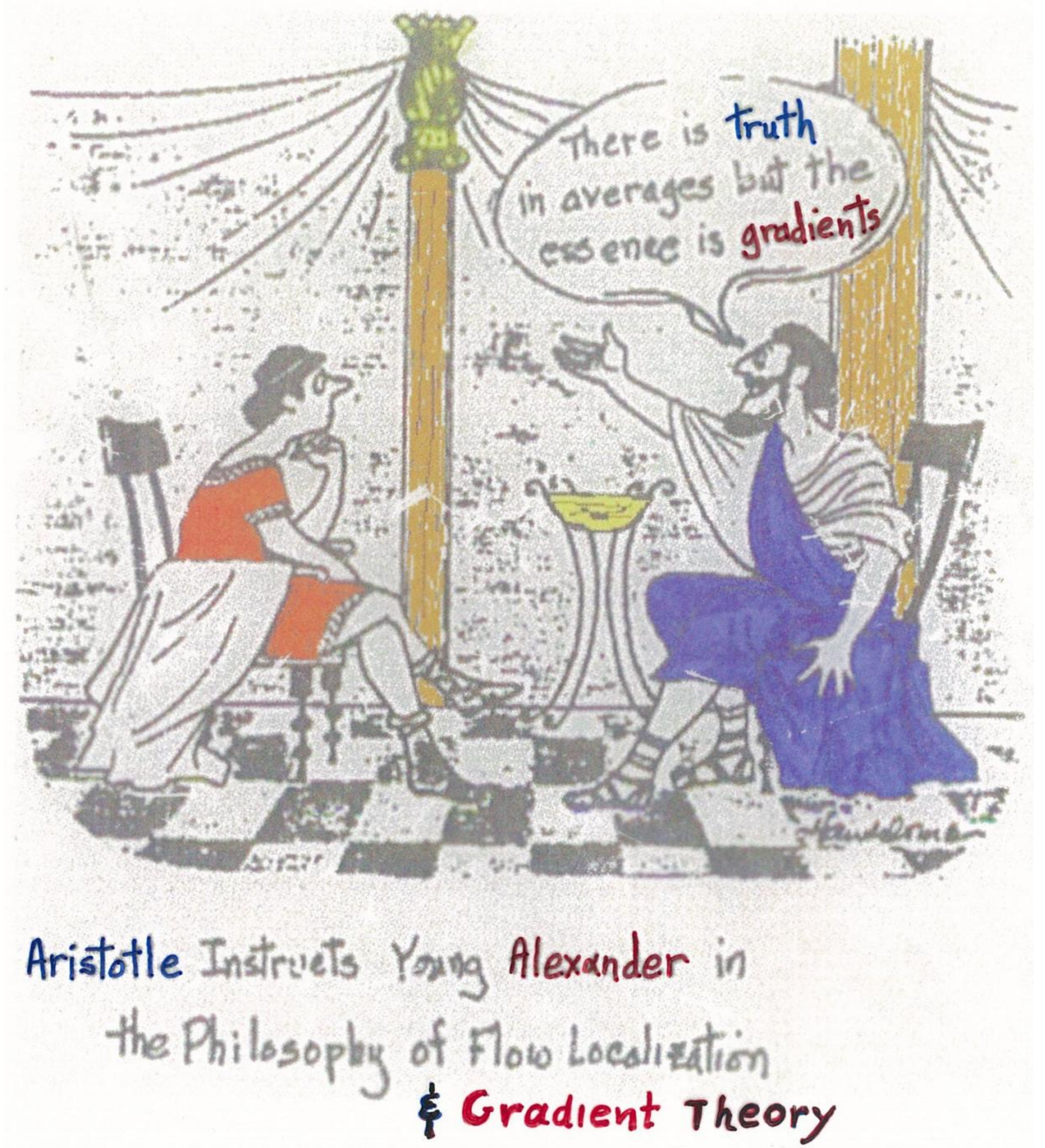
GRADIENT MECHANICS ACROSS TIME, SCALES, & MATERIALS

- ***Senior Collaborators*** →
  - Serrin / Minnesota
  - Walgraef / ULB
  - Romanov / Ioffe
  - Milligan – Hackney/MTU
- ***Senior PhD Students / Post Docs*** →
  - Bammann / Sandia – Mississippi State
  - Zbib / Washington State
  - Zaiser / U Edinburgh
  - Askes / U Sheffield
  - Konstantinidis - Kalampakas/ AUT
- ***Other Students/Faculty*** →
  - 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
- ***Children*** →
  - Katerina / Nanotechnology
  - Elias / Music
- ***The Forth/Crete Effect*** →
  - Economou/Kafatos/Fotakis
  - Flytzanis/Stratakis/Tsibidis

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.

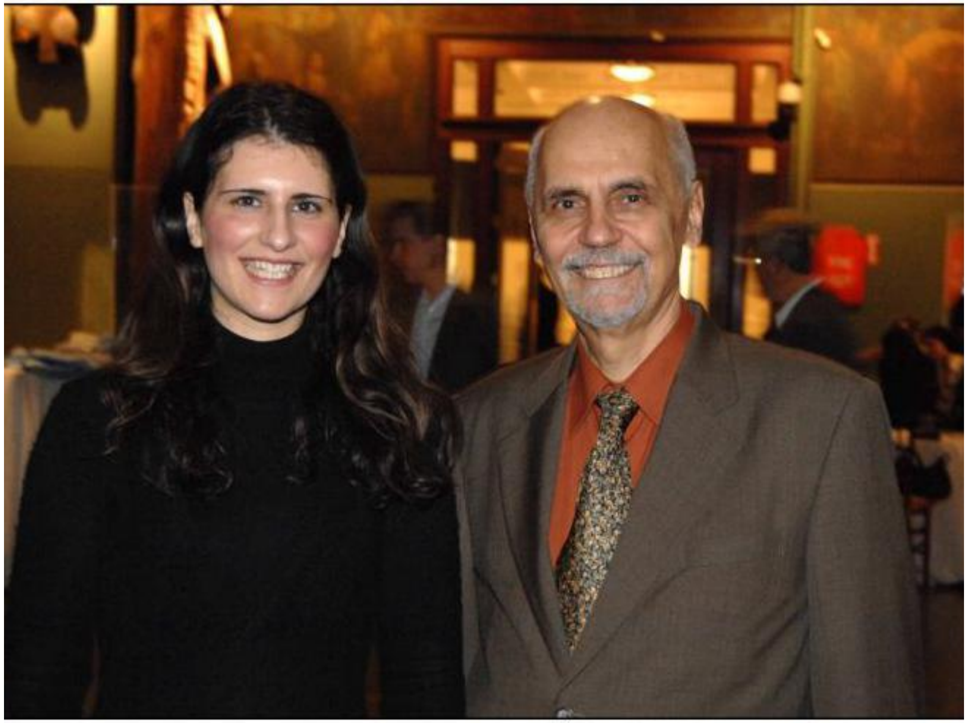
"She just beat everyone in the class," remembers Associate Professor Paul Charlesworth. "She's one of the finest students to ever take my general chemistry course."

ERC STARTING GRANT

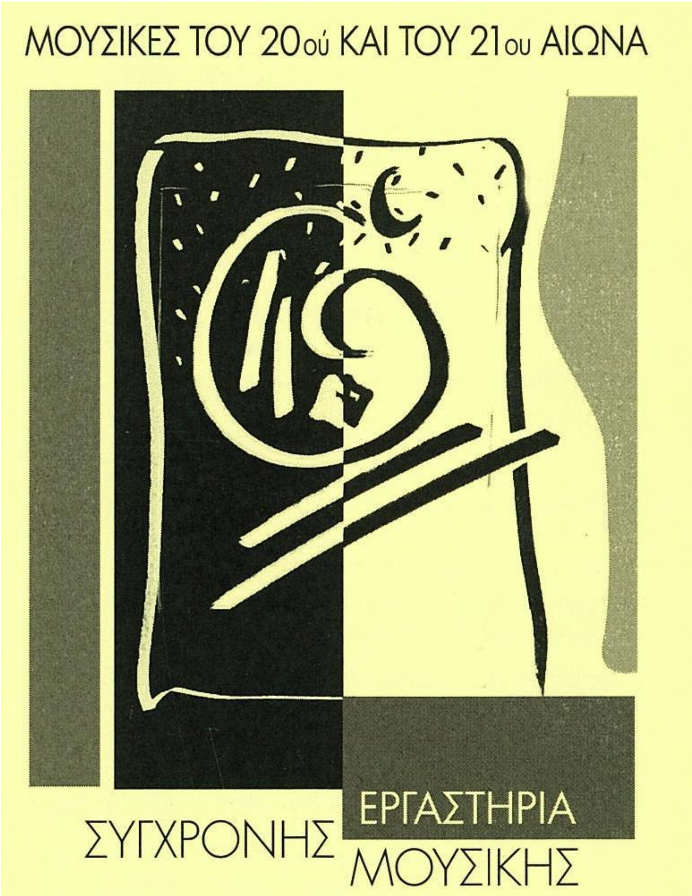
Probing the Micro-Nano Transition (MINATRAN): Theoretical and Experimental Foundations, Simulations and -Applications [1.3 Million Euros]

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.

A Glimpse at Mythology

▪ Prometheus' Legend

Hesiod's Theogony (800 bc) – Aeschylus Trilogy (500 bc)

- Prometheus "κλέπτει" (steals/arranges) fire/knowledge from Olympus/Zeus via Athena's helmet for miserable Humans

∴ **Survival**

- Humans survive but fight each other viciously/destruction Zeus sends Hermes to bring them consciousness/peace

∴ **Societies**

- Zeus sends Pandora (made by Hephaestus out of clay) Pandora's jar of gifts (evils/pain/diseases + hope)

  Humans are left with "hope" striving to free themselves from their troubled + mortal nature

∴ **Civilization**

■ Homer's Automata

- ***Iliad***

Ε 749: Hera opens the Gates automatically } → *telecontrol?*

Σ 372: Hephaestus' 20 golden self-moving tripods } → *telecontrol?*

Σ 468-473: Hephaestus' automated Lab → *modern casting unit?*

Σ 410-420: Young Servant Girls (made out of gold with mind/voice/movement) assisting "crippled" Hephaestus to walk → *human robots?*

- ***Odyssey***

Θ 555-563: Phaeacians' Ships possessing "mind of their own " traveling at extremely high speeds at night and in clouds without fear to sink → *modern auto-pilots?*

A Glimpse at Ancient Technology

- **800-700 bc:** Empirical Techniques imported from the East

- **700-200 bc:** Science/Mathematics ↔ **400 bc-100 ad:** Technology

- **Teacher / Student Sequences**
  - Thales – Anaximander – Pythagoras – Archytas
  - Socrates – Plato – Aristotle – Archimedes
  - Euclid – Aristarchus – Hipparchus – Ptolemy
  - Ctesibius – Philo - Heron

- **Geometry/Numbers/Forces/Compressed Air/Mirrors**
  – Geodesy/Astronomy; Mining/Metallurgy; Statics/Optics/Engineering
  – Buildings/Monuments, Aqueducts/Harbors, War/Musical Instruments

The Great Alexandria

- **Turning point in the History of Mankind**
  From a Top-Down to a Bottom-Up Approach

- **The search for the origin of the Universe**
  from first principles [e.g. the 4 elements – earth/water/fire/air] →
  search for unfolding the puzzle from everyday life observations
  ∴ measurement / fabrication / construction → *Modern Engineering*

- **Great Thinkers**
  are not Philosophers / Generals and Landlords / Merchants,
  BUT simple everyday men
  - *Ctecibius* (Aeroton, Hydraulic Pump, Hydraylis) - son of barber
  - *Heron* (Watt's Steam Engine, Siphons, Lamps) – shoemaker

∴ The Precursor of Renaissance: Da Vinci, Galileo, Newton

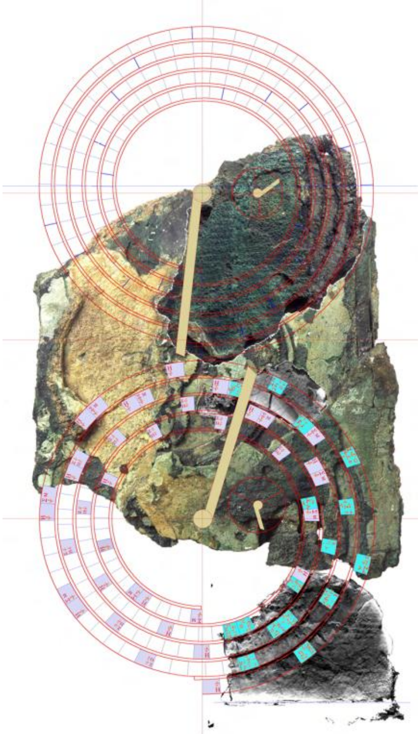
- **150-100 bc: Antikythera Mechanism** → The 1st Computer/GPS

– Ancient Mechanical Computer designed to calculate the positions of sun/moon/stars, eclipses, calendar – 1st astronomical clock

– Remarkable miniaturization/precision and complexity: 3 Dials & over 30 gears with teeth (comparable to 18th Century clocks)

– Designed after Hipparchos' theory of the Moon

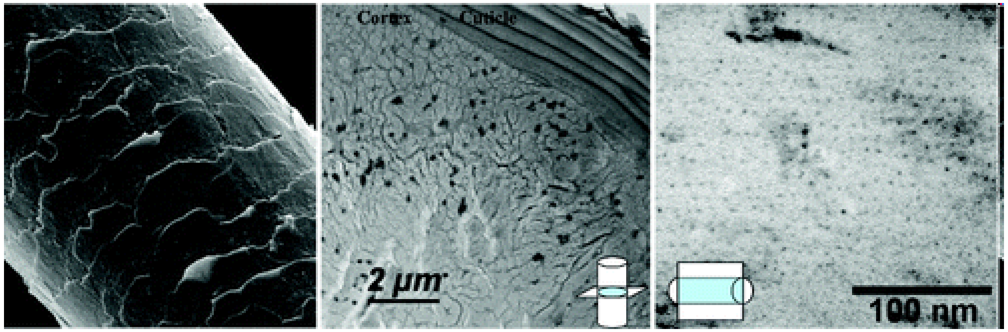
The Antikythera Mechanism main fragment: 32×16 ×10 cm



The Antikythera Mechanism's Reconstruction: Athens Archaeological Museum

A Glimpse at Ancient Nanotechnology

- Ancient Egyptians/Greeks (~2000 bc) used Pd-S Nanoparticles (5-200 nm) for hair coloring
- Ancient Thracians (~800 bc) used Au Nanoparticles (~70 nm) to change Glass Cup Color with Light (Green → Red)
- Damascus (Alexander/Ottomans) used swords containing C-Nanotubes developed during forging + heat treatment
- Roman Catholics used Au/Si Nanoparticles (~100 nm) in stained glass – Church Windows



Pd-S Nanoparticles (5-200 nm) for hair coloring

Au Nanoparticles change Glass Cup Color with Light (Green → Red)

Damascus steel swords

A Glimpse at Current Nanotechnology

R. Feynmann (1918-88) Prophet of Nanotechnology
Caltech's Lecture: Dec 29th 1959

"There's Plenty of Room at the Bottom"

Recent Examples of New Fields

- Kamerlingh Onnes: Low-Temperature physics
- Percy Bridgman: High-Pressure physics

New Emerging Field

- **Manipulating/controlling things on small scale**

  In 2000 we will wonder why it was not until 1960 that anybody began seriously moving in this direction

∴ Nanoscience / Nanotechnology

- Why cannot we write the entire 24 volumes of the *Encyclopedia Brittanica* on the head of a pin?
  - All necessary to do is to reduce the letters by 25,000 times
  - By Photoengraving to raise letters on a metal surface that are 1/25,000 of their ordinary size
  - Look through with an electron microscope and reverse the lenses to read (demagnify/magnify)

- 24 million volumes $\Rightarrow$ Need 1 million pinheads

i.e. 3 square yards or 35 pages of the Encyclopedia

- This does not involve New Physics

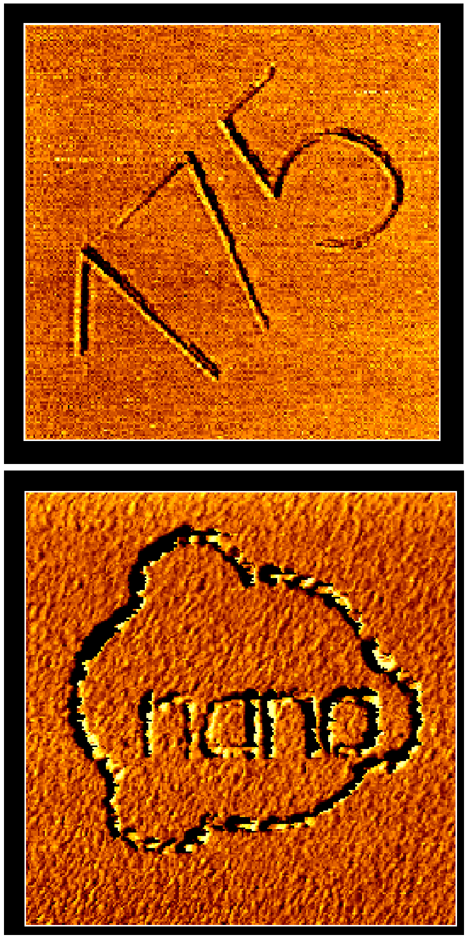
i.e. you can decrease size of things in a practical way, according to the laws of physics. I am not inventing anti-gravity, which is possible someday only if the laws are not what we think.

I am telling you what could be done if the laws are what we think; we are not doing it simply because we haven't yet gotten around to it.

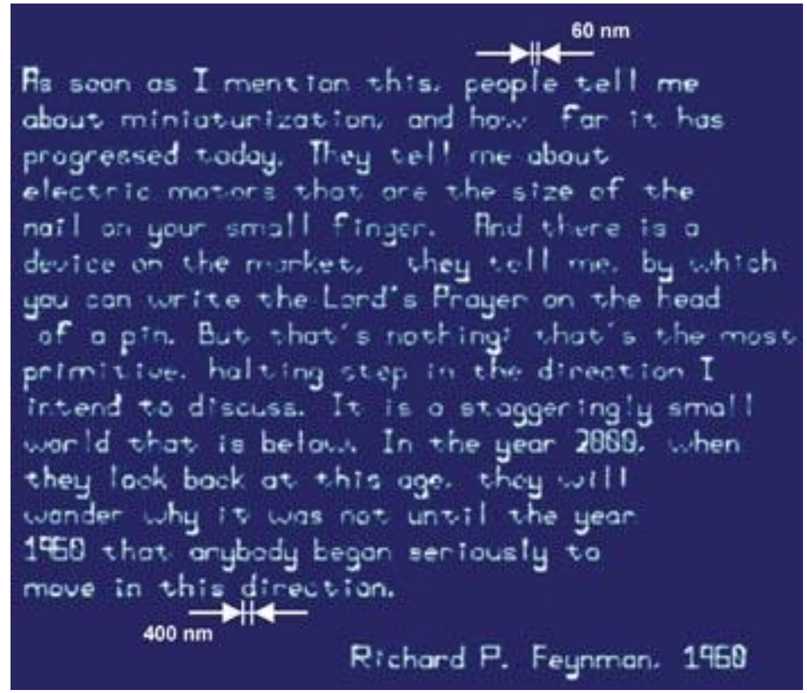
∴ Nanolithography

■ Nanolithography Today

- Chemical/electrochemical processes induced at predefined positions
  + AFM tip engraving on sample surface



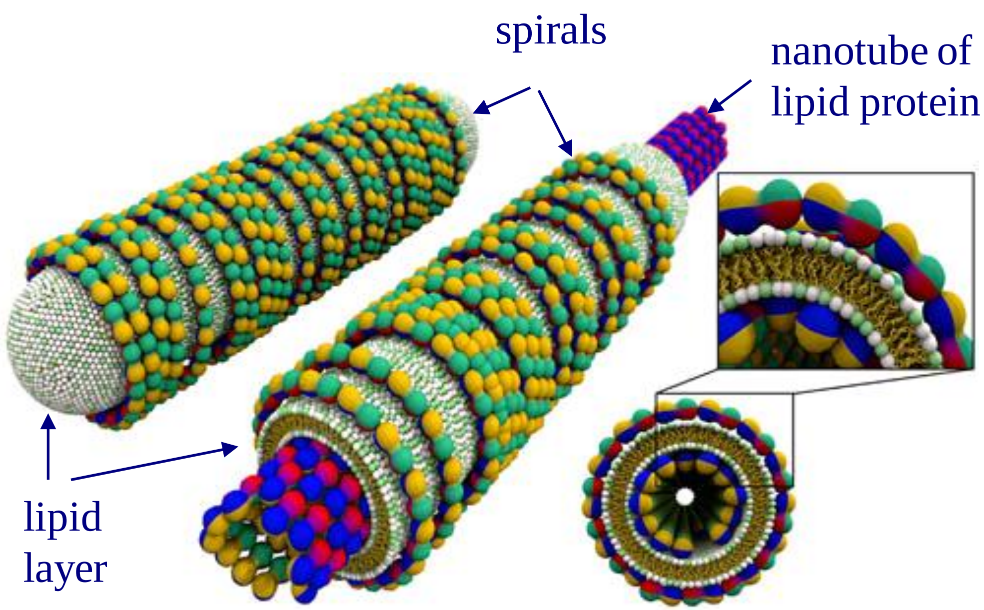
T. Schimmel et al, 2008



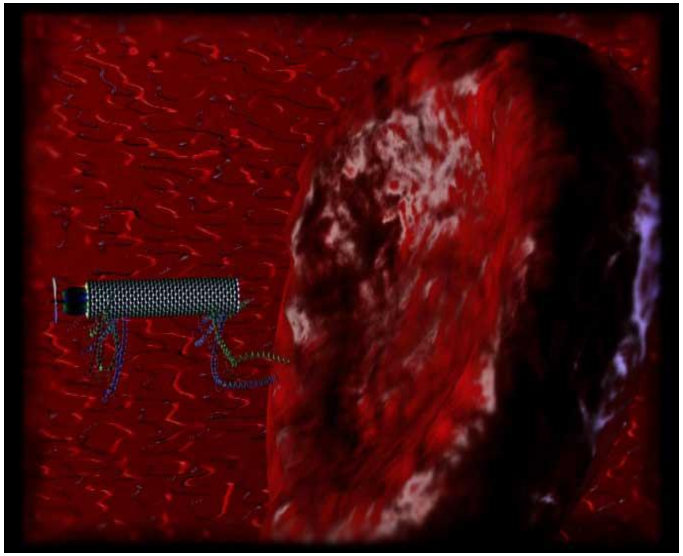
Text written by using Dip-Pen Nanolithography (DPL) and imaged by using AFM (Mirkin Group, Northwestern University)

■ Nanomedicine Today/Future

- Smart Bio-Nanotubes / Nanorobots

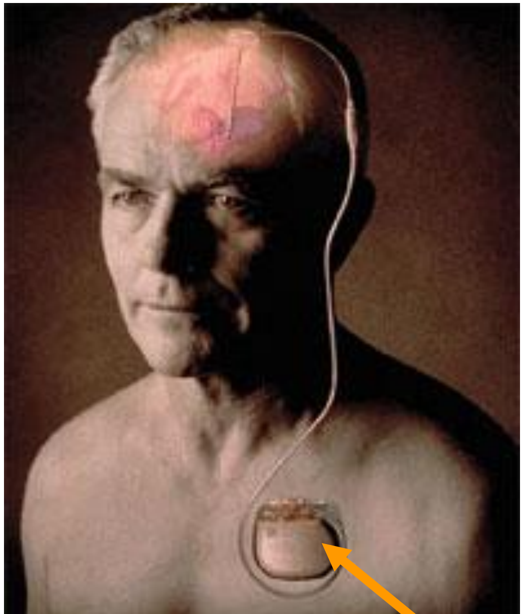


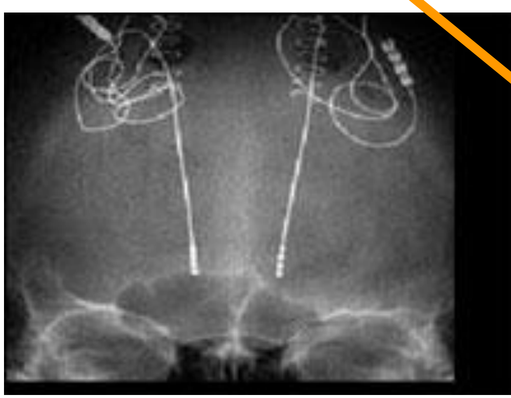
Bio-nanotube: Selective Storage/Release of Drugs
Nanotubes of lipid proteins encapsulated in a lipid layer covered by protein spirals
http://www.voyle.net



Bio-nanorobot:
Futuristic Targeted Drug Release
http://bionano.rutgers.edu/mru.html

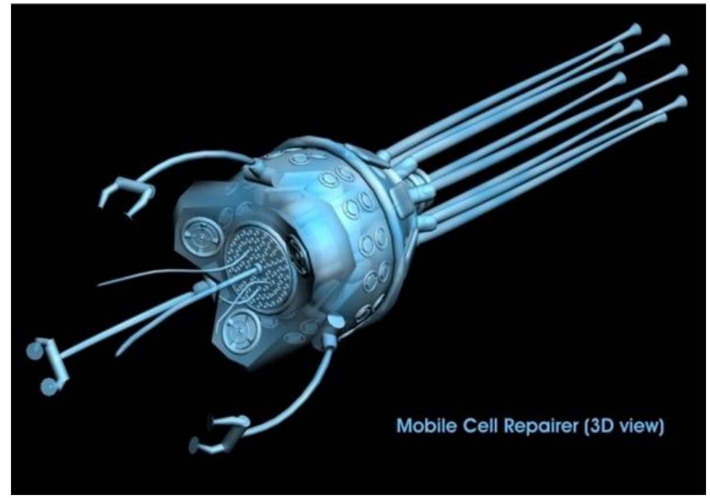
- Nanostructured Li-batteries / Nanosurgeons
  Cure of Alzheimer's/Parkinson Diseases and Brain Damage/Paralysis





Li-battery

Deep Brain Stimulation
Dr. H. Mayberg, Univ. Toronto

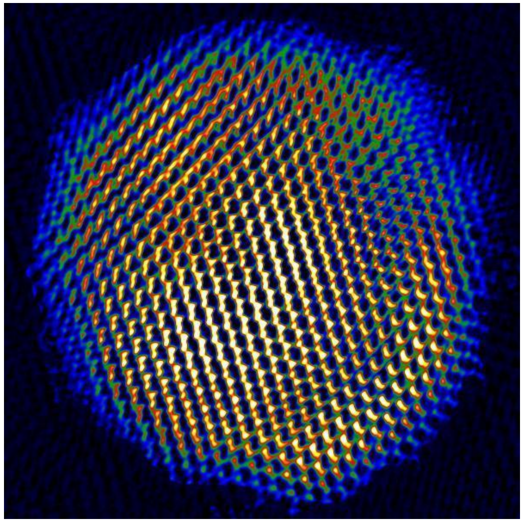


Mobile Cell Repairer
Y. Svidinenko, Nanotechnology News Network

Mobile Artery Cleaner

New Electron Microscopes / Super Imaging

- High-Resolution Transmission Electron Microscope (HRTEM/~0.8 Å) (C atoms imaged in diamond separated by only 0.89 Å/ Si at 0.78 Å)
- Scanning Electron Microscope (SEM/~0.4 nm)
- Scanning Tunneling Microscope (STM/Lateral ~0.1 nm, Depth ~0.1 Å)
- Atomic Force Microscope (AFM/Lateral ~0.1 nm, Depth ~0.1 Å)
- Most Recent Ultrahigh Resolution TEM /~1 Å
  New Technique overcoming the limit of diffraction

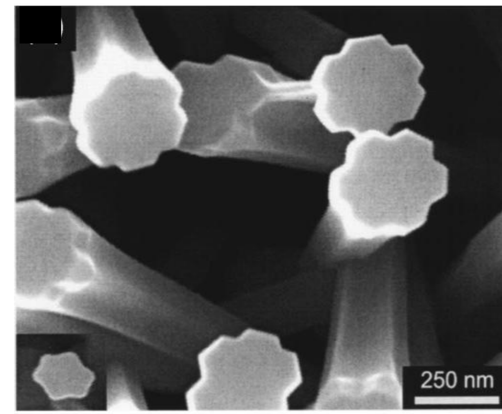


Reconstructed Image of a 9 nm diameter CdS quantum dot
Zuo et al, Univ. Illinois

■ Nanomanufacturing/Nanomechanics

- Nanoholes with diameters of a few nm were drilled in a stainless steel foil using intense electron beams of 2.4 nm nominal probe size from a field-emission electron gun in a HTREM

- Nanoscrews of ZnO were manufactured with an average diameter of the tops of about 250 nm, that of the roots of about 60 nm, and the average length in the order of several microns



SEM top view of the 18 sides of nanotips

- Nanostamping Parts with characteristic dimensions below 1 nm and up to 100 nm are used for magnetic memory storage

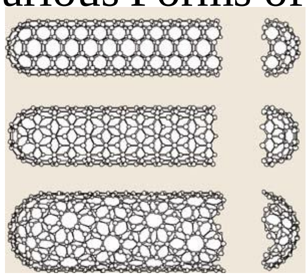
- Micro/Nano Motors

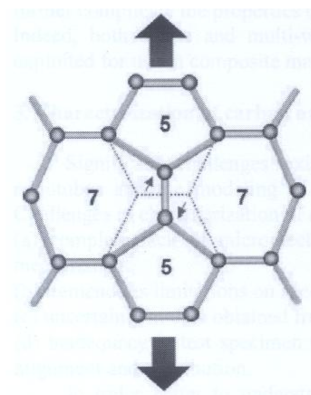
Outer rotor diameter: 10 mm
Length from mount: 14 mm

Popular Nanomechanics Topics

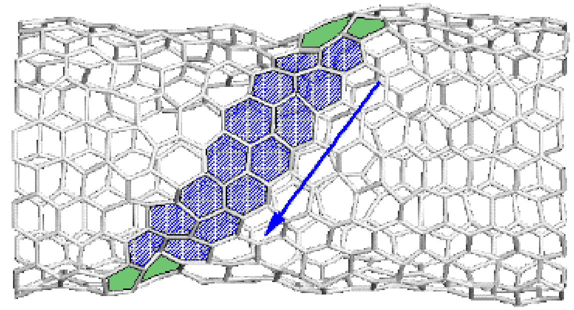
- Nanotubes

Various Forms of CNTs

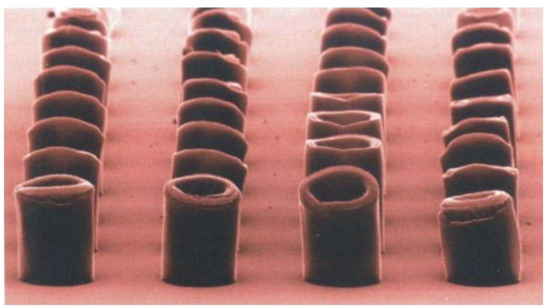




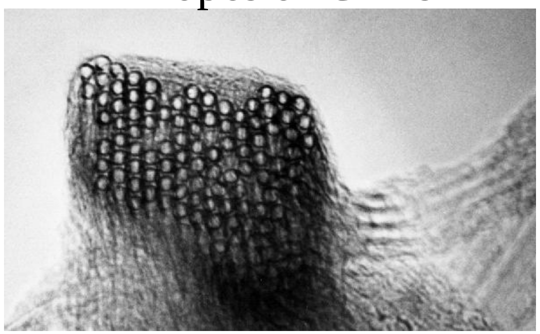
5/7 Dislocation-like Defects in CNTs



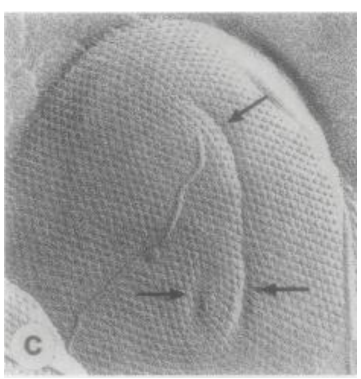
Multiwalled CNTs

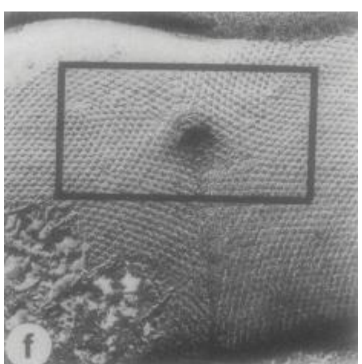


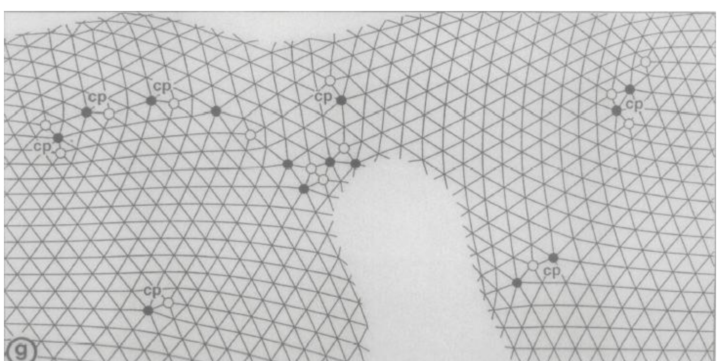
Ropes of CNTs



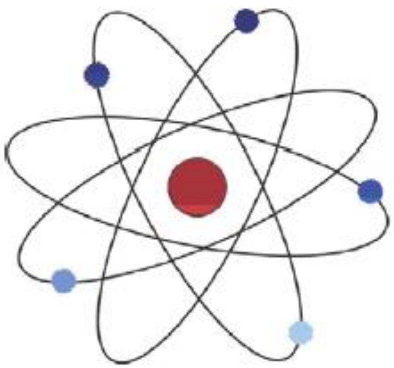
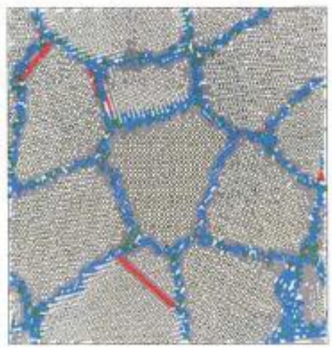
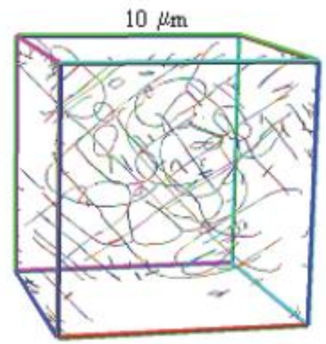
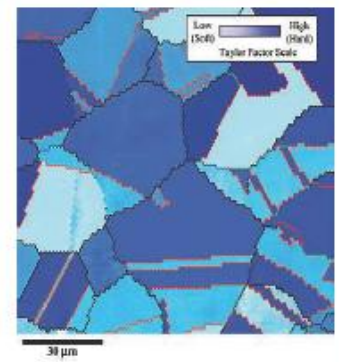
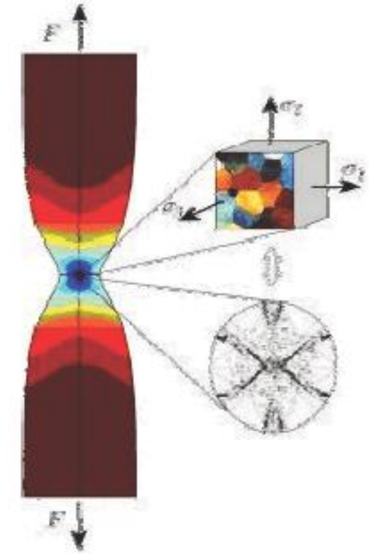
- Nanobiomembranes/M. sinense Cells



