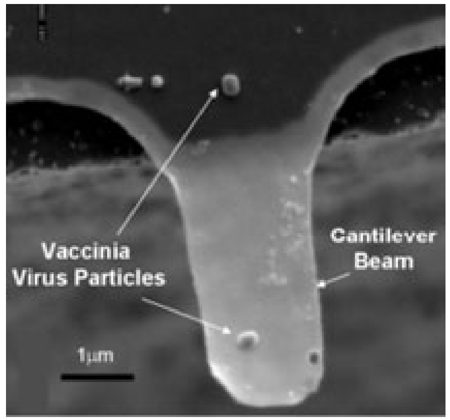


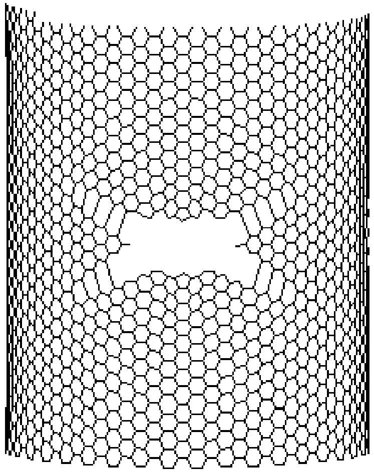
Cantilever with no detection



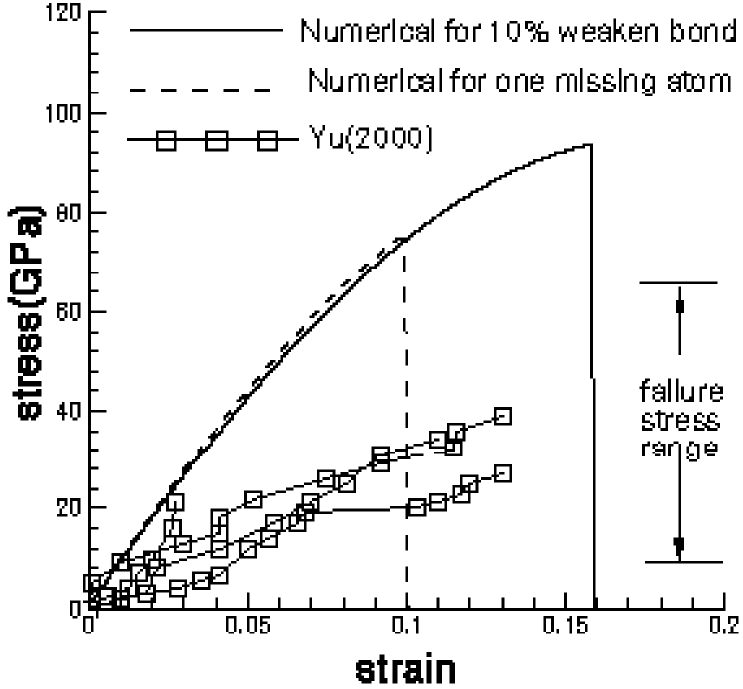
Cantilever with detection







Fracture with
5/7/7/5 dislocation of nanotube



Stress-strain curve for
experiment vs. computation

Fracture in the presence of a 5/7/7/5 defect (Stone-Wales type) nanotube and comparison of MM calculations with the Ruoff and co-workers experiments.

■ Flexural Wave Propagation in Nanotubes

- ***Gradient Constitutive Eqs***

$$\sigma = E\left(\varepsilon + \ell^2 \frac{\partial^2 \varepsilon}{\partial x^2}\right), \quad \tau = G\left(\gamma + \ell^2 \frac{\partial^2 \gamma}{\partial x^2}\right)$$

$$M = EI\left(\frac{\partial \varphi}{\partial x} + \ell^2 \frac{\partial^3 \varphi}{\partial x^3}\right)$$

$$\frac{\partial w}{\partial x} = \varphi - \gamma$$

where w – deflection, – slope, $\beta = 0.5$ – thin wall tube

- ***Timoshenko-like Beam***

$$\rho\frac{\partial^2 w}{\partial t^2}+\beta G\left[\left(\frac{\partial\varphi}{\partial x}-\frac{\partial^2 w}{\partial x^2}\right)+\ell^2\left(\frac{\partial^3\varphi}{\partial x^3}-\frac{\partial^4 w}{\partial x^4}\right)\right]=0$$

$$\rho I\frac{\partial^2\varphi}{\partial t^2}+\beta AG\left[\left(\varphi-\frac{\partial w}{\partial x}\right)+\ell^2\left(\frac{\partial^2\varphi}{\partial x^2}-\frac{\partial^3 w}{\partial x^3}\right)-EI\left(\frac{\partial^2\varphi}{\partial x^2}-\ell^2\frac{\partial^4\varphi}{\partial x^4}\right)\right]=0$$

$$c=\sqrt{\frac{-b_1\pm\sqrt{b_1^2-4a_1c_1}}{2a_1}}\qquad\text{. . . . .}\qquad\text{flexural wave speed}$$

where $a_1=\rho^2 Iq^2/\beta G,\quad c_1=EIq^2\left(1-\ell^2q^2\right)^2$

$$b_1=\left[\rho A+\rho I\left(1+E/\beta G\right)q^2\right]\left(\ell^2q^2-1\right)$$

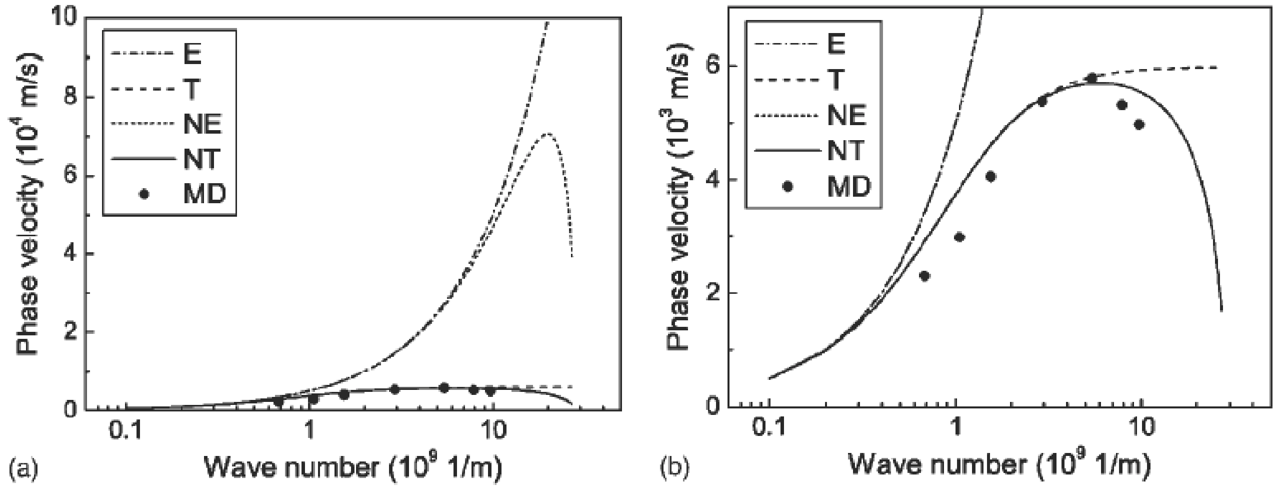
$\ell\to 0\qquad\Rightarrow$

$$\rho A\frac{\partial^2 w(x,t)}{\partial t^2}+EI\frac{\partial^4 w(x,t)}{\partial t^4}-\rho I\left(1+\frac{E}{\beta G}\right)\frac{\partial^4 w(x,t)}{\partial x^2\partial t^2}+\frac{\rho^2 I}{\beta G}\frac{\partial^4 w(x,t)}{\partial t^4}=0$$

- ***Euler-like Beam (neglect rotary inertia & shear)***

$$\rho A\frac{\partial^2 w(x,t)}{\partial t^2}+EI\left[\frac{\partial^4 w(x,t)}{\partial t^4}+\ell^2\frac{\partial^6 w(x,t)}{\partial t^6}\right]=0$$

$$c=q\sqrt{\frac{EI}{\rho A}\left(1-\ell^2 q^2\right)}\quad ; \qquad \ell\to 0 \qquad \Rightarrow \qquad c=q\sqrt{\frac{EI}{\rho A}}$$



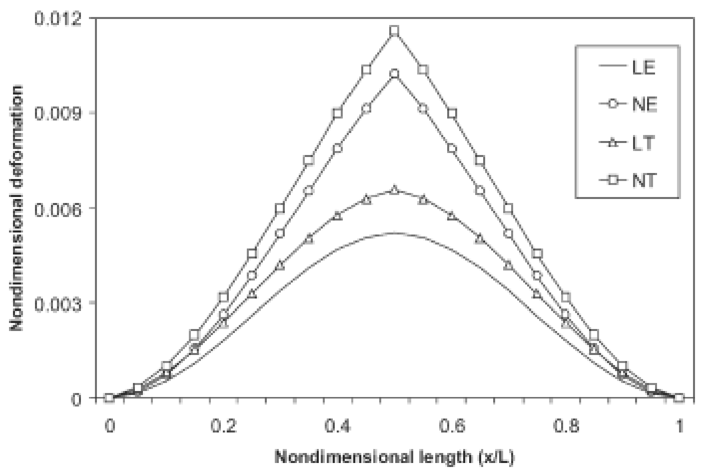
The dispersion relation of the armchair (5,5) carbon nanotube.
(a) The phase velocity of flexural wave versus wave number; (b) The zoom of (a).

- ***Cantilever/Simply supported Nanotubes***

$$\frac{\partial V}{\partial x} + q(x) = 0 \quad ; \quad V - \frac{\partial M}{\partial x} = 0$$

$$\sigma - \ell^2 \frac{\partial^2 \sigma}{\partial x^2} = E\varepsilon$$

$$M - \ell^2 \frac{\partial^2 M}{\partial x^2} = EI \frac{\partial^2 w}{\partial x^2}$$



Static deformation of a fixed–fixed structure subjected to a point force at the middle.

