ECA 1975-2015: A 40-year Academic/Life Journey

■ Pre-Academic/Formative Years

- ***1950-1967: High-School Education, Lamia, Greece***
  - ***Influences:***
    - Grand Father: Blacksmith Hard Working till 77
    - Father: Police Officer – Discipline vs. Liberalism
    - Mother/Grand Mother: Unconditional Love
    - Physics High School Teacher: Give Lectures for him
    - Math High School Teacher: Lessons Beyond Classroom
    - French High School Teacher: Encourage Poetry Writing
- ***1968-1973: Metallurgy & Mat. Sci. Nat. Techn. Univ. Athens***
  - ***Influences:***
    - Metallurgy Prof. Mousoulos/Academician: Arrange for interships to Finland/Belgium/Yugoslavia
    - Materials Science Professor Konofagos/Rector-Minister: Arrange for publishing my Poetry Book "Quest" in 1973/5000 copies
- ***1973-1975: PhD Chem. Eng. & Materials Sci. Univ. of Minnesota***
  - ***Influences:***
    - W.W. Gerberich/Advisor Materials Science
    - R. Fosdick/Co-Advisor Continuum Mechanics
    - N. Xystris and D. Beskos/G. Stephanopoulos: Graduating PhD and Starting Assistant Professors, respectively

■ Academic Posts

- ***1976-80: Assist. Prof. Univ. of Illinois Urbana-Champaign***
  - ***Influences:***
    - R. Shield, Chairman: Scientific conflicts
    - PhD Students: **D. Bammann**, D. Unger, P. Taylor, R. Wilson, M. Kahled and Visiting Scholars: N. Xystris and J. Hill ⇒ Great support/understanding
    - Cliff Astill: NSF Program Manager – 3 NSF Grants (simultaneously)
    - Maria Balogiannis/Aifantis: Lost **Marilia** during delivery
- ***1980-82: Visiting Prof. Univ. of Minnesota***
  - ***Influences:***
    - Jim Serrin – Regents Professor: Great Mentor
    - Rutherford Aris – Regents Professor: Unexpected Supporter
    - Bill Gerberich – Former Advisor: Offer Visiting Appointment
    - Dick Oriani – Director: Attended my Graduate Course Lectures
- ***1982: Michigan Tech (MTU), Full Professor with Tenure***
  - ***Influences:***
    - President Dale Stein – Materials Sci./US Academy of Engineering ⇒ Made it possible bending the MTU Bylaws
    - Mechanics Director Predebon, Chairmen Lord/Johnson
    - Deans: Krueger/Sikarskie/Kunz
    - Colleagues: W. Milligan/S. Hackney
- ***1990: Aristotle Univ., Prof. of Mechanics after Special Invitation***
  - ***Influences:***
    - Chairman/Director: G. Lazarides/N. Charalambakis
    - Rector: A. Mantis

■ Other Major Influences

- ***Nobel Laureate:*** Ilya Prigogine
- ***Continuum Mechanics Guru:*** Morton Gurtin
- ***Best/most dedicated PhD Students:*** **D. Bammann**, H. Zbib/T. Webb, **I. Tsagrakis**, **A. Konstantinidis**
- ***Closest Senior Collaborators:*** J. Serrin, D. Walgraef, **Y. Dafalias**, E. Gdoutos, D. Beskos/N. Triantafyllidis, S. Hackney/W. Milligan, I. Ovidko/**A. Romanov**, I. Vardoulakis/H. Muhlhaus, G. Frantziskonis/G. Voyiadjis, **K-Y. Xu**, **C. Qi**
- ***Closest Younger Collaborators/Post Docs:*** C. Ru, M. Gutkin, J. Ning, B. Altan, M. Zaiser, H. Askes, M. Lazar
- ***Current Collaborators/Post Docs:*** **A. Chattopadhyay**, **M. Mousavi**, C. Bagni/**D. Toennies**, G. Efremidis/M. Avlonitis, R. Yang/Y. Chen/Y. Yue, V. Tarasov
- ***Additional Strong Supporters/Co-authors & Mentors:*** E. Hart/J.C.M. Li/F. Nabarro, K. Valanis, **J. Kratochvil**/O. Dillon, L. Kubin/Y. Estrin, R. De Borst/B. Sluys, S. Forest/P. Steinmann/G. Maugin, J. Rice/J. Hutchinson/J. Willis, C. Polizzotto, Y. Bai/W. Yang, **J. De Hosson**, **V. Berdichevski**, **N. Morozov**, **I. Groma**, **A. Ngan**

■ Major Contributions to Early Careers of Excellent Researchers

• *Scientific Mentorship*

H. Zbib (Professor and Head - Washington State University - USA), **D. Bammann** (Professor - Mississippi State University/formerly at Sandia Labs - USA), D. Unger (Professor - University of Evansville - USA), A. Neimitz (Professor and Vice-Rector – Kielce University – Poland), C. Ru (Professor – Alberta – Canada), M. Zaiser/Edinburgh (Professor and Head), H. Askes/Sheffield (Professor and Head), M. Gutkin/St. Petersburg, M. Seefeldt/Leuven, M. Lazar/Darmstadt, **K.-Y. Xu** (Professor - Shanghai University - China), **X. Zhang** (Lecturer - Southwest Jiaotong University - China), I. Chasiotis (Associate Professor - University of Illinois at Urbana-Champaign - USA), I. Mastorakos (Research Professor - Washington State University - USA), K. Kalaitzidou (Assistant Professor - Georgia Tech - USA), **A. Konstantinidis** (Assistant Professor - Aristotle University of Thessaloniki - Greece), M. Avlonitis (Lecturer - Ionion University - Greece), G. Efremidis (Lecturer - University of Thessaly - Greece), **I. Tsagrakis** (Part time Lecturer - University of Crete - Greece). [Shorter term visitors through TMR/RTN fellowships in Academia include: M. Ferro/Torino, C. di Prisco/Milano, N. Pugno/Torino, P. Cornetti/Torino, G. Ribarik/Budapest, H.-P. Gänser/Leoben, P. Grammenoudis/Darmstadt, J.V. Andersen/Paris. Others in Research Institutions/Industry include: V. Gruetzun, F. Hagemann, Th. Putelat, G. Rambert, F. Tzschicholz.]