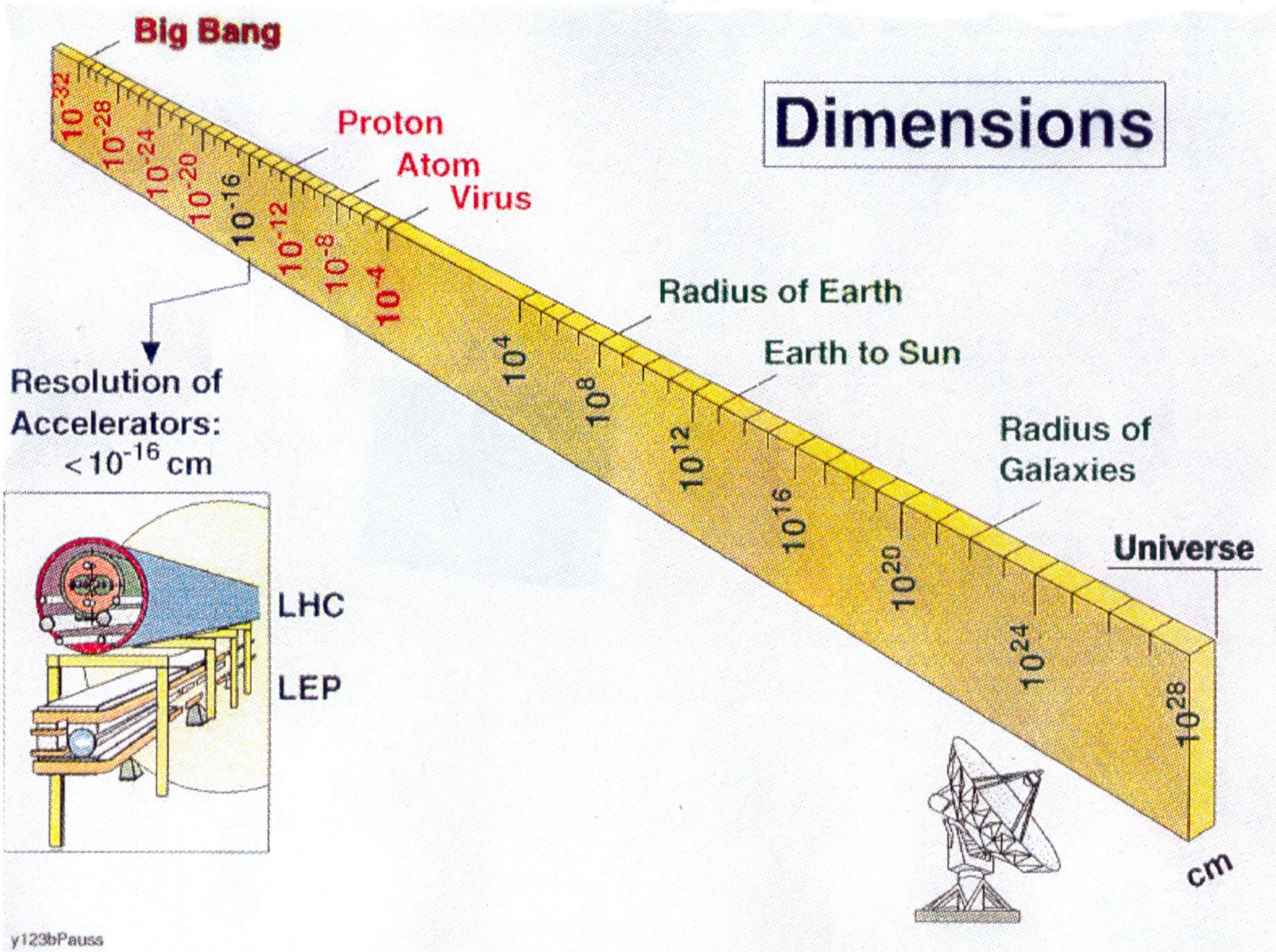




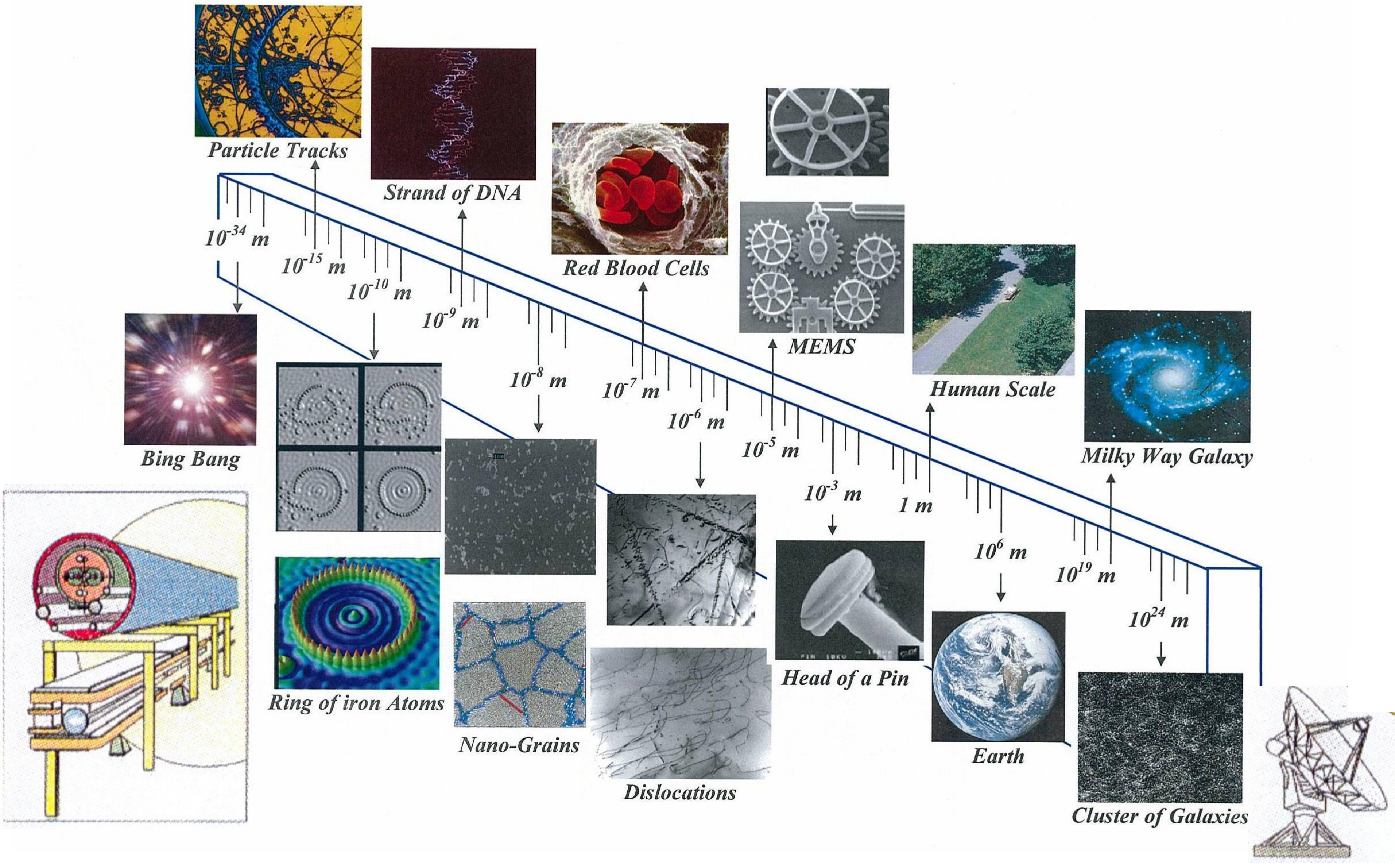
■ From Atomic/Nano to Micro/Macro

Quantum	Atomistic	Microscale	Mesoscale	Continuum
				
Quantum Mechanics	Molecular Dynamics	Dislocation Dynamics	Grain Boundary Mechanics	Continuum Mechanics
$10^{-11} – 10^{-10}$ m	$10^{-9} – 10^{-6}$ m	$10^{-8} – 10^{-5}$ m	$10^{-6} – 10^{-3}$ m	$> 10^{-3}$ m
$10^{-16} – 10^{-12}$ sec	$10^{-13} – 10^{-10}$ sec	$10^{-12} – 10^{-8}$ sec	$10^{-10} – 10^{-6}$ sec	$> 10^{-6}$ sec

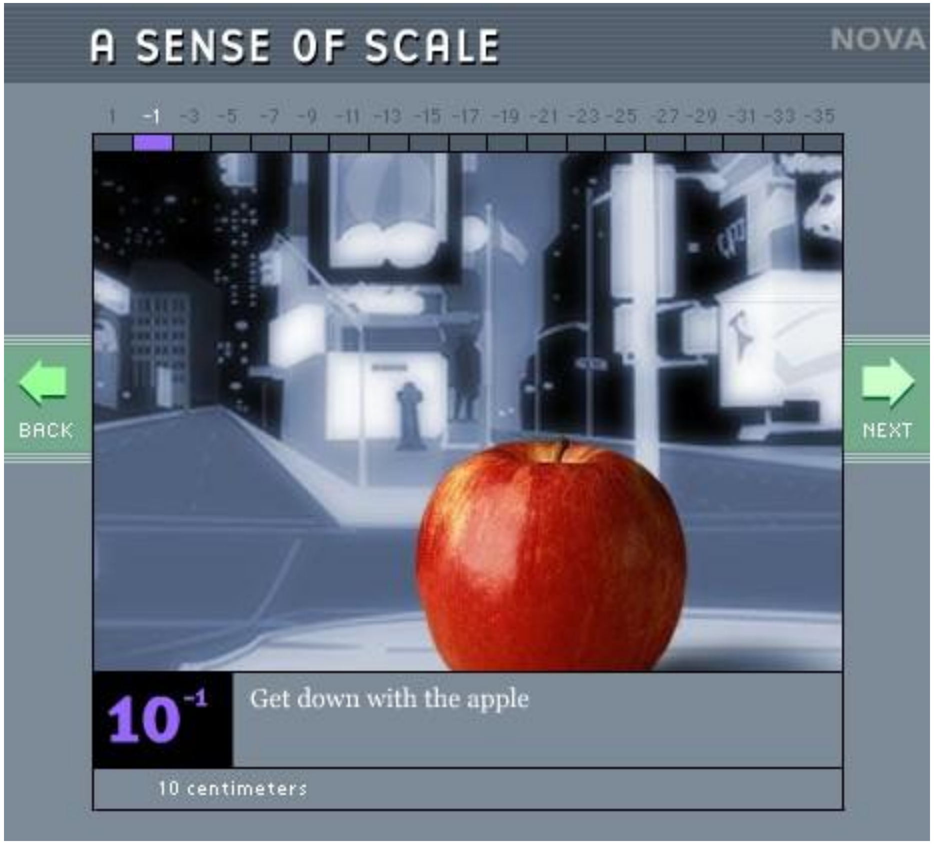
- A Sense of Scale: $10^{-32} – 10^{28}$ m

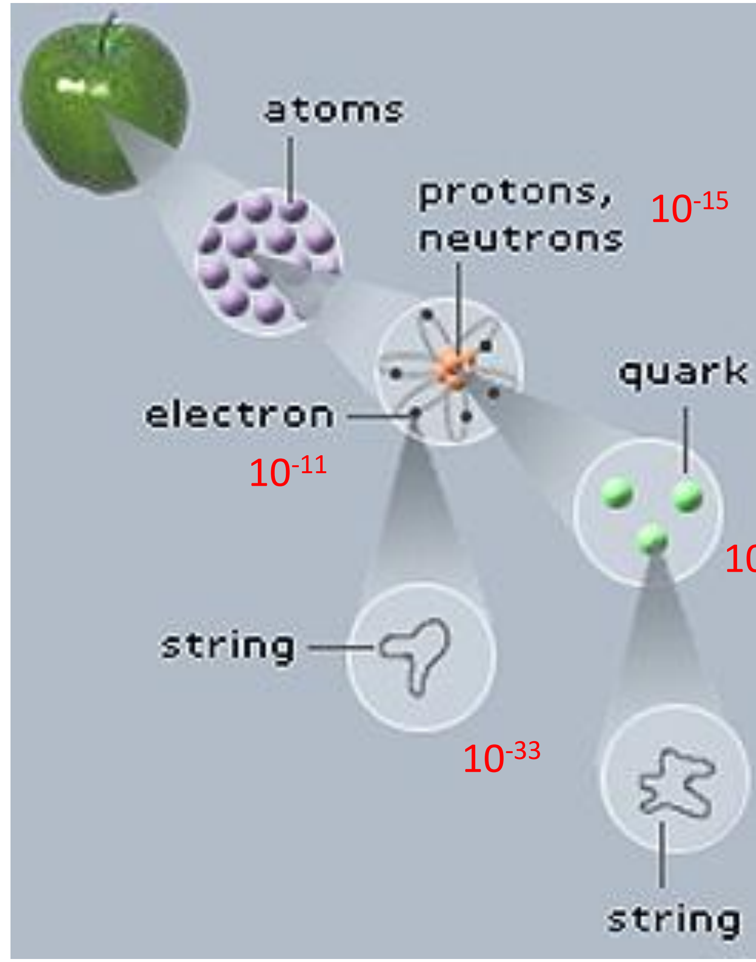


- A Sense of Scale: $10^{-34} – 10^{24}$ m



■ Below Newton's Apple

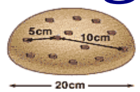


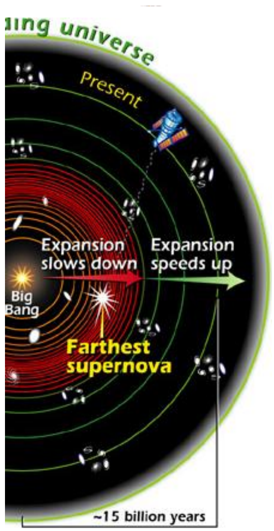


■ Interesting (?) Analogies

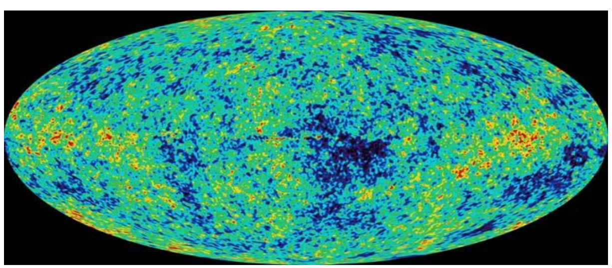
Hot Big Bang

Hubble : 1928



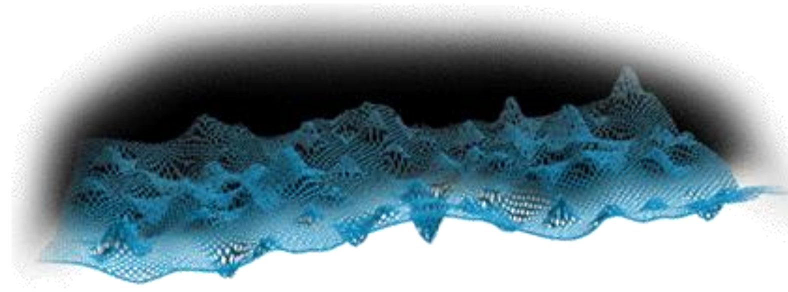


Penzias & Wilson : 1965



COBE : 1992 WMAP : 2003

Spacetime Foam



A Glimpse at Mechanics

■ Post-Newtonian (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 : $\mu\nabla^2\boldsymbol{u} + (\lambda + \mu)\nabla\, div\boldsymbol{u} = \rho\ddot{\mathbf{u}}$

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

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

$\boldsymbol{E}$ ... 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.

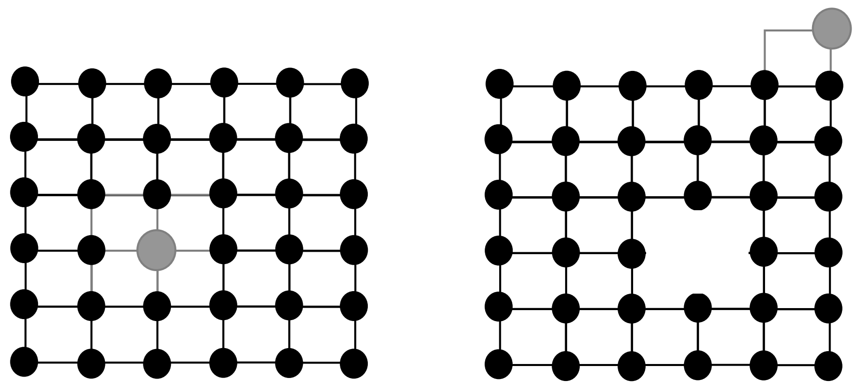
$$\frac{\partial \boldsymbol{B}}{\partial t} + \operatorname{curl}\boldsymbol{E} = 0 \quad ; \quad \operatorname{div}\boldsymbol{B} = 0$$

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

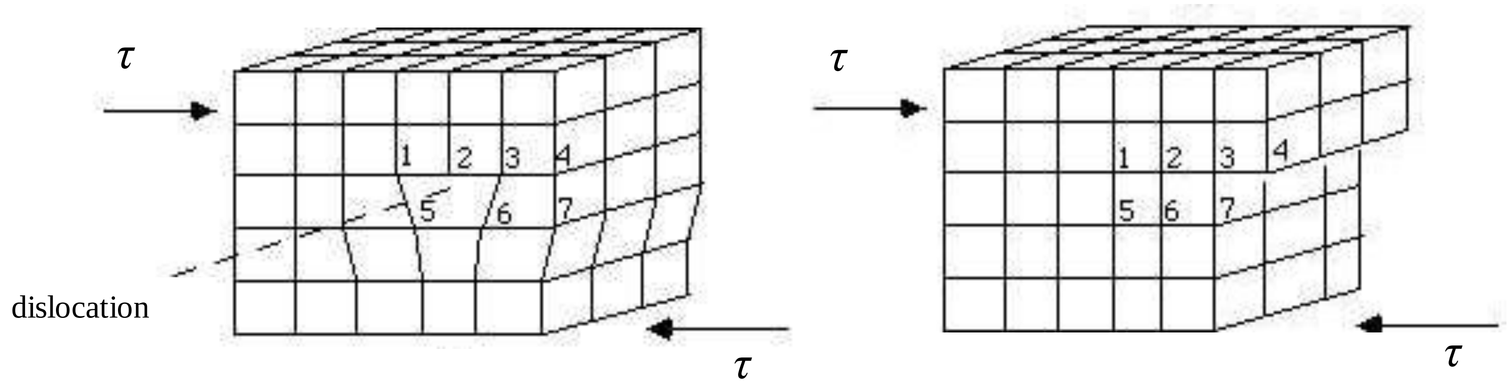
A Glimpse at Gradient Mechanics

■ Motivation

- ***Vacancies***

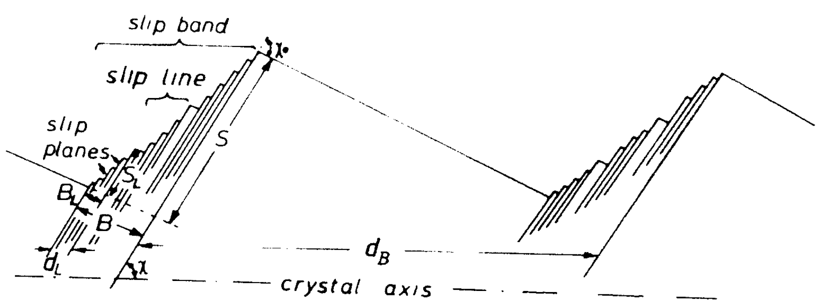


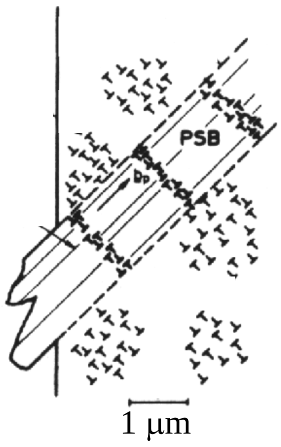
- ***Dislocations***

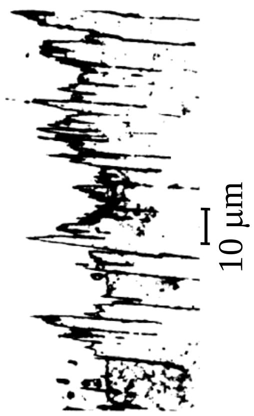


- A continuum with micro(nano)structure is viewed as a classical continuum which, in addition, can interchange mass, momentum, energy and entropy with its bounding surface. As a result, a surface region is excluded from the local (bulk) description; however, changes in the surface region are considered 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*)







■ Self-Diffusion in Solids

- ***Balance Laws***

$\rho = \rho^* \rho_s$ . . . . vacancy concentration

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

$\frac{\partial T}{\partial x} = \hat{f}$ . . . . 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

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

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

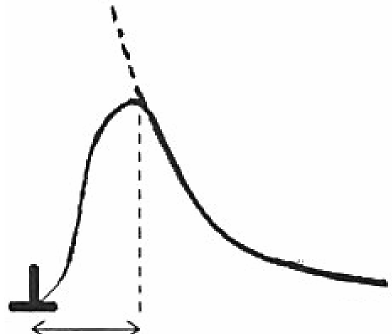
- Elasticity:

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

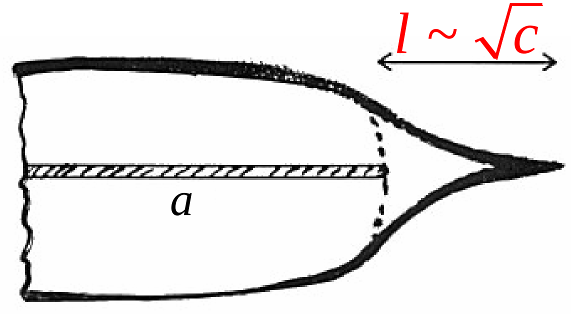
$$\boldsymbol{T}^{nano} = \lambda(\mathrm{tr}\boldsymbol{\varepsilon})\mathbf{1} + 2\mu\boldsymbol{\varepsilon} - c\nabla^2\left[\lambda(\mathrm{tr}\boldsymbol{\varepsilon})\mathbf{1} + 2\mu\boldsymbol{\varepsilon}\right]$$

i.e. Gradient Elasticity

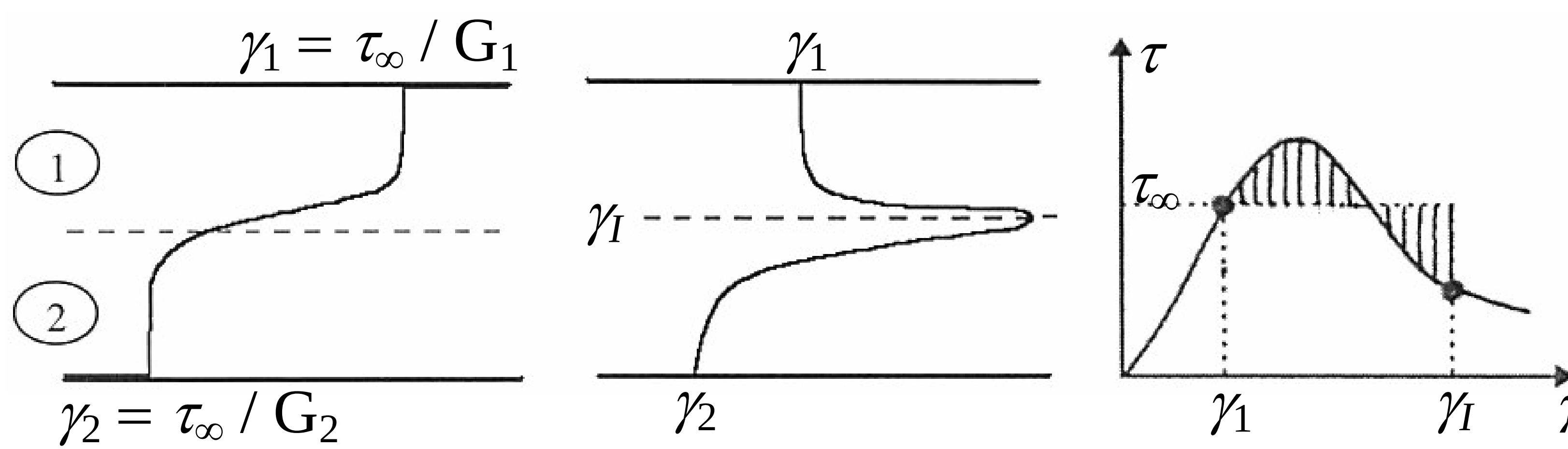
- $\boldsymbol{\sigma} = \lambda(\mathrm{tr}\,\boldsymbol{\varepsilon})\mathbf{1} + 2G\boldsymbol{\varepsilon} - c\nabla^2\left[\lambda(\mathrm{tr}\,\boldsymbol{\varepsilon})\mathbf{1} + 2G\boldsymbol{\varepsilon}\right]$ … Gradient Elasticity



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



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



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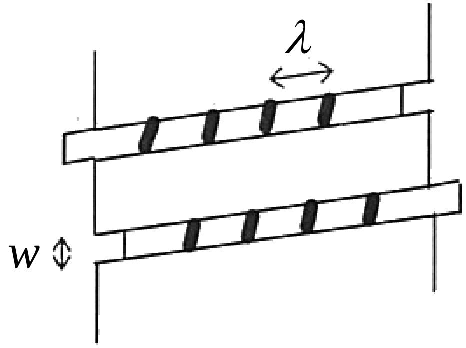
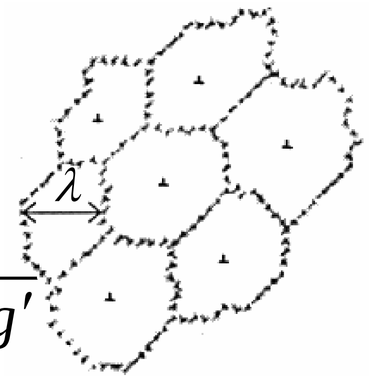
■ More on Gradient Benchmark Problems

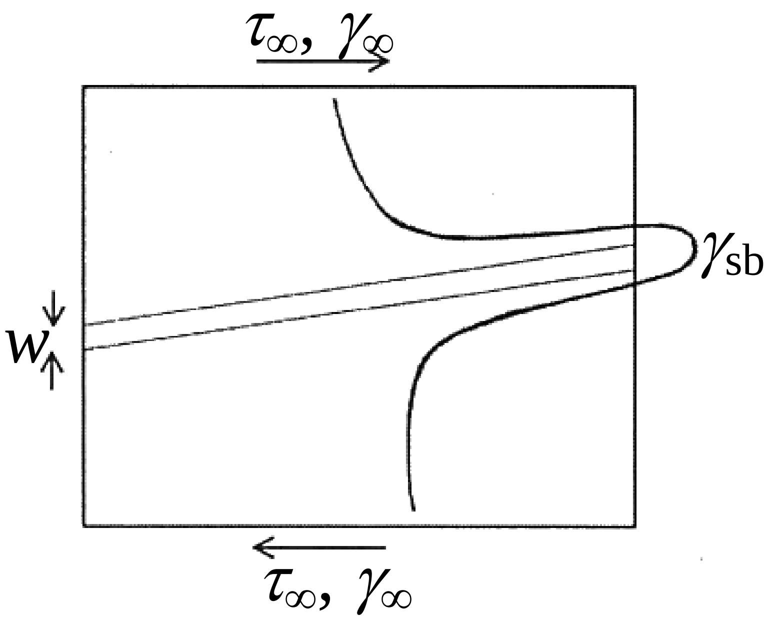
- $\dot{\rho} = g(\rho) + D\nabla^2\rho$ … Gradient Dislocation Dynamics

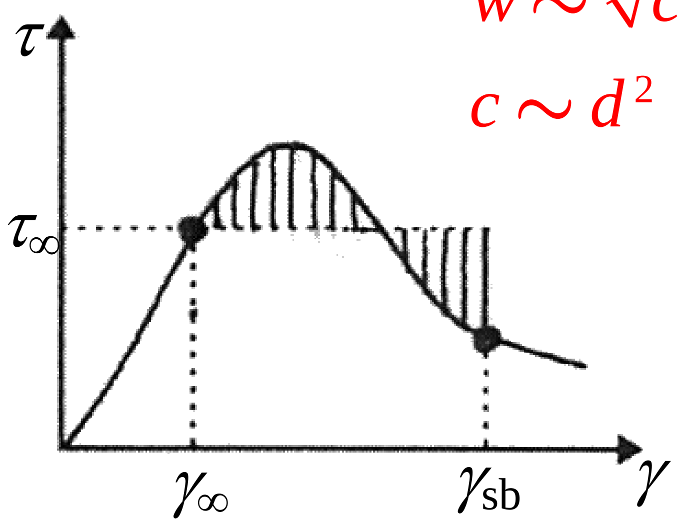




$\lambda \sim \sqrt{D/g'}$

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





$w \sim \sqrt{c}$

$c \sim d^2$

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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*

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

  - *Barenblatt 1963*

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

- *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 Nanopolycrystals

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

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

- ***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.***

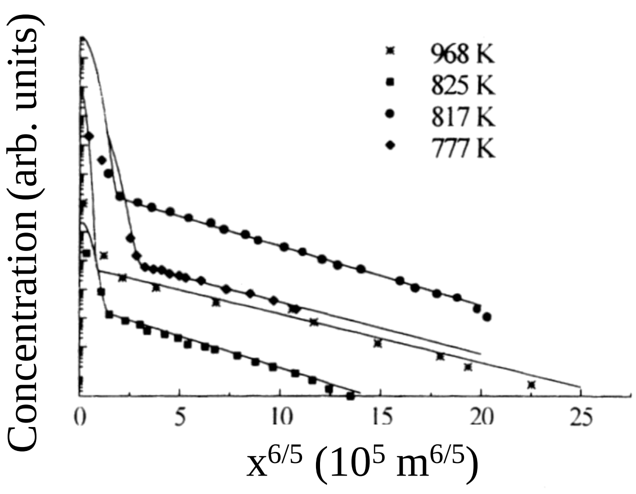
$$\frac{\partial \rho}{\partial t} + \tau \frac{\partial^2 \rho}{\partial t^2} = D\nabla^2 \rho + \bar{D}\frac{\partial}{\partial t}\nabla^2 \rho - \mathrm{E}\nabla^4 \rho$$

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

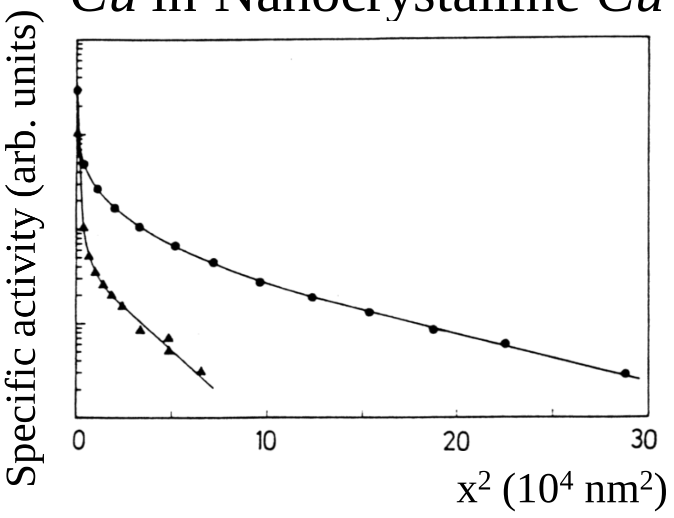
$$t \to \infty \Rightarrow \frac{\partial \rho}{\partial t} = D\nabla^2 \rho \quad ; \quad D = D_{eff} = \frac{\kappa_2}{\kappa_1 + \kappa_2} D_1 + \frac{\kappa_1}{\kappa_1 + \kappa_2} D_2$$
$$= f\, D_1 + (1 - f)D_2$$

- *Diffusion Penetration Profiles*

^{64}Cu in Polycrystalline Cu



^{67}Cu in Nanocrystalline Cu



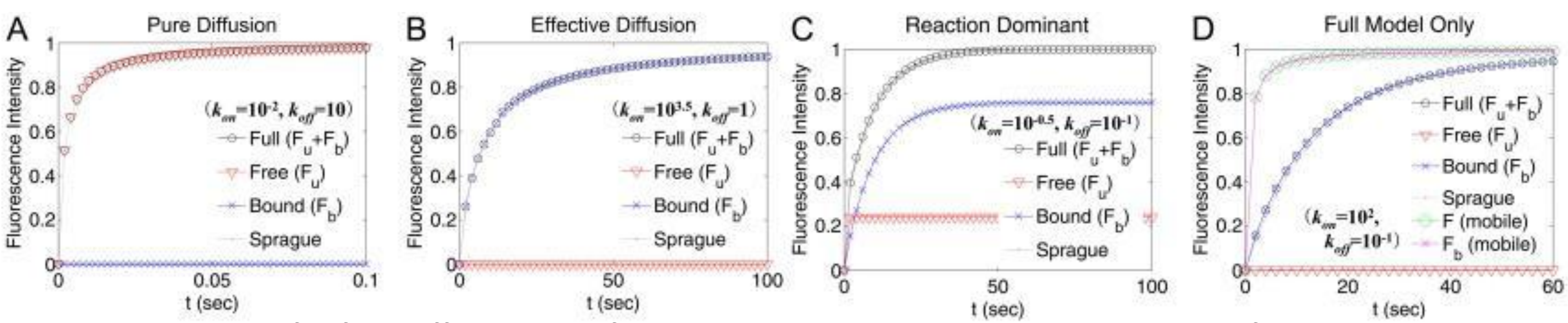
- **Rutherford Aris:** On the Permeability of Membranes with Parallel but Interconnected Pathways [*Math. Biosci.* **77**, 5-16 (1985)]

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

$$A_1 D_1 \frac{d^2 c_1}{dx^2} = k_1 p c_1 - k_2 p c_2 \quad ; \qquad A_2 D_2 \frac{d^2 c_2}{dx^2} = -k_1 p c_1 + k_2 p c_2$$

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

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



(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***

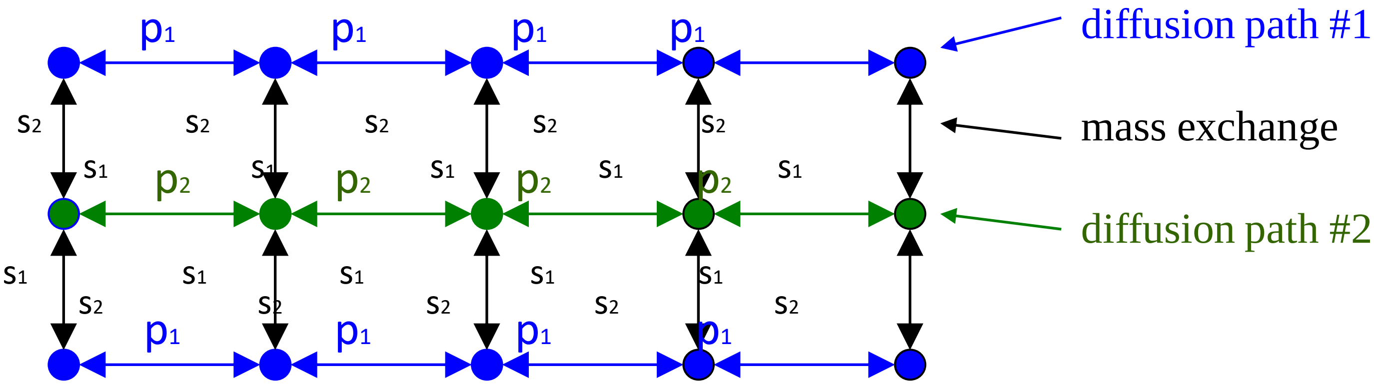
$$C_e \frac{\partial T_e}{\partial t} = \nabla(K_e \nabla T_e) - g(T_e - T_i) + S(r,z,t)$$

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

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

▪Random Walk Model

• Random Walk on Graphs



Graph: Two dimensional infinite grid

• Probabilities for jumps:

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

$$2p_1 + 2s_1 + r_1 = 1$$
$$2p_2 + 2s_2 + r_2 = 1$$

• Assumptions:

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

• *Discrete Version*

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

• *Continuous Version*

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

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

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

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

Special Case

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

$$\frac{\partial \rho_1}{\partial t} = D_1 \partial_{xx} \rho_1 - (\kappa_1 \rho_1 - \kappa_2 \rho_2) \quad , \quad \frac{\partial \rho_2}{\partial t} = D_2 \partial_{xx} \rho_2 + (\kappa_1 \rho_1 - \kappa_2 \rho_2)$$

- Extra condition

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

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

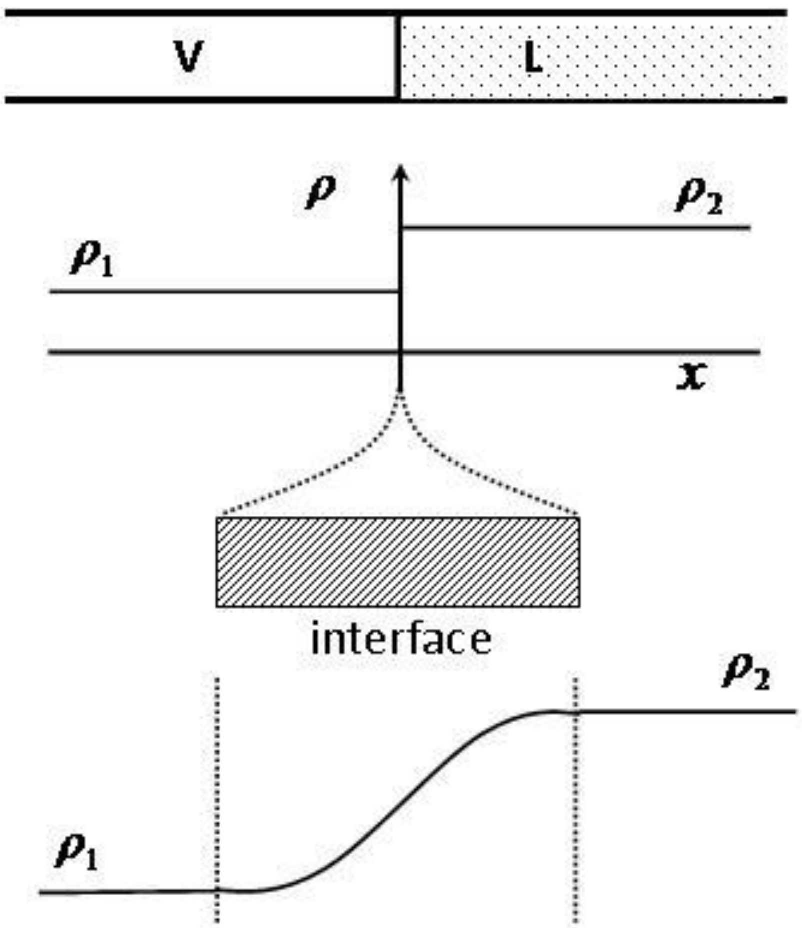
$$D_1 \approx 4.34 \times 10^{-9}, D_2 \approx 1.36 \times 10^{-11}, \kappa_1 \approx 4 \times 10^{-4}, \kappa_2 \approx 4 \times 10^{-7}$$
$$\Rightarrow \kappa_2 D_1 - \kappa_1 D_2 \approx 10^{-15}$$

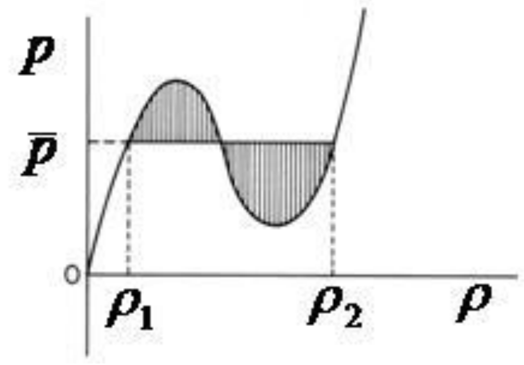
- Diffusion of Ca^{2+} in MgO single crystal

$$D_1 \approx 7.64 \times 10^{-17}, D_2 \approx 6.65 \times 10^{-20}, \kappa_1 \approx 5 \times 10^{-3}, \kappa_2 \approx 1.5 \times 10^{-6}$$
$$\Rightarrow \kappa_2 D_1 - \kappa_1 D_2 \approx 10^{-23}$$

INTERFACES
THE VdW/MAXWELL GRADIENT L-V INTERFACE

- **Van der Waals 1873 / Maxwell 1875: Thermodynamics**





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

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

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

■ 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:*** $\mathrm{MR} \Rightarrow \frac{1}{\rho^2} \to E(\rho) = \frac{1}{a}\exp\left(2\int\frac{b}{a}d\rho\right); \quad a \equiv \alpha+\gamma,\ b \equiv \beta+\delta$
- ***Note:*** Maxwell (1876) ; Korteweg (1901) ; Truesdell (1949)

■ Solution Details – Remarks

- ***Planar Interfaces***

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

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

  - *Analytical Solutions / Conditions for Existence*

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

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

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

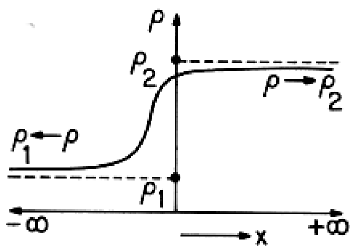
$$a = \frac{1}{16}\rho^2 u' + \frac{1}{2}\rho u\,, \quad b = \frac{1}{16}\rho^2 u'' + \frac{1}{4}\rho u' - \frac{1}{4}u\,, \quad c = \frac{1}{2}u + \frac{1}{4}\rho u'$$

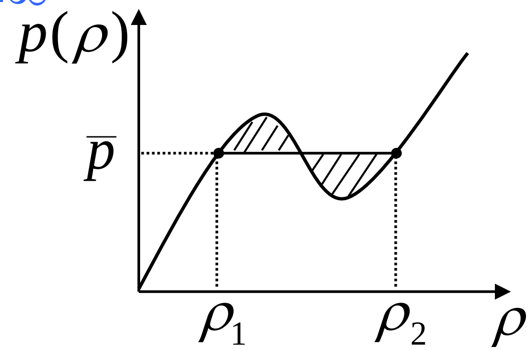
- *Validity of MR:* $\left(\frac{a}{\rho^2}\right)' = 2\left(\frac{b}{\rho^2}\right)$