GRADIENT PLASTICITY / SCALE INVARIANCE [PLASTICITY OF NANOPOLYCRYSTALS]

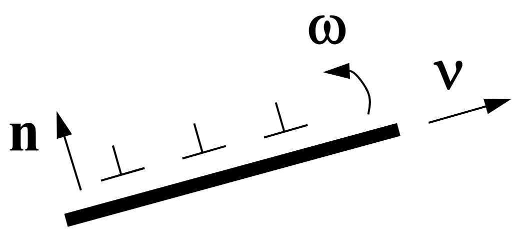
■ Gradient Plasticity: A Scale Invariance Argument

- ***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; $\hat{\mathbf{f}}$...dislocastion-lattice interaction force

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



$$\mathbf{M} = \left(\boldsymbol{\nu} \otimes \mathbf{n}\right)_{\mathrm{s}}, \quad \boldsymbol{\Omega} = \left(\boldsymbol{\nu} \otimes \mathbf{n}\right)_{\alpha}, \quad \dot{\boldsymbol{\nu}} = \boldsymbol{\omega}\boldsymbol{\nu}$$

$$\mathbf{D}^{\mathrm{p}} = \dot{\gamma}^{\mathrm{p}}\mathbf{M}, \quad \mathbf{W}^{\mathrm{p}} = \dot{\gamma}^{\mathrm{p}}\boldsymbol{\Omega}, \quad \mathbf{T}^{\mathrm{D}} = \mathrm{t_m}\mathbf{M} + \mathrm{t_n}\mathbf{N}$$

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

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

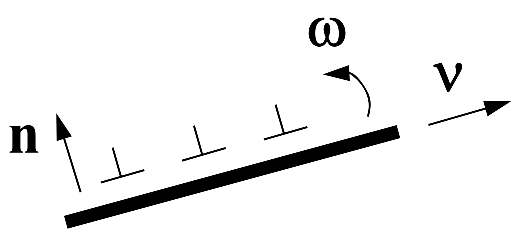
- ***Momentum Balance for Dislocated State***

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

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

- ***Recall***

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



$$\mathbf{M} = \left(\boldsymbol{\nu} \otimes \mathbf{n}\right)_{s}, \quad \boldsymbol{\Omega} = \left(\boldsymbol{\nu} \otimes \mathbf{n}\right)_{\alpha}, \quad \dot{\boldsymbol{\nu}} = \boldsymbol{\omega}\boldsymbol{\nu}$$

$$\mathbf{D}^{\mathrm{p}} = \dot{\gamma}^{\mathrm{p}}\mathbf{M}, \quad \mathbf{W}^{\mathrm{p}} = \dot{\gamma}^{\mathrm{p}}\boldsymbol{\Omega}, \quad \mathbf{T}^{\mathrm{D}} = t_{m}\mathbf{M} + t_{n}\mathbf{N}$$

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

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

- ***Structure of Macroscopic Anisotropic Hardening Plasticity***

$$\mathbf{D}^{p} = \frac{\dot{\gamma}^{p}}{2\sqrt{J}}\left(\sigma' - \alpha'\right)$$

$$\overset{o}{\alpha} = \left(\frac{\dot{t}_{m}}{\dot{\gamma}^{p}} - \frac{\dot{t}_{n} t_{m}}{t_{n}\dot{\gamma}^{p}}\right)\mathbf{D}^{\mathbf{p}} + \frac{\dot{t}_{n}}{t_{n}}\alpha, \qquad \overset{o}{\alpha} = \dot{\alpha} - \omega\alpha + \alpha\omega$$

$$\omega = \mathbf{W} - \mathbf{W}^{\mathbf{p}}, \qquad \mathbf{W}^{\mathbf{p}} = -\frac{1}{t_{n}}\left(\alpha\mathbf{D}^{\mathbf{p}} - \mathbf{D}^{\mathbf{p}}\alpha\right)$$

$$\dot{\gamma}^{p} = \frac{\sigma' \cdot \left(\sigma' - \alpha'\right)}{\kappa\left(t'_{m} + 2\kappa'\right)}; \qquad \begin{cases} \dot{f} = 0 \\ f = \frac{1}{2}\left(\sigma' - \alpha'\right)\cdot\left(\sigma' - \alpha'\right) - \kappa^{2} = 0 \end{cases}$$

- ***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 ($\boldsymbol{n}, \boldsymbol{\nu}$)*

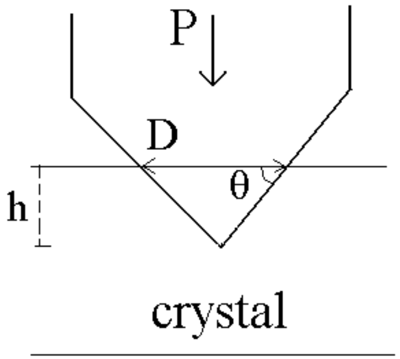
$$\therefore \quad \left(\mathrm{div}\mathbf{T}^{\mathbf{inh}}\right) \cdot \boldsymbol{\nu} \approx \nabla^{2}\gamma^{p}$$

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

ADDITIONAL BENCHMARK PROBLEMS

■ Size Effects in Micro/Nano indentation

- ***Definitions***



$$H = \frac{P}{A_p}, \ \tan\theta = \frac{2h}{D}$$

$$A_p = \pi\left(\frac{D}{2}\right)^2 = \frac{\pi}{(\tan\theta)^2}h^2$$

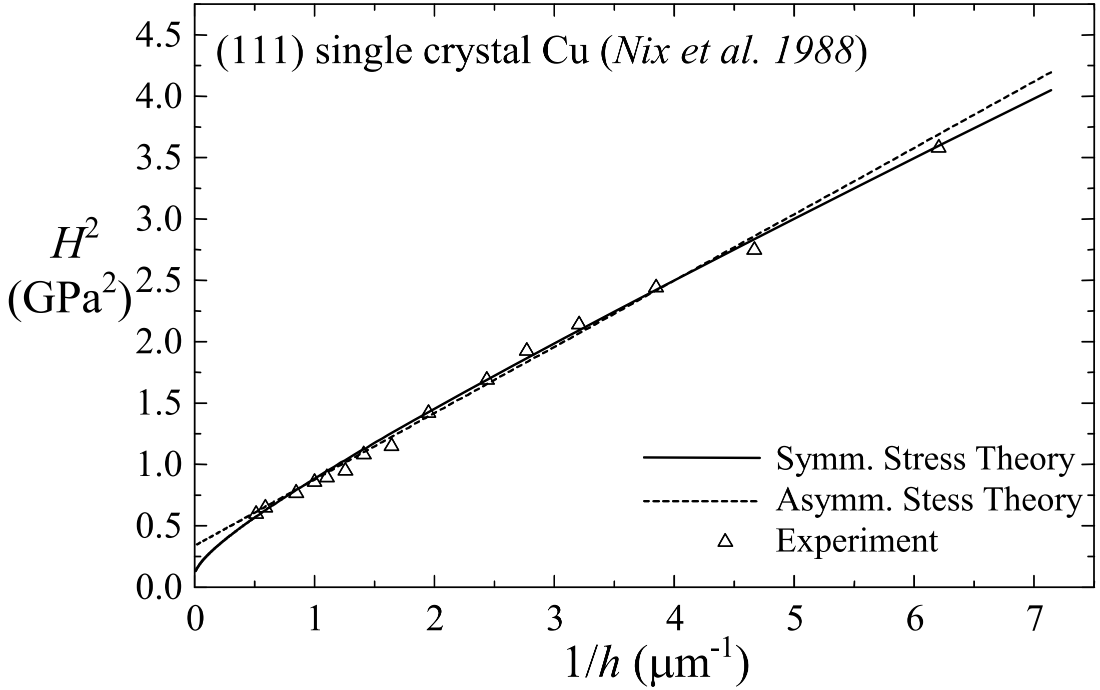
- ***Gradient Theory (Symmetric Stress) and Tabor's Rule***

$$\tau = \kappa(\gamma) + c\left|\nabla\gamma\right|^{1/2}; \qquad \gamma \sim \frac{2h}{D} = \tan\theta$$

$$\left|\nabla\gamma\right| \sim \frac{2\gamma}{D} = \frac{2\tan\theta}{D} = \frac{(\tan\theta)^2}{h}$$

$$H = 3\sigma \rightarrow H = 3\sqrt{3}\tau \Rightarrow H \sim H_0\left[1 + \sqrt{\frac{l}{h}}\right]; \qquad \sqrt{l} = 3\sqrt{3}c\frac{\tan\theta}{H_o}$$

• *Couple Stress Theory (Asymmetric Stress)*



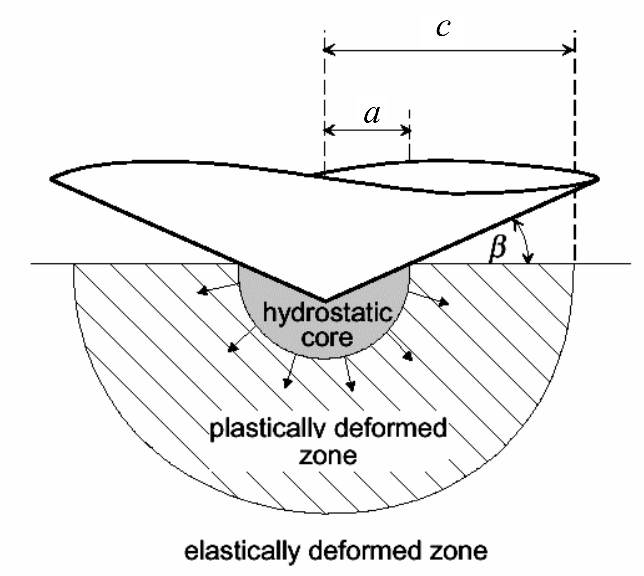
Gradient Theory → $H_o = 0.35$ GPa, $l = 4.6$ μm ⇒ $(c/G)^2 = 6.73\ 10^{-5}$ μm

Couple Stress Theory → $H_o = 0.581$ GPa, $l = 1.6$ μm

■ Johnson's Spherical Cavity Model Revisited

- ***Core Incompressibility***

$$2\pi a^2 du(a) = \pi a^2 dh = \pi a^2 \tan\beta da$$



- ***Geometric Similarity***

$$\frac{da}{dr_{ep}} = \frac{a}{r_{ep}}$$

- ***Constitutive Assumptions***

  – Rigid Perfect Plasticity $\left(\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^p, d\sigma_Y / d\bar{\varepsilon} = 0\right)$

  – Gradient Yield Condition: $\bar{\sigma} = \sigma_Y - c\nabla^2\varepsilon$

- ***Displacements / Stresses / Tractions***

$$u(r) = \frac{r_{ep}^3}{r^2}\frac{\sigma_Y(1+\nu)}{3E}\frac{r_{ep}^2}{r_{ep}^2+4l^2(1+\nu)}, \quad l^2 = \frac{c}{E}$$

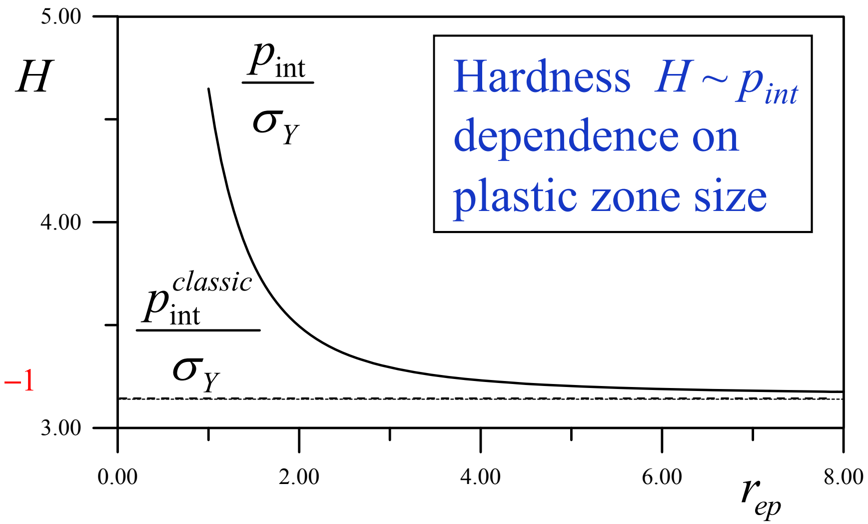
$$t(r) = -\frac{2\sigma_Y}{3} - 2\sigma_Y \log(\frac{r_{ep}}{r}) - \frac{4}{15}\sigma_Y(1+\nu)\frac{l^2}{r_{ep}^2+4l^2(1+\nu)}\left[9\left(\frac{r_{ep}}{r}\right)^5 - 19\right]$$