• *More …*

K. Aifantis (Arizona); N. Pugno (Trento); ERC Starting Grant Recipients in 2008 & 2011
(Lab Visitors at AUT)
A. Konstantopoulos: ERC Senior Grant Recipient – Director of CERTH
(Master Student at MTU – later Lab Visitor at AUT)

■ Other Notables

- Int. Symposium on Mechanics of Dislocations (ECA/Hirth), MTU 1983
- 1 mo Visit to USSR/US Academy of Sciences, 1986
- International Conference on Mechanics, Physics and Structure of Materials – "*A Celebration of Aristotle's 23 Centuries*", AUT ,1990
- 1 mo Visit to Japan/Japanese Government, 1996
- *Joint ASME/ASCE/SES Symposium* Organized in ECA's honor, Baton Rouge, 1-3 June 2005
- Adjunct Distinguished Professor/King Abdulaziz University – Jeddah, 2011-13
- Visiting Foreign Expert/ITMO University – St. Petersburg, 2014-15
- Distinguished Foreign Scientist/Southwest Jiaotong Univ. – Chengdu, 2015
- Included in the ISI Web of knowledge list of most highly cited authors in the world: ENGINEERING (3rd entry no. A0086-2010-N out of 262) [citations: ~8000, h-index 43 (SCOPUS), ~8100, h-index 44 (ISI)]
- Listed in G.A. Maugin's *Continuum Mechanics Through the Twentieth Century*, 2013, p. 157 (along with late Academicians P. Theocaris and P. Panagiotopoulos)

■ A McMat Symposium for ECA's 55

2005 Joint ASCE/ASME/SES Conference on Mechanics and Materials

June 1 – 3, 2005
Baton Rouge, Louisiana

McMat 2005

MECHANICS & MATERIALS CONFERENCE

Symposium Honoring the Contributions of Elias Aifantis

Organizers: Douglas J. Bammann, Hussein M. Zbib, Petros Sofronis

Every four years, the engineering mechanics and materials communities of the American Society of Civil Engineers (ASCE), the American Society of Mechanical Engineers (ASME), and the Society of Engineering Science (SES) hold a joint conference. In 1997, it was held at Northwestern University in Evanston, Illinois, and in 2001, it was held at University of California in San Diego, La Jolla, California. The 2005 Joint ASME/ASCE/SES Conference on Mechanics and Materials (McMat2005) will be held in Baton Rouge, Louisiana, on June 1-3, 2005. Activities will be hosted by Louisiana State University with Professor George Z. Voyiadjis as the Conference Chair. This important conference offers an exciting exchange of information that comes about through the congress of three major engineering mechanics and materials communities.

This special symposium within the McMat2005 conference is organized to recognize the contributions of Professor Elias Aifantis in the fields of mechanics and materials. In particular, the areas associated with diffusion-reaction theory, gradient theory, mixture theory and hydrogen embrittlement, plasticity and material instability.

Conference Location and Organization

McMat2005 will be held at the Holiday Inn Select located adjacent to Interstate I-10 in the middle of a new bustling area of Baton Rouge. Activities will be hosted by Louisiana State University, and many faculty and students are heavily involved with organizing the conference.

For more information, visit the conference web site at **www.McMat2005.eng.lsu.edu**. The full program and registration information should be available soon.

ASCE
American Society of Civil Engineers

ASME
SETTING THE STANDARD
1880 — 2005

■ **Most Significant Achievements**

- ***According to Berdichevsky***

  Katerina Aifantis/Daughter - Scientist

- ***According to Katerina***

  Elias Aifantis/Son - Musician

- ***According to me***

  Their Mother Maria Balogiannis/Aifantis

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

By Marcia Goodrich

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

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

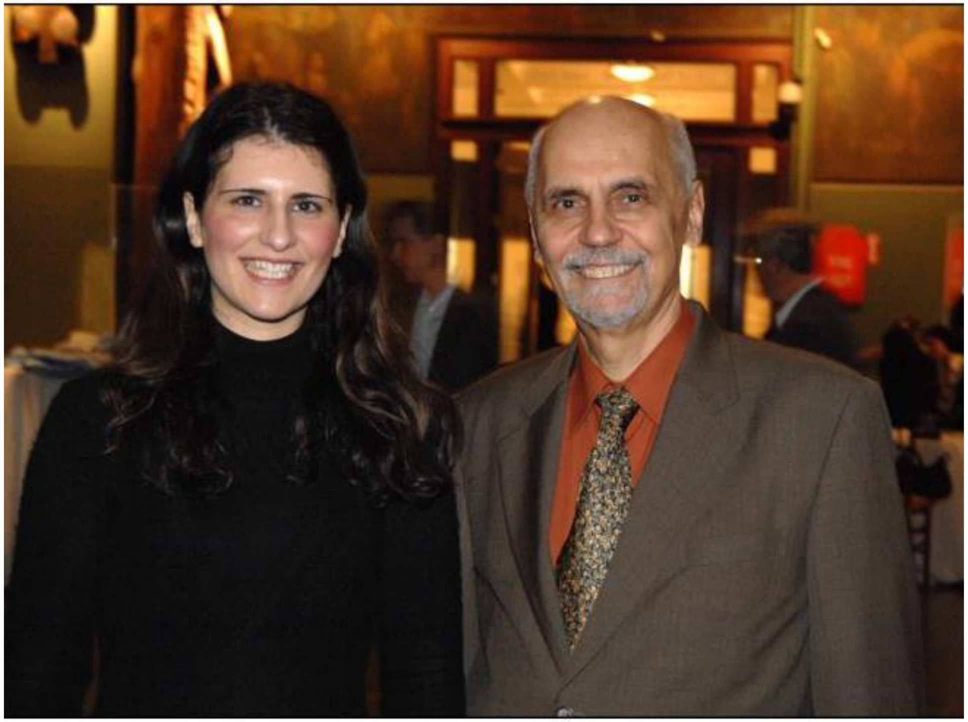
"She just beat everyone in the class," remembers Associate Professor Paul Charlesworth. "She's one of the finest students to ever take my general chemistry course."

ERC STARTING GRANT

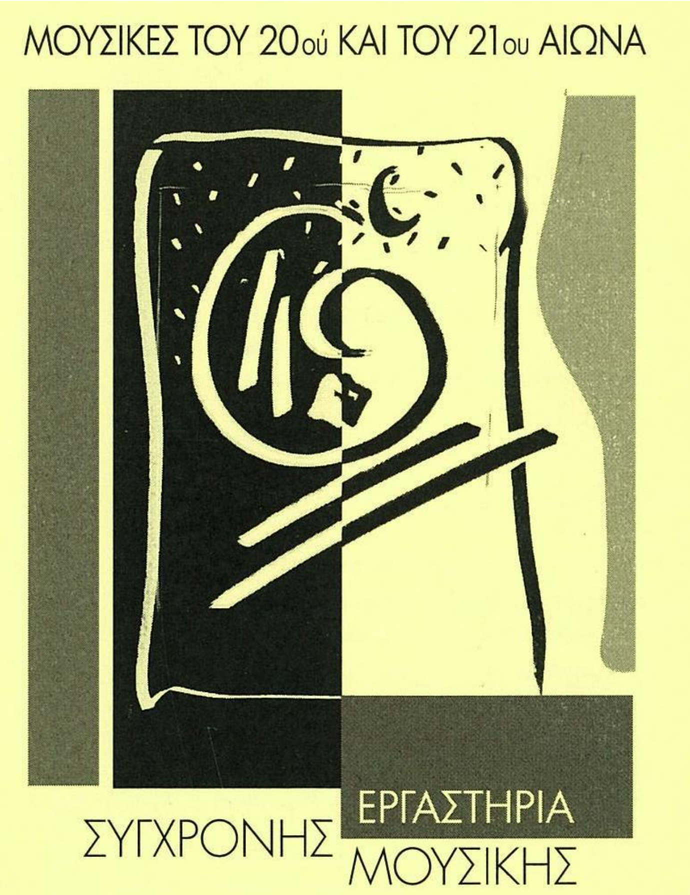
Probing the Micro-Nano Transition (MINATRAN): Theoretical and Experimental Foundations, Simulations and -Applications [1.3 Million Euros]