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

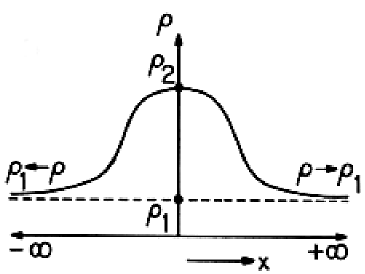
- ***Planar Interfaces / 1D Profiles***

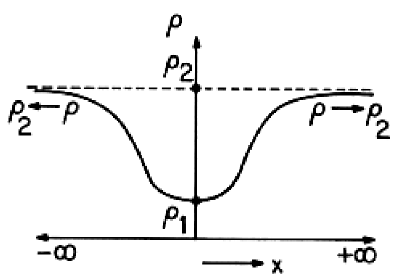
  - *Transitions (interfaces)* $\rho \rightarrow \rho_{1,2}$ *as* $x \rightarrow \mp\infty$

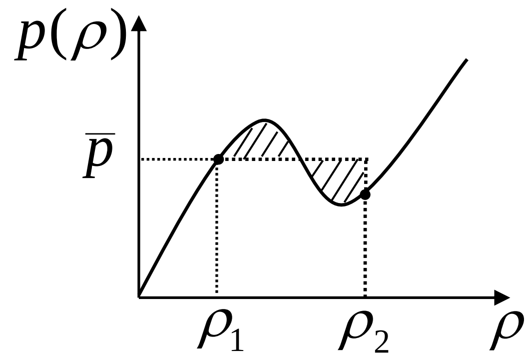




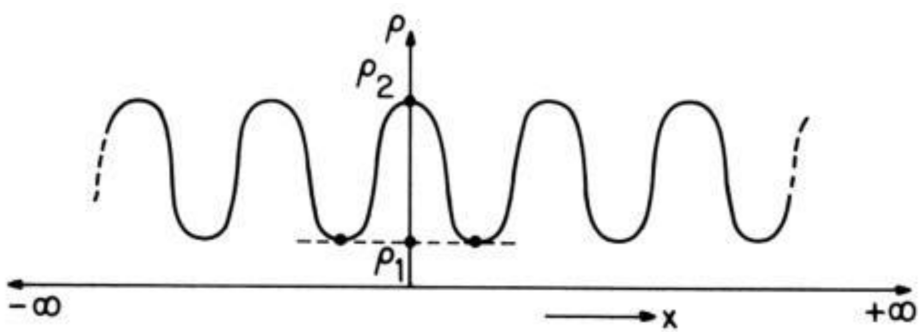
  - *Reversals (films)* $\rho \rightarrow \rho_1$ as $x \rightarrow \mp\infty$

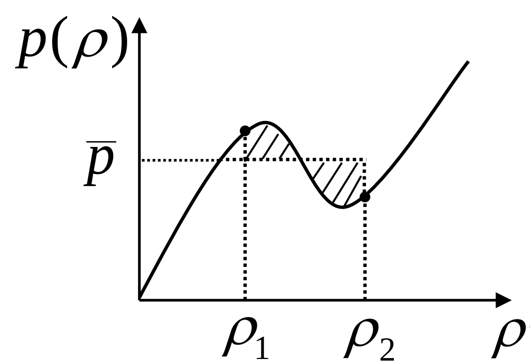






  - *Oscillations (layers)*

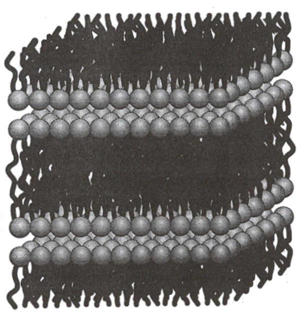




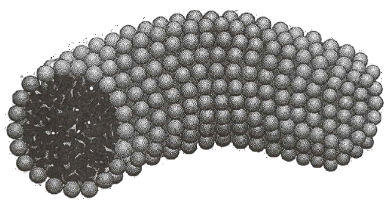
- ***General Interfaces / 3D Structures***

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

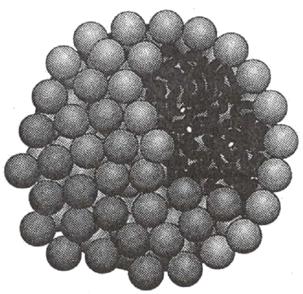
$$\tilde{b} \not\equiv 0 \;\Rightarrow\; \rho = \rho(x)\,; \qquad \rho = \rho(r)\,; \qquad \rho = \rho(R)$$



layers



cylinders

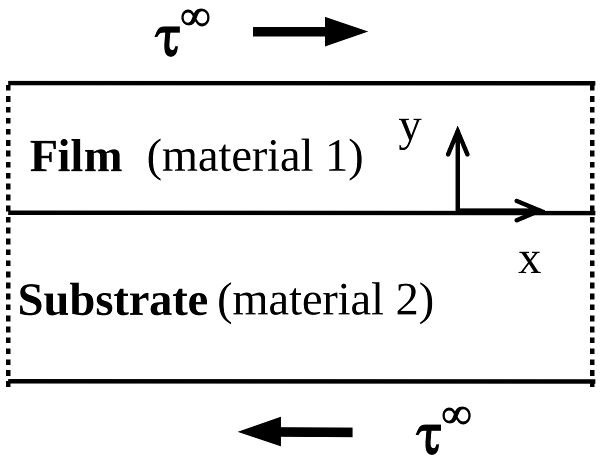


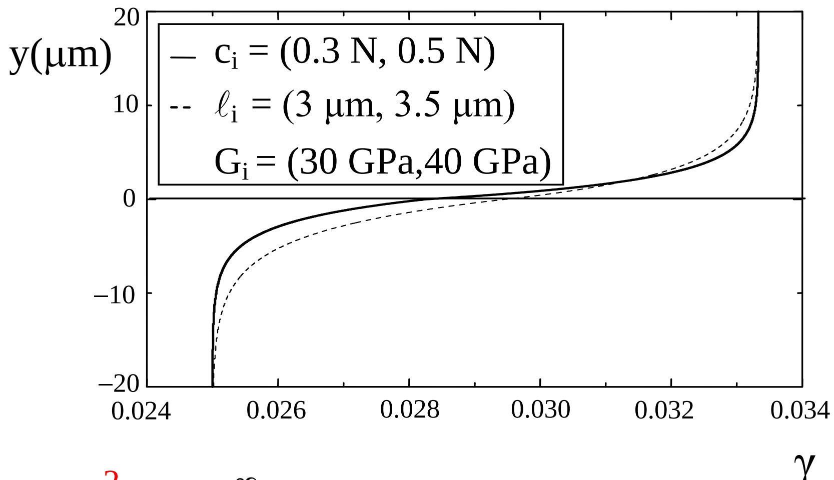
spheres

Micelle Structures

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:*** $\kappa_i = G_i \gamma$; $\tau_I = G_I \gamma_I$

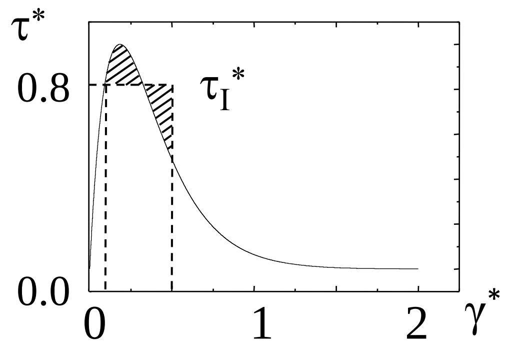
- *Aifantis (1984)* $\begin{cases} \gamma_1 = \gamma_2 \\ \partial\gamma_1 = \partial\gamma_2 \big|_{y=0} \end{cases} \Rightarrow G_I = \dfrac{G_1 G_2 \left(\sqrt{G_1/c_1} + \sqrt{G_2/c_2}\right)}{G_1\sqrt{G_2/c_2} + G_2\sqrt{G_1/c_1}}$

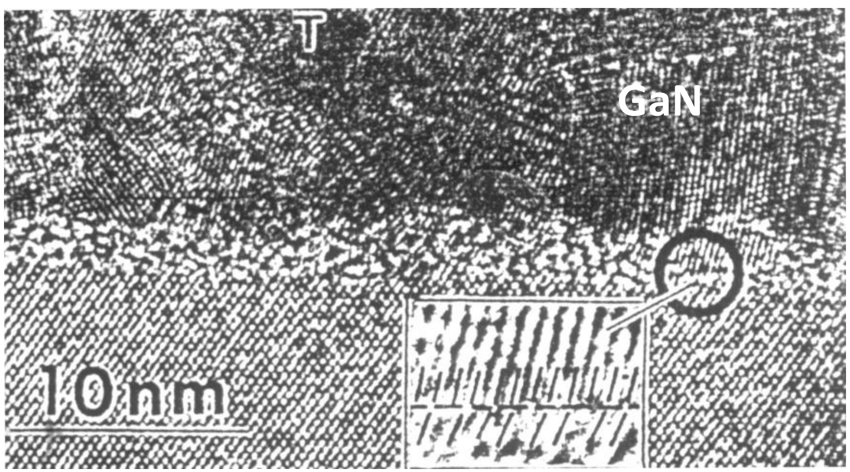
- *Fleck-H (1994)* $\begin{cases} \gamma_1 = \gamma_2 \\ \ell_1\partial\gamma_1 = \ell_2\partial\gamma_2 \big|_{y=0} \end{cases} \Rightarrow G_I = \dfrac{G_1 G_2 \left(\sqrt{G_1 c_1} + \sqrt{G_2 c_2}\right)}{G_1\sqrt{G_2 c_2} + G_2\sqrt{G_1 c_1}}$

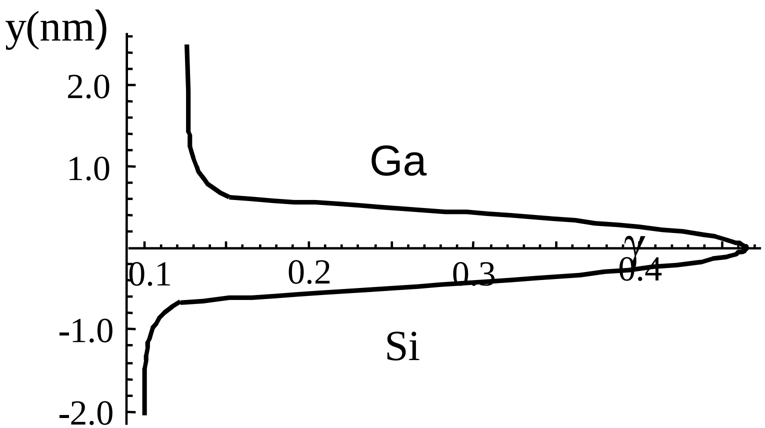
- ***Elastic Bimaterial / Inelastic Interface:*** $\kappa_i = G_i \gamma$; $\tau_I = G_I \gamma_I$

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

  - *Maxwell Rule:* $\int_{\gamma_\infty^*}^{\gamma_I^*} [\tau^*(\gamma^*) - \tau_I^*] d\gamma^* = 0$





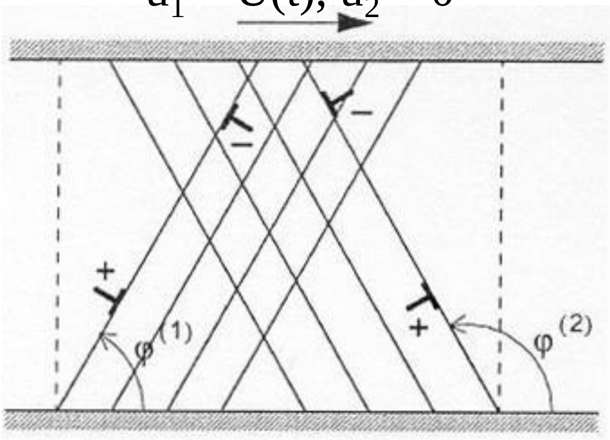


■ Plastic Boundary Layers

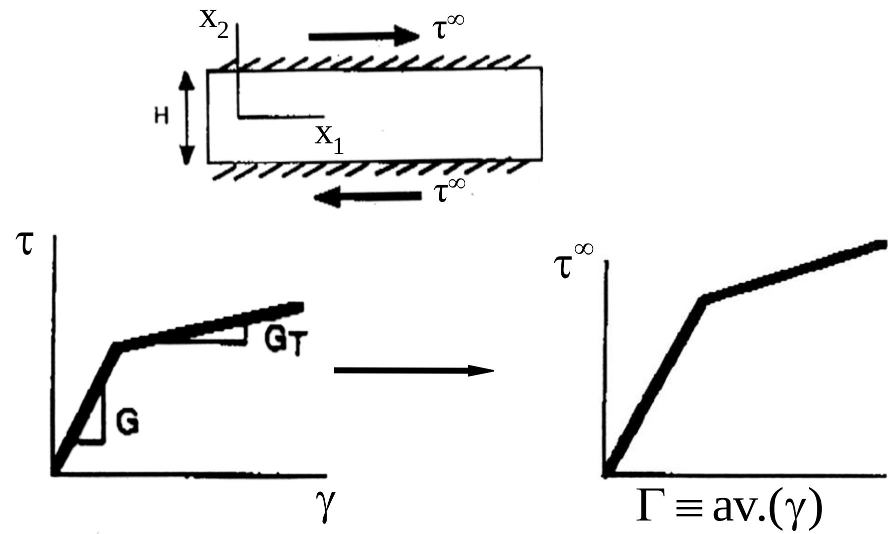
- ***Fleck/Van Der Giessen/Needleman (2000)***

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

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



$u_1 = 0,\ u_2 = 0$

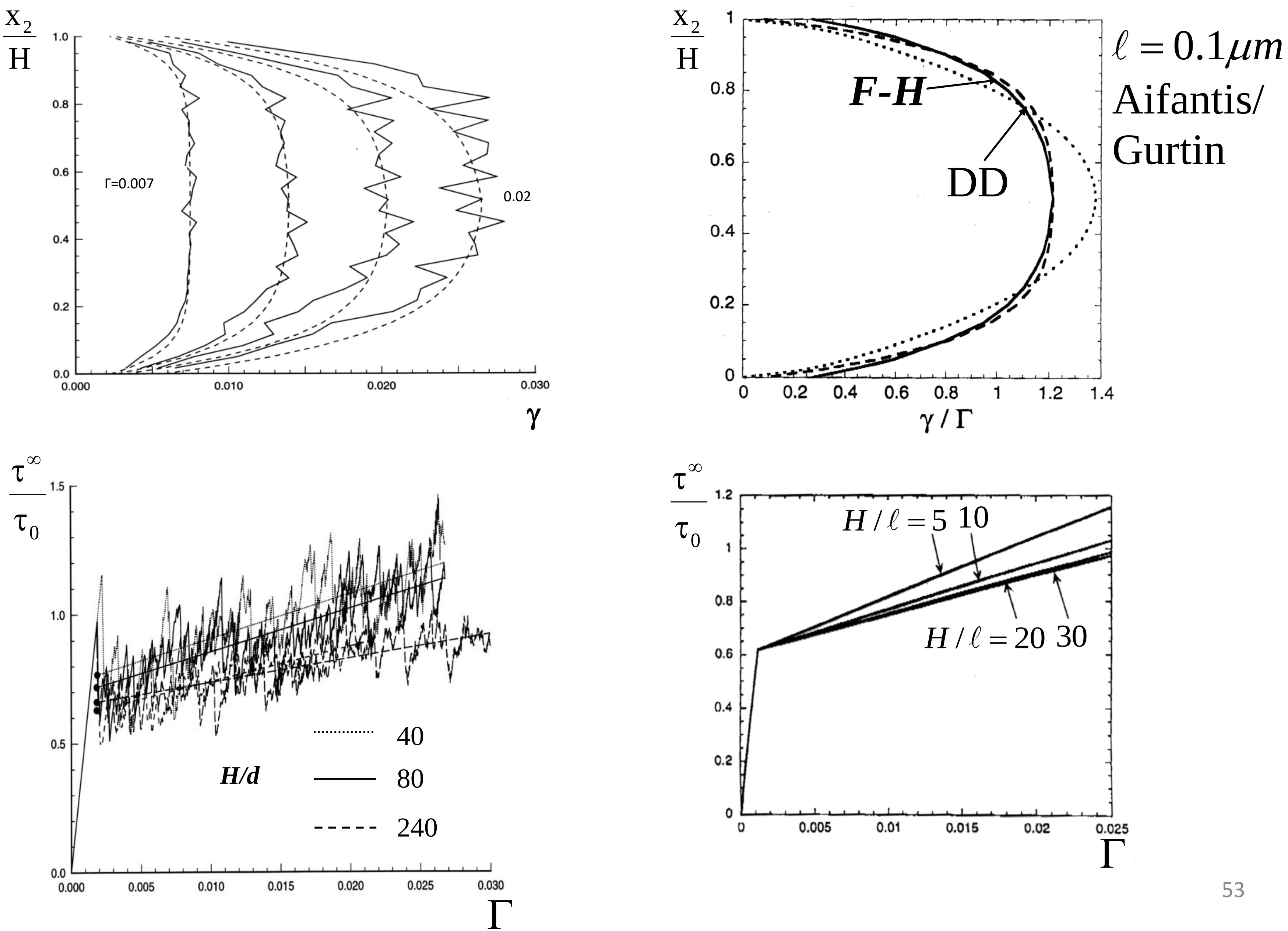


- ***Aifantis (1984) / Gurtin (2000)***

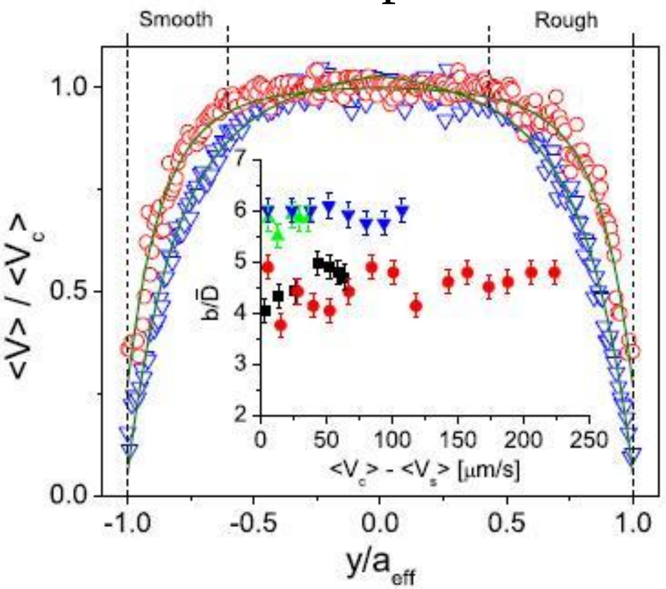
$$\tau = \tau_0 + G_T\gamma - G_T\ell^2\nabla^2\gamma = \tau^\infty \quad \Rightarrow \quad \gamma = \frac{\tau^\infty}{G} + \frac{\tau^\infty - \tau_0}{G_T}\left[1 - \frac{\cosh(x_2/\ell)}{\cosh(H/\ell)}\right]$$

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

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

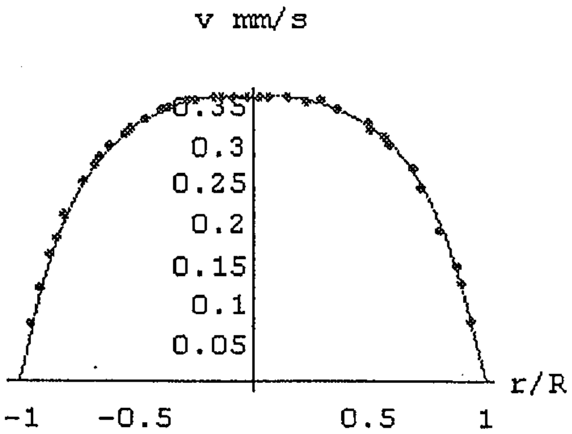


- **L. Isa, R. Besseling & W.C.K. Poon**, Shear Zones in the Capillary Flow of Colloidal Suspensions [*Phys. Rev. Lett.* **98**, 198305 (2007)]



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

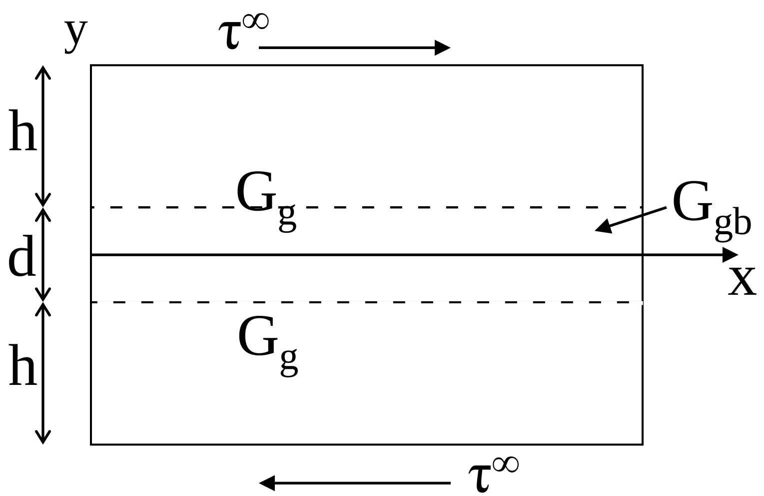
- **Silber et al / Goldsmith & Turitto Experiments**



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

■ Effective Moduli of Nanopolycrystals

- ***Idealized Unit Cell***



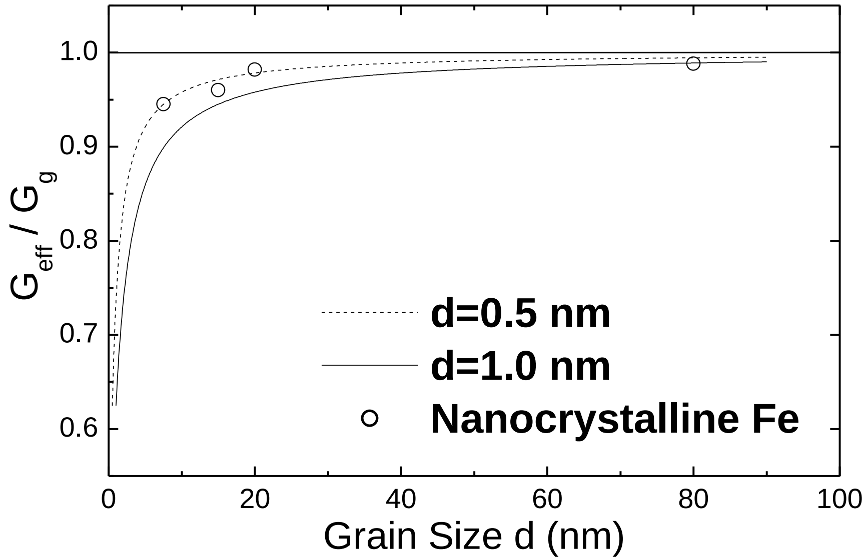
$$\text{Bc's}\quad \begin{cases} \partial_y \gamma_{gb} = 0 & , \; y=0 \\ \left.\begin{array}{l} \gamma_g = \gamma_{gb} \\ \partial_y \gamma_g = \partial_y \gamma_{gb} \end{array}\right\} & , \; |y| = d/2 \\ \gamma_g = \tau^\infty / G & , \; |y| = h + d/2 \end{cases}$$

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

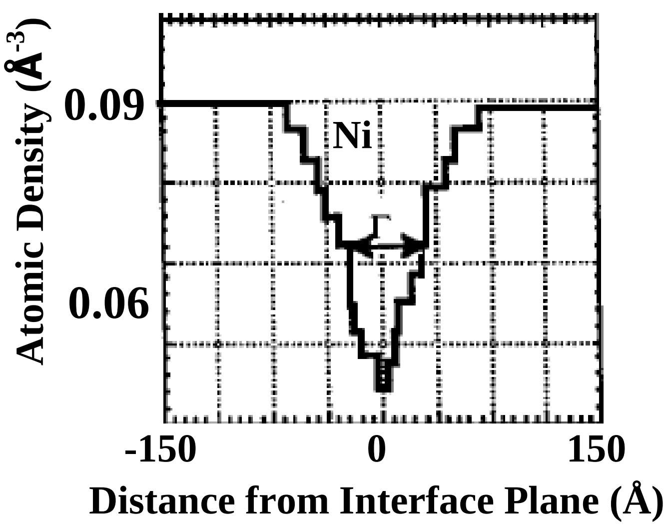
- ***Average Strain/Effective Modulus***

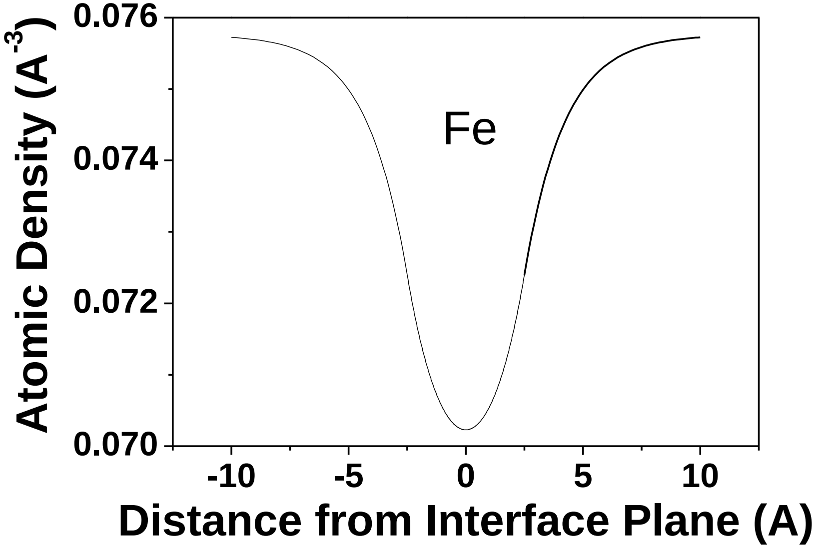
$$\Gamma = \frac{1}{(h+d/2)} \left(\int_0^{d/2} \gamma_{gb} dy + \int_0^{h+d/2} \gamma_g dy \right), \quad G_{eff} = \tau^\infty / \Gamma$$

- ***Size Dependence / Experiments***



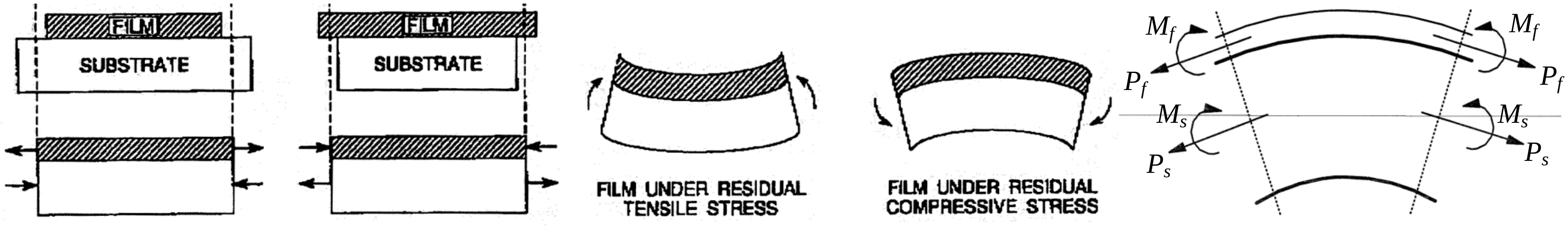
- ***Observations***





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

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

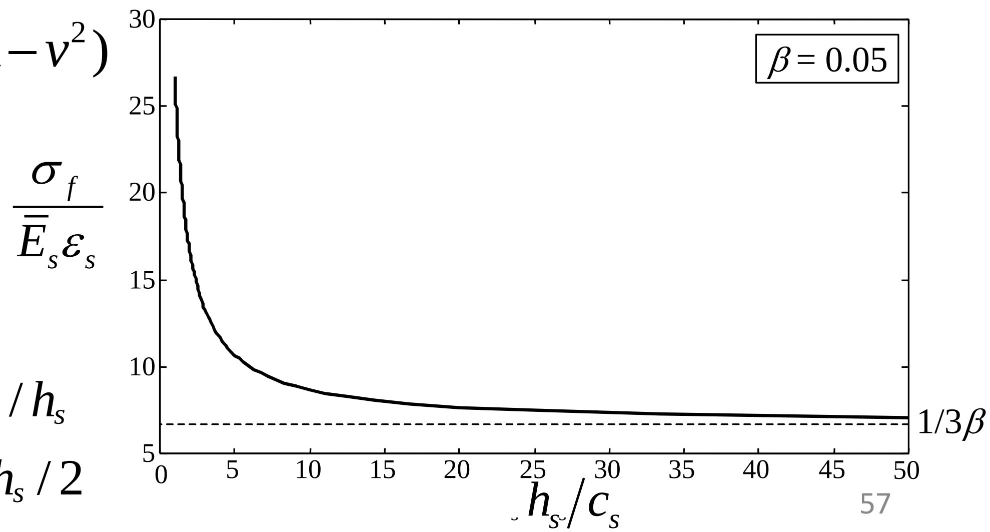
Gradient Elasticity:

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

Modified Stoney Formula:

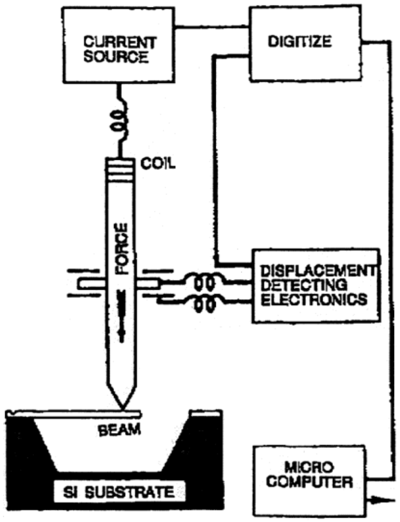
$$\therefore\ \sigma_f = \frac{P_f}{wh_f} = \kappa\frac{\bar{E}_s h_s^2}{6h_f}\left(1 + \frac{3c_s}{h_s}\right)$$

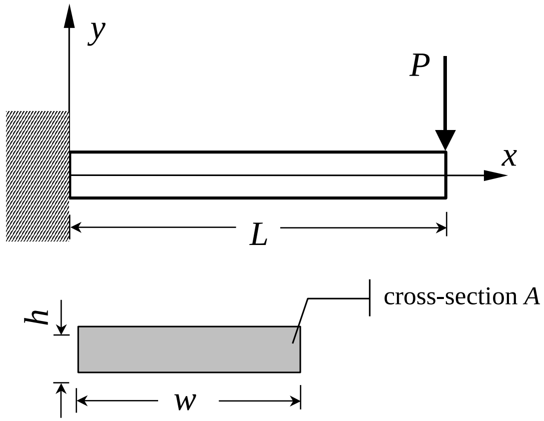
$$\Rightarrow\ \frac{\sigma_f}{\bar{E}_s\varepsilon_s} = \frac{1}{3\beta}\left[1 + 3\left(\frac{h_s}{c_s}\right)^{-1}\right] \;;\; \begin{cases}\beta = h_f/h_s \\ \varepsilon_s = \kappa h_s/2\end{cases}$$



■ Bending of Cantilever Microbeams

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





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

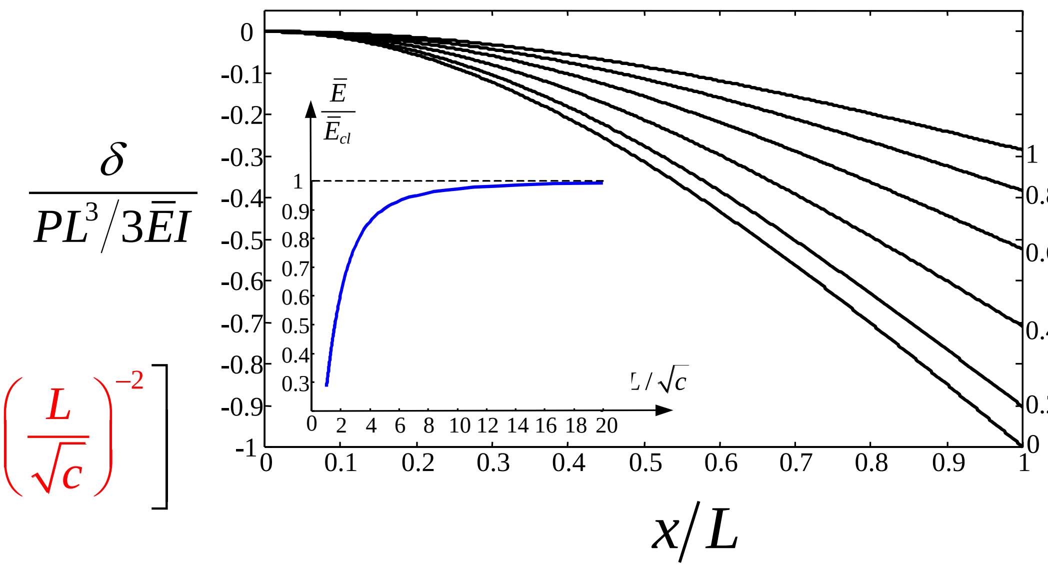
Axial Strain: $\varepsilon_{xx} = \kappa y; \ \kappa = \dfrac{d^2\delta}{dx^2}$

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

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

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

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



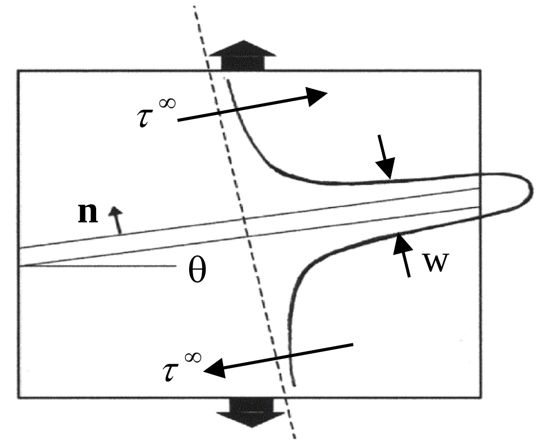
LOCALIZATION
SHEAR BANDS AND NECKS

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

- ***Constitutive Eq.***

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

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

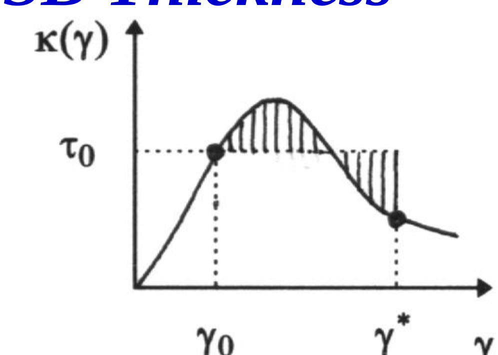


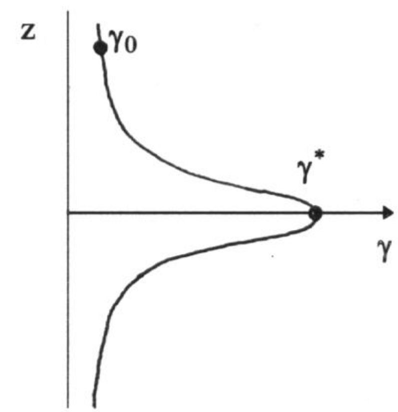
- ***Linear Stability / SB Orientation***

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

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

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



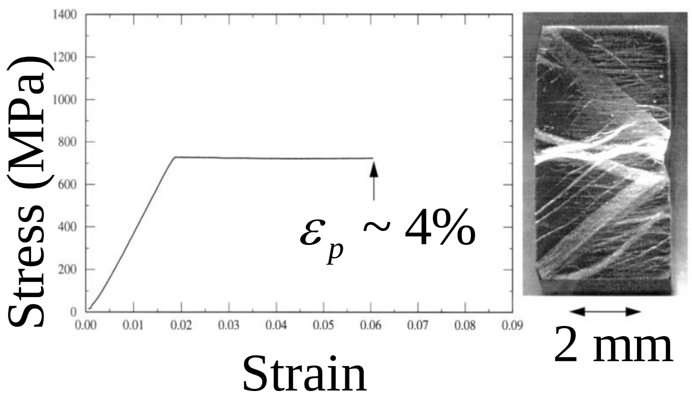


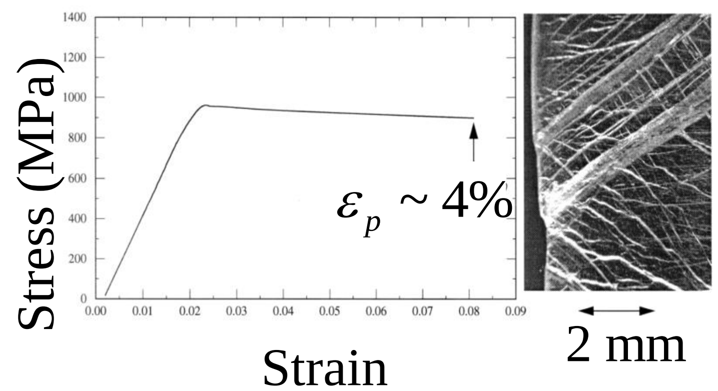
■ Bulk Nanostructured Fe – 10% Cu Polycrystals

- Compression tests

d ~1370 nm, σ_y ~750 Mpa
angle ~ 49^0

d ~540 nm, σ_y ~960 MPa
angle ~ 49^0





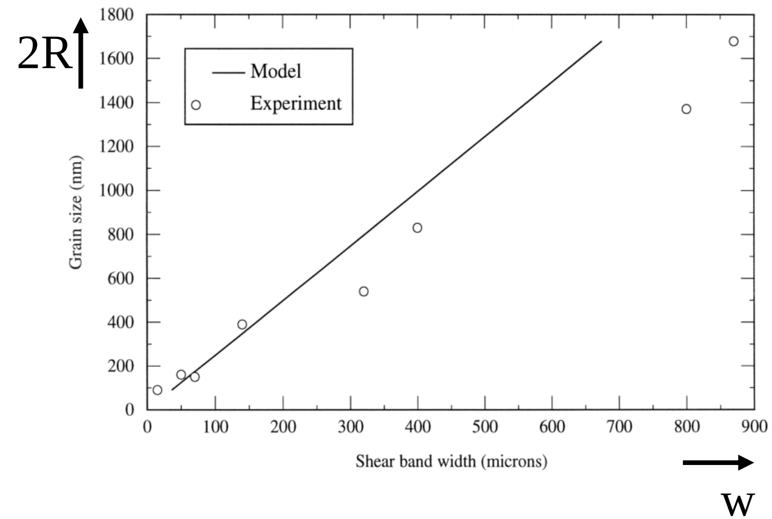
- Shear band width analysis

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

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

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

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



■ Statistical / Random Aspects

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

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

(σ, ε) ... random microscopic fields

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

- ***Taylor expansion + Averaging***

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

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

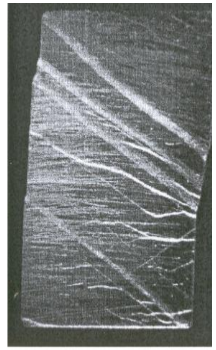
$\Lambda(r)$ ... correlation function ; h ... hardening coefficient