- ***Johnson's Modified Relations***

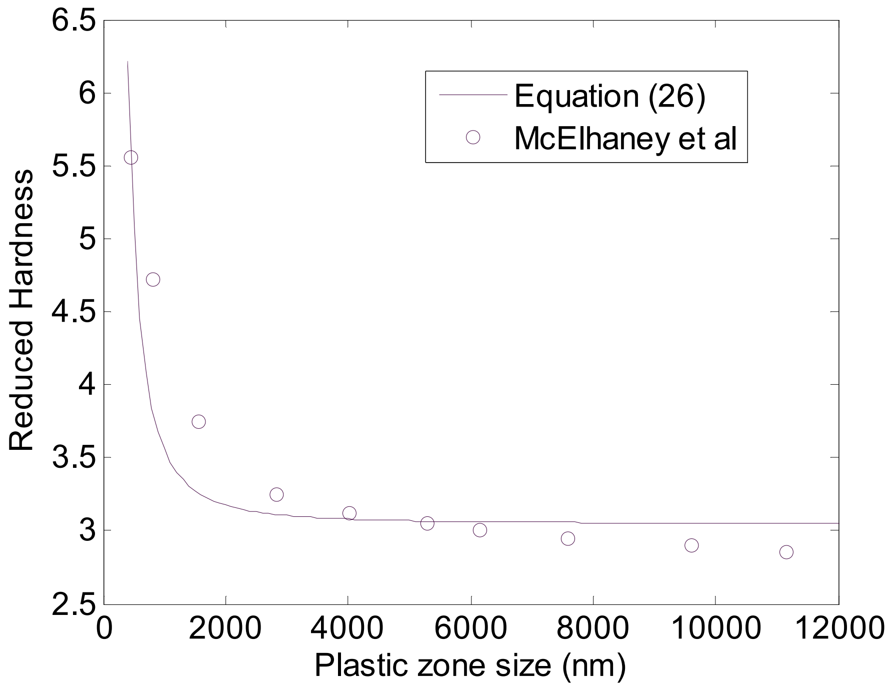
$$\frac{p_{\text{int}}}{\sigma_Y} = -\frac{t(\alpha)}{\sigma_Y} = \frac{2}{3} + 2\log(\frac{r_{ep}}{\alpha})$$

$$+\frac{4}{15}\frac{l^2(1+\nu)}{r_{ep}^2+4l^2(1+\nu)}\left[9\left(\frac{r_{ep}}{\alpha}\right)^5 - 19\right]$$

$$\left(\frac{r_{ep}}{a}\right)^3 = \frac{E\tan\beta}{2\sigma_Y(1+\nu)}\left(\frac{r_{ep}^2(3r_{ep}^2+20l^2(1+\nu))}{3(r_{ep}^2+4l^2(1+\nu))^2}\right)^{-1}$$



- ***Prediction of H/σ_Y vs r_{ep}***



$$E = 129.8\ GPa,\ v = 0.34,\ \sigma_Y = 0.36\ GPa$$

The fit determines the internal length $\ell \approx 15.77$ nm

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).

MICROMORPHIC/MICROFORCE FORMULATION [FOREST+ECA/IJSS (In Press)]

■ General Scalar Microstrain Gradient Plasticity

- ***Classical and Genaralized Plasticity***

$$DOF0 = \{\boldsymbol{u}\} \qquad STATE0 = \{\boldsymbol{\varepsilon}^e, p, \alpha\}$$

$$DOF = \{\boldsymbol{u}, {}^{\chi}p\} \qquad STATE = \{\boldsymbol{\varepsilon}^e, p, \alpha, {}^{\chi}p, \nabla{}^{\chi}p\}$$

- ***Extra Balance Eq***

$$p^{(i)} = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} + a\,{}^{\chi}\dot{p} + \boldsymbol{b}\,\nabla{}^{\chi}\dot{p}, \qquad p^{(c)} = \boldsymbol{t}\cdot\boldsymbol{u} + a^{c}\,{}^{\chi}\dot{p}$$

$$div\,\boldsymbol{b} - a = 0, \quad \forall \boldsymbol{x} \in \Omega, \qquad \boldsymbol{b}\cdot\boldsymbol{n} = a^{c}, \quad \forall \boldsymbol{x} \in \Omega$$

- ***State Laws***

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^p$$

$$\boldsymbol{\sigma} = \rho\frac{\partial\psi}{\partial\boldsymbol{\varepsilon}^e}, \quad R = \rho\frac{\partial\psi}{\partial p}, \quad X = \rho\frac{\partial\psi}{\partial\alpha}, \quad a = \rho\frac{\partial\psi}{\partial{}^{\chi}p}, \quad \boldsymbol{b} = \rho\frac{\partial\psi}{\partial\nabla{}^{\chi}p}$$

- ***Evolution Eqs***

$$D^{res} = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}^p - R\dot{p} - X\dot{\alpha} \geq 0$$

$$\dot{\varepsilon}^p = \dot{\lambda}\frac{\partial f}{\partial\boldsymbol{\sigma}}, \quad \dot{p} = -\dot{\lambda}\frac{\partial f}{\partial R}, \quad \dot{\alpha} = -\dot{\lambda}\frac{\partial f}{\partial X}$$

■ Link to Aifantis Strain Gradient Plasticity

- ***Yield Function***

$$f\left(\boldsymbol{\sigma}, R\right) = \sigma_{eq} - \sigma_Y - R$$

- ***Hardening***

$$R = \frac{\partial \psi}{\partial p} = \left(H + H_\chi\right) p - H_\chi {}^\chi p$$

- ***Under Plastic Loading***

$$\sigma_{eq} = \sigma_Y + H {}^\chi p - A\left(1 + \frac{H}{H_\chi}\right) \Delta {}^\chi p$$

– Compare with Aifantis model [Aifantis, 1987]

$$\sigma_{eq} = \sigma_Y + R\left(p\right) - c^{-} \Delta p$$

Equivalence obtained for $H_\chi = \infty$ (internal constraint):

$${}^\chi p \equiv p, \qquad A = c$$

■ Simplified Scalar Microstrain Gradient Plasticity

- ***Quadratic Free Energy Potential***

$$\rho\psi\left(\boldsymbol{\varepsilon}, p, {}^{\chi}p, \nabla {}^{\chi}p\right) = \frac{1}{2}\boldsymbol{\varepsilon}^{e} : \Lambda : \boldsymbol{\varepsilon}^{e} + \frac{1}{2}Hp^{2} + \frac{1}{2}H_{\chi}\left(p - {}^{\chi}p\right)^{2} + \frac{1}{2}\nabla {}^{\chi}p \cdot \boldsymbol{A} \cdot \nabla {}^{\chi}p$$

- ***Constitutive Eqs.***

$$\boldsymbol{\sigma} = \Lambda : \boldsymbol{\varepsilon}^{e}, \quad a = -H_{\chi}\left(p - {}^{\chi}p\right), \quad \boldsymbol{b} = \boldsymbol{A}\nabla {}^{\chi}p, \quad R = \left(H + H_{\chi}\right)p - H_{\chi}{}^{\chi}p$$

- ***Substitution of Constitutive Eq. into Extra Balance Eq.***

$${}^{\chi}p - \frac{1}{H_{\chi}} div\left(\boldsymbol{A} \cdot \nabla {}^{\chi}p\right) = p$$

- ***Homogeneous and Isotropic Materials*** $\quad \boldsymbol{A} = A\boldsymbol{1}$

$${}^{\chi}p - \frac{A}{H_{\chi}}\Delta {}^{\chi}p = p, \qquad \text{bc:} \quad \nabla {}^{\chi}p \cdot \boldsymbol{n} = a^{c}$$

Same partial differential eq. as in the implicit gradient-enhanced elastoplasticity with $a^{c} = 0$ [Engelen et al., 2003]

■ Hypertemperature

- ***Degrees of Freedom and State Space***

$$DOF = \{\boldsymbol{u}\,, T\}, \qquad STATE = \{\boldsymbol{\varepsilon}\,, T\,, \nabla T\}$$

- ***Extended Power of Internal Forces***

$$p^{(i)} = \boldsymbol{\sigma} : \boldsymbol{\varepsilon} + a\dot{T} + \boldsymbol{b}\cdot\nabla\dot{T}$$

- ***Generalized Balance of Momentum Eqs.***

$$div\boldsymbol{\sigma} + \boldsymbol{f} = 0\,, \qquad div\boldsymbol{b} - a = 0$$

- ***Energy Balance***

$$\dot{\in} = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} + a\dot{T} + \boldsymbol{b}\cdot\nabla\dot{T} - div\boldsymbol{q}$$

- ***Entropy Imbalance***

$$\rho\left(T\dot{\eta} - \dot{\in}\right) + p^{(i)} - \frac{\boldsymbol{q}}{T}\cdot\nabla T \geq 0$$

- ***Clausius-Duhem Inequality***

$$\psi(\boldsymbol{\varepsilon}, T, \nabla T)$$

$$\left(\boldsymbol{\sigma} - \rho\frac{\partial \psi}{\partial \boldsymbol{\varepsilon}}\right) : \dot{\boldsymbol{\varepsilon}} - \left(\rho\eta + \rho\frac{\partial \psi}{\partial T} - a\right)\dot{T} + \left(\boldsymbol{b} - \rho\frac{\partial \psi}{\partial \nabla T}\right)\cdot \nabla \dot{T} - \frac{\boldsymbol{q}}{T}\cdot \nabla T \geq 0$$

- ***State Laws***

$$\boldsymbol{\sigma} = \rho\frac{\partial \psi}{\partial \boldsymbol{\varepsilon}}, \qquad \rho\eta = -\rho\frac{\partial \psi}{\partial T} + a, \qquad \boldsymbol{b} = \rho\frac{\partial \psi}{\partial \nabla T}$$