2008-2013

Dr. Potocnik
European Commissioner for Research



Professor Kafatos
President of ERC



μέγαρο μουσικής αθηνών

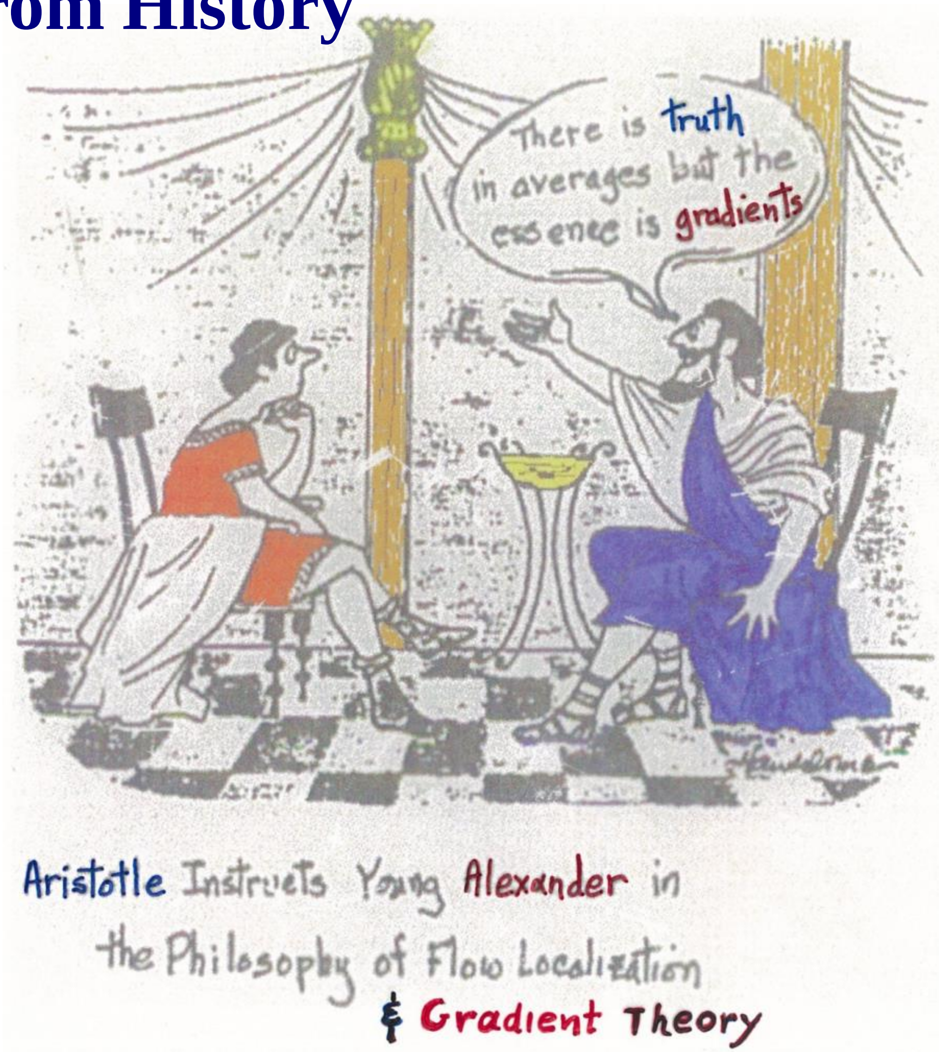
2008-2009

ΜΕ ΤΗΝ ΥΠΟΣΤΗΡΙΞΗ ΤΟΥ ΥΠΟΥΡΓΕΙΟΥ ΠΟΛΙΤΙΣΜΟΥ

Sounds Like Music (2008)

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

■ Motivation from History



❑ Slide from Owen Richmond (US) – Lev Pitaevskii (USSR)

[1990 Int. Conf. on Aristotle's 2300th Birthday]

- 50 USSR out of 300 International Participants
- 3 Chinese Academy Participants

■ Motivation from 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***

E 749: Hera opens the Gates automatically
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?*

Research Highlights

#1. Mechanical Theory of Diffusion (ECA 1980)

$\mathrm{div}\mathbf{T} = \hat{\mathbf{f}}$; $\mathbf{T}$ ... stress tensor of diffusing species

$\hat{\mathbf{f}}$ ... diffusive force

$$\{\mathbf{T}, \hat{\mathbf{f}}\} \rightarrow \{\rho, \nabla\rho, \nabla\dot{\rho}, \nabla^2\rho \ldots\}$$

$\Rightarrow$ Diffusion Classes/Non-universality of Fick Law

- $\dot{\rho} = D\nabla^2\rho$ ... Fick/parabolic
- $\dot{\rho} = D\nabla^2\rho + \bar{D}\nabla^2\dot{\rho}$ ... Barenblatt/pseudoparabolic
- $\dot{\rho} = D\nabla^2\rho - E\nabla^4\rho$ ... Cahn/spinodal
- $\dot{\rho} = (D + N\sigma)\nabla^2\rho - M\nabla\sigma \cdot \nabla\rho$ ... Cottrell/stress-assisted diffusion
- $\left\{\begin{aligned} \dot{\rho}_1 &= D_1\nabla^2\rho_1 + \kappa_1\rho_1 + \kappa_2\rho_2 \\ \dot{\rho}_2 &= D_2\nabla^2\rho_2 - \kappa_1\rho_1 - \kappa_2\rho_2 \end{aligned}\right\}$ ... 2ble Diffusion
- $\dot{\rho} + \tau\ddot{\rho} = D\nabla^2\rho + \bar{D}\nabla^2\dot{\rho} - E\nabla^4\rho$ ... Higher Order Diffusion/Nanodiffusion