■ Bulk Nanostructured Fe-10%Cu Polycrystals

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

$d = 150\text{nm}$

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



$d = 300\text{nm}$

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

$d = 830\text{nm}$

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

- ***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*

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

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

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

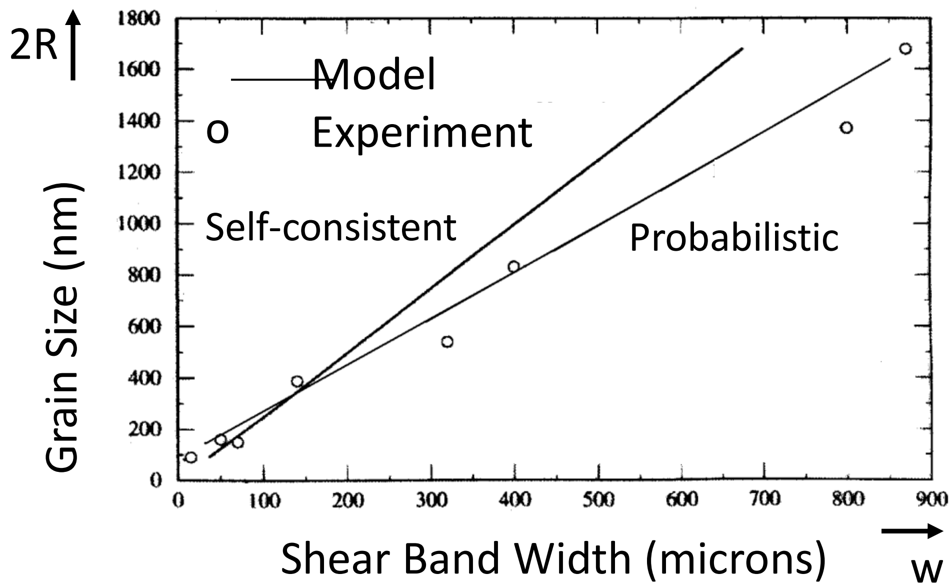
- *Shear band width analysis*

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

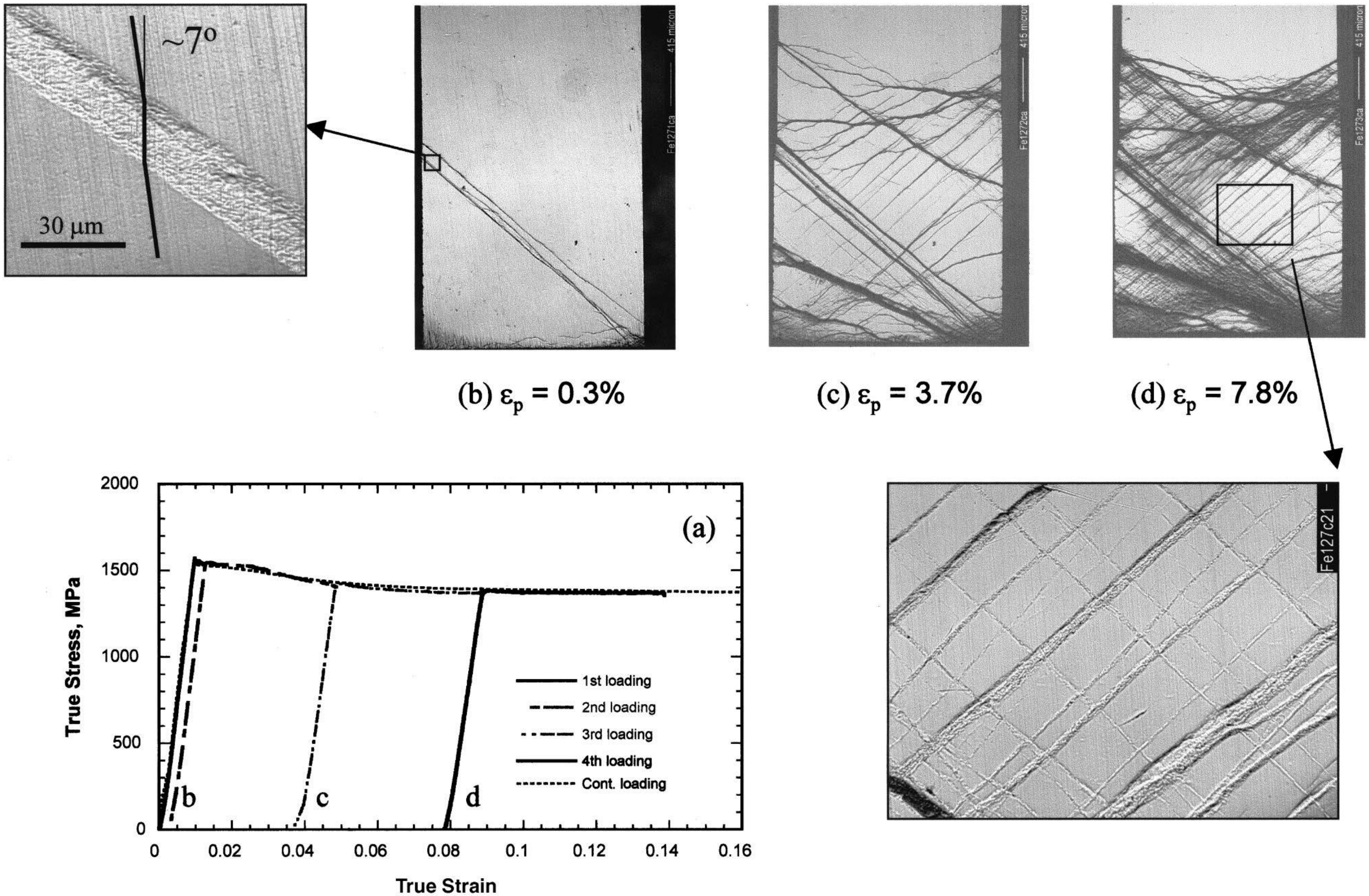
- *Calibration for 300nm grain size*

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

- *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%).

▪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

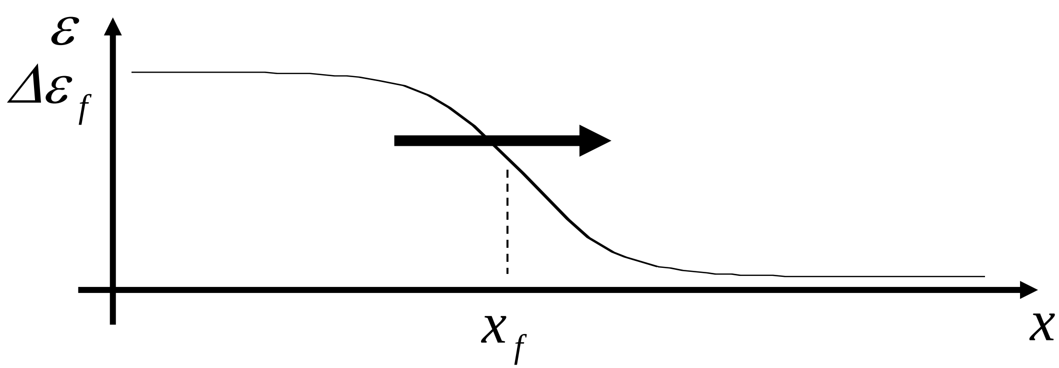
$$\therefore \quad \sigma_0 = \kappa(\varepsilon) + \delta\, f(\varepsilon, x) - c\frac{\partial^2 \varepsilon}{\partial x^2} \qquad (c = 1)$$

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

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

$$\Rightarrow\begin{cases}\dfrac{\varepsilon_{,x}^{2}}{2}+\sigma_{0}\,\varepsilon-V\left(\varepsilon\right)=0; \qquad V\left(\varepsilon\right)=\displaystyle\int_{-\infty}^{\infty}\kappa\left(\varepsilon\right)\varepsilon_{,x}dx \\ \delta\sigma_{1}=\dfrac{\delta}{\Delta\varepsilon_{f}}\displaystyle\int_{-\infty}^{\infty} f\left(\varepsilon,x\right)\varepsilon_{,x'}dx'\end{cases}$$

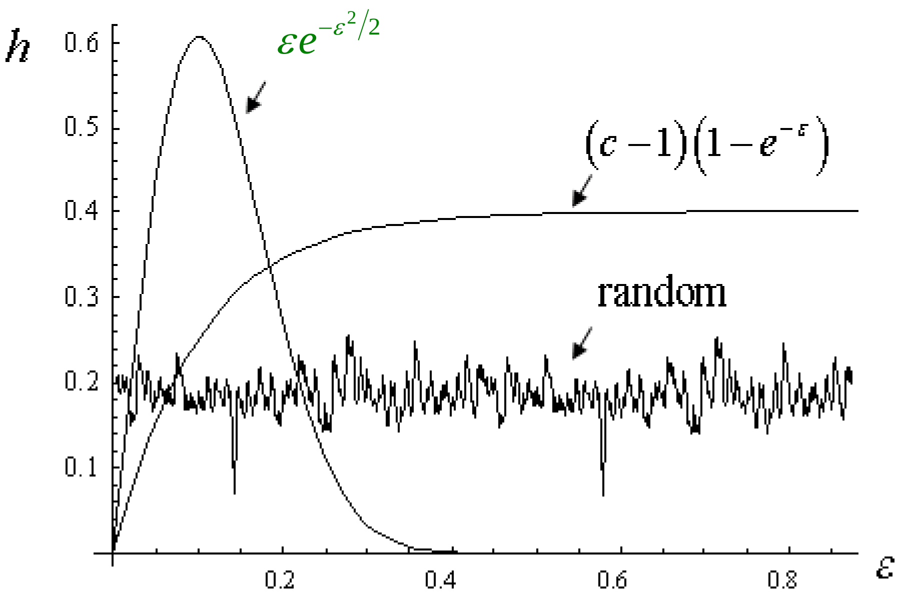
– *Front "locus" shifts along specimen* $\varepsilon=\varepsilon(x-x_{f})$



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

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

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



- ***Implementation***

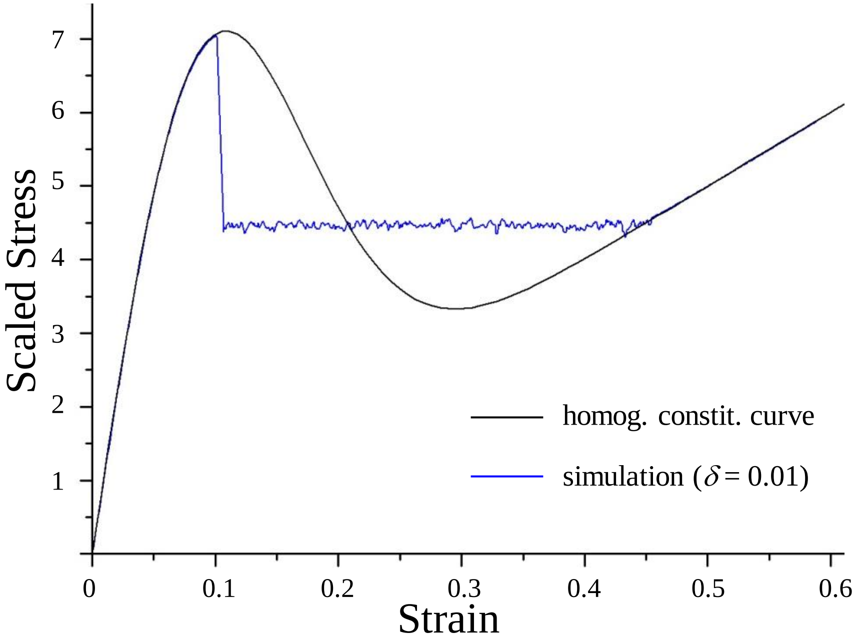
$$\kappa(\varepsilon)=\varepsilon\, e^{-\varepsilon^2/2}+\theta\varepsilon\,; \qquad \theta=\text{const.} \ \ldots\ \text{linear hardening}$$

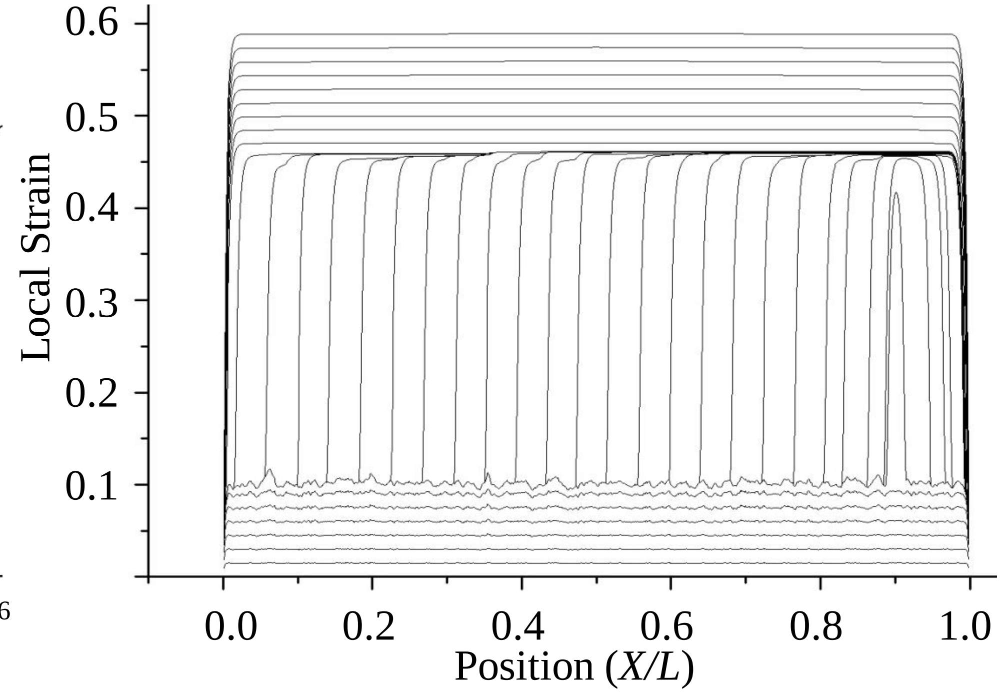
$$V(\varepsilon)=e^{-\varepsilon^2/2}-\frac{\theta}{2}\varepsilon^2$$

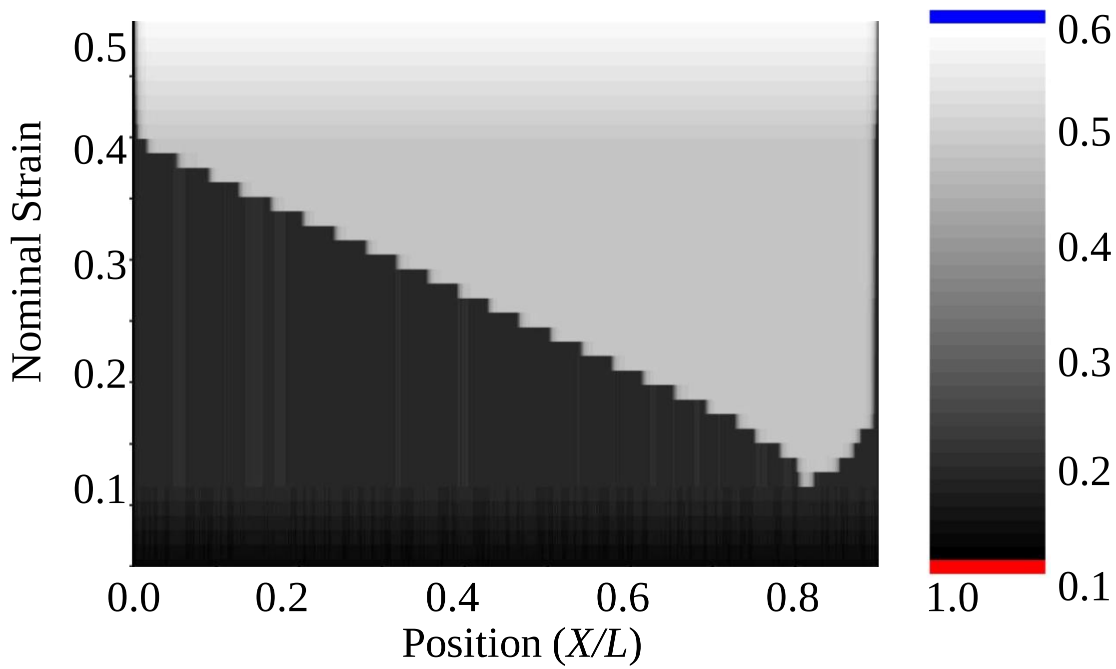
$$f(\varepsilon,x)=\delta\,\varepsilon\, e^{-\varepsilon^2/2}\,g(x)$$

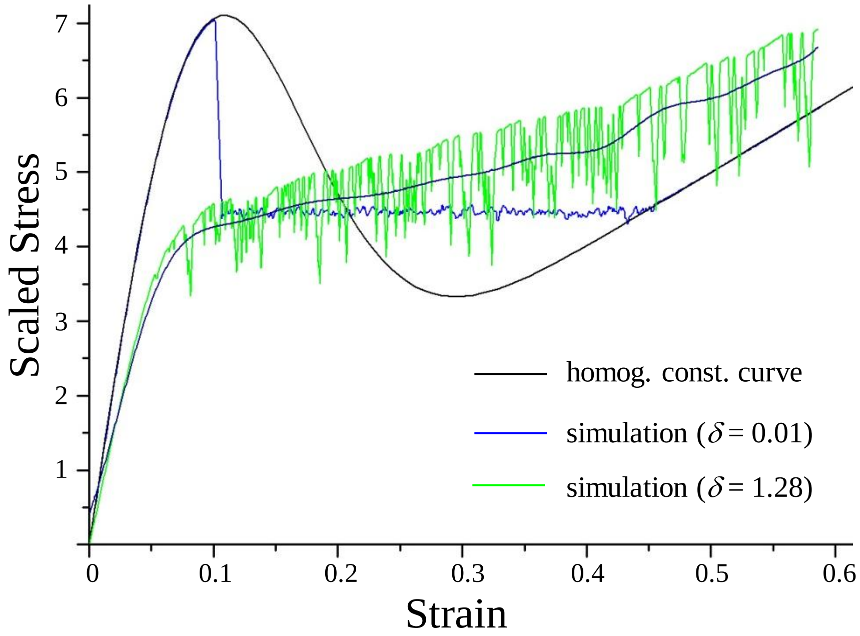
$$x-x_0=\int_{\varepsilon_{-\infty}}^{\varepsilon}\frac{d\varepsilon}{\sqrt{-2\left[e^{-\varepsilon^2/2}-\frac{\theta}{2}\varepsilon^2+\sigma_0\left(\varepsilon-\varepsilon_{-\infty}\right)\right]-V\left(\varepsilon-\varepsilon_{-\infty}\right)}}$$

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

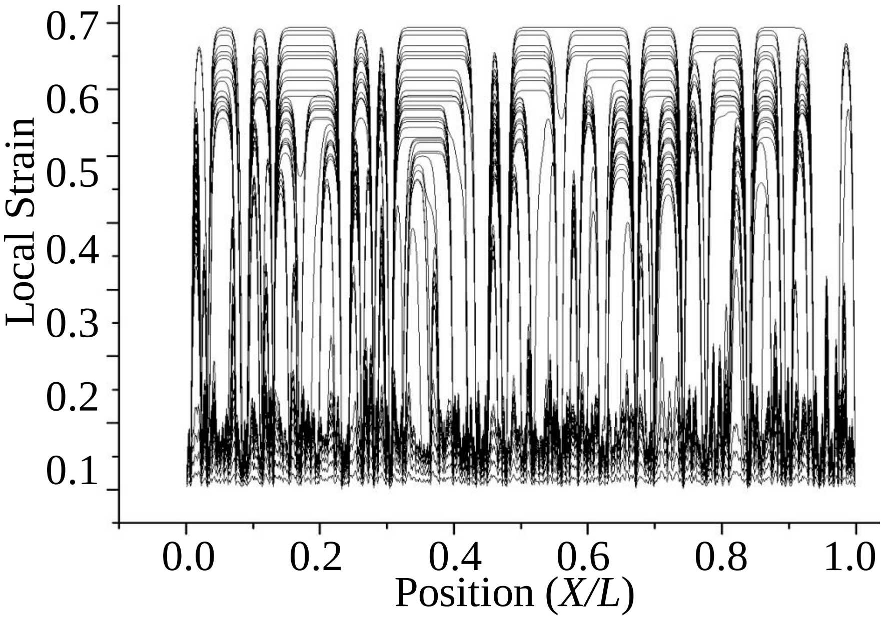

Scaled Stress
Strain
homog. constit. curve
simulation (δ = 0.01)
0
0.1
0.2
0.3
0.4
0.5
0.6
1
2
3
4
5
6
7


Local Strain
Position (*X/L*)
0.0
0.2
0.4
0.6
0.8
1.0
0.1
0.2
0.3
0.4
0.5
0.6

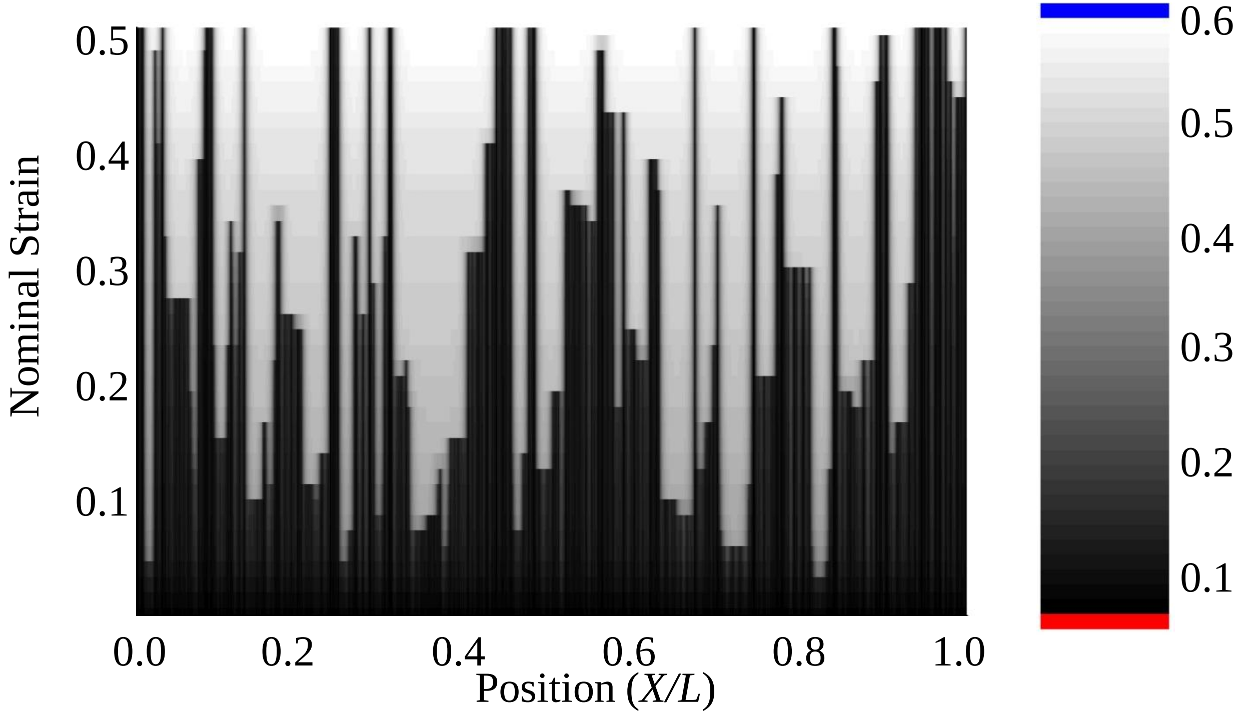

Nominal Strain
Position (*X/L*)
0.0
0.2
0.4
0.6
0.8
1.0
0.1
0.2
0.3
0.4
0.5
0.6



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



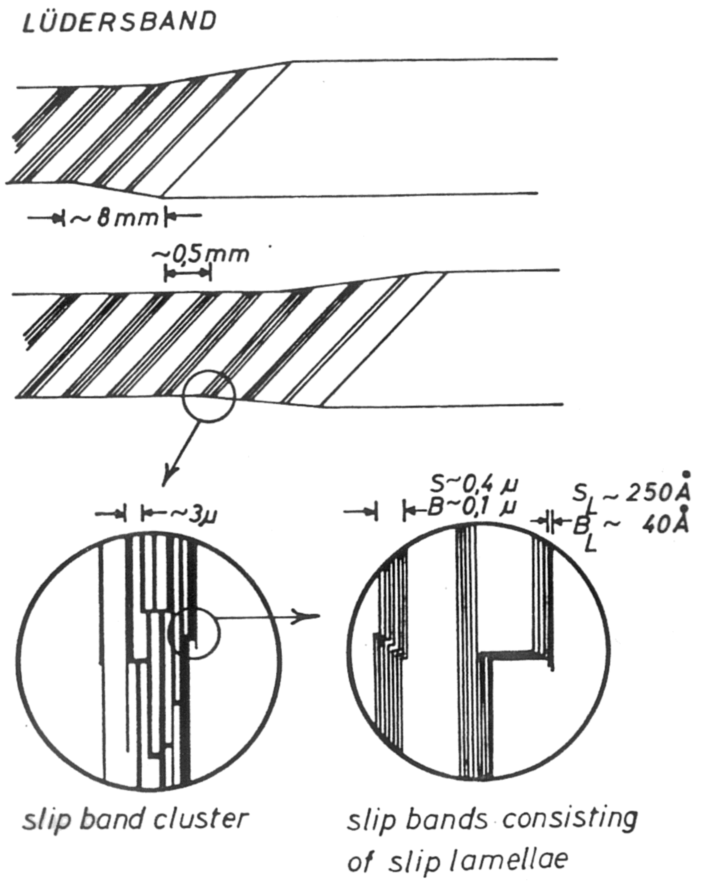
Local Strain
Position (X/L)

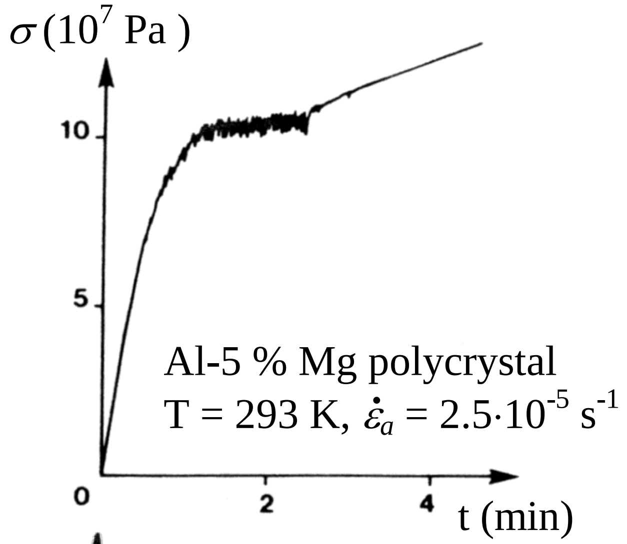


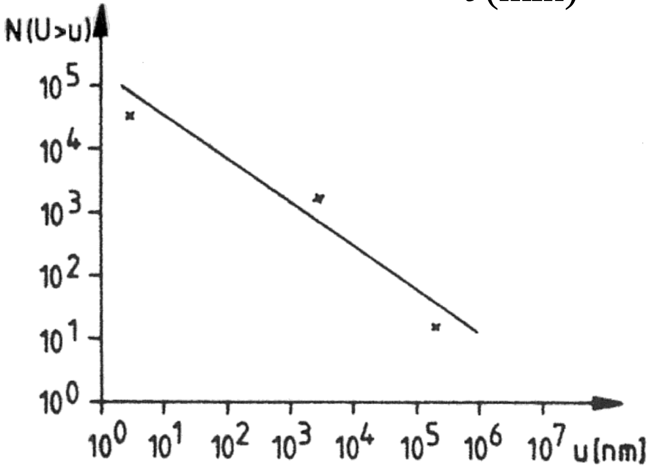
Nominal Strain
Position (X/L)

MORE ON TRAVELLING DEFORMATION BANDS

- **Lüders bands (LB)**

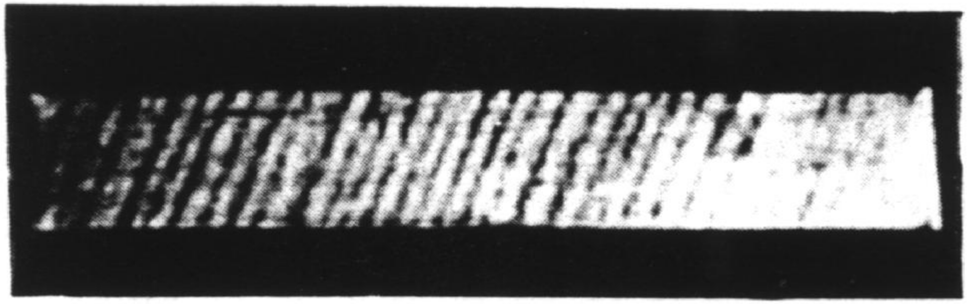


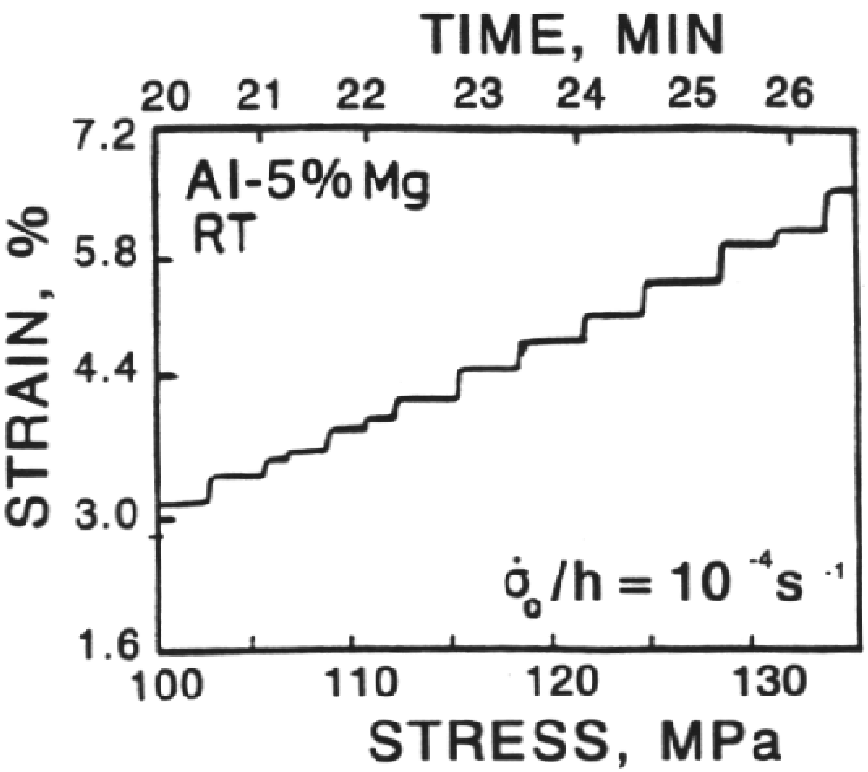


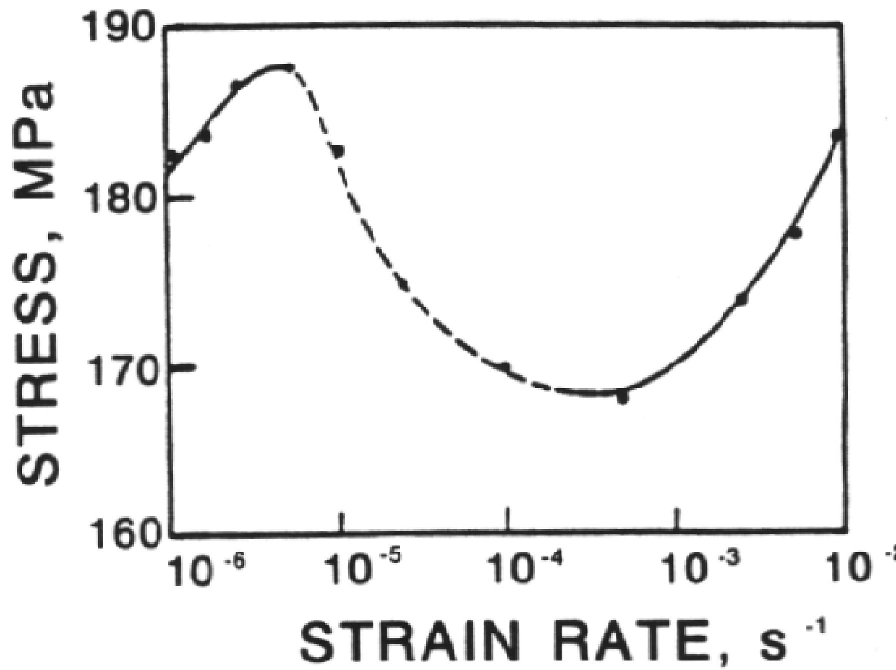


■ Portevin-Le Chatelier bands (PLC)

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







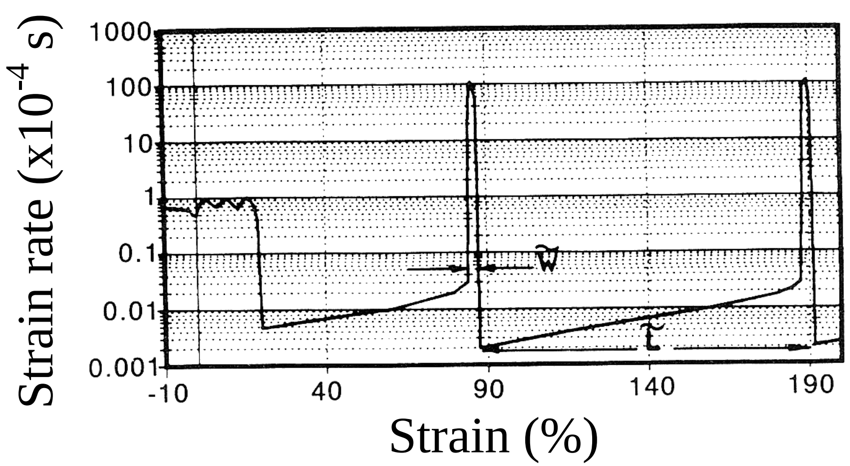
- ***PLC (Preliminary) Modeling***

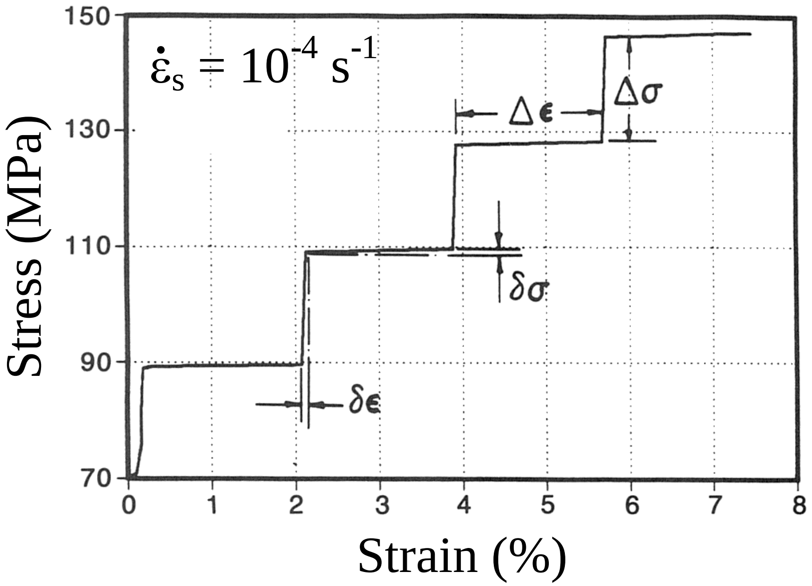
$$\sigma = h\varepsilon + f(\dot{\varepsilon}) + c\varepsilon_{xx}$$

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

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

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





■ A Note on the Origin of Gradients

- ***Self - Consistent Approximation***

  - *Simple Shear*

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

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

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

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

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

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

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

- *Various Models for α*

- Lin 1954

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

- Kroner (1958) / Budiansky – Wu (1962)

$$\alpha = 1$$

- Berveiller – Zaoui 1979
  (Secant Model)

$$\alpha = \frac{1}{1 + (\mu / 2H)}, \quad H = \frac{\bar{\tau}}{\bar{\gamma}}$$

- Hill (1965) / Hutchinson (1970)
  (Tangent Model)

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

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

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

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

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

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

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

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

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

NANOMATERIALS & NANOMECHANICS

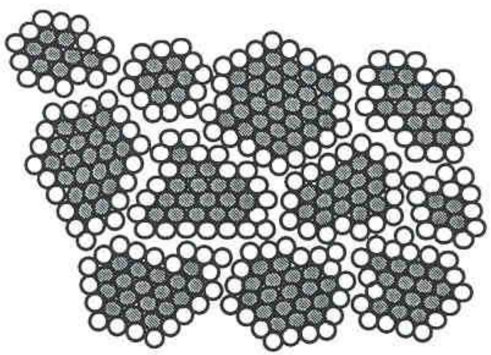
Nanopolycrystals: Observations/Metal Physics Aspects

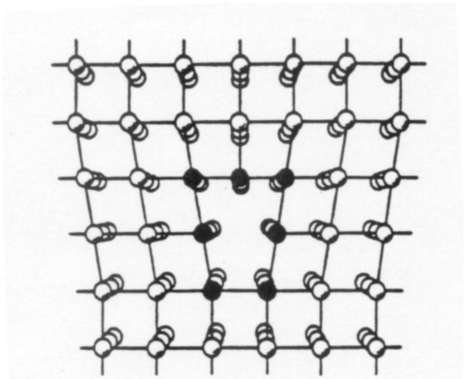
■ Grain Configuration at the Nanoscale

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

Grain d

1-50 nm



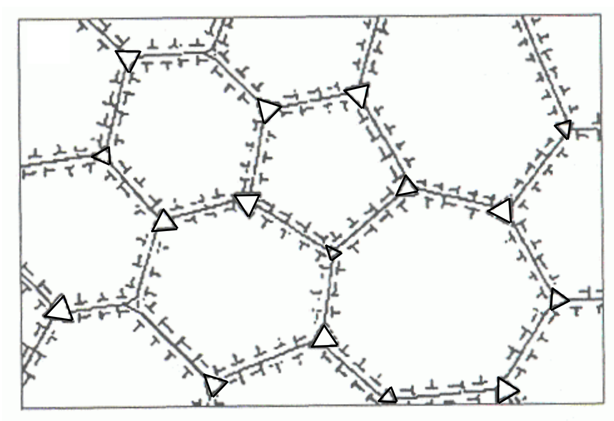


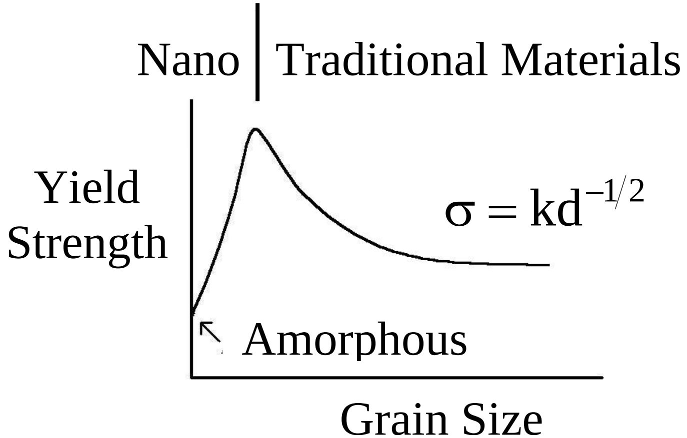
Core r_0

~1 nm

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

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





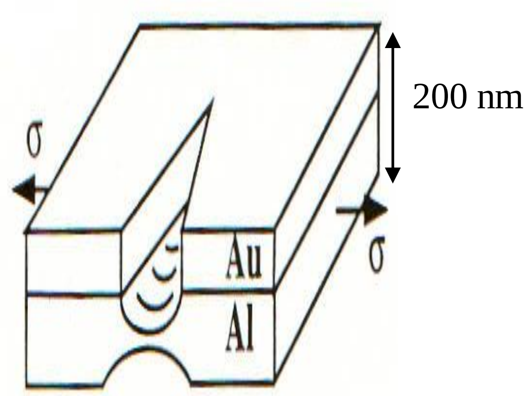
Plasticity Mechanisms ?