- ***Fourier Law***

$$\boldsymbol{q} = -\kappa \nabla T$$

- ***Heat Equation***

$$\rho T \dot{\eta} = -div\boldsymbol{q}$$

- ***Linear Model***

$$\rho\psi_T(T, \nabla T) = -\rho(T - T_0)\eta_0 - \frac{1}{2}\frac{\rho C_\varepsilon}{T_0}(T - T_0)^2 + \frac{1}{2}A\nabla T \cdot \nabla T$$

$$\rho C_\varepsilon \dot{T} = \kappa \Delta T - T_0 A \Delta \dot{T}$$

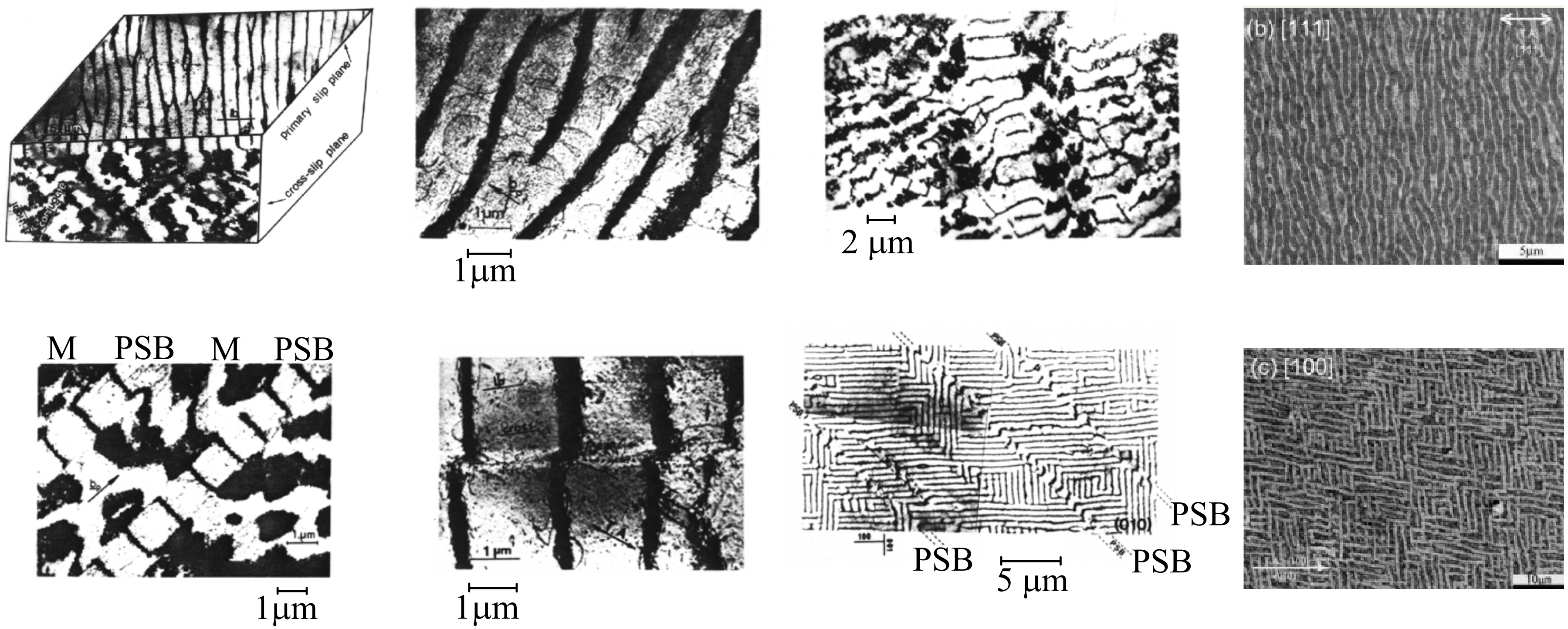
Called first Cattaneo Eq. [Müller and Ruggeri, 1993]

DISLOCATION PATTERNING: THE W–A MODEL

[Nicolis & Prigogine Book *Exploring Complexity* (1989), Chapter 5]

■ PSBs Ladder/Labyrinth Structures in Cyclic Deformation

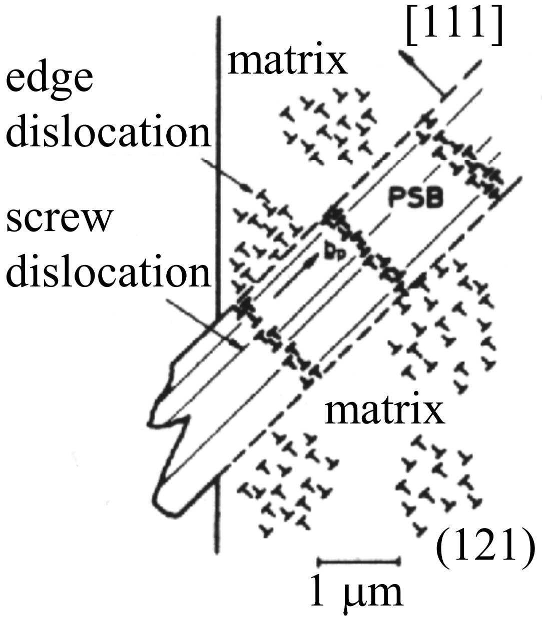
- ***The Initial Motivation for Dislocation Patterning Developments***

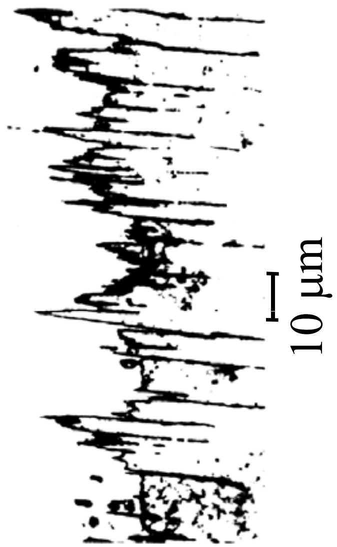


– *Winter-Mughrabi-Laird; Tabata et al; Kaneko-Hashimoto*

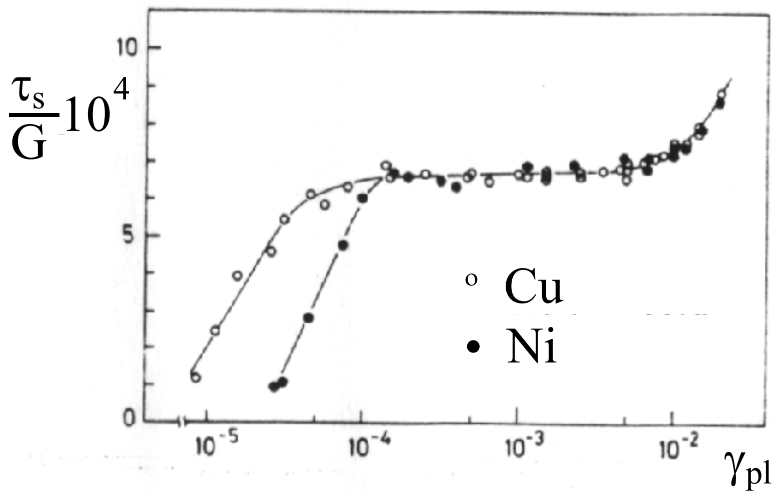
TEM and SEM micrographs

- ***More Pictures on PSB's***
  - *- Vein / Ladder structure – specimen surface*





  - *- Stress – strain graph*



■ Pre W–A Dislocation Evolution Models

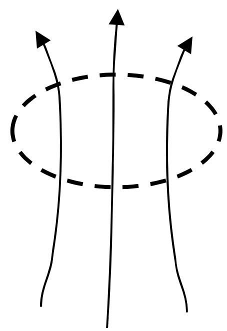
- ***Gilman/Metal Physics Dislocation Dynamics ('50s)***

$$\dot{\rho} = g(\rho); \qquad g(\rho) = a\rho\text{-}b\rho^2$$

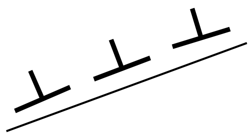
$\therefore$ Hardening / softening, Creep, etc.

- ***Kroner/Mura/Kosevich Continuous Distributions (60's)***

$$\dot{\boldsymbol{\alpha}} + \mathrm{curl}\,\mathbf{J}^{\mathbf{T}} = 0$$



$$\boldsymbol{\alpha} \equiv \int (\mathbf{t} \otimes \mathbf{b})\, \rho \; d\Omega\,, \qquad \mathbf{J} \equiv \int (\mathbf{t} \times \mathbf{j}) \otimes \mathbf{b} \; d\Omega$$

Single Slip:  $\Rightarrow$ $\dot{\rho} + \mathrm{div}\,\mathbf{j} = 0\,, \qquad \mathbf{j} = \rho\, \boldsymbol{\upsilon}$

i.e. "particle-like" conservation law

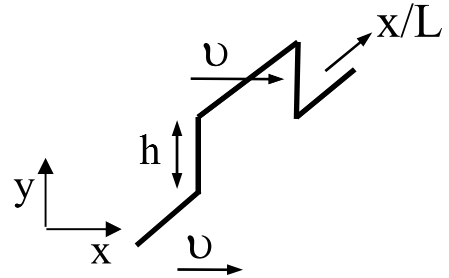
- ***ECA Compromise for Single Slip (80's)***
  - *Complete Balance Law:* $\dot{\rho} + \mathrm{div}\mathbf{J} = g$; $\begin{cases} \mathbf{J} = -D\nabla_y \rho + \ldots \\ g = a\rho - b\rho^2 + \ldots \end{cases}$
  - *Dislocation Effective Diffusion:* $\dot{\rho} = D\nabla^2_{yy}\rho + \ldots + g(\rho)$, $D \simeq D_{cs} + D_g$
    - Cross slip (D_{cs})

      $$D_{cs} \sim q_{cs} \frac{h^2}{d} \langle \upsilon \rangle$$

      q_{cs} … cross-slip probability parameter

      d … average glide distance

      (Malygin, Kubin, et al.)



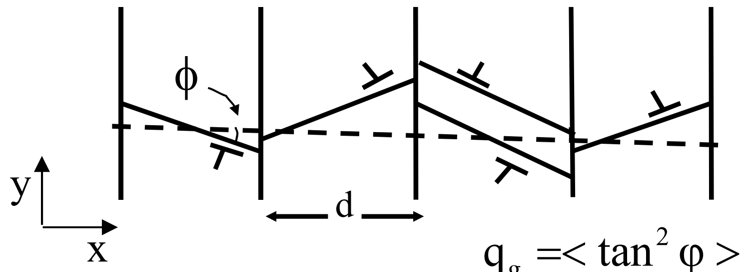
    - Glide (D_g)

      $$D_g \sim q_g d \langle \upsilon \rangle$$

      q_g … average over all glide planes/grain orientation parameter

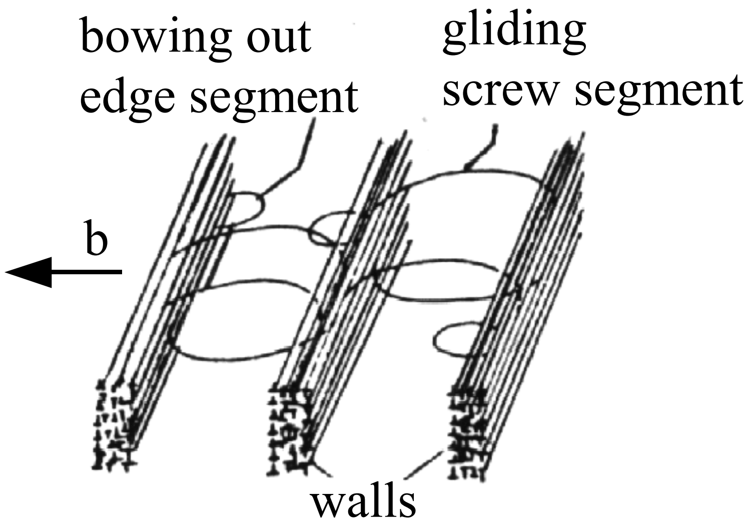
      d … average grain size

      (Hahner, et al)