• ***Higher-order Diffusion Equation***

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

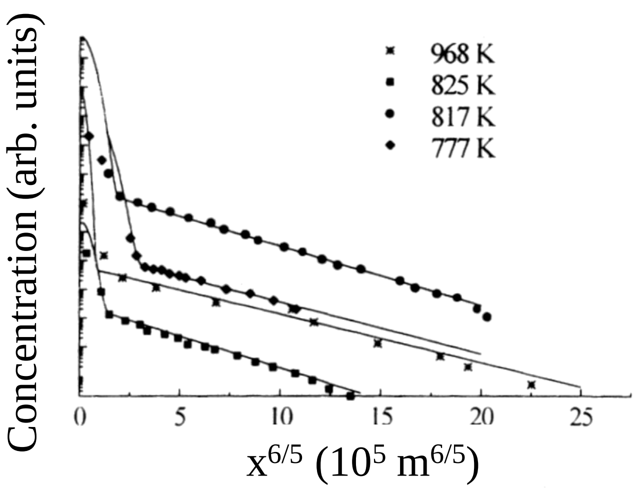
$$\tau = (\kappa_1 + \kappa_2)^{-1} \;,\; D = \tau(\kappa_1 D_2 + \kappa_2 D_1) \;,\; \bar{D} = \tau(D_1 + D_2) \;,\; \mathrm{E} = \tau D_1 D_2$$

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

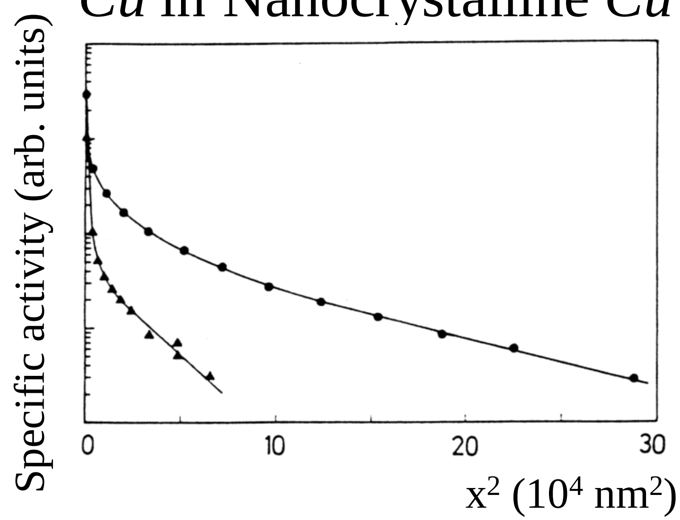
$$= f\, D_1 + (1 - f)D_2$$

- *Diffusion Penetration Profiles*

^{64}Cu in Polycrystalline Cu



^{67}Cu in Nanocrystalline Cu



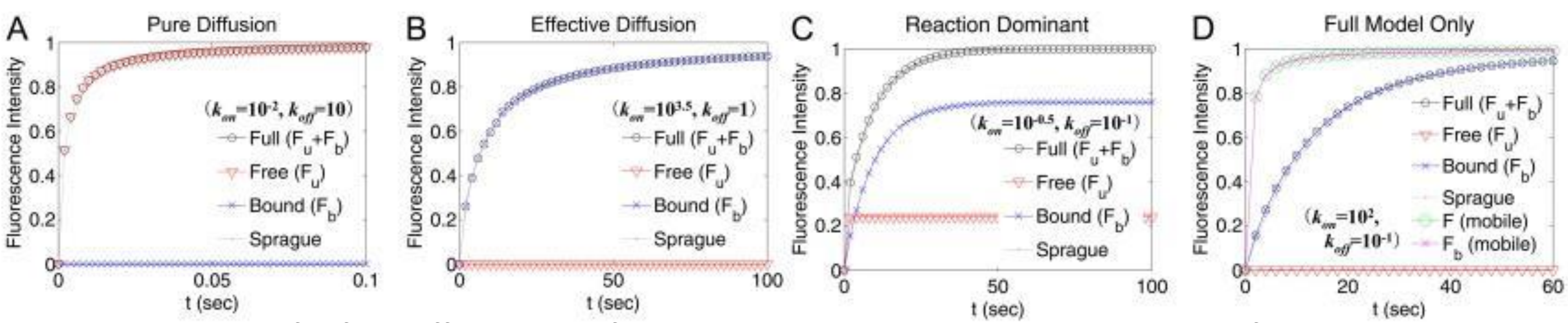
- **Rutherford Aris:** On the Permeability of Membranes with Parallel but Interconnected Pathways [*Math. Biosci.* **77**, 5-16 (1985)]

*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)]

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



(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***

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

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

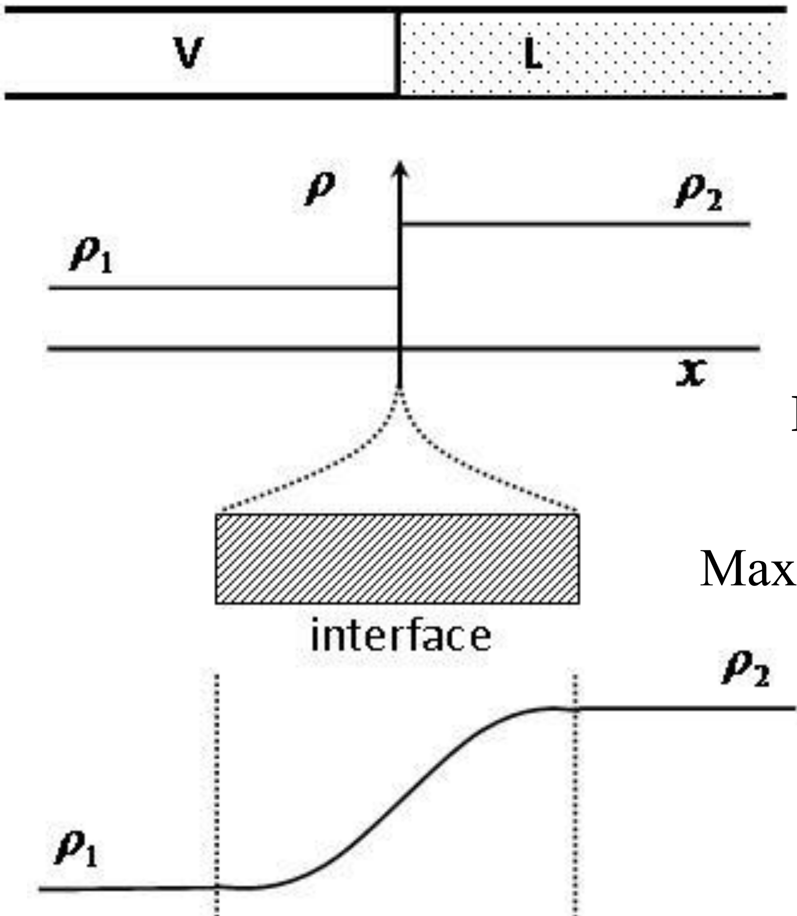
T_e ... temperature of electron gas; T_i ... temperature of ions/phonon bath