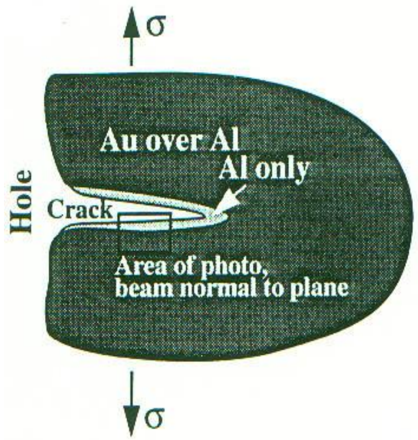
Inverse Hall-Petch Relation ?

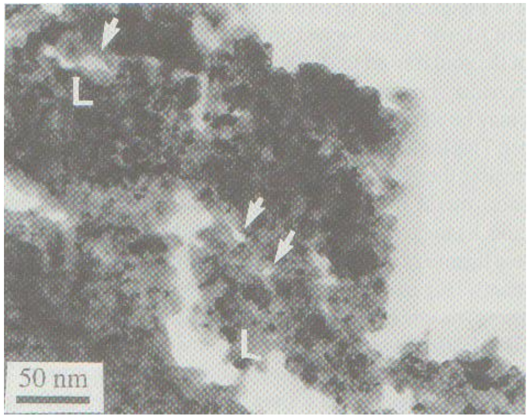
Improved/Engineered Properties: Examples

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.



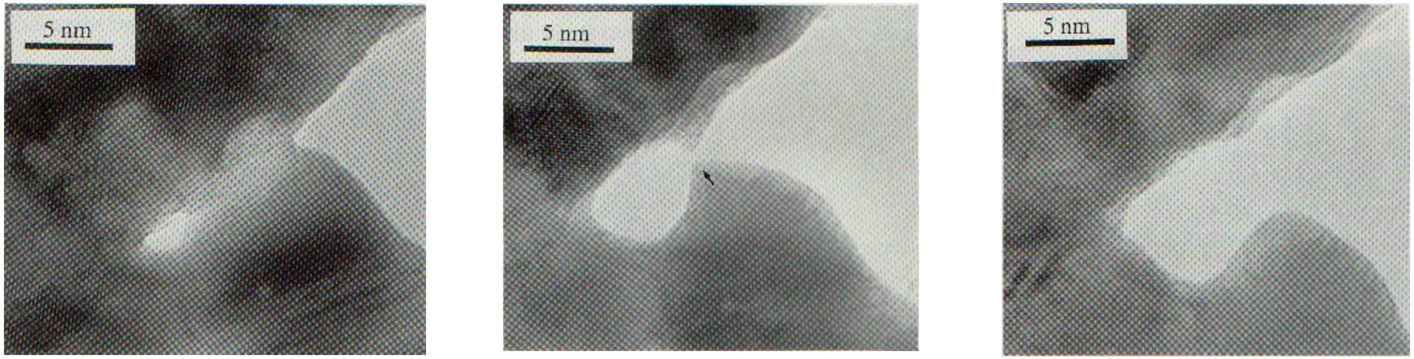




Schematics

8 nm Au on Al: Nanovoid Coalescense

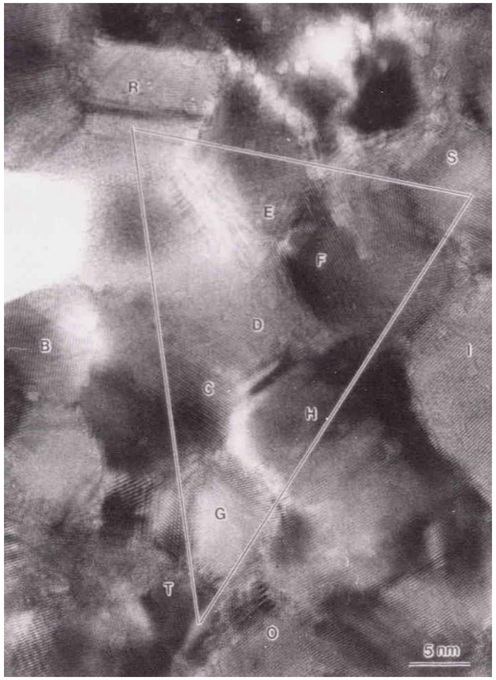
- ***Nanovoid Nucleation***



8 nm Au on C: Nanocrack growth via nanopore formation

25 nm Au on C: Periodic Crack profiles and bifurcation

• *Grain Rotation / Dislocation Emergence*

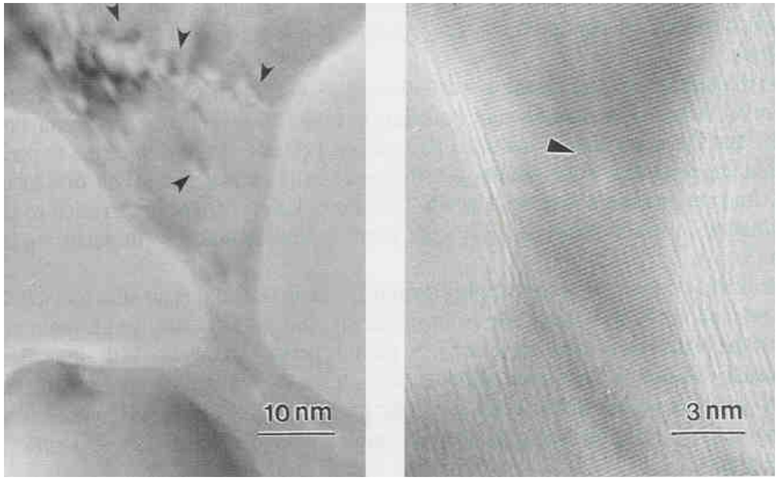


10 nm Au: 6-15 degrees relative grain rotation

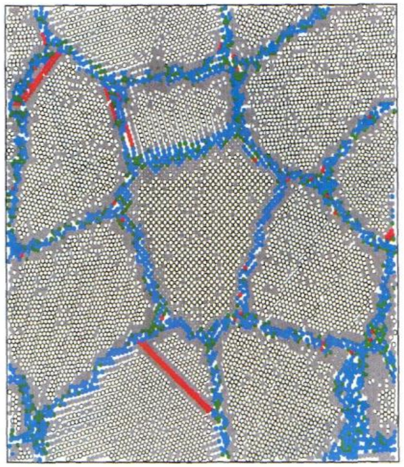
Elementary Rosette Analysis

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



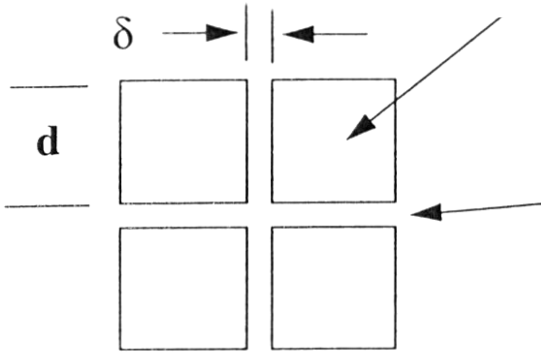
100 nm Au film



~12 nm Ni nanopolycrystals

■ Initial Simple – Minded Models

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



"Bulk" Phase, Hall – Petch relation

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

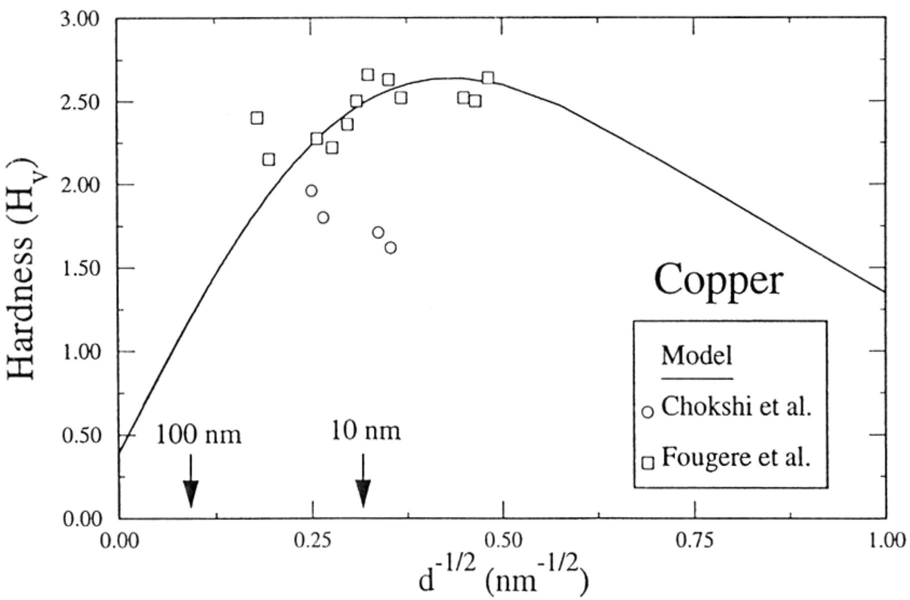
"Boundary" Phase, Constant strength related to amorphous material or grain boundary sliding (σ_{GB})

- 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

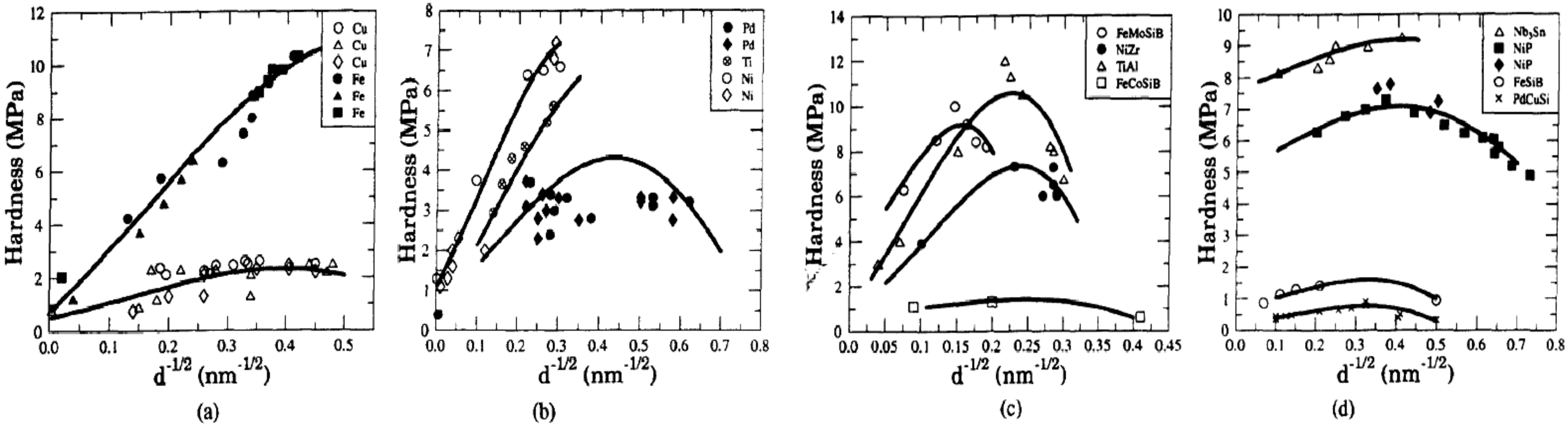
•Continuum elasticity Model has also been developed, which shows the importance of gradients in elasticity of nanophase materials

■ Improved Inverse Hall-Petch Relation

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

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

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

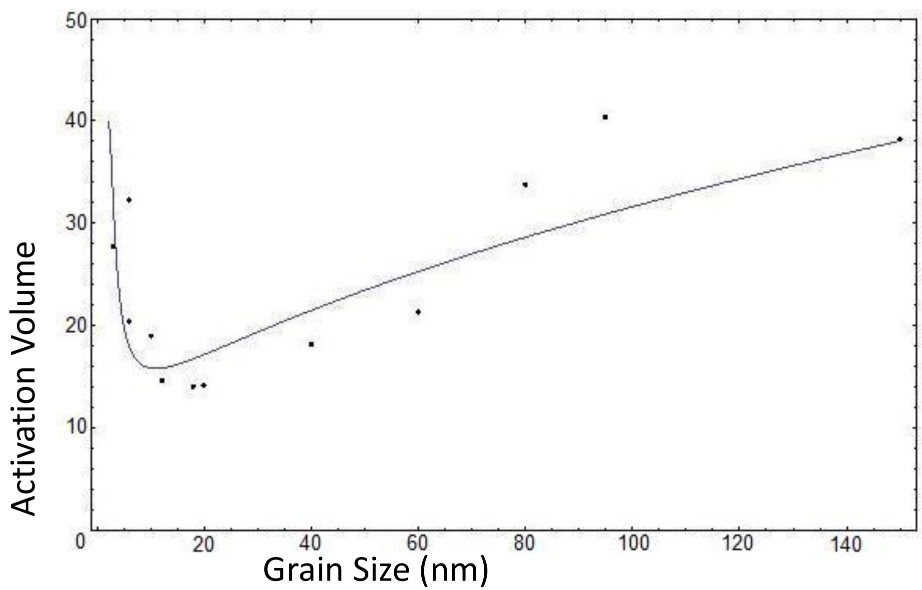


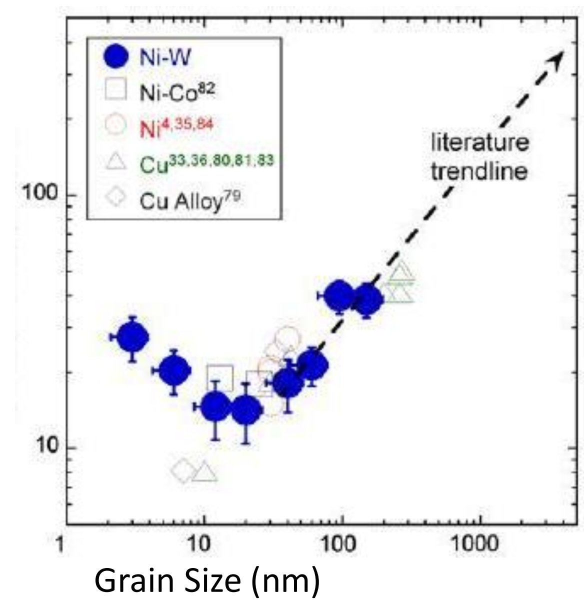
(a) & (b): nanocrystalline metals; (c) & (d): intermetallics

■ Activation Volume (υ)

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

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





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

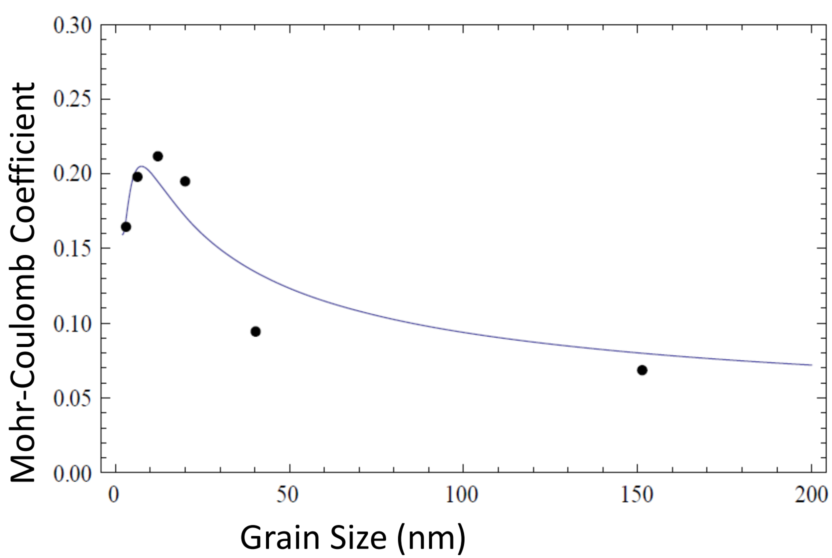
■ Pressure – Sensitivity Parameter (α)

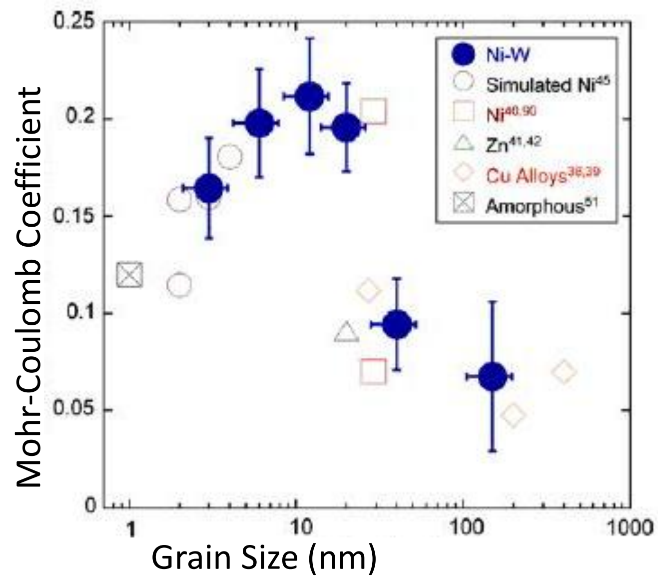
- $$\sqrt{J} + \alpha p - \kappa = 0$$

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

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

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



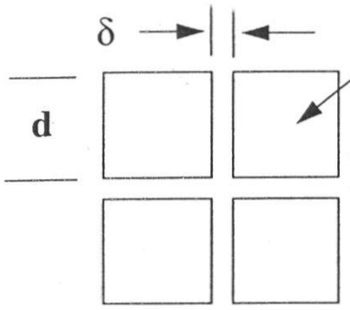


$$\alpha_g^0 = 0.02, \quad \alpha_{gb} = 0.16, \quad \delta = 2\,nm, \quad k_g = 0.7\sqrt{nm}$$

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***

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

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

- ***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

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

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

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***

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

Gradela: A Scale Invariance Argument

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

- Strain:

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

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

$$\mathrm{e}\ldots \quad \text{atomic lattice chain strain}$$

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

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

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

- Stress:

$$\sigma = \hat{\sigma}(\mathbf{n},\boldsymbol{\nu};\ \mathrm{s})$$

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

$$\mathrm{s}\ldots \quad \text{atomic lattice chain stress};\quad (\mathrm{a,b})\ldots \quad \text{constants}$$

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

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

k ... lattice atomic chain elastic modulus

c ... gradient coefficient

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

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

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

■ Gradela Dynamics:Euler–Bernoulli Beam(EBB)

- ***Standard Relations***

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

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

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

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

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

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

l_s^2 ... static internal length

l_d^2 ... dynamic internal length

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

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

- ***Wave Solution***

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

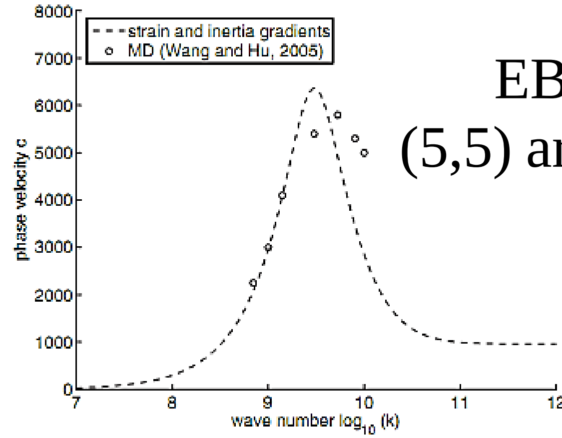
- ***Comparison with MD***

$\hat{u}$ amplitude

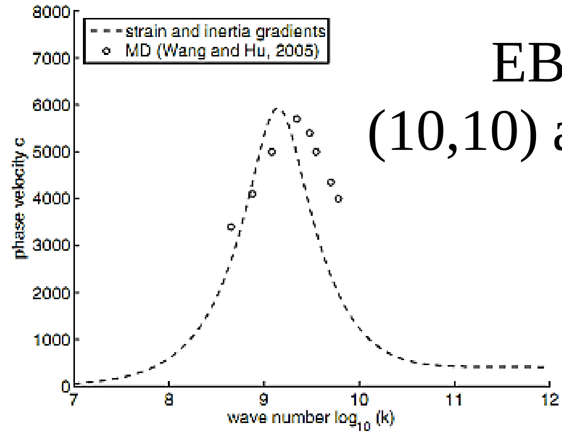
k wave number

c phase velocity

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



EBB theory
(5,5) armchair CNT



EBB theory
(10,10) armchair CNT

■ Gradela Dislocation Nanomechanics

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

- ***Screw Dislocation :***

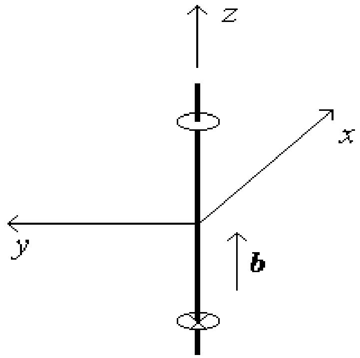
- Stress / Strain :

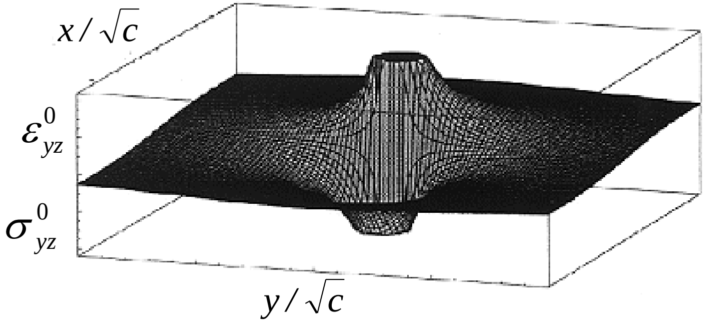
$$\begin{cases}\sigma_{xz}=\dfrac{\mu b_z}{4\pi}\left[-\dfrac{y}{r^2}+\dfrac{y}{r\sqrt{c}}K_1\left(r/\sqrt{c}\right)\right]; & \sigma_{yz}=\ldots\\ \varepsilon_{xz}=\dfrac{b_z}{4\pi}\left[-\dfrac{y}{r^2}+\dfrac{y}{r\sqrt{c}}K_1\left(r/\sqrt{c}\right)\right]; & \varepsilon_{yz}=\ldots\end{cases}$$

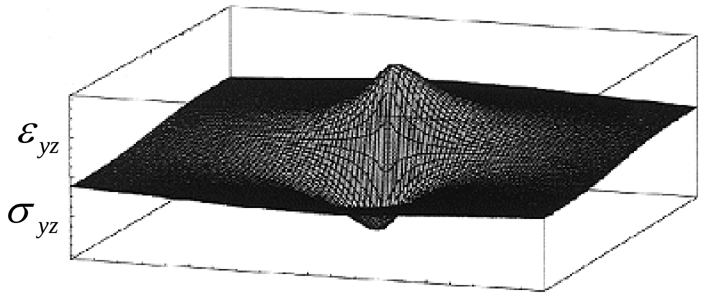
$$\therefore\quad \mathbf{r}\to 0 \;\Rightarrow\; \mathbf{K_1}\left(\mathbf{r}/\sqrt{\mathbf{c}}\right)\to\frac{\sqrt{\mathbf{c}}}{\mathbf{r}} \;\Rightarrow\; \left(\boldsymbol{\sigma}_{\mathbf{xz}},\boldsymbol{\varepsilon}_{\mathbf{yz}}\right)\to \mathbf{0}$$

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

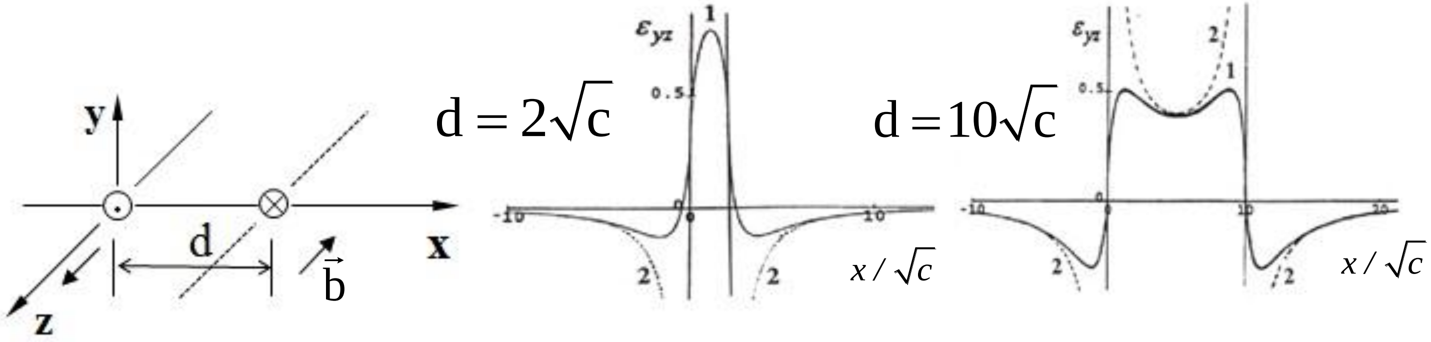
$$\therefore\quad \mathbf{r}\to 0 \;\Rightarrow\; \textbf{no need for ad hoc dislocation core } \mathbf{r_0}$$





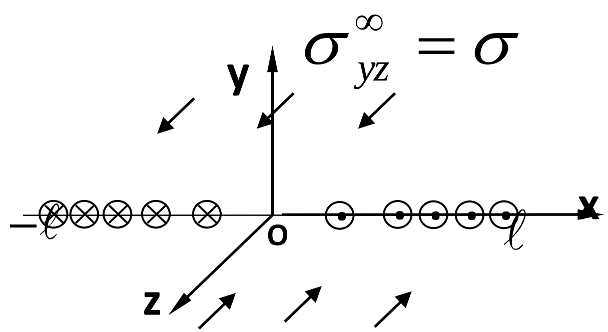


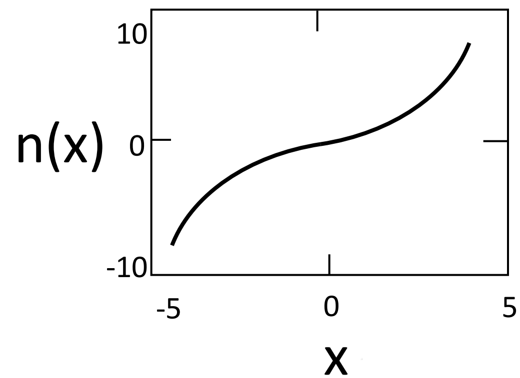
• *Dislocation Dipoles [insight to nucleation / annihilation]*

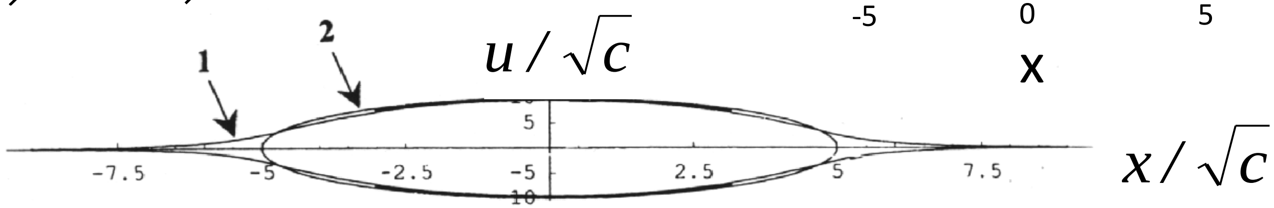


$\therefore \quad d \approx 10\sqrt{c}$.. *characteristic distance of “strong” interaction*

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





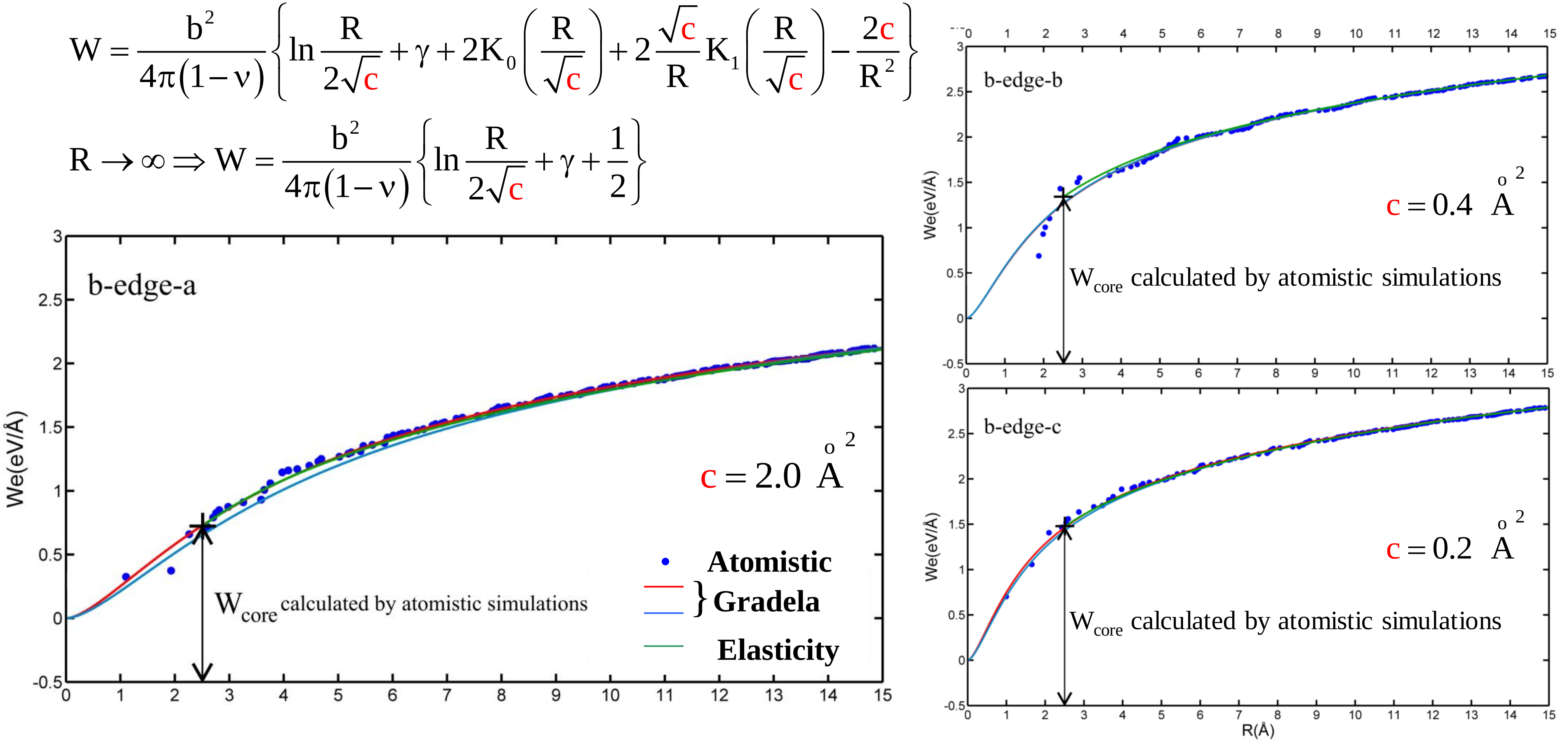


$\therefore$ *Barenblatt’s “smooth closure” condition*

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

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

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



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

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

- ***X-ray Line Profile Analysis***

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

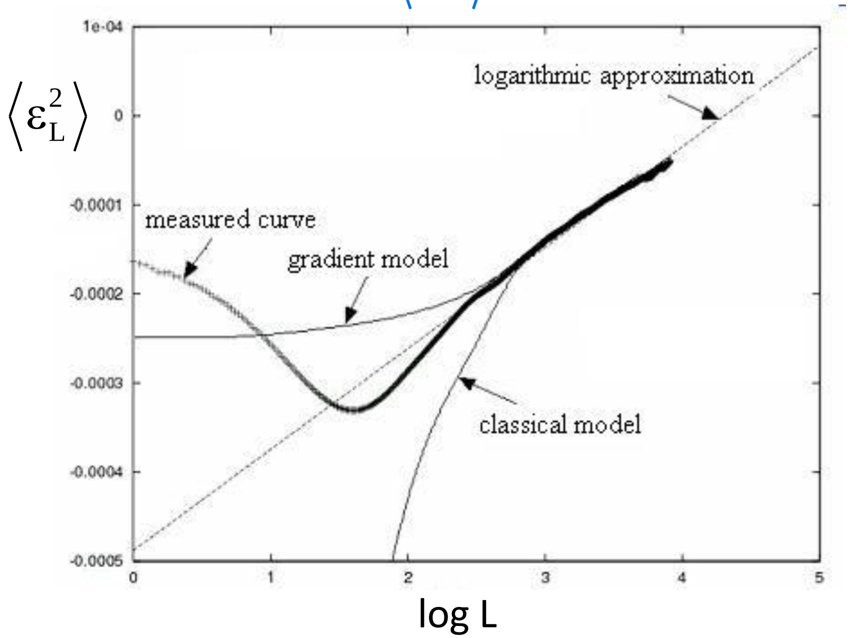
According to Gradela (e.g. ECA 2003) the ε_{xx} component of the strain tensor corresponding to an edge dislocation with Burgers vector $\mathbf{b} = b\,\mathbf{e_x}$ is

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

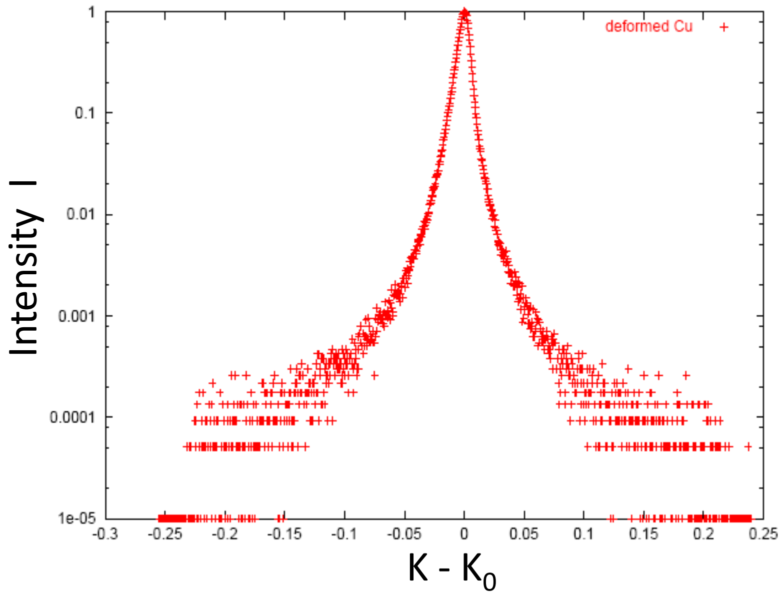
where

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

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

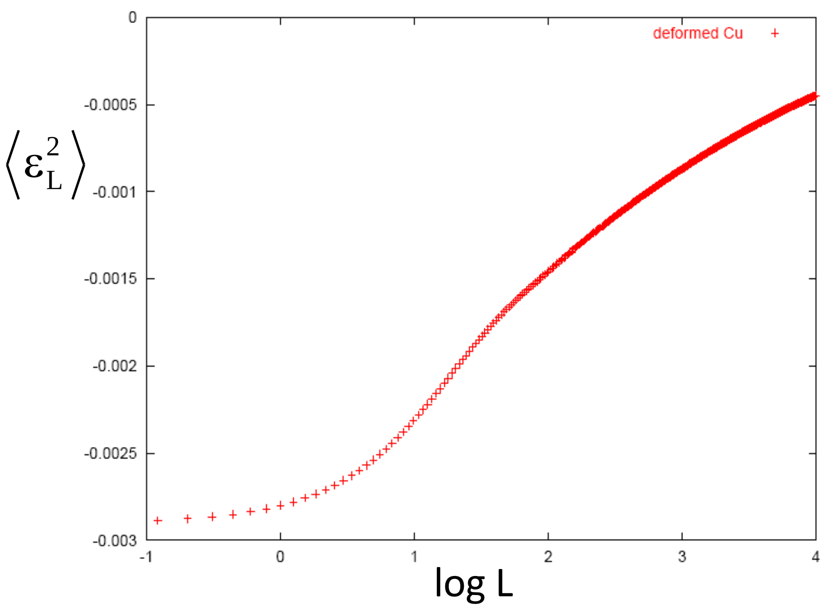


- *X-ray line profile for deformed Cu single crystal*



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 $L \rightarrow 0$

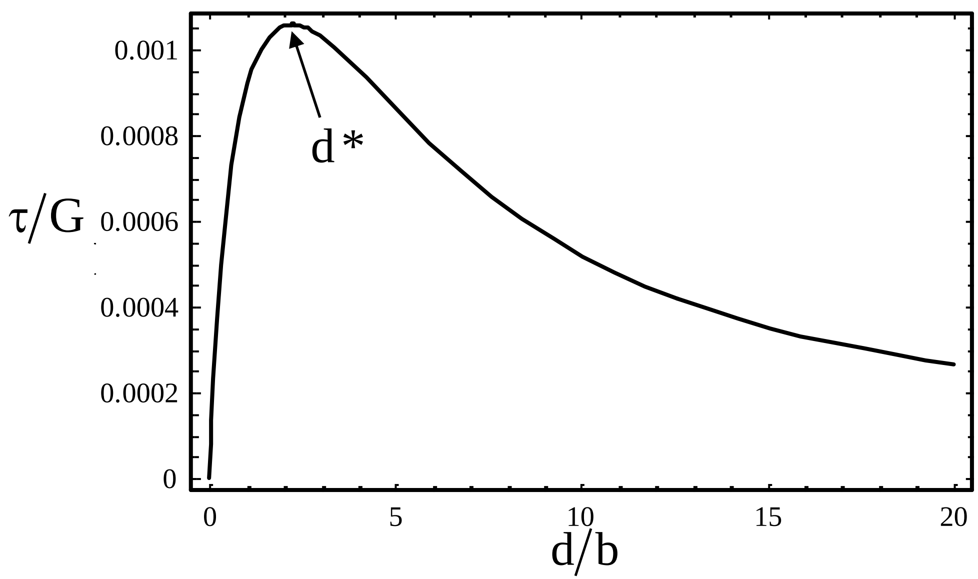
- ***Image Force – Inverse Hall Petch Behavior***