$q_g = < \tan^2 \varphi >$

■ The (In)Famous W-A Model: 1D Reaction-Diffusion Scheme



$$\dot{\rho}_i = g(\rho_i) + D_i \nabla^2_{xx} \rho_i - h(\rho_i, \rho_m)$$

$$\dot{\rho}_m = D_m \nabla^2_{xx} \rho_m + h(\rho_i, \rho_m)$$

$$h(\rho_i, \rho_m) = \beta \rho_i - \gamma \rho_m^2 \quad ; \quad -g'(\rho_i^o) = \alpha > 0$$

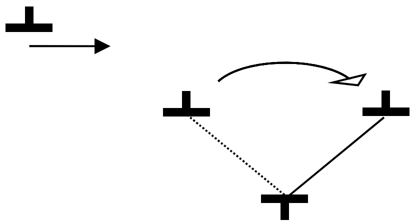
(ρ_i, ρ_m) … (immobile, mobile) dislocation density

$\beta = \beta(\tau)$ … bifurcation parameter

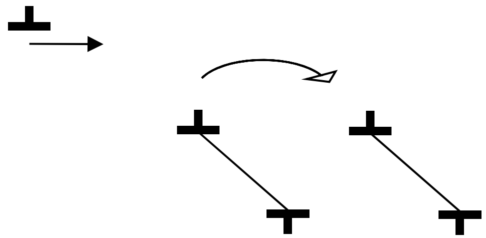
(α, γ) … reaction cross-section parameters

- ***The Underlying Diffusive – Reaction Mechanisms***

  - *Diffusive Mechanisms (D_i)*

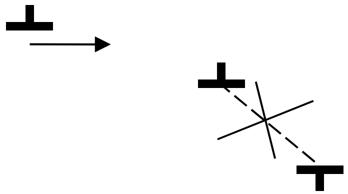


Dipole “switching“



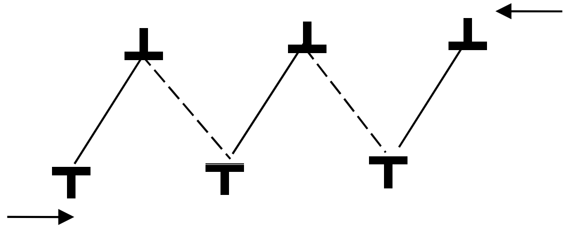
Dipole “sweeping“

  - *Dipole Dissolution ($\beta\,\rho_i$)*



$$\left(\frac{\partial \rho_i}{\partial t}\right)^{-} \sim \beta\,\dot{\gamma}^{pl}\,\rho_i$$

  - *Cubic Term ($\gamma\,\rho_m\,\rho_i^2$)*

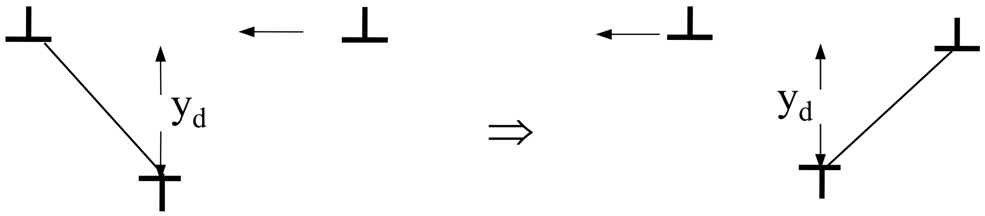


$$\left(\frac{\partial \rho_i}{\partial t}\right)^{+} \sim \gamma\,\dot{\gamma}^{pl}\,\rho_m\,\rho_i^2$$

- ***More on the Origin of the Diffusion-like Terms D_i , D_m***

– *Diffusion coefficient of immobile dislocations D_i*

Dipole exchange mechanism (Differt – Essmann 1993)



$$\Rightarrow \quad D_i \sim \frac{y_d^2}{t_d} \sim \rho_m \upsilon y_d^3$$

y_d … mean dipole height $\qquad$ t_d … average time between two successive events

– *Diffusion-like coefficient of mobile dislocations D_m*

Distinction between $\rho_m^{\pm}$ (Walgraef-Aifantis 1985)

$$\rho_m = \rho_m^+ + \rho_m^- \qquad\qquad \Rightarrow \begin{cases} \dot{\rho}_m = -\upsilon \partial_x k_m + \beta \rho_i - \gamma \rho_m \rho_i^2 \\ \dot{k}_m = \upsilon \partial_x \rho_m - \gamma k_m \rho_i^2 \end{cases}$$

$$k_m = \rho_m^+ - \rho_m^- \quad \left(\ldots = \rho_{GND} \right)$$

Adiabatic elimination of k_m $\left(\dot{k}_m \approx 0 \right)$

$$\therefore \quad \dot{\rho}_m = D_m \partial_{xx}^2 \rho_m + \beta \rho_i - \gamma \rho_m \rho_i^2 \quad , \qquad D_m = \frac{\upsilon^2}{2 \gamma \rho_i^2}$$

- ***Linear Stability Analysis of the 1D W–A Model***

– *Hopf:* $\beta = \beta_H = \alpha + \gamma \rho_i^2$ … bursts (Neumann)

– *Turing:* $\beta = \beta_T = \left(\sqrt{\alpha} + \sqrt{\gamma \rho_i^2 D_i / D_m} \right)^2$ … layers (Mughrabi)

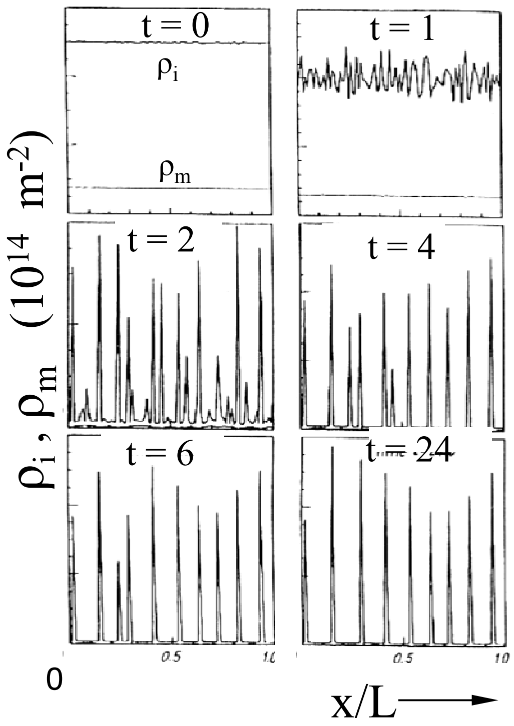
$$\therefore \; q_{critical} = q_c = \frac{2\pi}{\lambda_c} = \left(\frac{\alpha \gamma \rho_i^2}{D_i D_m} \right)^{1/4}$$

– *Ladder Wavelength:* λ_c

$$D_m \sim \frac{\upsilon^2}{\gamma \rho_i^2} \;,\quad \sqrt{D_i/\alpha} \approx \ell_c \;,\quad \dot{\gamma}^{pl} = b \rho_m \upsilon$$

$$\therefore \; \lambda_c = d \cong \frac{16}{\sqrt{\rho_i}} \quad \Rightarrow \quad \rho_i \sim \frac{256}{d^2}$$

i.e. same estimate as Mughrabi for Cu



Temporal evolution of the system within a grain of size L=13 μm. Stable spatially periodic patterns for ρ_i are developed (Walgraef et al, Glazov et al)

- ***2D Considerations – Nonlinear Regime***
  - *Governing Evolution Eqs*

$$\dot{\rho}_i = g(\rho_i) + D_{ix}\nabla^2_{xx}\rho_i + D_{iy}\nabla^2_{yy}\rho_i - h(\rho_i, \rho_m)$$

$$\dot{\rho}_m = D_{mx}\nabla^2_{xx}\rho_m - h(\rho_i, \rho_m)$$

  - *Slow-mode Dynamics*

2-time scales near bifurcation (Haken's Slaving Principle; central manifold thm.)

$\omega_s \approx 0 \quad \rightarrow \quad \sigma_q$ … slow modes in Fourier Space

$\omega_R < 0 \quad \rightarrow \quad R_q$ … fast modes in Fourier Space $\dot{R}_q \approx 0$

$$\partial_t \sigma = \left[\varepsilon - d_x\left(q_c + \nabla^2_{xx}\right)^2 + d_y\nabla^2_{yy}\right]\sigma - \upsilon\sigma^2 - u\sigma^3$$

$\varepsilon \sim (\beta - \beta_c)/\beta_c$, $\sigma \sim R\exp\left[i(q_c x + \phi)\right]$, $(d_x, d_y;\ \upsilon, u) = \text{consts}$

$\sigma_o = 2R_o\cos(q_c x + \phi_o)$, $R_o = \sqrt{\varepsilon/3u}$, $\phi_o =$ *const.*

$R = R_o + \tilde{R}$, $\phi = \phi_o + \tilde{\phi}$

$\therefore \quad R \rightarrow R_o$, $\dot{\phi} = D_{\parallel}\nabla^2_{xx}\phi + D_{\perp}\nabla^2_{yy}\phi$

- ***3D Considerations – The Bifurcation Diagram***
  - *Governing Evolution Eqs*

$$\dot{\rho}_i = g(\rho_i) - \left(D_\parallel \nabla_\parallel^2 + D_\perp \nabla_\perp^2\right)\left(1 + E\nabla^2\right)\rho_i - h(\rho_i, \rho_m)$$

$$\dot{\rho}_m = D_{mx} \nabla_{xx}^2 \rho_m + h(\rho_i, \rho_m)$$

$$\nabla_\parallel^2 = \nabla_{xx}^2 + \nabla_{yy}^2, \quad \nabla_\perp^2 = \nabla_{zz}^2 \quad ; \quad D_\parallel = M_{xx}\left|J^o\right| = M_{yy}\left|J^o\right| >> D_\perp = M_{zz}\left|J^o\right|, \quad E = \frac{J^1}{J^o}$$

  - *Holt-like Energetic Treatment of ρ_i*

$$\mathbf{J}_i = -\mathbf{M}\nabla\mu_i, \quad \mu_i(\mathbf{r}) = E_c + \int J\left(\left|\mathbf{r}-\mathbf{r}'\right| f(\mathbf{r}') \rho_i(\mathbf{r}')\right) d\mathbf{r}' \simeq E_c + J^o \rho_i(\mathbf{r}) + J^1 \nabla^2 \rho_i$$

$$J^o = \int J(\mathbf{r}) f(\mathbf{r}) d\mathbf{r} \quad ; \quad J^1 = \frac{1}{2}\int J(\mathbf{r}) f(\mathbf{r}) \left|\mathbf{r}\right|^2 d\mathbf{r}$$

i.e. the first two moments of nonlocal interaction $J(\mathbf{r})$

$\mathbf{M}$ mobility tensor; E_c core energy; f dislocation distribution fct

  - *Amplification Factor ω_q*

$$\omega_q = r - d_\parallel\left(q_x^2 + q_y^2 - q_o^2\right) - d_\perp q_z^2 + \beta \frac{q_x^2}{q_x^2 + q_*^2}$$

$$r = \left(D_\parallel / 4E\right) - \alpha, \; q_o = 1/2E, \; q_* = \gamma \rho_i^{o2} / D_m, \; d_\parallel = D_\parallel E, \; d_\perp = \left(D_\parallel - D_\perp\right)/2$$

- ***Stability Diagram: The Competition between Veins and Ladders***
  - *Low values of stress* $(\beta \simeq 0)$