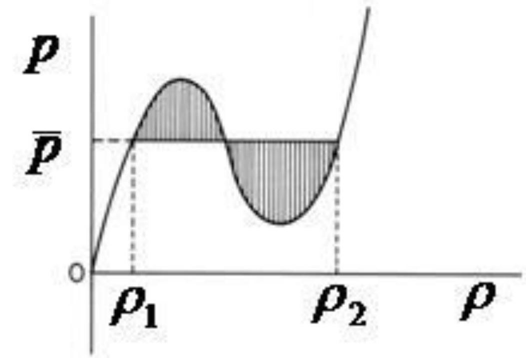
#2. Mechanical Theory of Interfaces (ECA & Serrin 1982)

- ***Revisit Van der Waals/Maxwell's Thermodynamics***

$$\mathrm{div}\,\mathbf{T} = \mathbf{0}$$

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





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

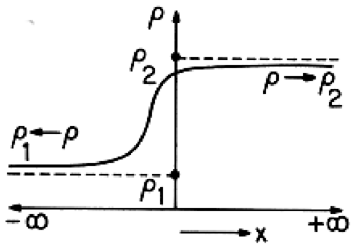
Maxwell's Rule (MR): $\displaystyle\int_{\rho_1}^{\rho_2}\left[p(\rho) - \bar{p}\right]\frac{d\rho}{\rho^2} = 0$

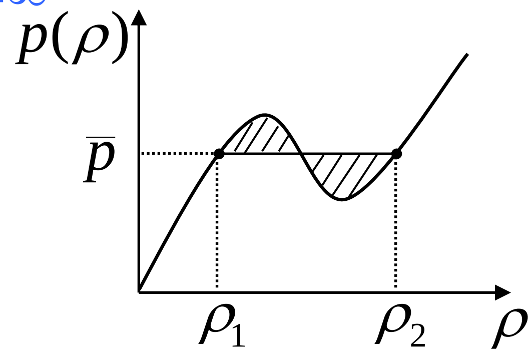
$$1/\rho^2 \rightarrow E(\rho) = \frac{1}{a}\exp\left(2\frac{b}{a}d\rho\right)$$

$$a = \alpha + \gamma\,; \quad b = \beta + \delta$$

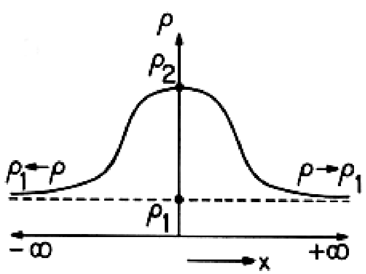
• Planar Interfaces / 1D Profiles

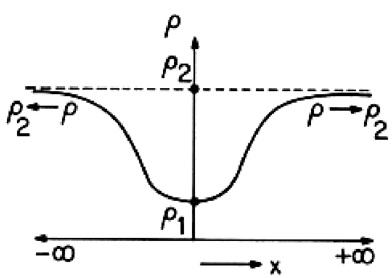
- *Transitions (interfaces)* $\rho \to \rho_{1,2}$ *as* $x \to \mp\infty$

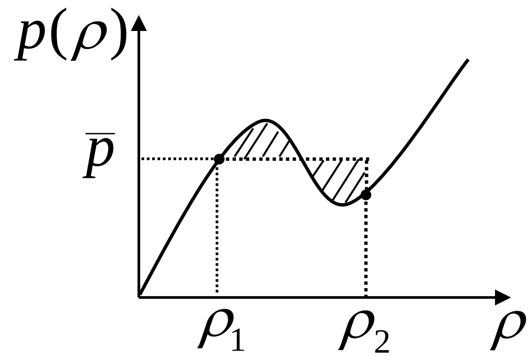




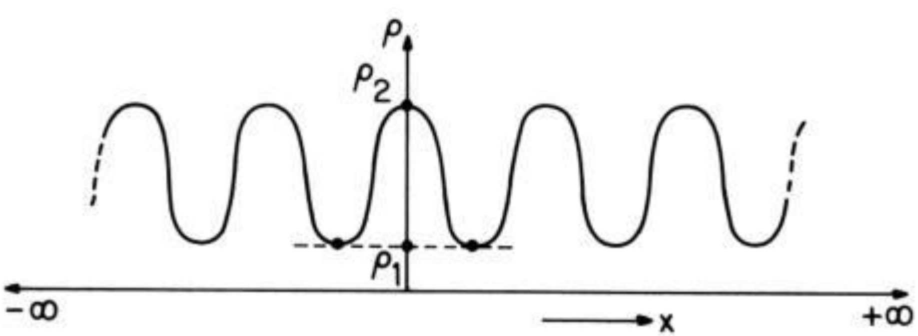
- *Reversals (films)* $\rho \to \rho_1$ as $x \to \mp\infty$

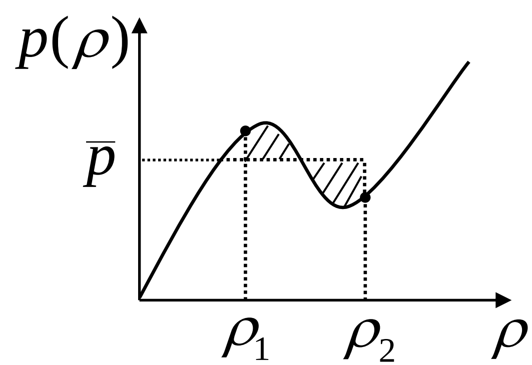






- *Oscillations (layers)*

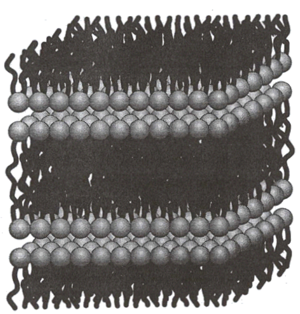




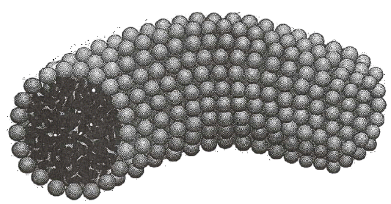
- ***General Interfaces / 3D Structures***

$$\nabla(-p + a\Box\rho + \tilde{b}\left|\nabla\rho\right|^2) = (c\Box\rho)\nabla\rho\,; \quad \begin{cases} \tilde{b} = b + \dfrac{1}{2}\left(c - a\dfrac{c'}{c}\right) \;\ldots\; (\equiv 0 \Rightarrow MR) \\ \Box\rho \equiv \nabla^2\rho + \dfrac{1}{2}\dfrac{c'}{c}\left|\nabla\rho\right|^2 \end{cases}$$

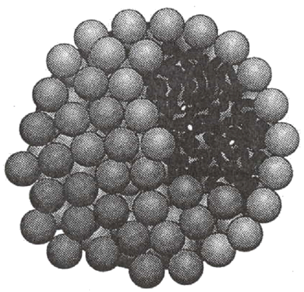
$$\tilde{b} \not\equiv 0 \;\Rightarrow \rho = \rho(x)\,; \qquad \rho = \rho(r)\,; \qquad \rho = \rho(R)$$



layers



cylinders



spheres

Micelle Structures

#3. Gradient Plasticity (Bammann/ECA 1982; ECA 1984)