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

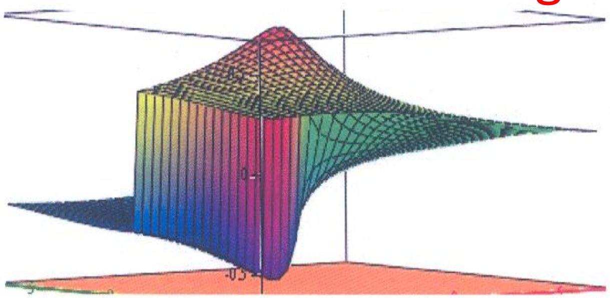
Vanishing of stresses at the origin: $\lim_{\mathbf{r}\to 0} \boldsymbol{\sigma}_{ij} = 0$

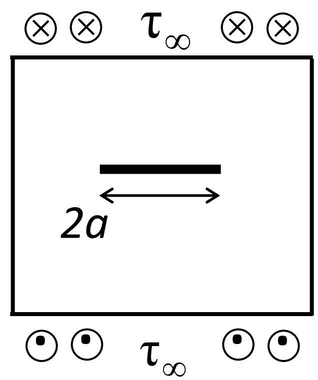
Zero tractions on crack surfaces: $\sigma_{zy}(x, 0^{\pm}) = 0 \quad ; \quad |x| \le a$

• *Nonsingular stress distribution in Mode III*

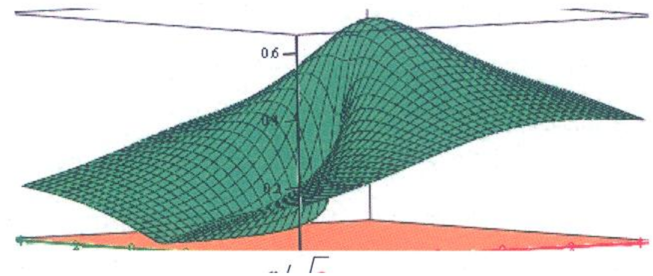
$$\sigma_{xz} = -\frac{K_{III}}{\sqrt{2\pi r}}\left[\sin\frac{\theta}{2}\left(1-\exp\left[-r/\sqrt{c}\right]\right)\right] \qquad \sigma_{yz} = \frac{K_{III}}{\sqrt{2\pi r}}\left[\cos\frac{\theta}{2}\left(1-\exp\left[-r/\sqrt{c}\right]\right)\right]$$

Gradient Stress non-singular

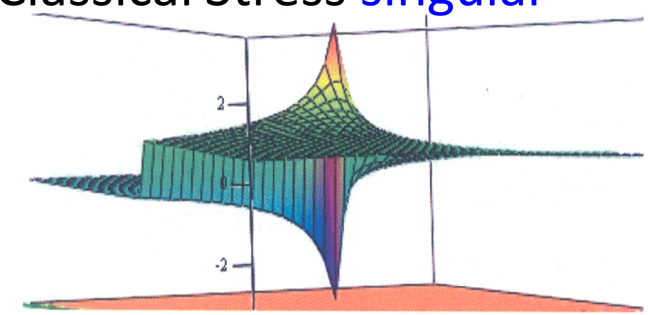




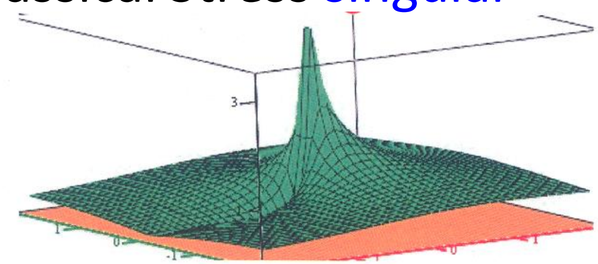
Gradient Stress non-singular



Classical Stress singular



Classical Stress singular



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

$$\therefore \ \sigma_{yz}^{max} = \sigma_{xz}^{max} \cong 0.254\frac{K_{III}}{\sqrt[4]{c}} \cong \frac{K_{III}}{4\sqrt[4]{c}}$$

(Stress Fracture Criterion) $K_{III} = \tau_{\infty}\sqrt{\pi a}$

■ Gradela Crack Nanomechanics (Mode I)

- ***Gradela: Mode I 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: $\lim\limits_{\mathbf{r}\to 0}\boldsymbol{\sigma}_{ij}=0$

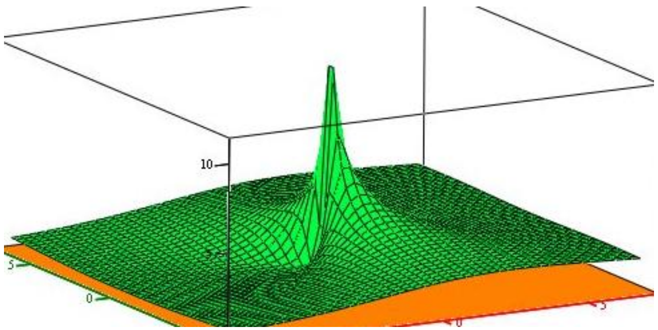
Zero tractions on crack surfaces

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

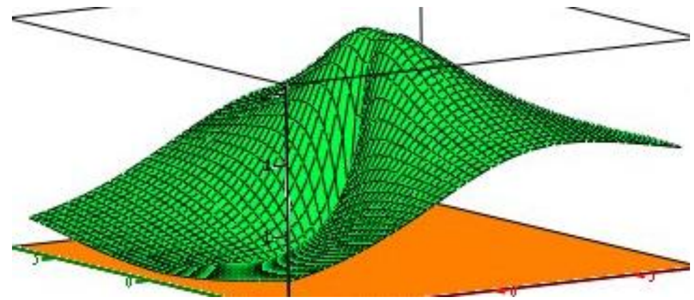
• *Nonsingular stress distribution in Mode I*

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

Classical Stress singular

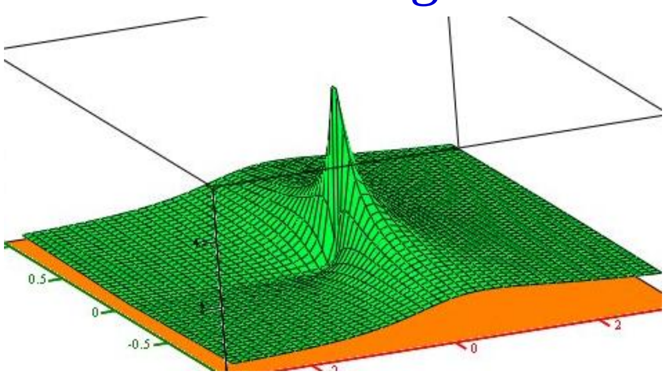


Gradient Stress non-singular

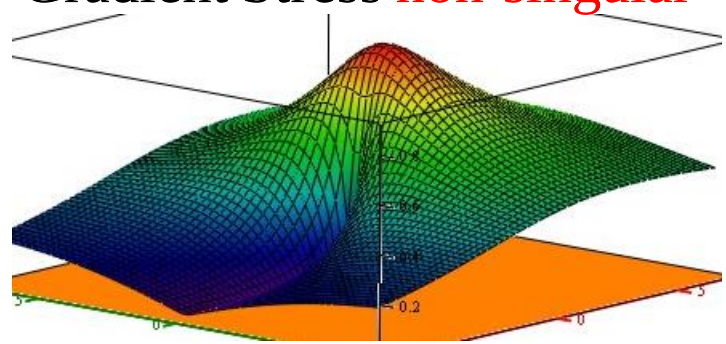


$$\sigma_{zz} = \frac{K_I \nu \sqrt{2}}{\sqrt{\pi r}}\cos\frac{\theta}{2}\left(1-e^{-r/\sqrt{c}}\right)$$

Classical Stress singular



Gradient Stress non-singular



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

▪ A Note on Mindlin's Strain Gradient Theory

- ***Strain Energy Density***

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

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

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

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

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

σ^E_{ij} ... elastic – like stress ; $\sigma^E_{ij} = \sigma^E_{ji}$ ... 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*

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

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

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

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

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

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

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

i.e.

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

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

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

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

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

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

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

A note on 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

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

<u>Kohn-Sham</u>: (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

GRADIENT PLASTICITY
[Plasticity of Nanopolycrystals]

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).

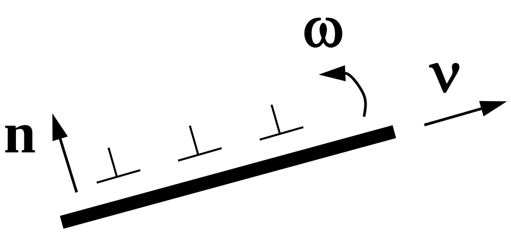
■ Gradient Plasticity: A Scale Invariance Argument

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

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

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

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



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

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

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

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

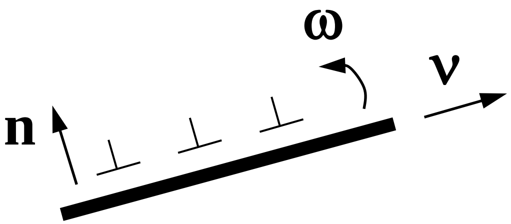
- ***Momentum Balance for Dislocated State***

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

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

- ***Recall***

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



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

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

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

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

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

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

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

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

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

- ***Inhomogeneous Back Stress:*** $T^D = \alpha + T^{inh}$
  - α = *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* $(\boldsymbol{n}, \boldsymbol{\nu})$

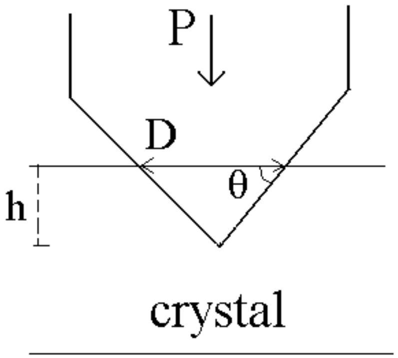
$$\therefore \quad \left(\mathrm{div}\mathbf{T}^{\mathbf{inh}}\right) \cdot \boldsymbol{\nu} \approx \nabla^{2}\gamma^{p}$$

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

ADDITIONAL BENCHMARK PROBLEMS

■ Size Effects in Micro/Nano indentation

- ***Definitions***



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

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

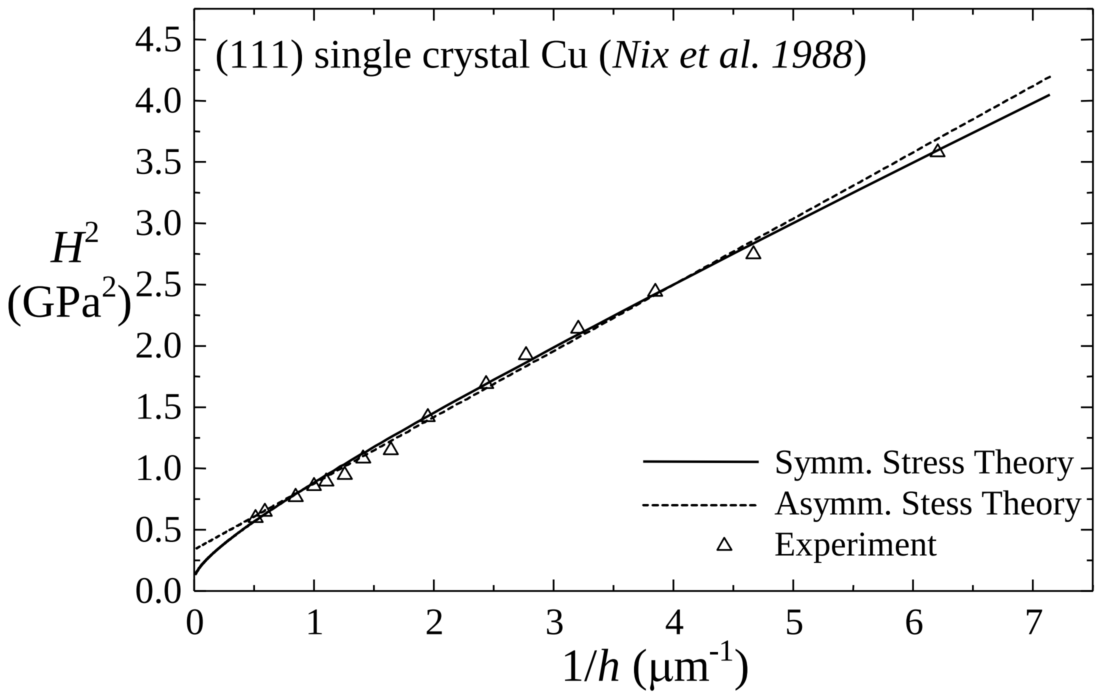
- ***Gradient Theory (Symmetric Stress) and Tabor's Rule***

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

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

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

- ***Couple Stress Theory (Asymmetric Stress)***



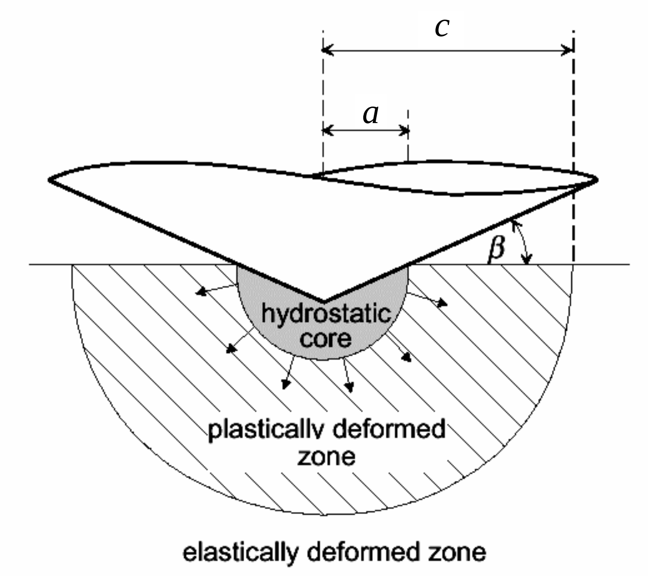
Gradient Theory $\rightarrow H_o = 0.35$ GPa, $l = 4.6$ μm $\Rightarrow (c/G)^2 = 6.73\ 10^{-5}$ μm

Couple Stress Theory $\rightarrow H_o = 0.581$ 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***

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

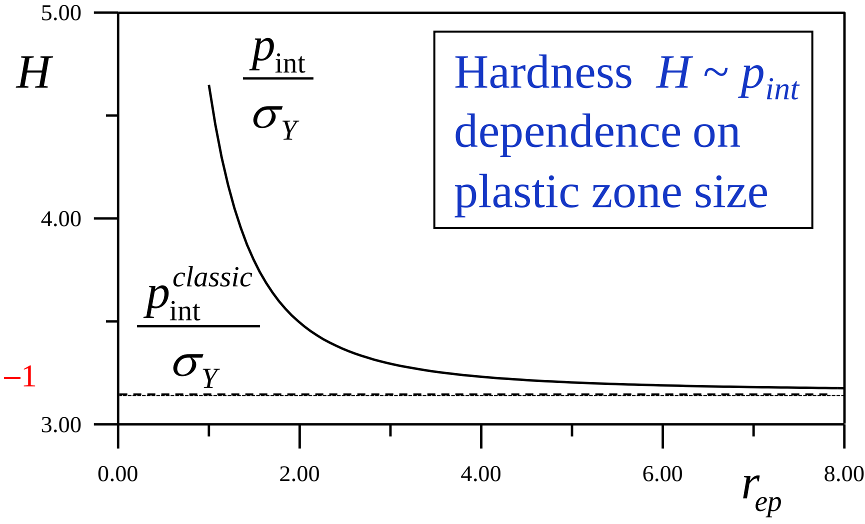
$$t(r) = -\frac{2\sigma_Y}{3} - 2\sigma_Y \log(\frac{r_{ep}}{r}) - \frac{4}{15}\sigma_Y(1+\nu)\frac{l^2}{r_{ep}^2+4l^2(1+\nu)}\left[9\left(\frac{r_{ep}}{r}\right)^5 - 19\right]$$

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

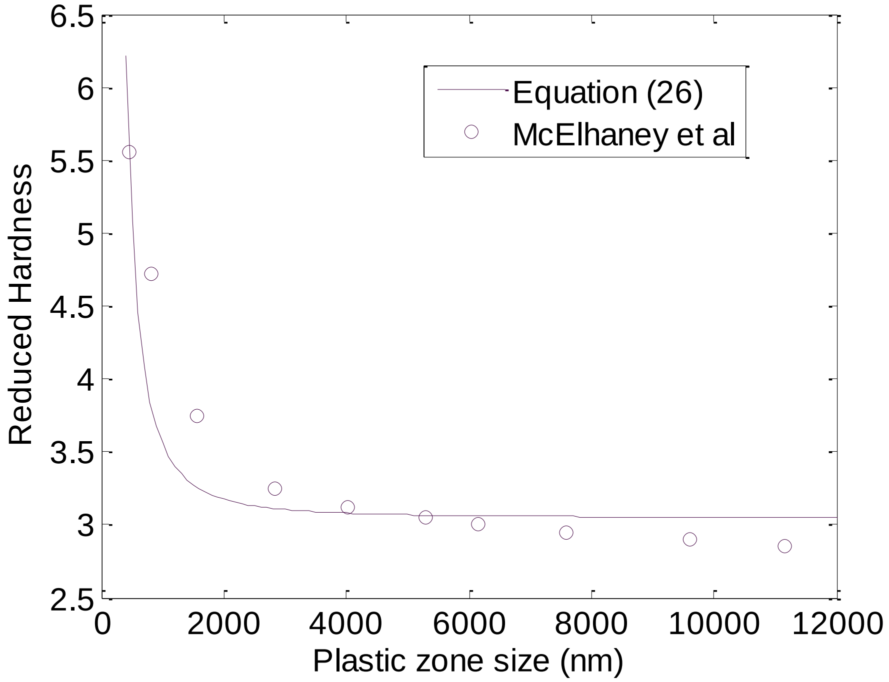
$$\frac{p_{\text{int}}}{\sigma_Y} = -\frac{t(\alpha)}{\sigma_Y} = \frac{2}{3} + 2\log(\frac{r_{ep}}{\alpha})$$

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

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



- ***Prediction of H/σ_Y vs r_{ep}***



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

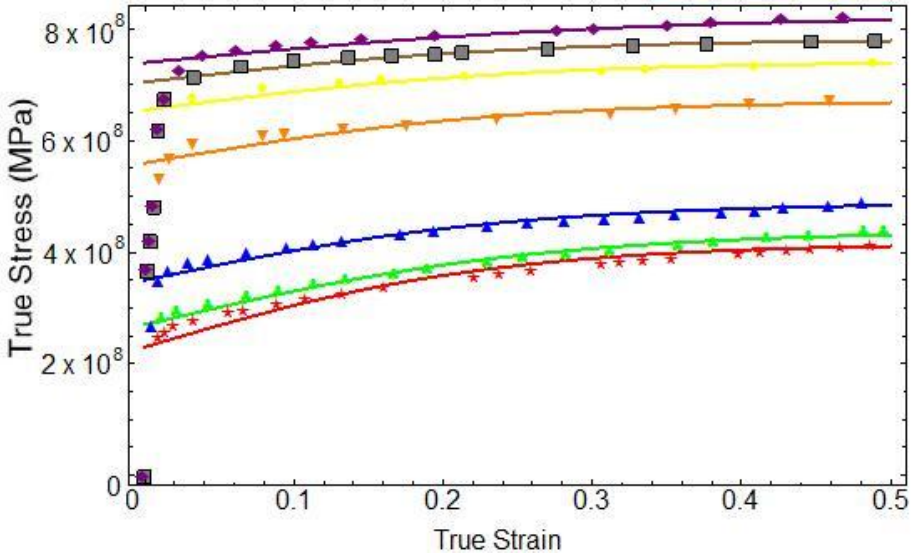
The fit determines the internal length $\ell \approx 15.77$ nm

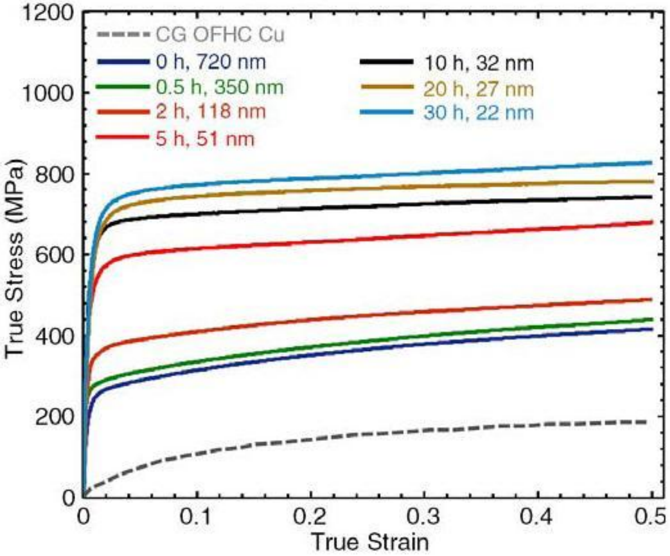
■ Stress-Strain Curves for Nanopolycrystals

- ***H-P Type Behavior***

$$\sigma = \sigma_f + \left(\sigma_s - \sigma_f\right)\tanh\left[\frac{h\varepsilon^p}{\sigma_s - \sigma_f}\right]$$

$$\sigma_{s,f} = \sigma_{s,f}^0 + k_{s,f} d^{-1/2}, \qquad h = h_0 - k_h d^{-1/2}$$



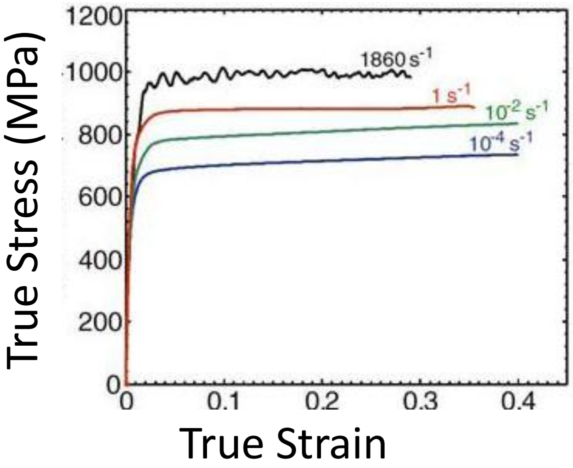


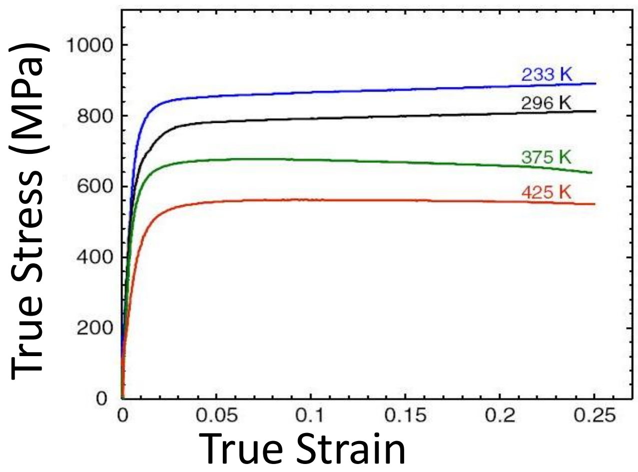
$$\sigma_s^0 = 230\,\text{MPa}, \quad k_s = 92.5\,\text{kPa}\sqrt{\text{m}}, \quad \sigma_f^0 = 70\,\text{MPa},$$

$$k_f = 104\,\text{kPa}\sqrt{\text{m}}, \quad h_0 = 827\,\text{MPa}, \quad k_h = 86\,\text{kPa}\sqrt{\text{m}}$$

• *Strain Rate & Temperature Effects*

$$\sigma_s \quad \rightarrow \quad \propto \left(1 + c\ln\frac{\dot{\varepsilon}}{\dot{\varepsilon}_0}\right) \qquad \sigma \quad \rightarrow \quad \left\{1 - \left[\left(T - T_{ref}\right)/\left(T_{melt} - T_{ref}\right)\right]^m\right\}$$





$$\sigma_s = 890 + 15\ln\dot{\varepsilon} \quad (\mathrm{MPa})$$

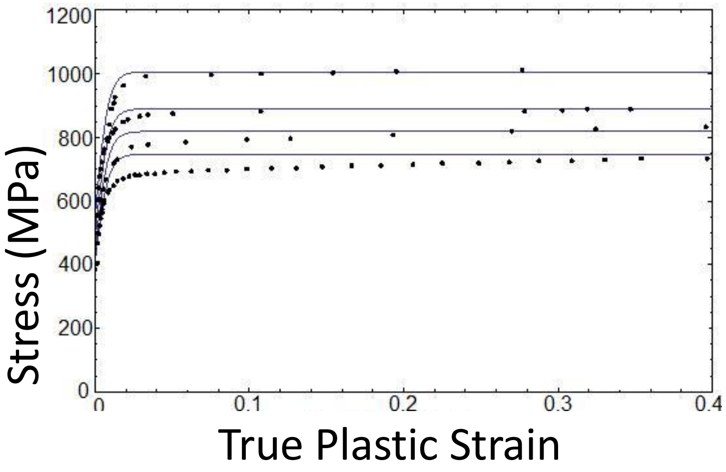
$$\sigma_f = 383\,(\mathrm{MPa})$$

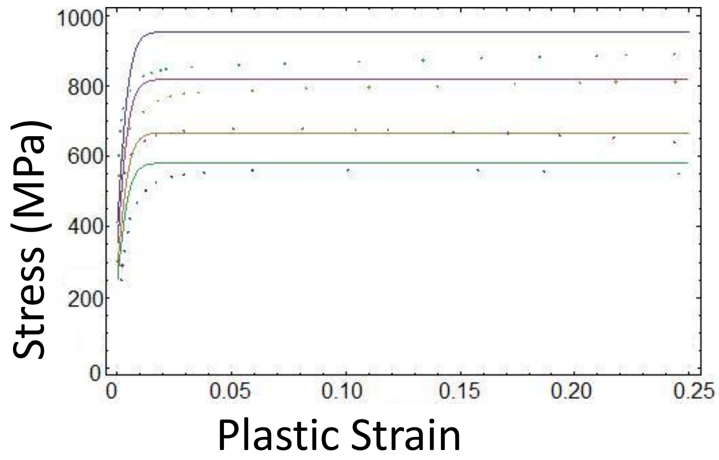
$$h = 95\,\mathrm{GPa}$$

$$T_{ref} = 296\mathrm{K}$$

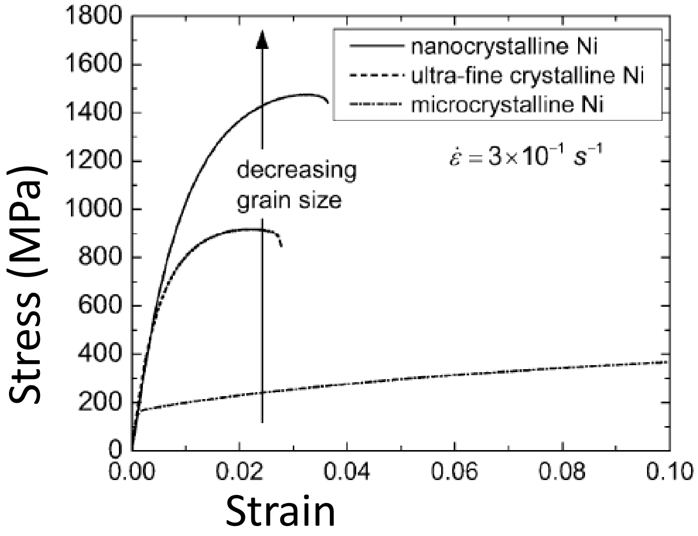
$$T_{melt} = 1356\mathrm{K}$$

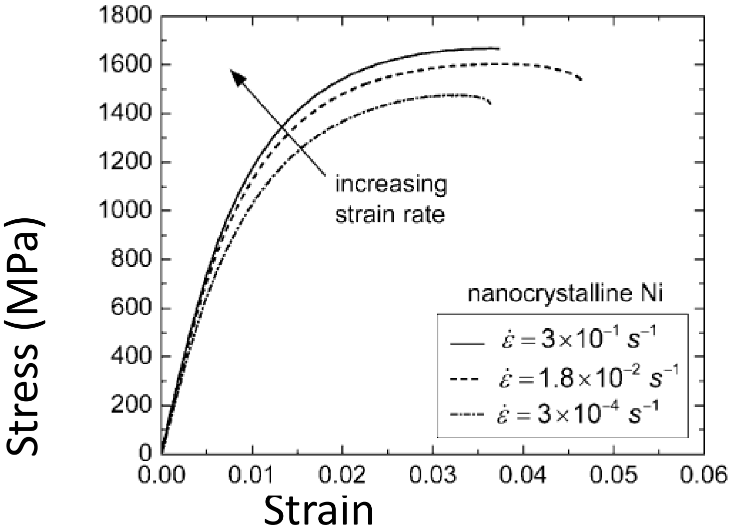
$$m = 2.6$$

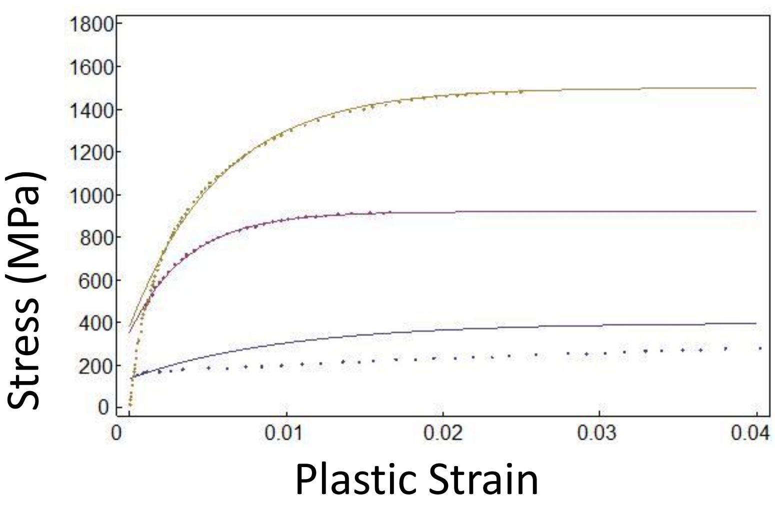


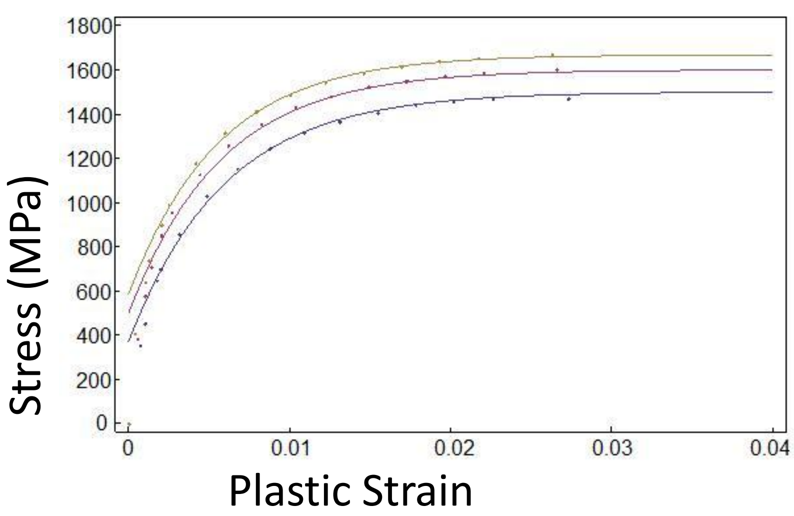


• Simultaneous Grain Size & Strain Rate Dependence







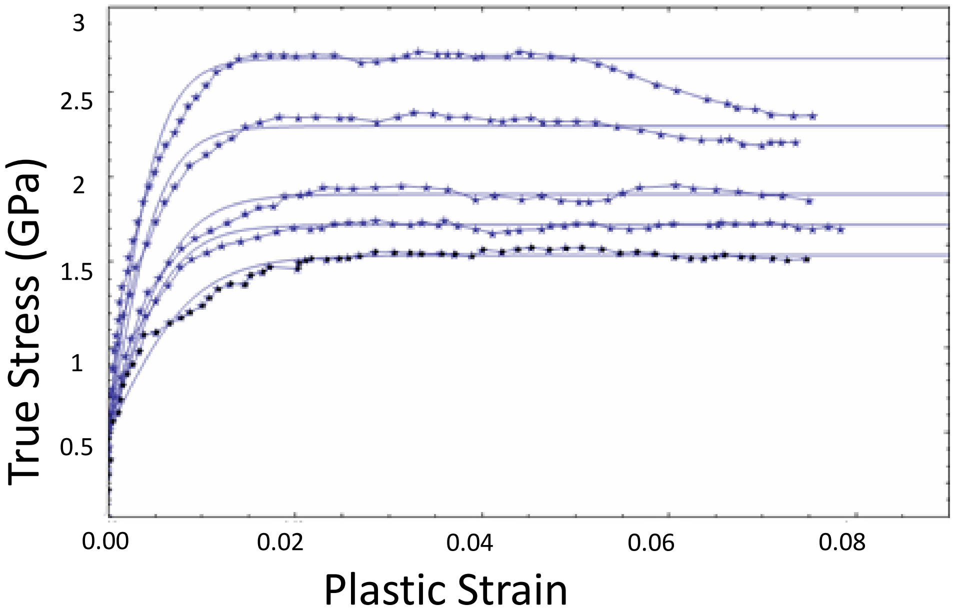


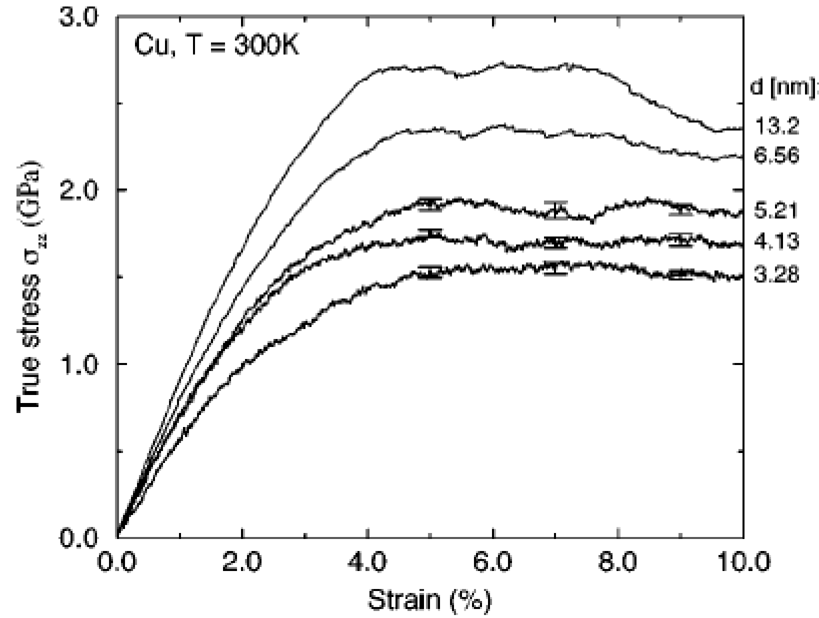
$$\sigma_f = \left(\sigma_f^0 + \frac{k_1}{\sqrt{d}} - \frac{k_2}{d} \right) \left(1 + m_f \ln\left(\frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_p^0} \right) \right)$$

$$\sigma_s = \left(\sigma_s^0 + \frac{k_3}{\sqrt{d}} - \frac{k_4}{d} \right) \left(1 + m_s \ln\left(\frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_p^0} \right) \right)$$

σ_f^0			σ_s^0			h_0	
70MPa			265MPa			3GPa	
k_1 $kPa\sqrt{m}$	k_2 $kPa\sqrt{m}$	m_f	k_3 $kPa\sqrt{m}$	k_4 $kPa\sqrt{m}$	m_s	k_5 $kPa\sqrt{m}$	k_6 $kPa\sqrt{m}$
386	1634	0.045	437	1207	0.016	60851	216646

• *Inverse H-P Type Behavior*





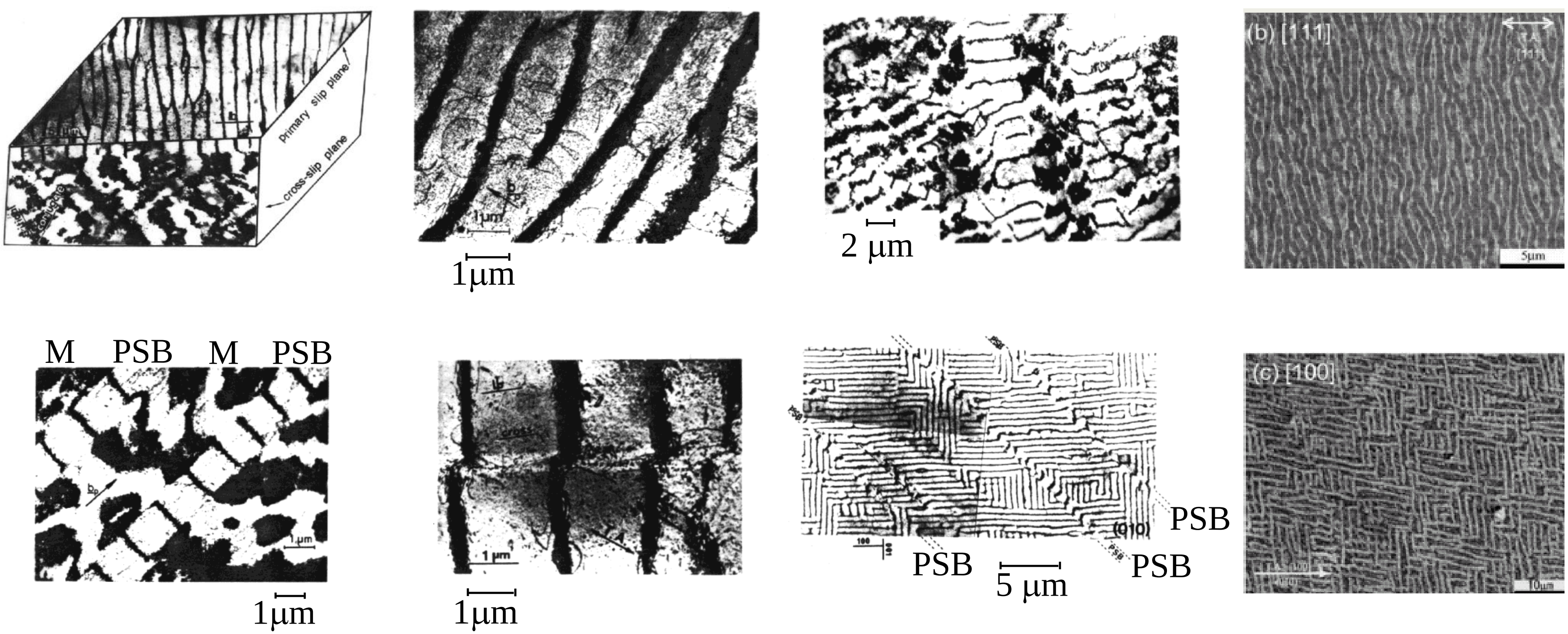
$$\sigma_f = 0.5\text{GPa}, \quad \sigma_s^0 = 4\text{GPa}, \quad k_s = -140\text{kPa}\sqrt{\text{m}}$$