    $r < 0$

    $\therefore$ homogeneous states $(\rho_i = \rho_i^o\,, \quad \rho_m = 0)$ stable

  - *Increasing stress* $(\beta < \beta_c)$

    $r - d_{\parallel}\left(q_x^2 + q_y^2 - q_o^2\right)^2 - d_{\perp} q_z^2 > 0$

    $\therefore$ veins with wavevector-like structure $\mathbf{q} = \left(q_x, q_y, q_z\right)$

    fastest growing $\mathbf{q}$: $q_x^2 + q_y^2 = q_o^2\,, \quad q_z = 0$

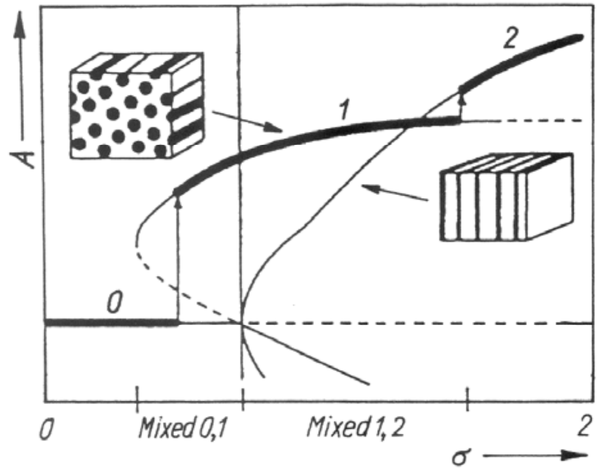
  - *Higher values of stress* $(\beta \geq \beta_c)$

    $r - d_{\parallel}\left(q_x^2 - q_o^2\right)^2 + \beta \dfrac{q_x^2}{q_x^2 + q_*^2} \geq 0$

    $\therefore$ ladders with wavevector $\mathbf{q} = \left(q_x, 0, 0\right)$

    preferred wavevector q_c: $2d_{\parallel}\left(q_c^2 - q_o^2\right) - \beta \dfrac{q_c^2}{\left(q_c^2 + q_*^2\right)^2} = 0$

    i.e. $q_c > q_0$



Bifurcation diagram for patterning in fatigue. The preferred stable states are given in heavy lines. A is the amplitude of modulation of the spatial pattern, and σ the absolute value of maximum stress per cycle

- ***Extension of W-A Model to 2ble Slip – Labyrinth Structures***

  - *Governing Evolution Eqs*

$$\dot{\rho}_i = D_i \nabla^2 \rho_i + \upsilon_c \rho_i \sqrt{\rho_i} - \upsilon_c \ell_c \rho_i^2 - \left(\beta_x + \beta_y\right)\rho_i + \gamma \rho_i^2 \left(\rho_{mx} + \rho_{my}\right)$$

$$\dot{\rho}_{mx}^+ = -\nabla_x\left(\upsilon_g \rho_{mx}^+\right) + \frac{1}{2}\beta_x \rho_i - \gamma \rho_i^2 \rho_{mx}^+ \quad ; \quad \dot{\rho}_{mx}^- = \nabla_x\left(\upsilon_g \rho_{mx}^-\right) + \frac{1}{2}\beta_x \rho_i - \gamma \rho_i^2 \rho_{mx}^-$$

$$\dot{\rho}_{my}^+ = -\nabla_y\left(\upsilon_g \rho_{my}^+\right) + \frac{1}{2}\beta_y \rho_i - \gamma \rho_i^2 \rho_{my}^+ \quad ; \quad \dot{\rho}_{my}^- = \nabla_y\left(\upsilon_g \rho_{my}^-\right) + \frac{1}{2}\beta_y \rho_i - \gamma \rho_i^2 \rho_{my}^-$$

υ_c ~ climb velocity (const) ; υ_g … glide velocity (spatially dependent)

  - *Adiabatic Elimination*

$$\dot{\rho}_i = D_i \nabla^2 \rho_i + \upsilon_c \rho_i \sqrt{\rho_i} - \upsilon_c \ell_c \rho_i^2 - \left(\beta_x + \beta_y\right)\rho_i + \gamma \rho_i^2 \left(\rho_{mx} + \rho_{my}\right)$$

$$\dot{\rho}_{mx} = \nabla_x\left[\left(\upsilon_g / \gamma \rho_i^2\right)\nabla_x\left(\upsilon_g \rho_{mx}\right)\right] + \beta_x \rho_i - \gamma \rho_i^2 \rho_{mx} \quad ; \quad k_{mx} = \frac{1}{\gamma \rho_i^2}\nabla_x\left(\upsilon_g \rho_{mx}\right)$$

$$\dot{\rho}_{my} = \nabla_y\left[\left(\upsilon_g / \gamma \rho_i^2\right)\nabla_y\left(\upsilon_g \rho_{my}\right)\right] + \beta_y \rho_i - \gamma \rho_i^2 \rho_{my} \quad ; \quad k_{my} = \frac{1}{\gamma \rho_i^2}\nabla_y\left(\upsilon_g \rho_{my}\right)$$

  - *Instability Threshold*

$$\mathbf{q_c} = \begin{cases} q_c \mathbf{e_x} \\ \text{or} \\ q_c \mathbf{e_y} \end{cases} \quad ; \quad q_c = \left(\frac{\gamma \rho_i^{o2}}{D_m D_i \tau}\right)^{1/4}, \quad \beta_c = \left(\sqrt{\frac{1}{\tau}} + \sqrt{\gamma \rho_i^{o2} \frac{D_i}{D_m}}\right)^2, \quad \tau \equiv \frac{2\ell_c}{\upsilon_c}$$

- ***Nonlinear Analysis of 2ble Slip W-A Model***

  - *Slow-mode Dynamics*

$$\tau_0\partial_t\sigma = \left[\varepsilon - d_0\left(q_c^2+\nabla^2\right)^2 - d_\perp\nabla_x^2\nabla_y^2\right]\sigma + \upsilon\sigma^2 - u\sigma^3$$

$$\tau_0 = \frac{\gamma\rho_i^{o2}}{\rho_c^2 D_m\beta_c},\quad \varepsilon = \frac{\beta-\beta_c}{\beta_c},\quad d_0 = \frac{D_m}{q_c^2\gamma\rho_i^{o2}},\quad d_\perp = \frac{\gamma\rho_m^{o\,2}}{q_c^4\left(\gamma\rho_i^{o2}+D_m q_c^2\right)},\quad \upsilon \simeq \frac{\gamma\rho_i^o}{q_c^2 D_m},\quad u \simeq \frac{\gamma}{q_c^2 D_m}$$

  - *Amplitude Eqs*

$$\sigma = A_x(x,y)e^{iq_cx} + A_y(x,y)e^{iq_cy} + A_x^*(x,y)e^{-iq_cx} + A_y^*(x,y)e^{-iq_cy}$$

$$\tau_0\partial_t A_x = \left[\varepsilon + 4d_0q_c^2\nabla_x^2 + d_\perp q_c^2\nabla_y^2\right]A_x - 3u\left(\left|A_x\right|^2 + g\left|A_y\right|^2\right)A_x$$

$$\tau_0\partial_t A_y = \left[\varepsilon + 4d_0q_c^2\nabla_y^2 + d_\perp q_c^2\nabla_x^2\right]A_y - 3u\left(\left|A_y\right|^2 + g\left|A_x\right|^2\right)A_y$$

- *Steady-states*

$$|A_x| = \frac{\varepsilon}{3u}, \quad A_y = 0 \quad ; \quad |A_y| = \frac{\varepsilon}{3u}, \quad A_x = 0$$ … i.e. walls ⊥ to x,y directions - stable

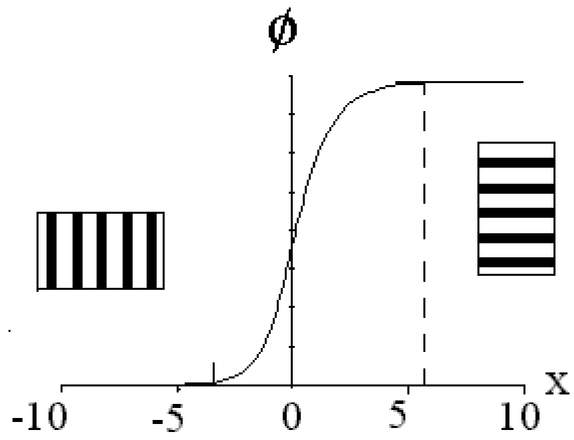
$$|A_x| = |A_y| = \frac{\varepsilon}{3u(1+g)}, \quad g \geq 2$$ … i.e. square patterns - unstable

- *Transients – Phase Dynamics*

$$A = A_x + iA_y \sim R\exp(i\varphi)$$

$$R \to R_0 = \frac{\sqrt{\varepsilon}}{3u}, \quad \varphi \to \varphi_0 = n\frac{\pi}{2}$$

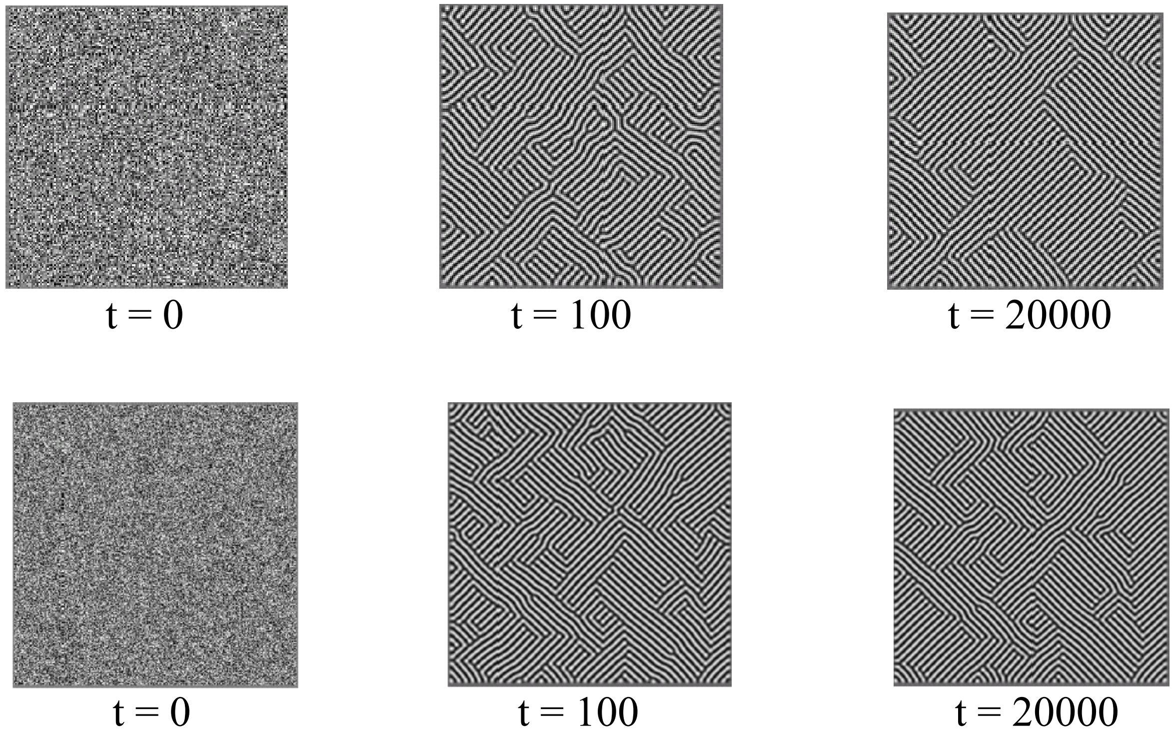
$$\varphi = \arctan\left[\exp\sqrt{\frac{3uR_0^2}{d_\perp q_c^2}}\right]$$