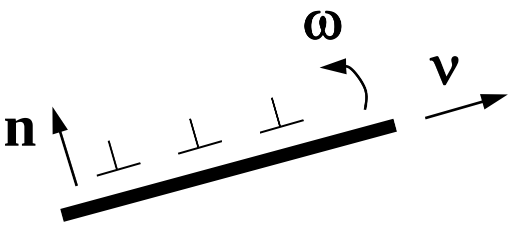
- ***Momentum Balance for Dislocated State***

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

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

- ***Yield Condition***

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



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

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

- ***Scale Invariance Argument***

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

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

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

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

  - $\mathring{\boldsymbol{\alpha}} = \left(\dfrac{\dot{\mathrm{t}}_{\mathrm{m}}}{\dot{\gamma}^{\mathrm{p}}} - \dfrac{\dot{\mathrm{t}}_{\mathrm{n}}\mathrm{t}_{\mathrm{m}}}{\mathrm{t}_{\mathrm{n}}\dot{\gamma}^{\mathrm{p}}}\right)\mathbf{D}^{\mathbf{p}} + \dfrac{\dot{\mathrm{t}}_{\mathrm{n}}}{\mathrm{t}_{\mathrm{n}}}\boldsymbol{\alpha}$ ... Armstrong-Frederick

    $\mathring{\boldsymbol{\alpha}} = \dot{\boldsymbol{\alpha}} - \boldsymbol{\omega}\boldsymbol{\alpha} + \boldsymbol{\alpha}\boldsymbol{\omega}$

    $\boldsymbol{\omega} = \mathbf{W} - \mathbf{W}^{\mathbf{p}}, \quad \mathbf{W}^{\mathbf{p}} = -\dfrac{1}{\mathrm{t}_{\mathrm{n}}}\left(\boldsymbol{\alpha}\mathbf{D}^{\mathbf{p}} - \mathbf{D}^{\mathbf{p}}\boldsymbol{\alpha}\right)$ ... Dafalias Plastic Spin

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

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

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

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

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

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

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

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

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

■ A Note on Consistency with Continuum Thermodynamics

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

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

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

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

Refs

- E.C. Aifantis, On the microstructural origin of certain inelastic models, *Trans. ASME, J. Engng. Mat. Tech.* **106**, 326-330 (1984).
- E.C. Aifantis, The physics of plastic deformation, *Int. J. Plasticity* **3**, 211-247 (1987).
- N.A. Fleck and J.W. Hutchinson, A reformulation of strain gradient plasticity, *J. Mech. Phys. Solids* **49**, 2245-2271 (2001).

■ A Note on Gradient/Laplacian Flow Stress

- ***Adiabatic Approximation for Defect/Dislocation Density***

▪ $\tau = \kappa(\gamma, \alpha) \quad ; \quad \dot{\alpha} = D\nabla^2\alpha + g(\gamma, \alpha) \quad \rightarrow \quad \tau = \kappa^*(\gamma) - c\nabla^2\gamma$

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

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

$$\Rightarrow \quad \tau = \kappa(\gamma) - c\gamma_{xx} \quad ; \quad \kappa(\gamma) \equiv \hat{\kappa}(\gamma) - (\lambda\Lambda/M)\gamma\,, \quad c \equiv \lambda\Lambda D/M^2$$

- ***Non-Local Approximation for Strain***

▪ $\bar{\gamma} = (1/V)\int_V \gamma(\boldsymbol{x}+\boldsymbol{r})dV,\; V = (4/3)\pi R^3 \;\Longrightarrow\; \bar{\gamma} \approx \gamma + \frac{R^2}{10}\nabla^2\gamma\,,\;\; R = d/2$

▪ $\bar{\tau} = \kappa(\bar{\gamma})\,, \quad \tau = \bar{\tau} - \beta\Delta\gamma \quad ; \quad \Delta\gamma = \gamma - \bar{\gamma}$

$$\therefore \quad \tau = \kappa(\gamma) - c\nabla^2\gamma\,; \quad c = Cd^2,\; C = R^2(\beta + h)/10,\; \beta = \alpha\mu(7-5\nu)/15(1-\nu)$$

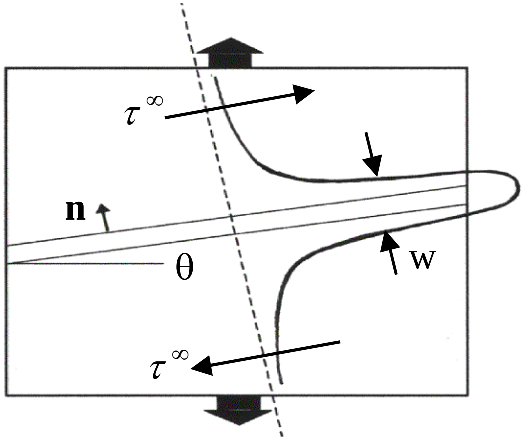
▪ ***Note:*** Maxwell's 1871 Interpretation of the Laplacian

■ A Note on Shear Band Widths/Spacings

- ***Constitutive Eq.***

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

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

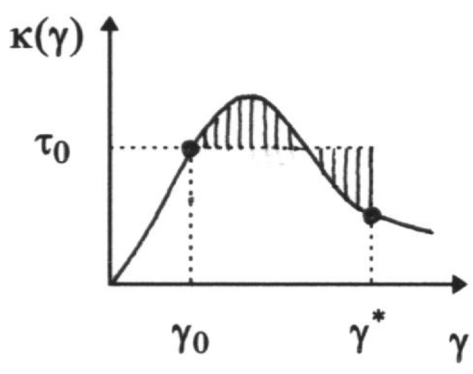


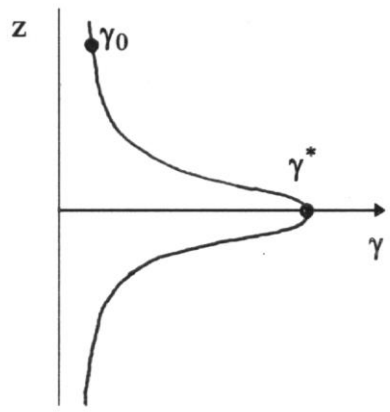
- ***Linear Stability / SB Orientation***