DISLOCATION PATTERNING: THE W–A MODEL

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

■ PSBs Ladder/Labyrinth Structures in Cyclic Deformation

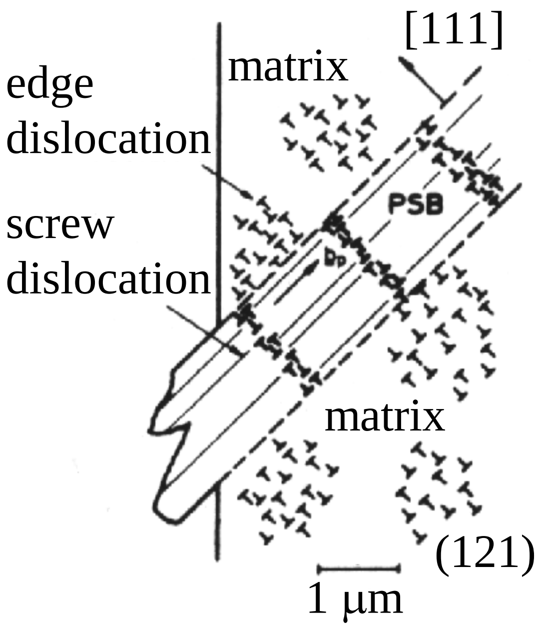
- ***The Initial Motivation for Dislocation Patterning Developments***

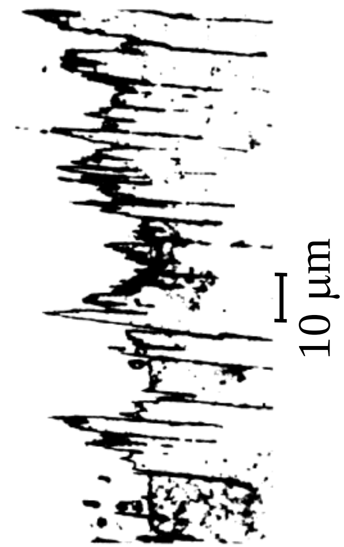


– *Winter-Mughrabi-Laird; Tabata et al; Kaneko-Hashimoto*

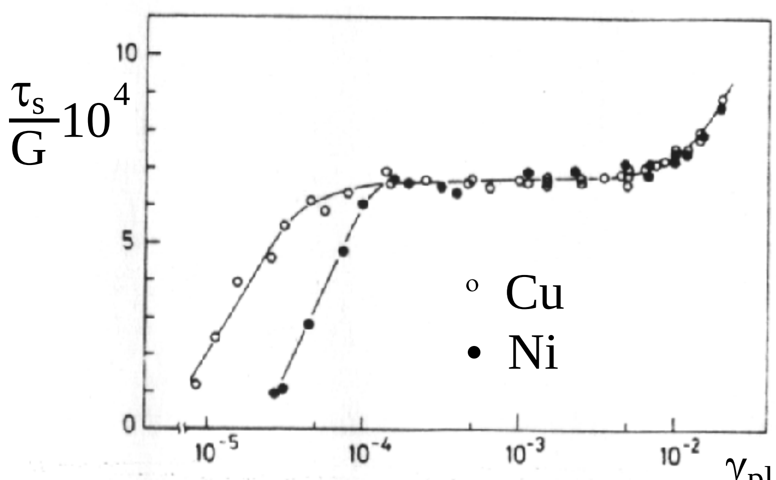
TEM and SEM micrographs

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

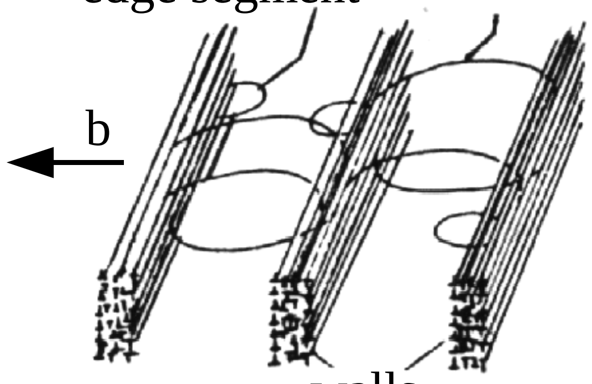




  - *Stress – strain graph*



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



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

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

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

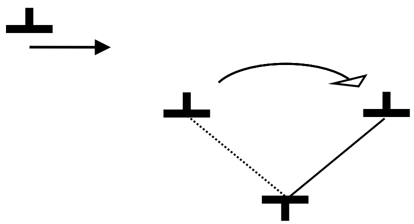
(ρ_i, ρ_m) … (immobile, mobile) dislocation density

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

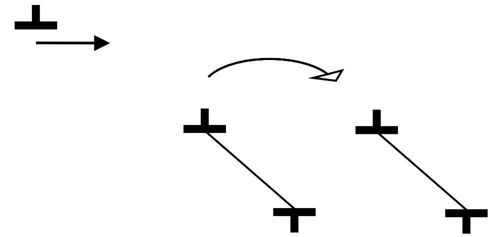
(α, γ) … reaction cross-section parameters

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

  - *Diffusive Mechanisms (D_i)*

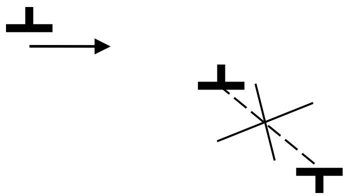


Dipole “switching“



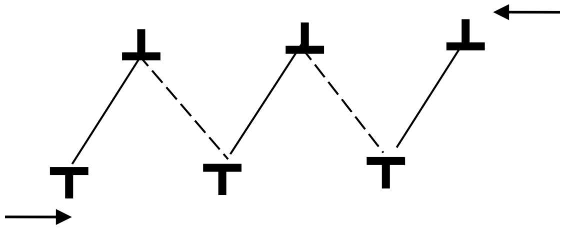
Dipole “sweeping“

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



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

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

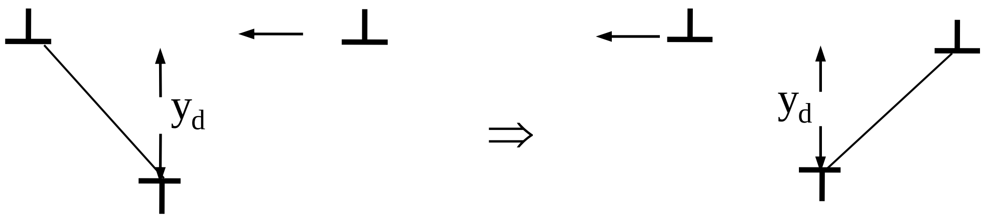


$$\left(\frac{\partial \rho_i}{\partial t}\right)^{+} \sim \gamma\, \dot{\gamma}^{pl}\, \rho_m\, \rho_i^2$$

- ***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 t_d … average time between two successive events

– *Diffusion-like coefficient of mobile dislocations D_m*

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

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

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

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)

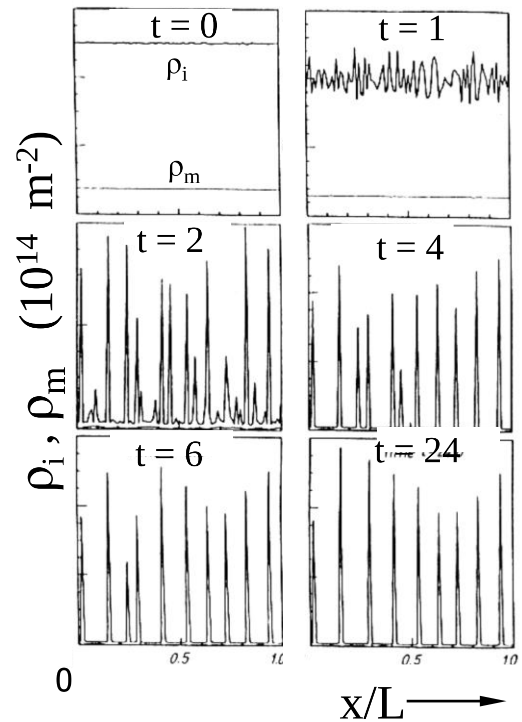
$$\therefore \; q_{critical} = q_c = \frac{2\pi}{\lambda_c} = \left(\frac{\alpha\gamma\rho_i^2}{D_i D_m}\right)^{1/4}$$

  – *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 $\dot{R}_q \approx 0$

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

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

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

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

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

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

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

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

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

  - *Holt-like Energetic Treatment of ρ_i*

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

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

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*

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

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

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

    $r < 0$

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

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

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

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

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

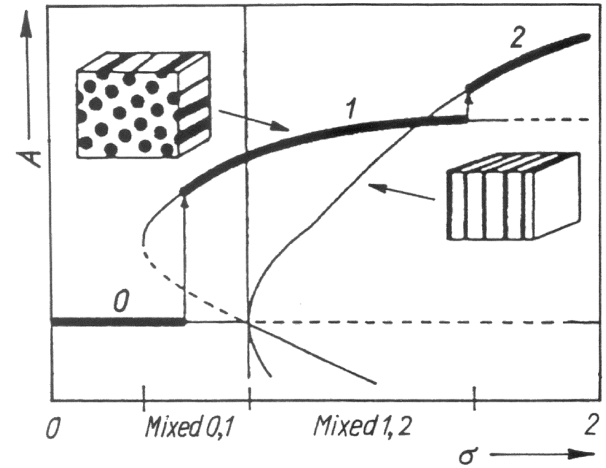
  - *Higher values of stress* $(\beta \geq \beta_c)$

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

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

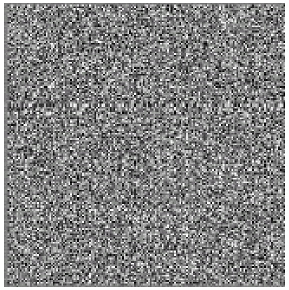
    preferred wavevector q_c: $2d_{//}\left(q_c^2 - q_o^2\right) - \beta\frac{q_c^2}{\left(q_c^2 + q_*^2\right)^2} = 0$

    i.e. $q_c > q_0$

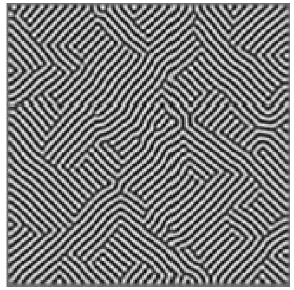


Bifurcation diagram for patterning in fatigue. The preferred stable states are given in heavy lines. *A* is the amplitude of modulation of the spatial pattern, and σ the absolute value of maximum stress per cycle

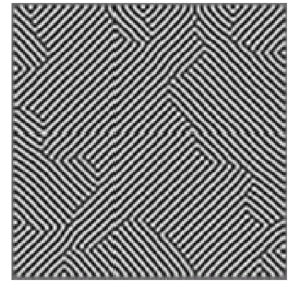
- *Simulation Results*



t = 0



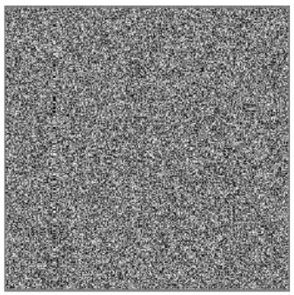
t = 100



t = 20000

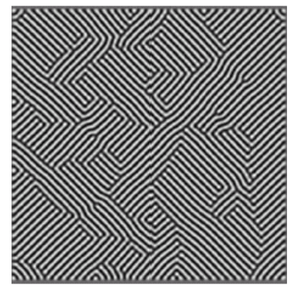
7.5% anisotropy

(a)



t = 0

t = 100

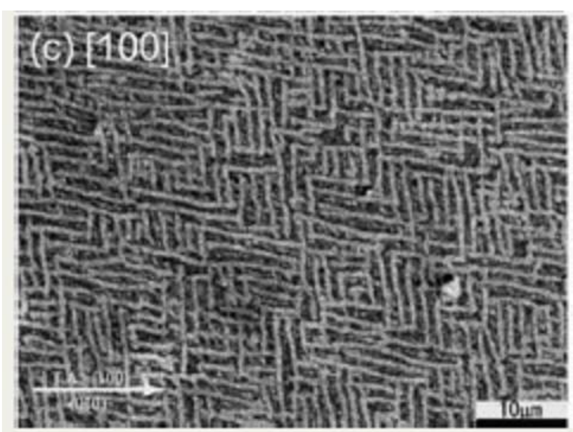


t = 20000

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)

■ Micro/Nano Defect Kinetics – Patterns

- ***The W–A Dislocation Patterning Model***

$$\frac{\partial \rho_1}{\partial t} = I\left(\rho_i, \rho_j\right) + D_i \nabla^2 \rho_i$$

- ***Application to Nanopolycrystals***

$$\frac{\partial \rho}{\partial t} = A_\rho \rho - B_\rho \rho^2 - C_0 \frac{\rho}{d} + C_3 \rho \varphi + \omega M \vartheta + N \frac{\psi}{d} + D_\rho \nabla^2 \rho$$

$$\frac{\partial \varphi}{\partial t} = A_\varphi \rho - B_\varphi \rho^2 - C_4 \rho \varphi - K \varphi + D_\varphi \nabla^2 \varphi$$

$$\frac{\partial \psi}{\partial t} = C_1 \frac{\rho}{d} + A_\psi \psi - B_\psi \psi^2 + D_\psi \nabla^2 \psi$$

$$\frac{\partial \vartheta}{\partial t} = C_2 \frac{\rho}{\omega d^2} - P_1 \rho \vartheta - P_2 \psi \vartheta - G \vartheta + D_\vartheta \nabla^2 \vartheta$$

ρ – mobile dislocations

φ – low-mobility (immobile) dislocations

ϑ – junction disclinations

ψ – grain boundary sliding dislocations

- ***Twinning in Nanopolycrystals***

$$\frac{\partial \rho}{\partial t} = A_\rho \rho - A_1 \rho^2 - B_1 \rho \xi + F_1 \theta \xi - G_1 \theta \xi \rho - K_1 \rho \phi + N_1 \theta \phi + D_\rho \frac{\partial^2 \rho}{\partial x^2}$$

$$\frac{\partial \theta}{\partial t} = B_2 \rho \xi + G_2 \theta \xi \rho + K_2 \rho \phi - R \theta^2 + D_\theta \frac{\partial^2 \theta}{\partial x^2}$$

$$\frac{\partial \phi}{\partial t} = E_0 \theta - K_3 \rho \phi - N_2 \theta \phi$$

$$\frac{\partial \xi}{\partial t} = A_2 \rho^2 - F_2 \theta \xi$$

ρ – mobile dislocations

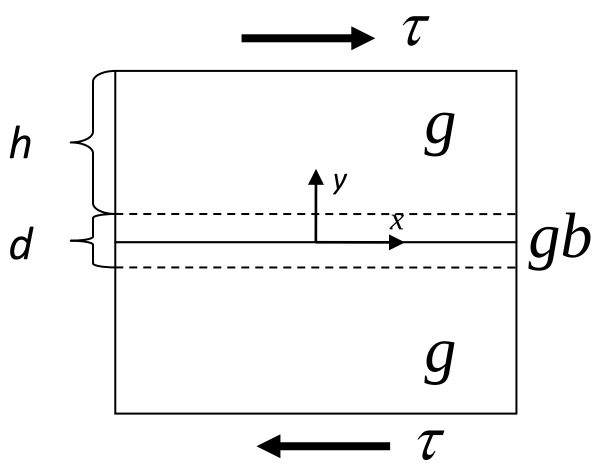
ϕ – twin lamellae

ϑ – disclination dipoles (twin fronts)

ξ – sessile Lomer-Cotrell dislocations

AN APPENDIX ON SIZE EFFECTS

Elastic Moduli of nc's



$$\tau = G_i\gamma_i - c_i\nabla_y^2\gamma_i \quad ; \quad i = (g, gb)$$

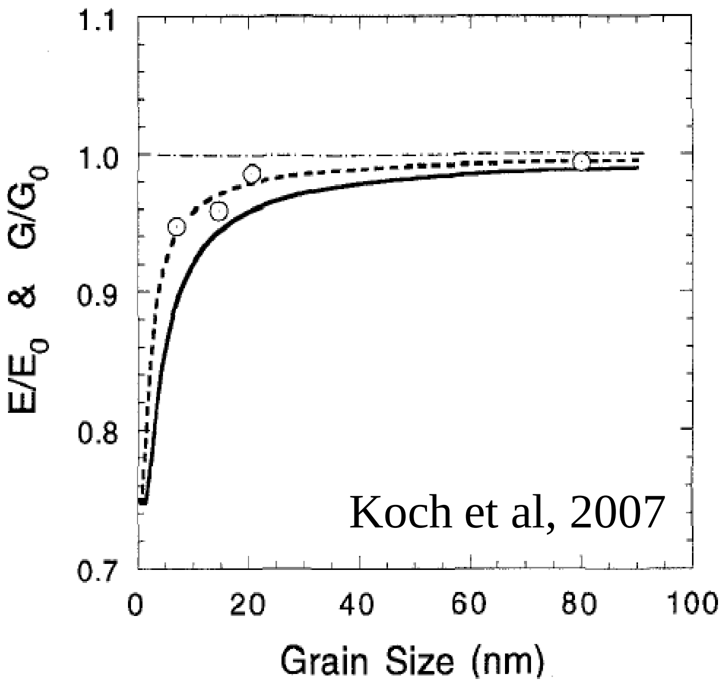
$$\Rightarrow \gamma_i = \frac{\tau}{G_i} + A_i e^{\sqrt{\frac{G_i}{c_i}}y} + B_i e^{-\sqrt{\frac{G_i}{c_i}}y}$$

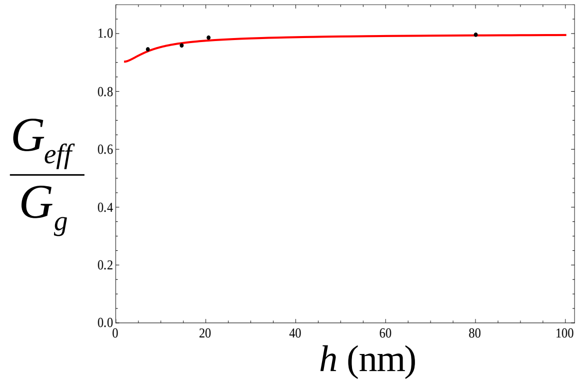
Bc's: γ & $\partial_y\gamma$ continuous at $\gamma = \frac{d}{2}$

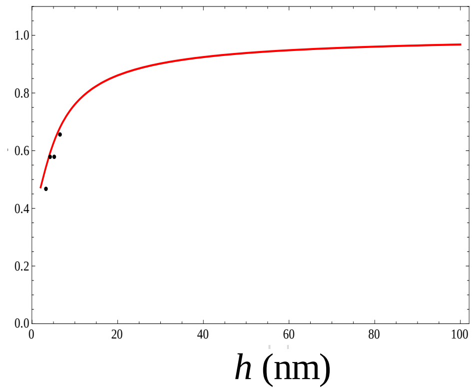
$$\partial_y\gamma_{gb}\Big|_{y=0} = 0 \quad \& \quad \gamma_g\Big|_{y=h+\frac{d}{2}} = \frac{\tau}{G_g}$$

$$\bar{\gamma} = \frac{1}{h+d/2}\left[\int_0^{d/2}\gamma_{gb}dy + \int_{d/2}^{h+d/2}\gamma_g dy\right]$$

$$G_{eff} = \tau/\bar{\gamma}$$



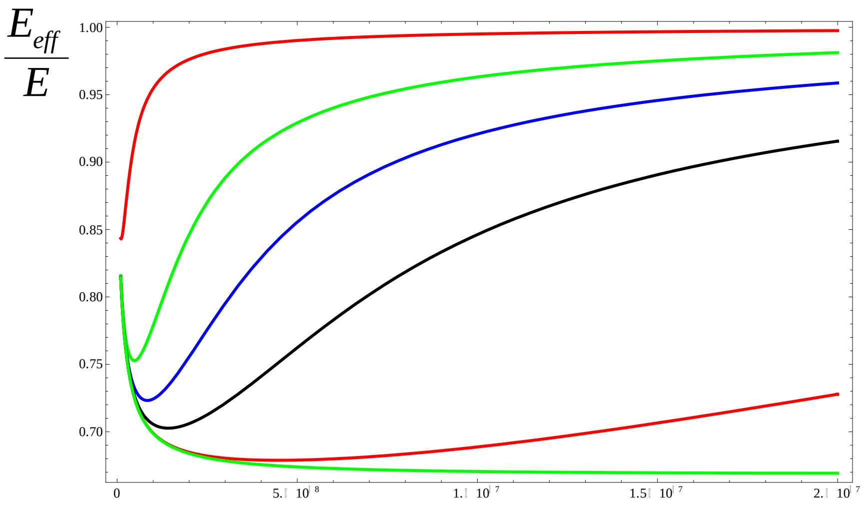




▪ Playing with the parameters

$$\left[c, \quad d, \quad h, \quad E_{gb}/E_g \right]$$

• Effect of d/h on E



(1)

• Effect of surface waviness on E

$\frac{E_{eff}}{E}$

wavelength/film thickness

(2)

- Initial decrease of $\frac{E_{eff}}{E}$ than increase
- (1) Simple gradient argument
- (2) FE calculation for polysilica film {Chasiotis + Knauss}
- Similar results for (nano)plates and (nano)wires using MD or surface tension theories

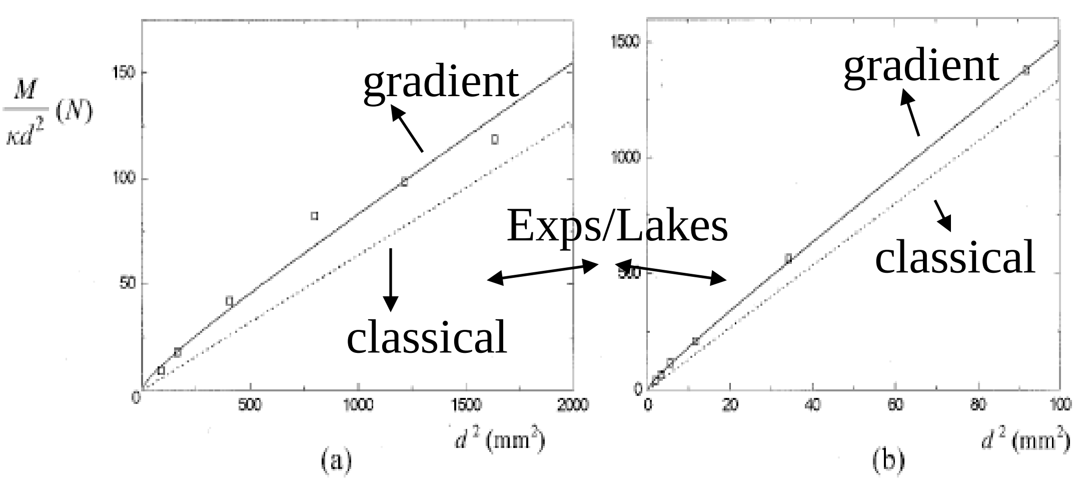
Pure Elastic Bending

$$\varepsilon = \kappa y \quad , \quad M = \int_A \sigma y dA = 2 \int_{-d/2}^{d/2} \int_0^{\sqrt{d^2/4 - z^2}} \sigma y dy dz$$ cylindrical bar (diameter d)

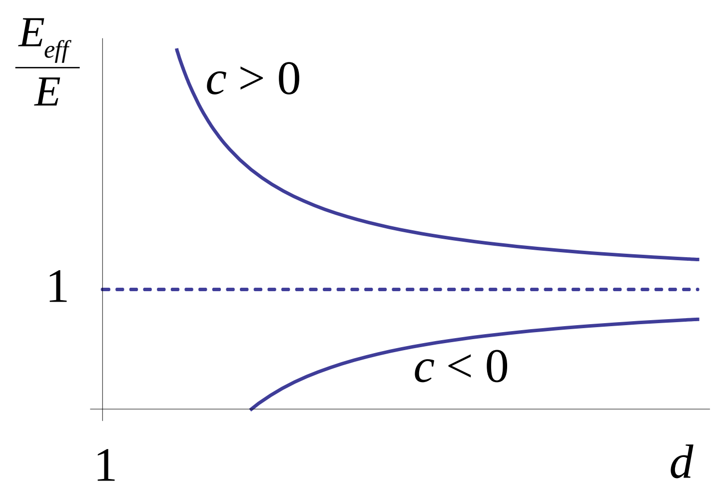
$$\sigma = E\left(\varepsilon + c\,\mathrm{sgn}(\varepsilon)\left|\nabla \varepsilon\right|\right)$$

$$\therefore \ \sigma = E\kappa\left(y + c\right) \quad ; \quad \frac{M}{\kappa d^2} = E\left(\frac{\pi d^2}{64} + c\frac{d}{6}\right) \ (*)$$

NOTE: $\frac{E_{eff}}{E} = 1 + \frac{\ell}{d}; \quad \ell \cong 7c \quad (**)$

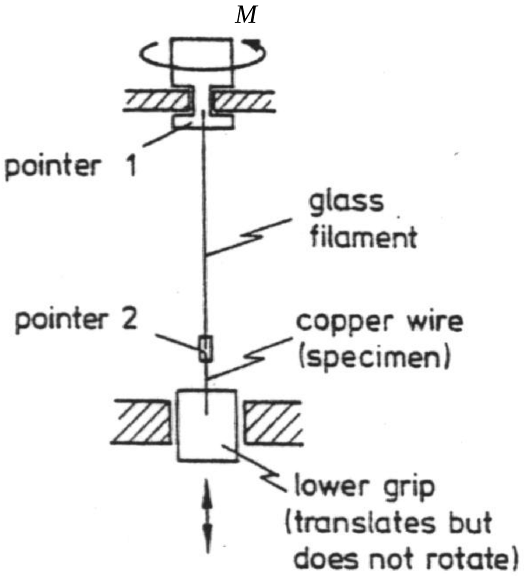


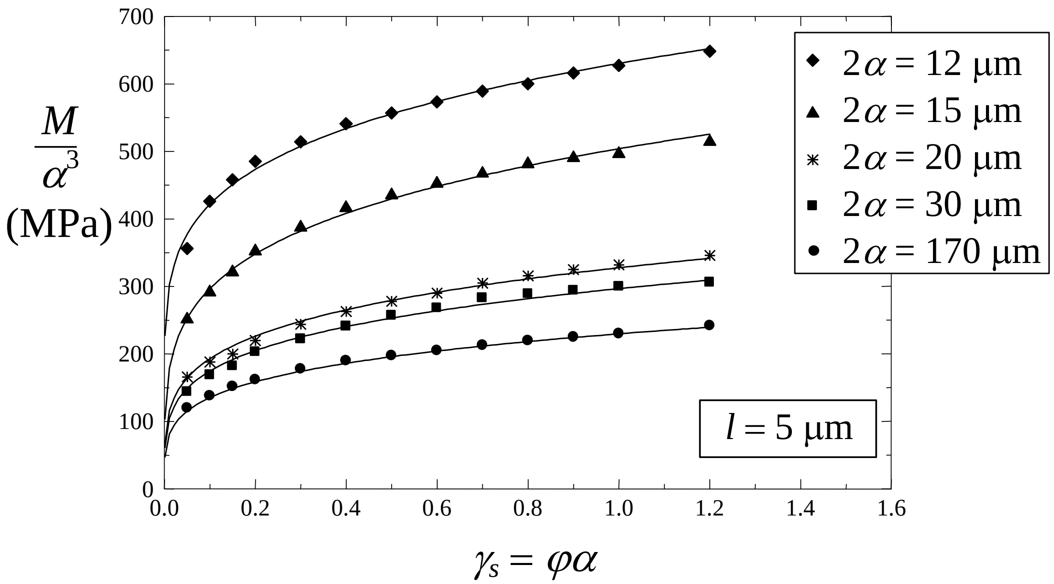
(a) Polymeric foam; (b) polyurethane foam (Aifantis, 1999)



Similar behavior from MD & Surface tension theories

Plastic Microtorsion

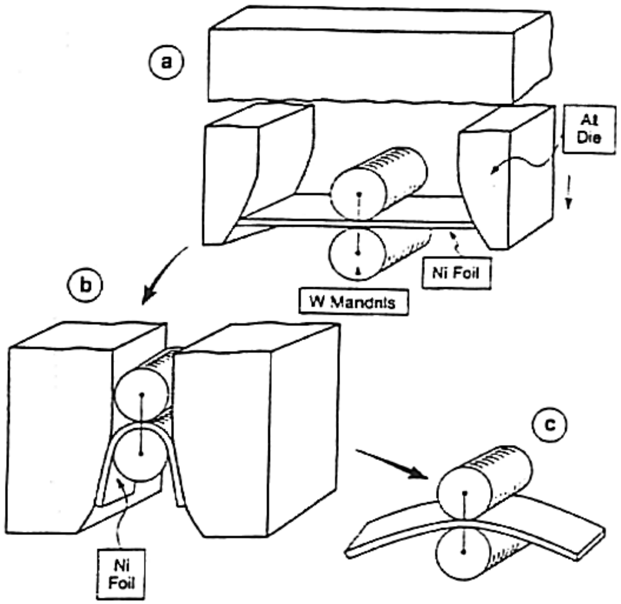


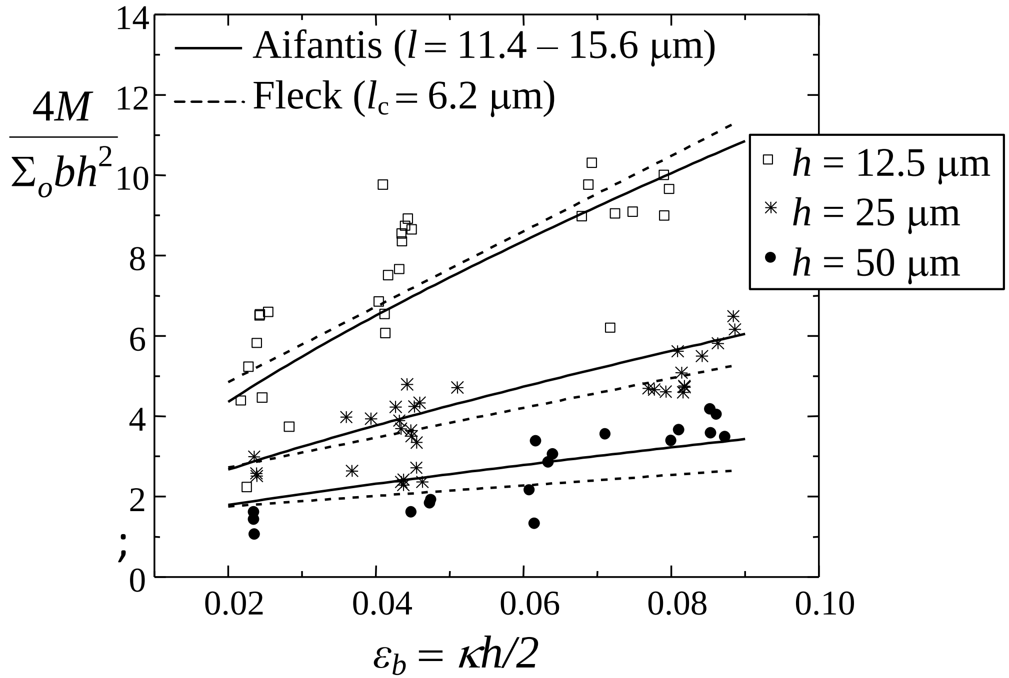


$$\tau = \tau_o + k(\gamma) + c(\gamma)\nabla^2\gamma\,, \qquad k(\gamma) = k_o\gamma^N\,, \qquad c(\gamma) = \bar{c}\gamma^{N-1}$$

$$\frac{M}{\alpha^3} = 2\pi\left\{\frac{\tau_o}{3} + k_o\frac{\gamma_s^N}{N+3}\left[1 + \frac{N+3}{N+1}\left(\frac{l}{\alpha}\right)^2\right]\right\}, \qquad l = \sqrt{\bar{c}/k_o}$$

Plastic Microbending





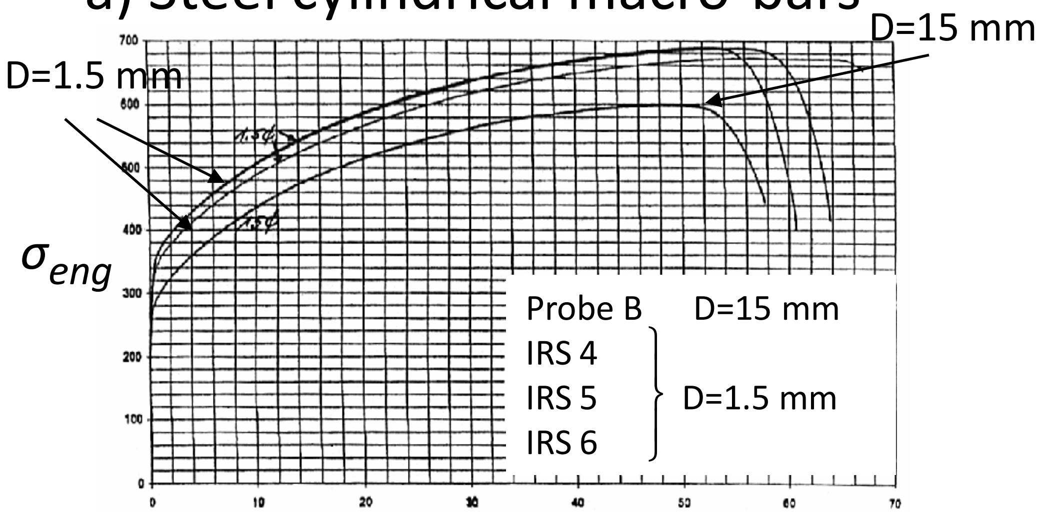
$$\bar{\sigma} = k(\bar{\varepsilon}) + c_1(\nabla\bar{\varepsilon}\cdot\nabla\bar{\varepsilon})^m + c_2\nabla^2\bar{\varepsilon};\quad k(\bar{\varepsilon}) = \frac{\sqrt{3}}{2}\Sigma_o + \frac{3}{4}E_p\bar{\varepsilon},\quad m = 0.34$$

$$\frac{4M}{\Sigma_o bh^2} = 1 + \frac{2E_p}{3\Sigma_o}\left[1 + \frac{2^{4m}}{(\sqrt{3})^{2m-1}}\left(\frac{l}{h}\right)^{2m}\varepsilon_b^{2m-1}\right]\varepsilon_b \qquad l = (c_1/E_p)^{1/2m}$$

Microtension (Gradients or Not?)

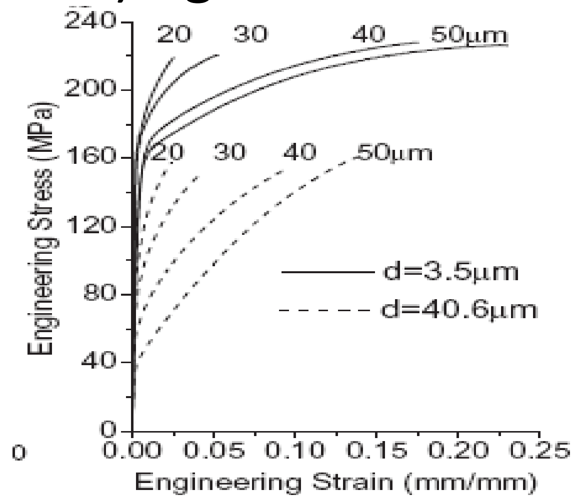
- ***Experiments***

a) Steel cylindrical macro-bars



Data from ECA et al 1998 ε_{eng}

b) Ag micro-wires



Data from Ngan 2011

NO macroscopic gradients; Size effect modeling?