Spatial variation of phase variable $\varphi(x)$ for a domain boundary separating a wall structure with walls parallel to the y direction from a structure with walls parallel to the x direction, for $d_\perp / d_0 = 0.3$ (lengths scaled by $\sqrt{(4d_0 q_c^2)/(3uR_0^2)}$)

- *Simulation Results*

(a)

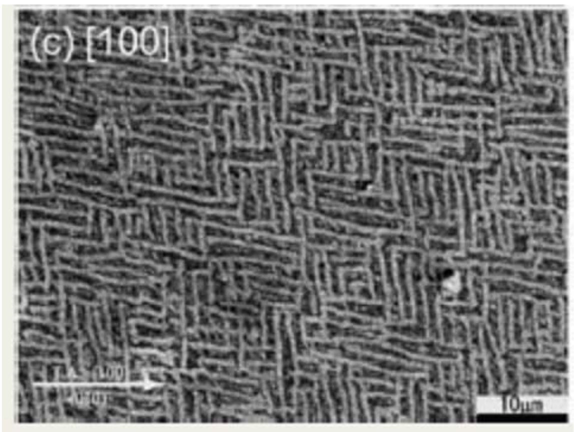


7.5% anisotropy

10% anisotropy

- *Experimental Observations*

(b)



(a) Temporal evolution of ρ starting from a random initial condition. Primary slip directions are parallel to box diagonals. Walls develop locally perpendicular to each slip direction, domains form and coarsen, finally reaching a steady state which consists in coexisting domains for each wall direction and with most of the domain walls perpendicular to the two slip directions

(b) Experimental "labyrinth" or "maze" dislocation wall patterns in Cu-single crystal under cyclic loading and oriented for multiple slip (Kaneko – Hashimoto)

- ***The ± of the W–A Model***

- *First time* to depart from quasi-equilibrium thermodynamic-like considerations (e.g. LEDS / Kuhlman-Wilsdorf) and consider "dislocation patterning" (ECA 1985) as a dynamical system
  - Motivated directly new *Stochastic/Statistical dislocation models* (Hahner-Zaiser, Groma, El Azab, et al) and *DDD simulations* (Ghoniem, Kubin, Zbib, Bulatov et al)
  - Motivated directly recent *Gradient Plasticity* constitutive models (Aifantis, Fleck-Hutchinson, Gao-Nix, Gurtin-Anand, et al)
  - Motivated directly a *Chemical-like Kinetics Framework for Defects* (vacancies-dislocations-disclinations-microcracks); Re: The (un)known R-A model for defect kinetics (1993), and other Russian work (Romanov, Ovid'ko, Malygin et al)
- *First time* to introduce/utilize the *Balance Eqn* for dislocation densities $\dot{\rho} + \mathrm{div}(\rho\upsilon) = g$ All subsequent developments (Kratochvil, Groma, El-Azab, Zaiser, Willis et al) built on this "particle-like" conservation law
- *First time* to introduce (ρ^+, ρ^-) or (ρ, k) , as well as $(\rho_i\ , \rho_m)$
- *The only model* todate to *predict* the competition of vein/ladder structures and their wavelengthts
- *Open questions* about the diffusion-like & reaction-like terms. Needs the input and additional / continuous work by experts in metal physics, statistical mechanics, and DDD simulations

DISLOCATION PATTERNING: THE W-A-G MODEL

- ***Revisiting the Groma-Zaiser et al Approach***

  - *Basic Assumptions*

    Parallel straight edge dislocations with $\mathbf{b} = b\hat{\mathbf{e}}_{\mathbf{x}}\ ,\quad \mathbf{t} = \hat{\mathbf{e}}_{\mathbf{z}}\ ,\quad r_i = (x_i, y_i)$

    - $\dot{\rho} + \mathrm{div}(\rho\upsilon) = 0\ ;\quad \upsilon = \mathbf{b}B\left[\tau^{int}(\mathbf{r}) + \tau^{ext}\right]^{1/m}\ ,\quad m = 1$

    - $\dot{\rho}^{\pm}(\mathbf{r},t) \pm b\nabla\left\{B\rho^{\pm}(\mathbf{r},t)\left[\tau^{int}(\mathbf{r}) + \tau^{ext}\right]\right\} = 0 \qquad \left(\rho^{+} \to b, \rho^{-} \to -b\right)$

    - $\rho = \rho^{+} + \rho^{-}\ ,\qquad k = \rho^{+} - \rho^{-}$

  - *Governing Eqs*

$$\begin{cases} \dot{\rho} = -b\nabla\left\{Bk(\mathbf{r},t)\left[\tau^{int}(\mathbf{r}) + \tau^{ext}\right]\right\} \\ \dot{k} = -b\nabla\left\{B\rho(\mathbf{r},t)\left[\tau^{int}(\mathbf{r}) + \tau^{ext}\right]\right\} \end{cases}$$

They may be viewed as the *Langevin Equations* in a stochastic scheme

- ***Mean Field Version***
  - *Governing Eqs*

$$\begin{cases} \dot{\rho}(\mathbf{r},t) = -b\nabla\left\{Bk(\mathbf{r},t)\left[\overline{\tau}^{int}(\mathbf{r},t)+\tau^{ext}\right]\right\} \\ \dot{k}(\mathbf{r},t) = -b\nabla\left\{B\rho(\mathbf{r},t)\left[\overline{\tau}^{int}(\mathbf{r},t)+\tau^{ext}\right]\right\} \end{cases}$$

$$\overline{\tau}^{int}(\mathbf{r},t) = \int k(\mathbf{r_1},t)\,\tau^{ind}(\mathbf{r}-\mathbf{r_1})\,d\mathbf{r_1} \quad ; \qquad \Delta^2\overline{\tau}^{int} = \frac{\mu b}{(1-\nu)}\frac{\partial^3}{\partial x\,\partial y^2}k(\mathbf{r},t)$$

$$\tau^{ind} = -\frac{\mu b}{2\pi(1-\nu)}\frac{x\left(x^2-y^2\right)}{\left(x^2+y^2\right)^2} = -\frac{\mu b}{2\pi(1-\nu)}\frac{\partial^3}{\partial x\,\partial y^2}g(r) \;;\quad g(r)=\frac{1}{2}r^2\ln r$$

  - *Linear Stability* $\left(\rho=\rho^o,\,k=0\right)$

$$\omega^2+\omega\frac{q_x^2q_y^2}{q^4}\Lambda+q_x^2\left(b\,B\,\tau^{ext}\right)^2=0\,; \qquad \Lambda=\frac{\mu b^2 B\rho^o}{2\pi(1-\nu)} \quad \Rightarrow \qquad \mathrm{Re}[\omega]\ \text{never} > 0$$

- $\omega = 0$ for $q_x = 0$ … modulations $\perp$ to glide direction
- $\omega = \pm i q_x b B \tau^{ext}$ for $q_y = 0$ … modulations $/\!/$ to glide direction

$\therefore$ Elastic interactions $\not\Rightarrow$ patterning; need stochasticity/correlations

- ***Stochastic Version***

Introduce the stochastic version for $\overline{\tau}^{\text{int}}$ into *Langevin Eqs* $\Rightarrow$

$$\begin{cases} \dot{\rho}(\mathbf{r},t) = -bB\nabla\left[k(\mathbf{r},t)\tau^{\text{ext}} + \int\left\langle k(\mathbf{r},t)k(\mathbf{r}_1,t)\right\rangle \tau^{\text{ind}}(\mathbf{r}-\mathbf{r}_1)d\mathbf{r}_1\right] \\ \dot{k}(\mathbf{r},t) = -bB\nabla\left[\rho(\mathbf{r},t)\tau^{\text{ext}} + \int\left\langle \rho(\mathbf{r},t)k(\mathbf{r}_1,t)\right\rangle \tau^{\text{ind}}(\mathbf{r}-\mathbf{r}_1)d\mathbf{r}_1\right] \end{cases}$$

$\left\langle \rho_\alpha(\mathbf{r},t)\rho_\beta(\mathbf{r}_1,t)\right\rangle = \rho_\alpha(\mathbf{r},t)\rho_\beta(\mathbf{r}_1,t)\left[1+d_{\alpha\beta}(\mathbf{r},\mathbf{r}_1)\right]$; $d_{\alpha\beta}$ are scaled pair correlation functions for dislocations of sign $(\alpha,\beta)=(+,-)$ with $d_{++}=d_{--}$, $d_{+-}=d_{-+}$

$$\therefore \begin{cases} \dot{\rho} = -bB\nabla\left[k\tau^{\text{ext}} + \int\left[k k_1(1+d_k)+\rho\rho_1 d_\rho\right]\tau^{\text{ind}}(\mathbf{r}-\mathbf{r}_1)d\mathbf{r}_1\right] \\ \dot{k} = -bB\nabla\left[\rho\tau^{\text{ext}} + \int\left[\rho k_1(1+d_k)+k\rho_1 d_\rho\right]\tau^{\text{ind}}(\mathbf{r}-\mathbf{r}_1)d\mathbf{r}_1\right] \end{cases}$$

$$\rho=\rho(\mathbf{r},t),\quad k=k(\mathbf{r},t),\quad \rho_1=\rho(\mathbf{r}_1,t),\quad k_1=k(\mathbf{r}_1,t)$$

$$d_k=d_k(\mathbf{r},\mathbf{r}_1)=1/2\left[d_{++}(\mathbf{r},\mathbf{r}_1)+d_{+-}(\mathbf{r},\mathbf{r}_1)\right],\ d_\rho=d_\rho(\mathbf{r},\mathbf{r}_1)=1/2\left[d_{++}(\mathbf{r},\mathbf{r}_1)-d_{+-}(\mathbf{r},\mathbf{r}_1)\right]$$

Note: The correlation fcts (d_ρ, d_k) scale with $\tilde{\mathbf{r}}=\mathbf{r}\sqrt{\rho^o}$ exhibiting $1/r$ singularity at "small" separations and exponential decay at "large" separations (Zaiser)

- ***Linear Evolution Eqs*** $\left(\hat{\rho} = \rho - \rho^o, \hat{k} = k - 0\right)$

$$\begin{cases} \dot{\hat{\rho}} = -bB\nabla\left\{\hat{k}\tau^{ext} + \rho^o \int \hat{\rho}\left(\mathbf{r} - \mathbf{r}_1, t\right) d_\rho\left(\mathbf{r}_1\right) \tau^{ind}(\mathbf{r}_1) d\mathbf{r}_1\right\} \\ \dot{\hat{k}} = -bB\nabla\left\{\hat{\rho}\tau^{ext} + \rho^o \int \hat{k}\left(\mathbf{r} - \mathbf{r}_1, t\right)\left[1 + d_k\left(\mathbf{r}_1\right)\right] \tau^{ind}(\mathbf{r}_1) d\mathbf{r}_1\right\} \end{cases}$$