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

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

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

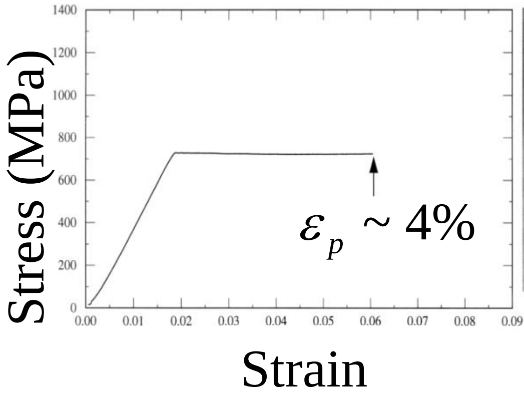


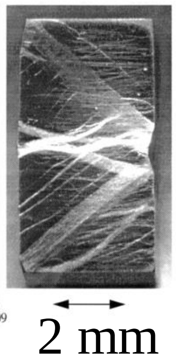


■ A Note on Bulk Nanostructured Fe–10% Cu Polycrystals

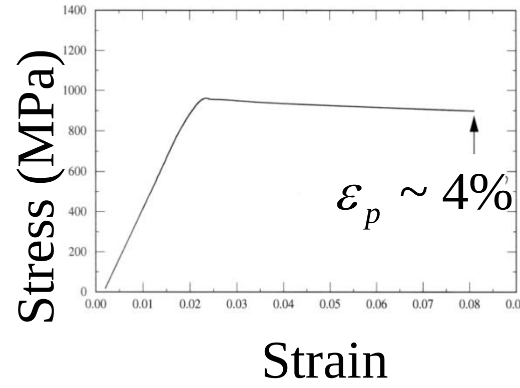
- Compression tests

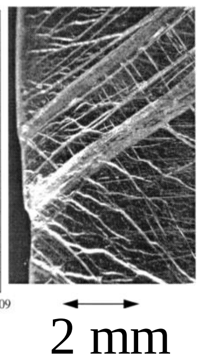
d ~1370 nm, σ_y ~750 Mpa
angle ~ 49^0





d ~540 nm, σ_y ~960 MPa
angle ~ 49^0





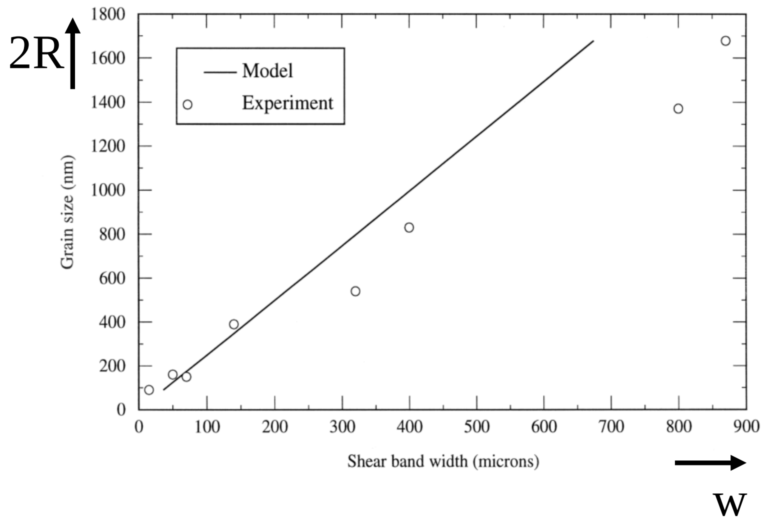
- Shear band width analysis

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

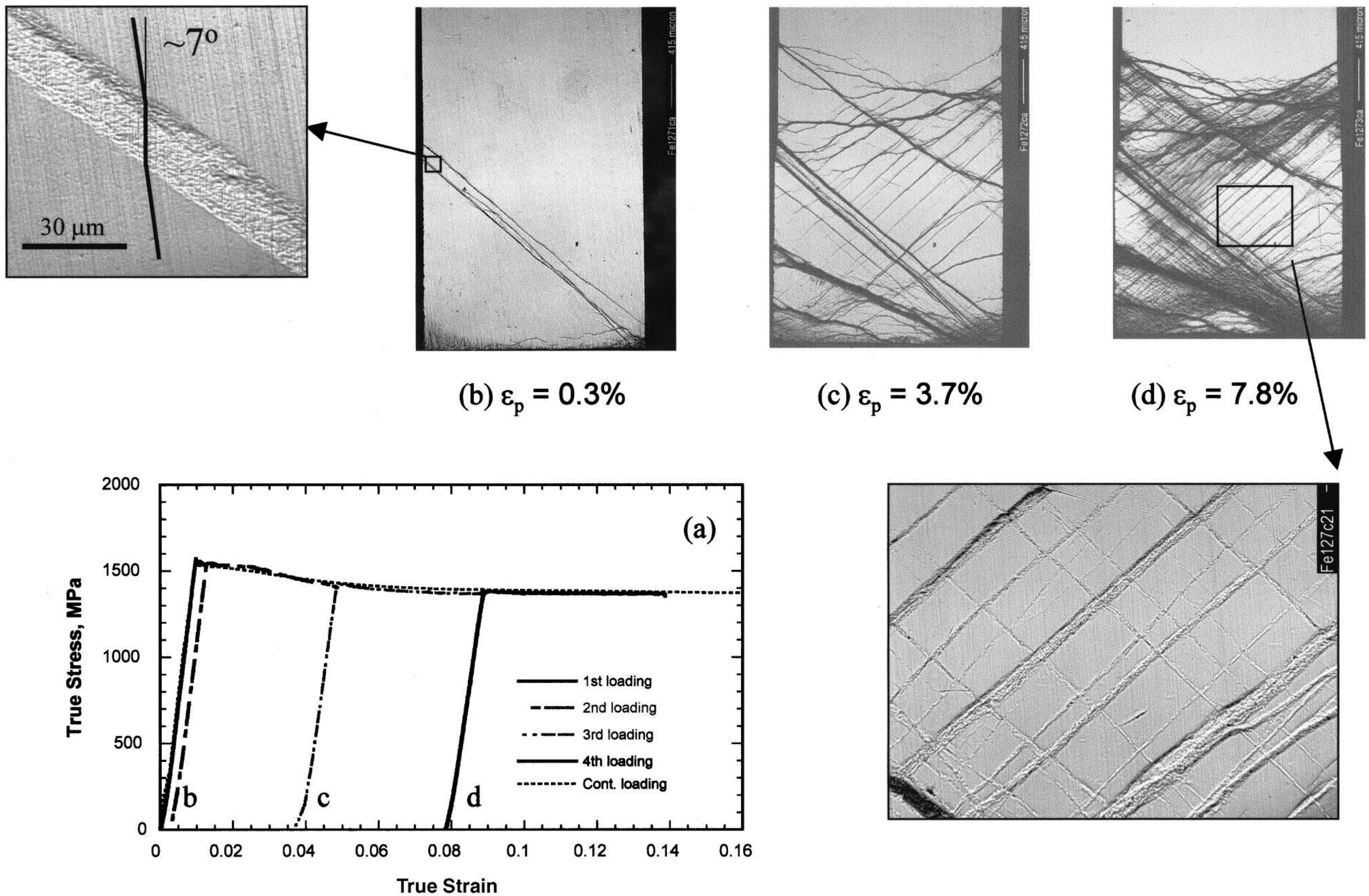
$$w \sim 0.4\sqrt{c}$$

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

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

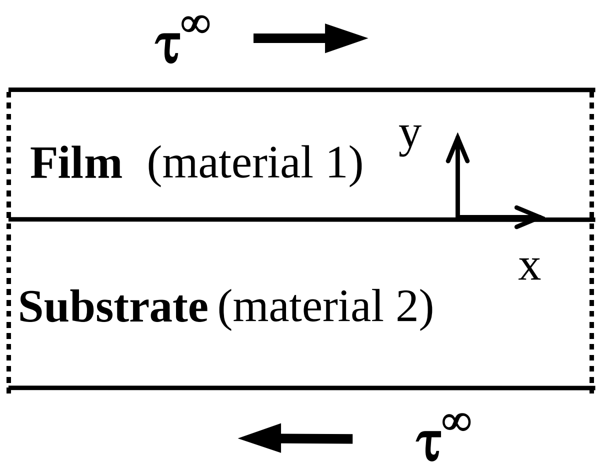


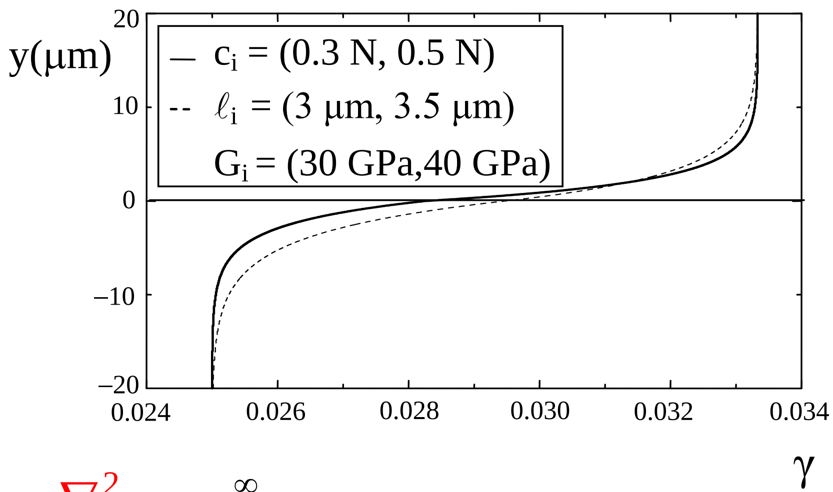
■ A Note on Nano Shear Bands: n-Fe (Ma et al)



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%).