- ***Modeling***

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

i.e. σ depends on ε and an internal variable α which evolves inhomogeneously through a ∇^2 diffusive transport term

- ***Adiabatic Elimination ($\dot{\alpha} = 0$)***

$\alpha = \alpha(r)$ reaches steady states much faster than ε

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

Bc's: α finite as $r \to 0 \Rightarrow A \equiv 0$

zero flux of α at $r = R$ $\Rightarrow -D\left.\frac{\partial \alpha}{\partial r}\right|_{r=R} = \frac{\alpha_c}{\sqrt{c}} = \frac{g\varepsilon^q}{\sqrt{c}}$

Assume Ludwig type relations: $\kappa(\varepsilon) = Y + k_0\varepsilon^n; \quad \lambda(\hat{\alpha}) = \lambda_0\hat{\alpha}^m$

$$\therefore \quad \bar{\sigma} = \frac{Y + k_0\left[\ln\left(1+\bar{\varepsilon}\right)\right]^n + \lambda_0\left[g\left(2\beta+1\right)\right]^m\left[\ln\left(1+\bar{\varepsilon}\right)\right]^{qm}}{1+\bar{\varepsilon}}$$

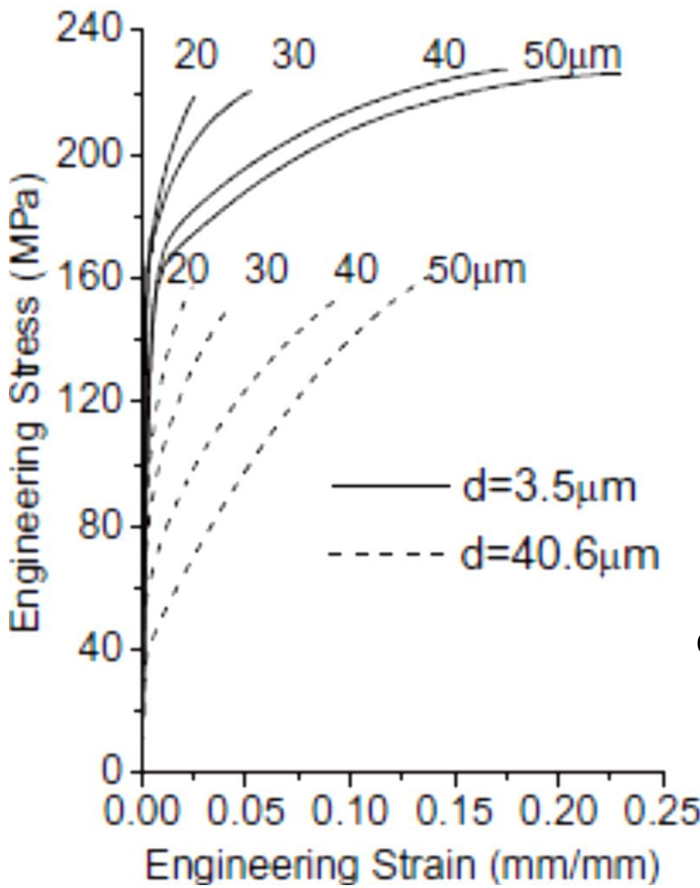
$\therefore$ Models specimen size effects in tension for steel macrocylinders

- ***Extrinsic vs Intrinsic Size Effects***

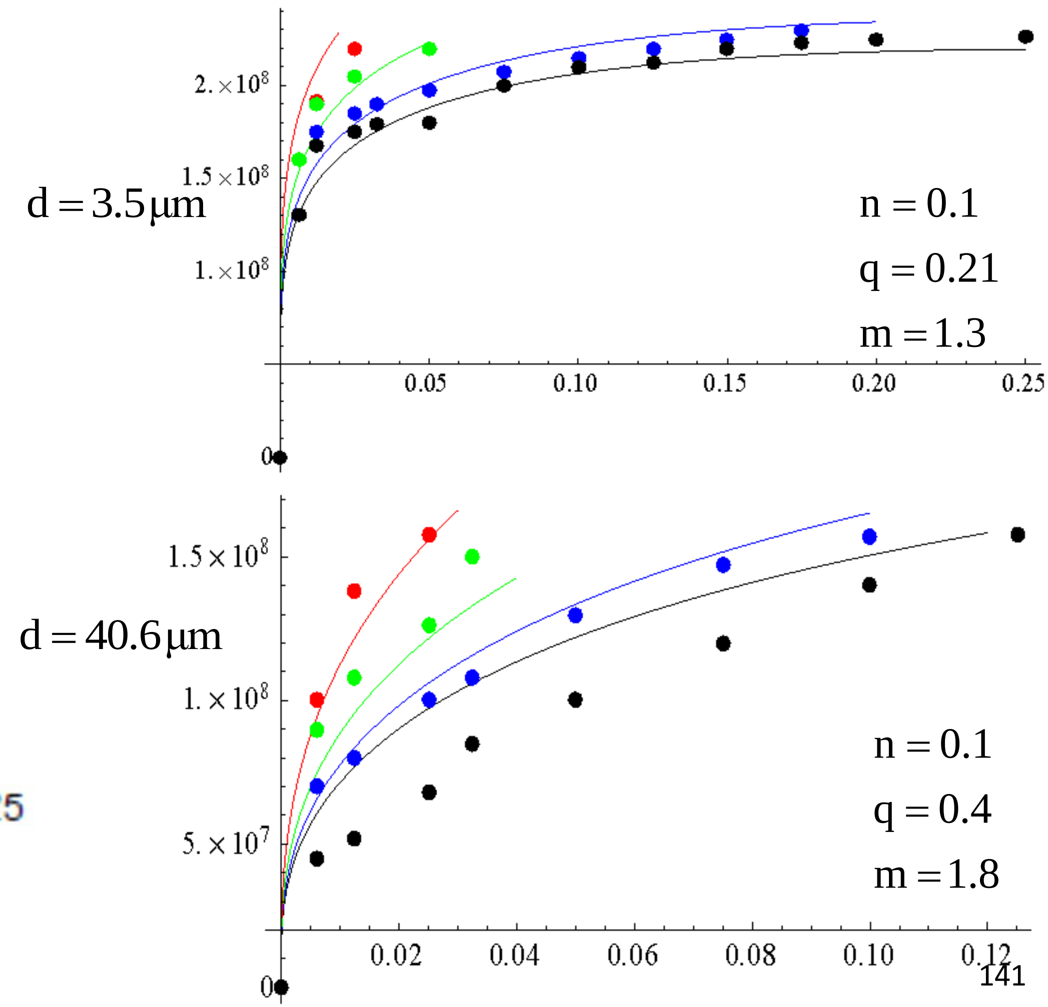
Grain size dependence can be introduced according to H-P relation to model combined extrinsic (specimen size D) – intrinsic (grain size d) scale effects

- ***Size Effects on the Tensile Strength of Ag Microwires***

$$Y = 10 + \frac{10^{-4}}{\sqrt{d}}[\text{MPa}]; \quad k_0 = 0.1 + \frac{5 10^{-3}}{\sqrt{d}}[\text{MPa}]; \quad \lambda_0 = 250 + \frac{5 10^{-3}}{\sqrt{d}}[\text{MPa}]$$

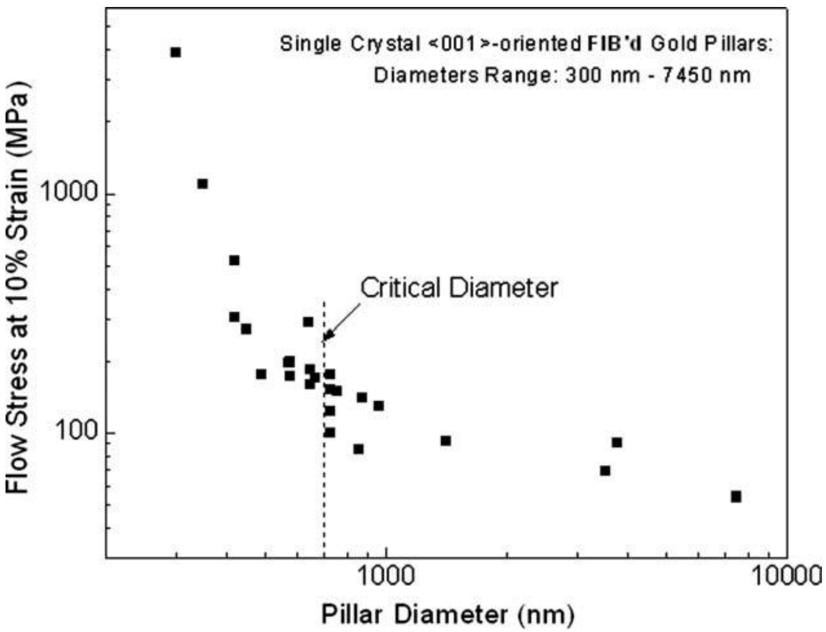


(Chen & Ngan, 2011)

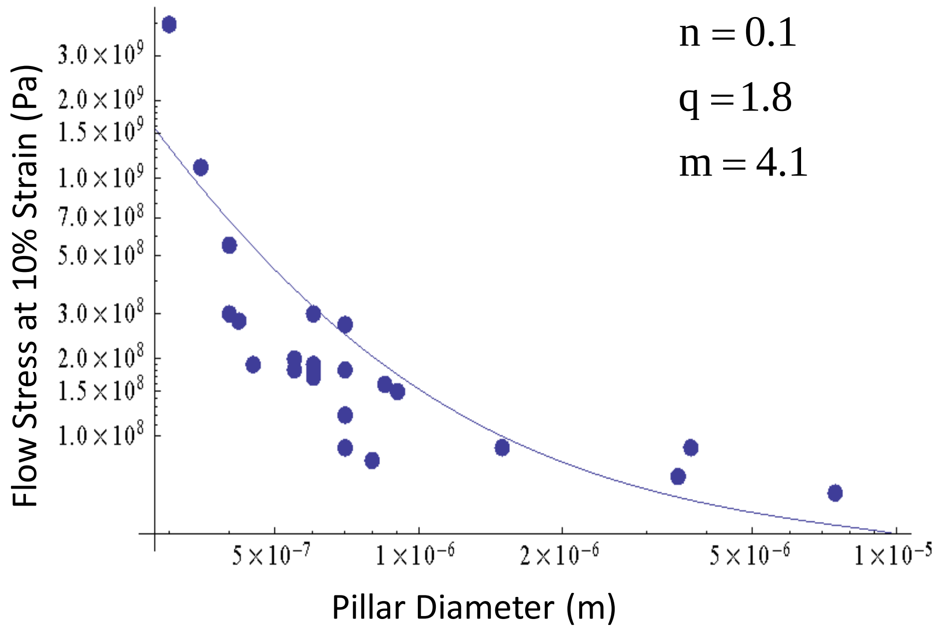


• *Size Effects on the Compressive Flow Stress of Au Micropillars*

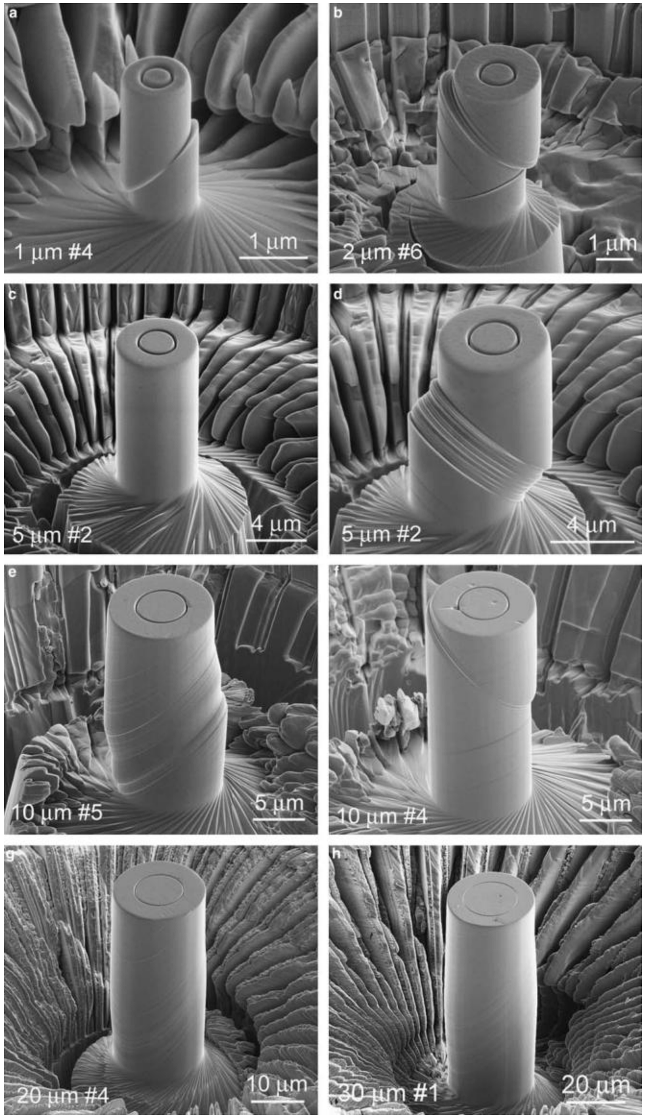
$$\bar{\varepsilon} = 0.1; \quad k_0 = 0.1 + \frac{210^{-3}}{\sqrt{d}}[\mathrm{MPa}]; \quad \lambda_0 = 250 + \frac{0.1}{\sqrt{d}}[\mathrm{MPa}]$$

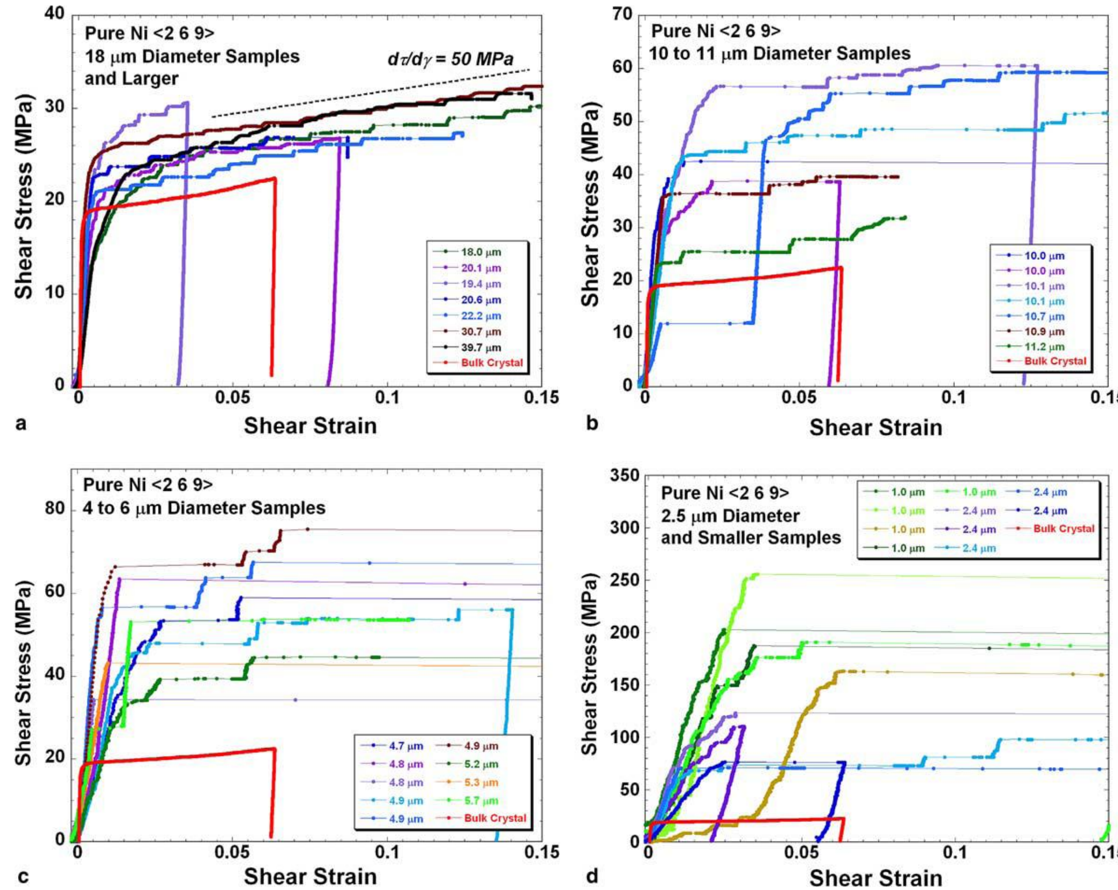


(Greer et al, 2005)



Compression of Micropillars



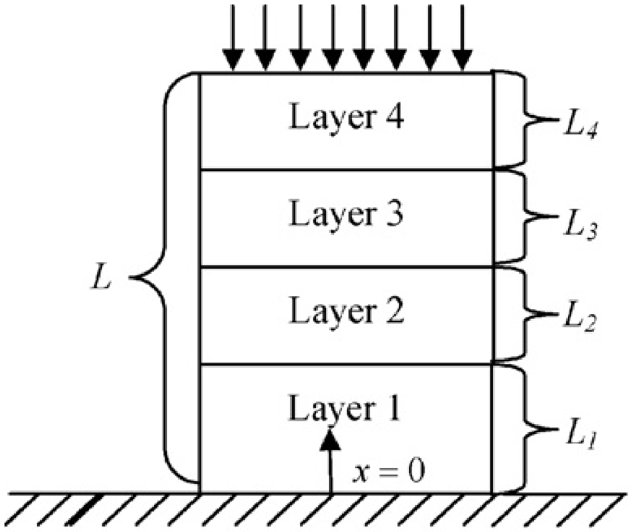


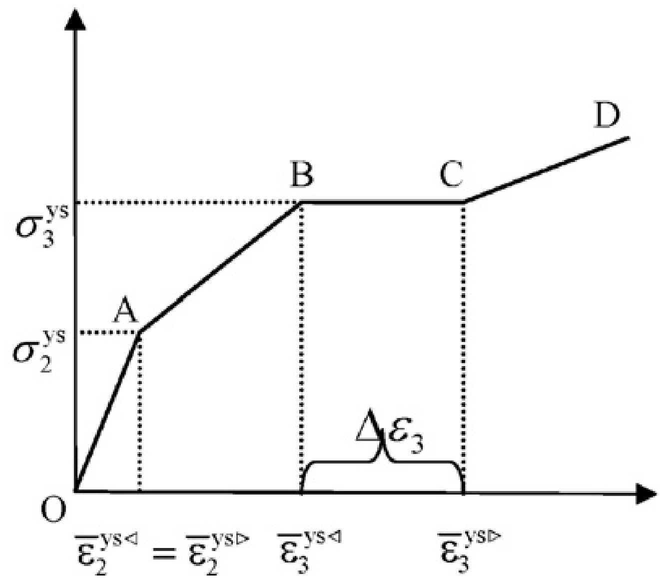
Dimiduk et al, 2005

- **Deterministic Gradient Plasticity (GP) Concept**

  (Katerina Aifantis & Zhang, 2011)

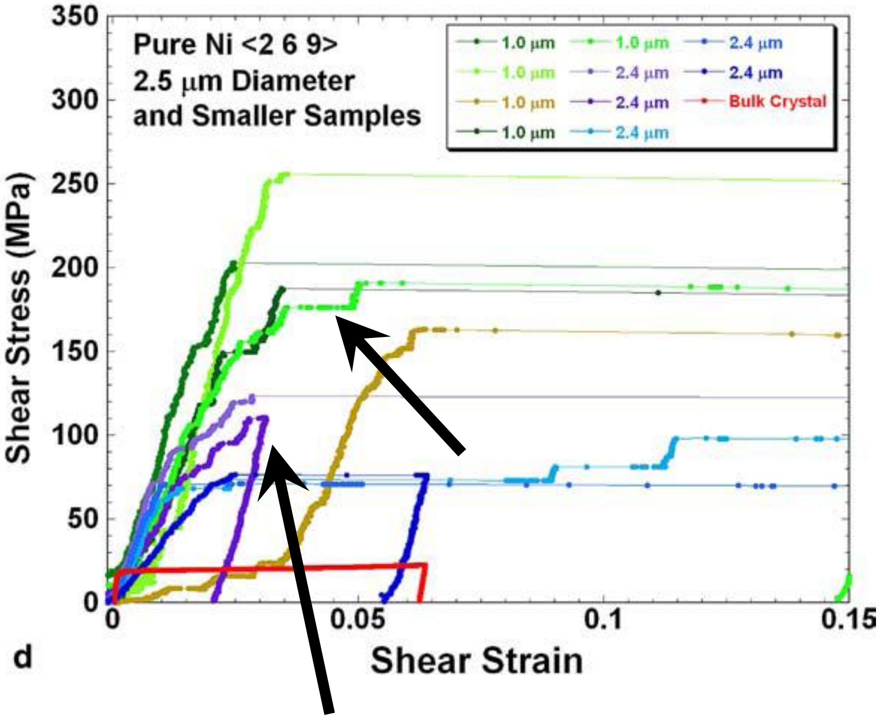
  - Pillars divided in elastic and plastic zones (different yield stress, moduli)
  - Solve 1-D boundary value problems for each zone

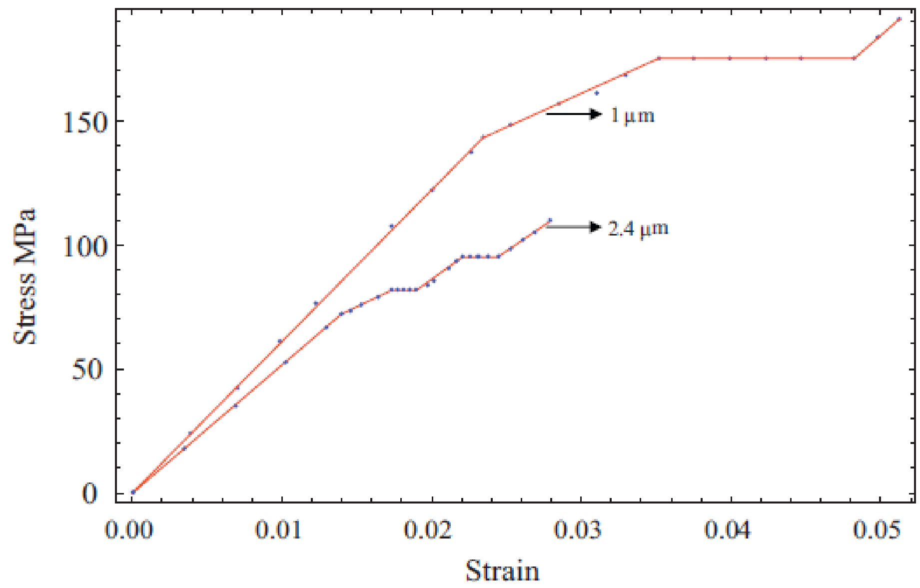




■ Deterministic GP Results

(Katerina Aifantis & Zhang, 2011)





Stochastic Gradient plasticity (GP) Concept

- Cellular Automaton Implementation (1-D case)

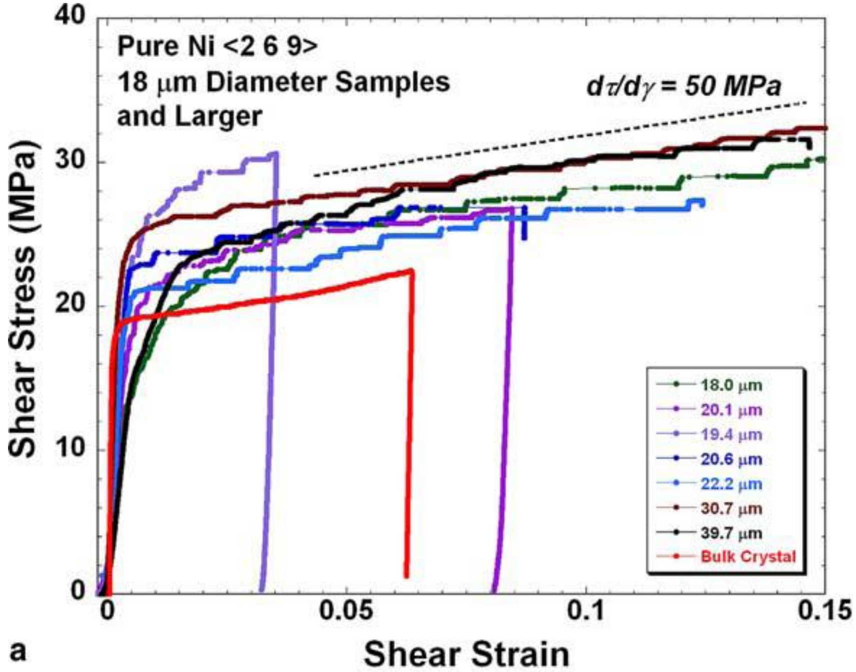
  - Random variations of cell yield stress (Gaussian distributed random variables with mean $\langle \sigma_y \rangle$ and variance $\delta\sigma_y^2$)
  - The coefficient of variation $CV = \delta\sigma_y / \langle \sigma_y \rangle$ is taken larger for larger diameters to take into account the pronounced difference from the mean
  - Constitutive relation: $\sigma_{EXT} - \beta\varepsilon^p + \beta\ell^2 \dfrac{d^2\varepsilon^p}{dx^2} = \sigma_y$

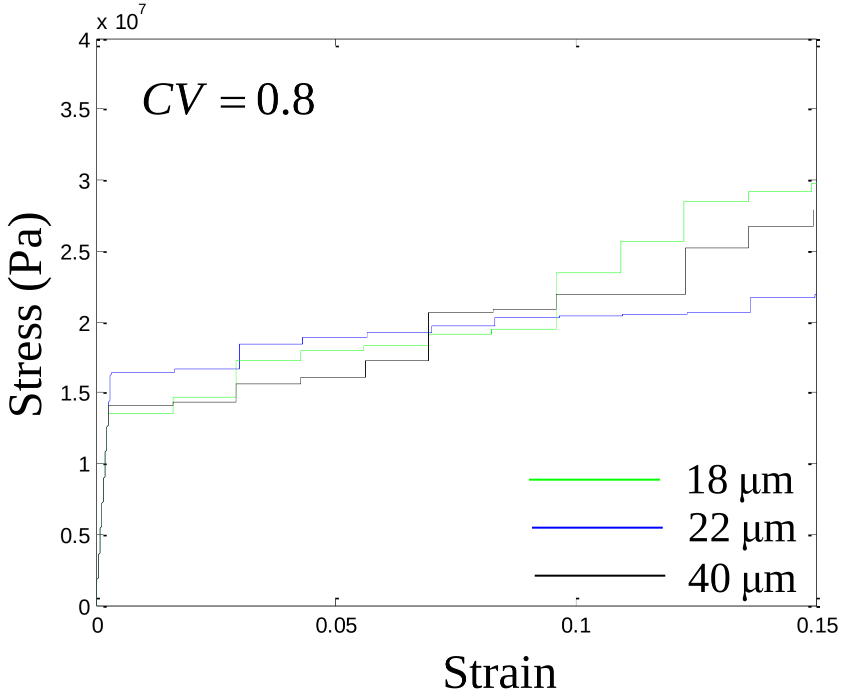
- Simulation Procedure

  - "Force controlled" simulations. External force f_{EXT} increased from 0 by steps of Δf
  - External stress at each cell $\sigma_{EXT} = f_{EXT} / \left(\pi r^2\right)$
  - Cells yield when $\sigma_{EXT} + \sigma_{INT} > \sigma_y$. Increase of cell strain by $\Delta\varepsilon$
  - Compute again internal stresses. Repeat until new stable configuration. Record values of σ_{EXT} and mean strain
  - Repeat the whole procedure until a certain strain level

Cellular Automaton Results

$$\langle \sigma_y \rangle = 81\,\text{MPa}; \qquad \beta = 6.4\,\text{GPa}; \qquad \ell = 0.9\,\mu\text{m}; \quad \Delta f = 0.08\,\mu\text{N}; \quad \Delta\varepsilon = 0.4;$$





AN APPENDIX ON ENTROPY & POWER LAWS

- Boltzmann-Gibbs Entropy

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

- Tsallis Entropy

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

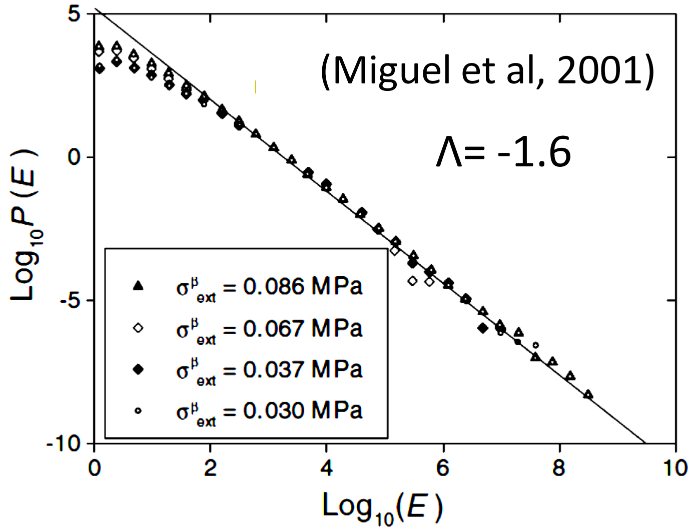
- Exponential Relaxation

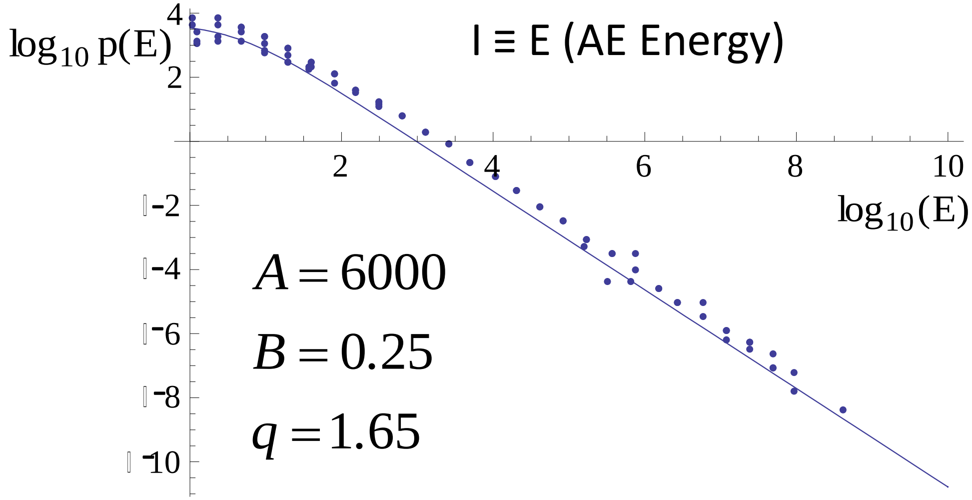
$$\frac{d\xi}{dt} = -\lambda_1 \xi \rightarrow \xi = e^{-\lambda_1 t} \quad ; \quad \lambda \geq 0 \; :$$ Lyapunov exponent

- Presence of fractality $\quad \frac{d\xi}{dt} = -\lambda_q \xi^q \longrightarrow \xi = \frac{1}{\left[1 + (q-1)\lambda_q t\right]^{\frac{1}{q-1}}}$

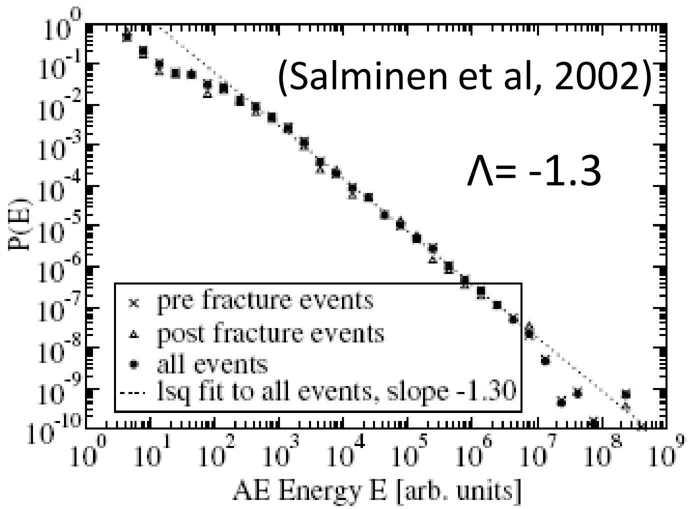
$\therefore \quad p(I) = \frac{A}{\left[1 + B(q-1)I\right]^{1/(q-1)}}$ (instead of $p(I) \sim I^{-\Lambda}$ as commonly done)

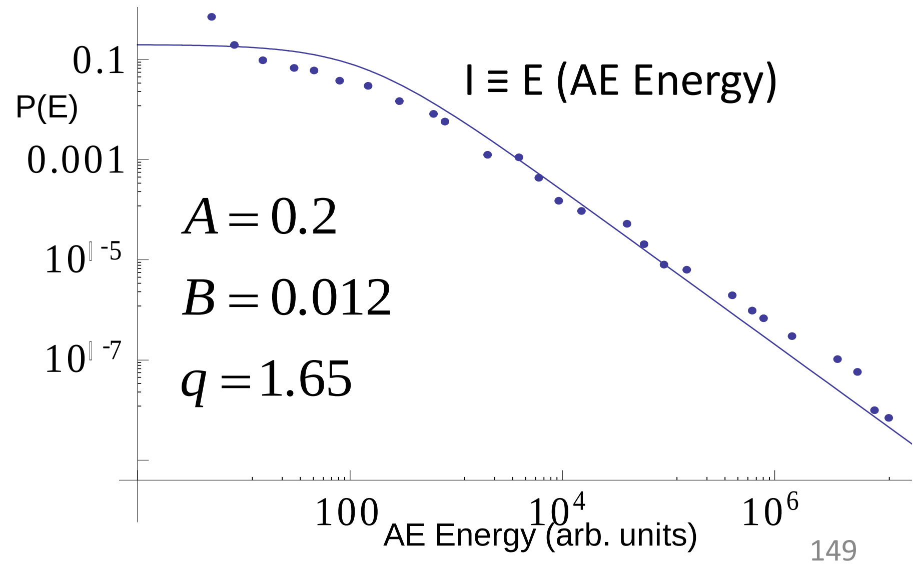
- Acoustic emission during creep of ice single crystals



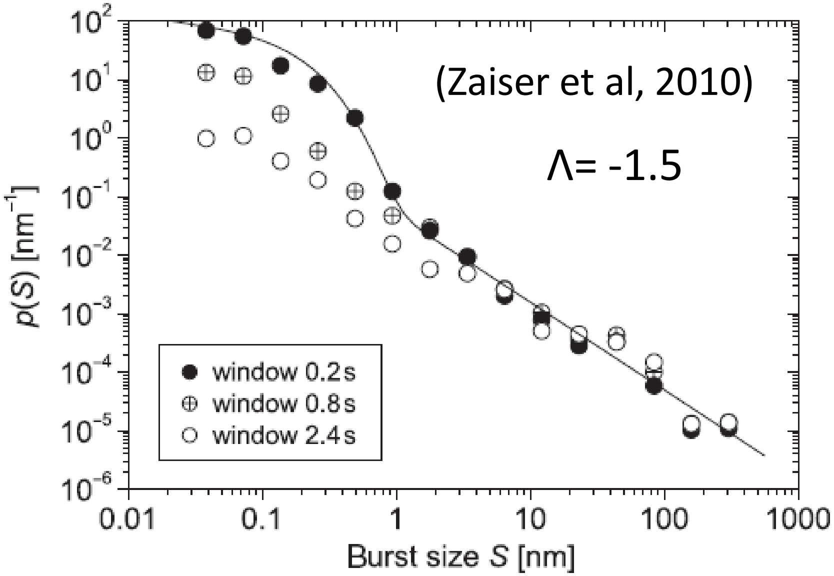


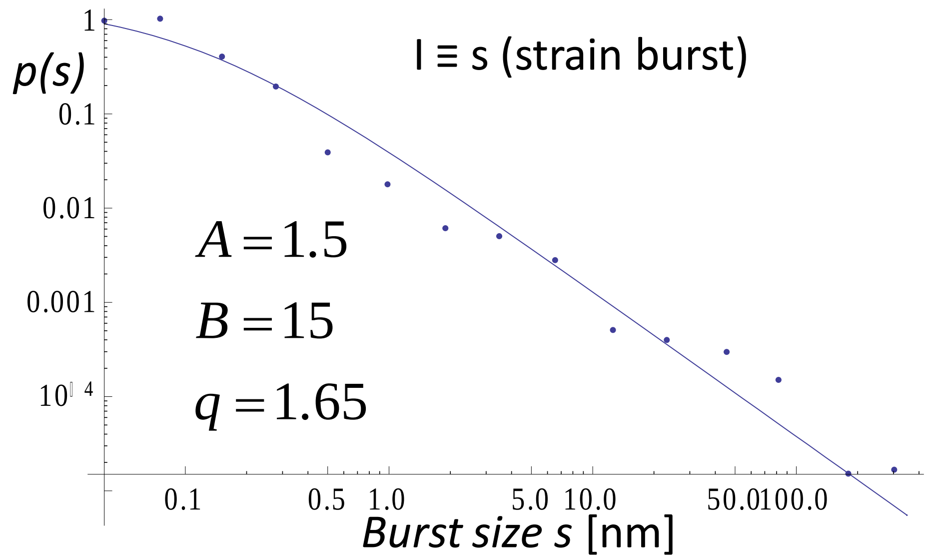
- Acoustic emission during paper fracture



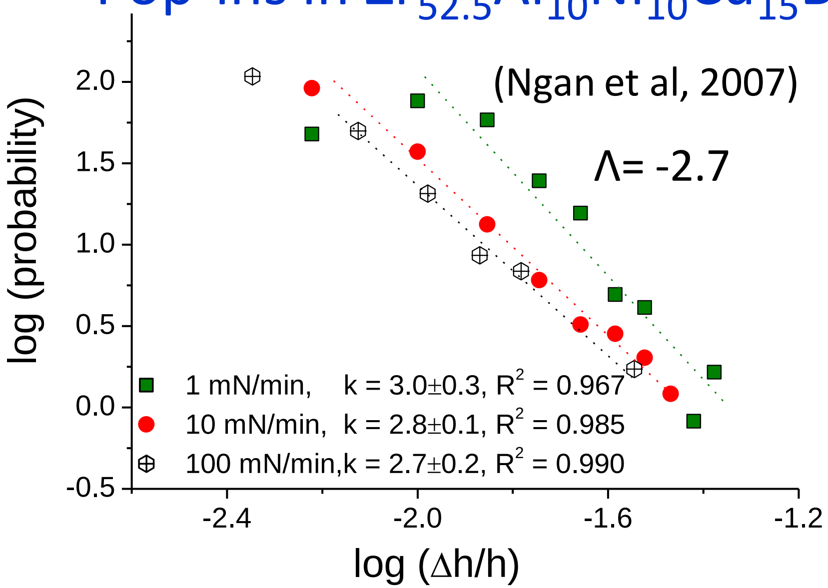


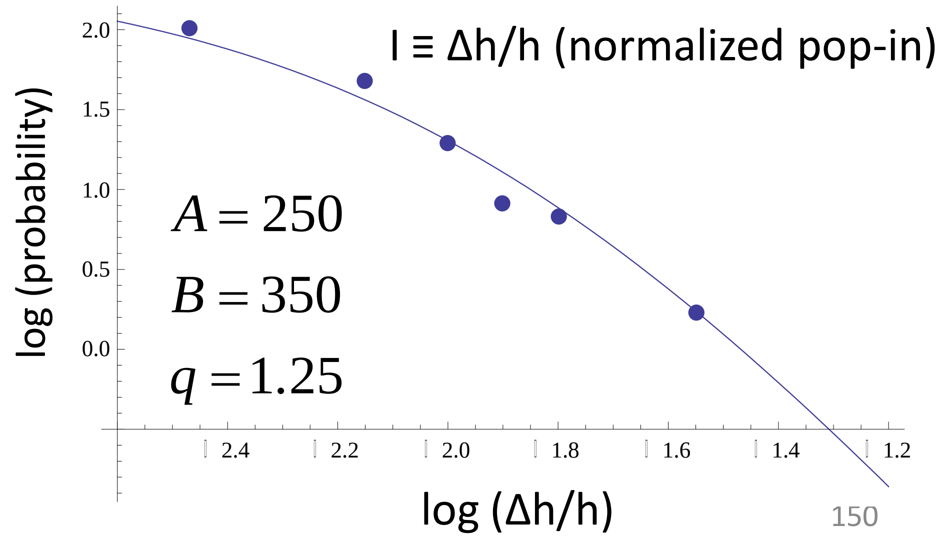
- Strain bursts in Mo micropillars under compression





- Pop-ins in $Zr_{52.5}Al_{10}Ni_{10}Cu_{15}Be_{12.5}$ glasses under indentation





- Slip Avalanches

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

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