- $$\rho^o \int \hat{\rho}\left(\mathbf{r} - \mathbf{r}_1, t\right) d_\rho\left(\mathbf{r}_1\right) \tau^{ind}(\mathbf{r}_1) d\mathbf{r}_1 = -\frac{\mu b \rho^o}{2\pi(1-\nu)} \int \hat{\rho}\left(\mathbf{r} - \mathbf{r}_1, t\right) d_\rho\left(\mathbf{r}_1\right) \frac{\partial^3}{\partial_{x_1}\partial^2_{y_1}} g(\mathbf{r}_1) d\mathbf{r}_1$$

$$\simeq \frac{\mu b \rho^o}{2\pi(1-\nu)}\left[D_\rho \partial^2_x + E_\rho \partial^3_x + F_\rho \partial_x \partial^2_y + \ldots\right]\hat{\rho}\left(\mathbf{r}, t\right)$$

$$D_\rho \equiv \frac{1}{\rho^o} \iint \frac{\partial^3 g\left(\tilde{\mathbf{r}}\right)}{\partial_{\tilde{x}} \partial^2_{\tilde{y}}} d_\rho\left(\tilde{\mathbf{r}}\right) \tilde{x}\, d\tilde{x}\, d\tilde{y}, \quad E_\rho \equiv \frac{1}{6\rho^{o2}} \iint \frac{\partial^3 g\left(\tilde{\mathbf{r}}\right)}{\partial_{\tilde{x}} \partial^2_{\tilde{y}}} d_\rho\left(\tilde{\mathbf{r}}\right) \tilde{x}^3\, d\tilde{x}\, d\tilde{y},$$

$$F_\rho \equiv \frac{1}{2\rho^{o2}} \iint \frac{\partial^3 g\left(\tilde{\mathbf{r}}\right)}{\partial_{\tilde{x}} \partial^2_{\tilde{y}}} d_\rho\left(\tilde{\mathbf{r}}\right) \tilde{x}\, \tilde{y}^2 d\tilde{x}\, d\tilde{y}$$

- $$\rho^o \int \hat{k}\left(\mathbf{r} - \mathbf{r}_1, t\right) d_k\left(\mathbf{r}_1\right) \tau^{ind}(\mathbf{r}_1) d\mathbf{r}_1 \simeq \frac{\mu b \rho^o}{2\pi(1-\nu)}\left[D_k \partial^2_x + E_k \partial^3_x + F_k \partial_x \partial^2_y + \ldots\right]\hat{k}\left(\mathbf{r}, t\right)$$

- ***Stability Analysis*** ***(without source terms)***

$$\omega = \frac{\Lambda}{2}\left(q_x^2 D_+ - q_x^4 E_+ - q_x^2 q_y^2 F_+ - \frac{q_x^2 q_y^2}{q^4}\right) \pm \sqrt{\frac{\Lambda^2}{4}\left(q_x^2 D_- - q_x^4 E_- - q_x^2 q_y^2 F_- + \frac{q_x^2 q_y^2}{q^4}\right)^2 - q_x^2 \left(bB\tau^{ext}\right)^2}$$

$$D_\pm = D_\rho \pm D_k \simeq D_\rho\,, \quad E_\pm = E_\rho \pm E_k \simeq E_\rho\,, \quad F_\pm = F_\rho \pm F_k \simeq F_\rho$$

- $\tau^{ext} = 0$: Eqs decouple; both $\hat{\rho}$ and $\hat{k}$ have positive growth rates in finite domains of the **q**-space. In particular, $\hat{\rho}$ has maximum growth rate for $q_y = 0$ and $q_x = \sqrt{D_\rho / 2E_\rho} \propto \sqrt{\rho^o}$; i.e. Dislocation walls $\perp$ to glide direction are expected to grow first; this is in accordance to the numerical results of Bako & Groma

- $\tau^{ext} \neq 0$: Perturbations with $q_x = 0$ are always marginally stable. Perturbations with $q_y = 0$ are unstable for $0 < q_x^2 < q_M^2 = D_+ / E_+$ with $\omega \simeq 1/2\left(q_x^2 D_+ - q_x^4 E_+\right) \pm i\, q_x bB\tau^{ext}$. Thus, for each q between 0 and q_M, there is a $\tau^{ext}_{threshold}$ below which the instability is of the spinodal decomposition type, and above which is of wave type with walls perpendicular to the glide direction-x with fastest growth for $q_x^2 = q_0^2 = \left(D_+ / 2E_+\right)$ and corresponding velocity $\upsilon_0 \simeq \pm q_0 bB\tau^{ext}$. Perturbations with $q_y \neq 0$ are unstable

- ***Source Terms***

$$\dot{\rho} = (\text{as before}) + \alpha - \beta\left(\rho^2 - k^2\right) \quad ; \qquad \dot{k} = (\text{as before})$$

$$2\omega = -\left[\omega_0 + \Lambda\left(\frac{q_x^2 q_y^2}{q^4} - q_x^2 D_+ + q_x^4 E_+ + q_x^2 q_y^2 F_+\right)\right]$$

$$\pm\sqrt{\left[\omega_0 - \Lambda\left(q_x^2 D_- - q_x^4 E_- - q_x^2 q_y^2 F_- + \frac{q_x^2 q_y^2}{q^4}\right)\right]^2 - 4q_x^2\left(bB\tau^{ext}\right)^2}$$

ω_0 … linear relaxation rate of uniform perturbations related directly to $\alpha = \alpha(\rho, \tau)$

[ω_0^{-1}: may be viewed as an effective dislocation lifetime]

– Perturbations with $q_x = 0$ remain marginally stable, while other ones become stable for short individual dislocation lifetimes. Instability still occurs for $\tau^{ext} \neq 0$ for long dislocation lifetimes with $\omega_0 < \left(D_+^2/4E_+\right)$. The maximum rate still corresponds to $\left(q_x^2 = q_0^2 = \left(D_+/2E_+\right);\ q_y = 0\right)$, but the spectrum of unstable q's is now given by $q_x = 0$ and the band

$$\left(D_+/2E_+\right)\left[1 - \sqrt{1 - \left(4E_+\omega_0/D_+^2\right)}\right] < q_x^2 < \left(D_+/2E_+\right)\left[1 + \sqrt{1 - \left(4E_+\omega_0/D_+^2\right)}\right]$$

– Speculative nonlinear behavior: The initial periodic perturbations of the unstable state are quickly expected to destabilize w.r. to modes with larger wave lengths. Small clusters shrink and disappear, while larger clusters grow

- ***The Combined W-A-G Model***

  - *Governing Eqs*

$$\begin{cases} \dot{\rho} + bB\nabla\left(k\tau^{ext}\right) = \int\left[k\,k_1\left(1+d_k\right)+\rho\,\rho_1 d\rho\right]\tau^{ind}(\mathbf{r}-\mathbf{r}_1)d\mathbf{r}_1 + \alpha + \beta\rho_i - \gamma\rho_i^2\rho \\ \dot{k} + bB\nabla\left(\rho\tau^{ext}\right) = \int\left[\rho\,k_1\left(1+d_k\right)+k\,\rho_1 d\rho\right]\tau^{ind}(\mathbf{r}-\mathbf{r}_1)d\mathbf{r}_1 - \gamma\rho_i^2 k \\ \dot{\rho}_i = D_i\nabla^2\rho_i + g\left(\rho_i\right) - \beta\rho_i + \gamma\rho_i^2\rho \end{cases}$$

  - *Linear Evolution Eqs in Fourier Space*

$$\begin{cases} \dot{\hat{\rho}}\left(\mathbf{q},t\right) = -i\,q_x bB\tau^{ext}\hat{k}\left(\mathbf{q},t\right) - \beta^*\hat{\rho}_i\left(\mathbf{q},t\right) + \left[\Lambda\left(q_x^2 D_\rho - q_x^4 E_\rho - q_x^2 q_y^2 F_\rho\right) - \gamma^*\right]\hat{\rho}\left(\mathbf{q},t\right) \\ \dot{\hat{k}}\left(\mathbf{q},t\right) = -i\,q_x bB\tau^{ext}\hat{\rho}\left(\mathbf{q},t\right) - \left[\Lambda\dfrac{q_x^2 q_y^2}{q^4} + \gamma^*\right]\hat{k}\left(\mathbf{q},t\right) \\ \dot{\hat{\rho}}_i = \left(\beta^* - \omega_i - q^2 D_i\right)\hat{\rho}_i\left(\mathbf{q},t\right) + \gamma^*\hat{\rho}\left(\mathbf{q},t\right) \end{cases}$$

$$\beta^* = \beta + 2\left(\alpha/\rho_i^o\right),\quad \gamma^* = \gamma\rho_i^{o2},\quad \alpha = -g\left(\rho_i^o\right),\quad \rho^o = \left(\alpha + \beta\rho_i^o\right)/\gamma\rho_i^{o2}$$

- ***Adiabatic Elimination of*** $\hat{k}$ **:** $\hat{k}(\mathbf{q},t) = -i\, q_x bB\tau^{ext} \Big/ \left[\gamma^* + \Lambda\left(q_x^2 q_y^2 / q^4\right)\right]$

$$\begin{cases} \dot{\hat{\rho}}(\mathbf{q},t) = -\beta^* \hat{\rho}_i(\mathbf{q},t) - \left[\Lambda\left(q_x^2 D_T - q_x^4 E_\rho - q_x^2 q_y^2 F_\rho\right) + \gamma^*\right] \hat{\rho}(\mathbf{q},t) \\ \dot{\hat{\rho}}_i = \left(\beta - \omega_i - q^2 D_i\right) \hat{\rho}_i(\mathbf{q},t) + \gamma^* \hat{\rho}(\mathbf{q},t) \end{cases}$$

where $D_T = \left(bB\tau^{ext}\right)^2 \Big/ \left[\gamma^* + \Lambda\left(q_x^2 q_y^2 / q^4\right)\right] - D_\rho$ … new effective diffusivity

- *As before (W-A)* for $\tau^{ext} < \tau_{threshold} \Rightarrow D_T < 0 \quad \Rightarrow$

  a spinodal-like instability sets in leading to dislocation clusters (vein structures)

- *As before (W-A)* for $\tau^{ext} > \tau_{threshold} \Rightarrow D_T > 0 \quad \Rightarrow$

  a Turing-like instability sets in leading to dislocation walls (ladder structures)

- *New Feature:* $D_i = D_i(x)$ is now spatially-dependent through $\rho_i(x)$ since the adiabatic elimination of geometrically necessary dislocations $\rho_{GND} = k(\mathbf{r},t) \simeq -\nabla_x \left[\left(bB\tau^{ext}/\gamma\rho_i^2\right) + \ldots\right]$ leads to an effective diffusion for the immobile state with coefficient $\left(bB\tau^{ext}\right)^2 \Big/ \gamma\rho_i^2$

  i.e. in the presence of inhomogeneous vein structure the instability threshold for the ladder structure decreases in regions of low $\rho_i \quad \Rightarrow$

  ladders nucleate preferentially in the soft regions