■ A Note on Gradient Solid / Solid Interface





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

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

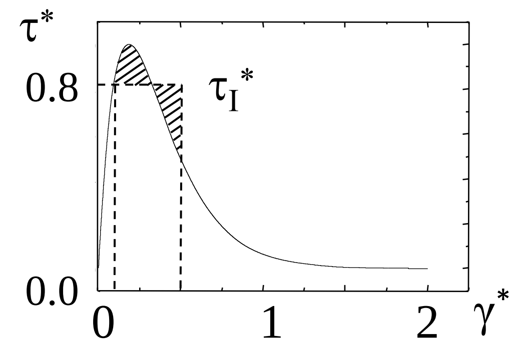
- *Aifantis (1984)* $\begin{cases} \gamma_1 = \gamma_2 \\ \partial\gamma_1 = \partial\gamma_2 \big|_{y=0} \end{cases} \Rightarrow \quad G_I = \dfrac{G_1 G_2\left(\sqrt{G_1/c_1} + \sqrt{G_2/c_2}\right)}{G_1\sqrt{G_2/c_2} + G_2\sqrt{G_1/c_1}}$

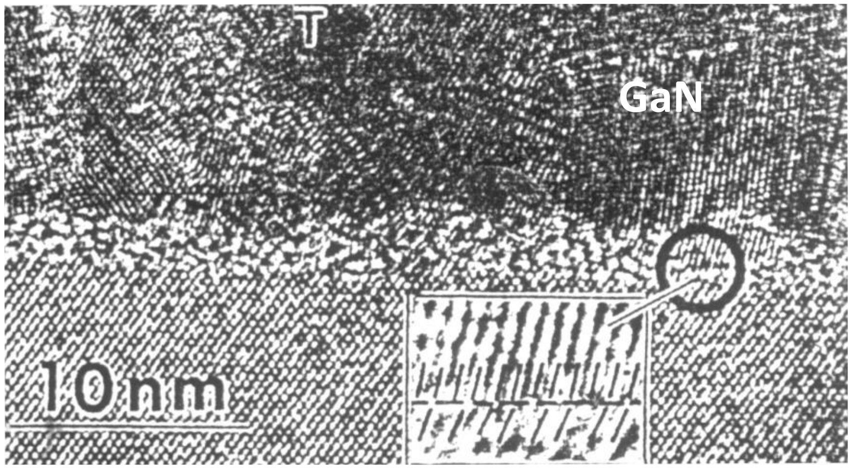
- *Fleck-H (1994)* $\begin{cases} \gamma_1 = \gamma_2 \\ \ell_1\partial\gamma_1 = \ell_2\partial\gamma_2 \big|_{y=0} \end{cases} \Rightarrow \quad G_I = \dfrac{G_1 G_2\left(\sqrt{G_1 c_1} + \sqrt{G_2 c_2}\right)}{G_1\sqrt{G_2 c_2} + G_2\sqrt{G_1 c_1}}$

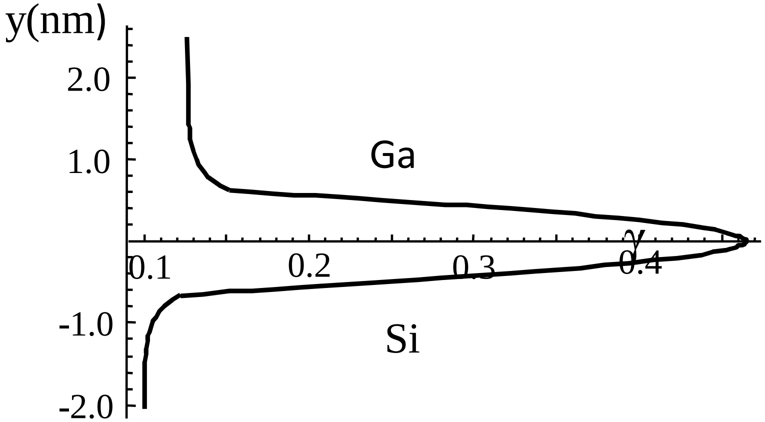
- ***Elastic Bimaterial / Inelastic Interface:*** $\kappa_i = G_i \gamma$; $\tau_I = G_I \gamma_I$

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

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



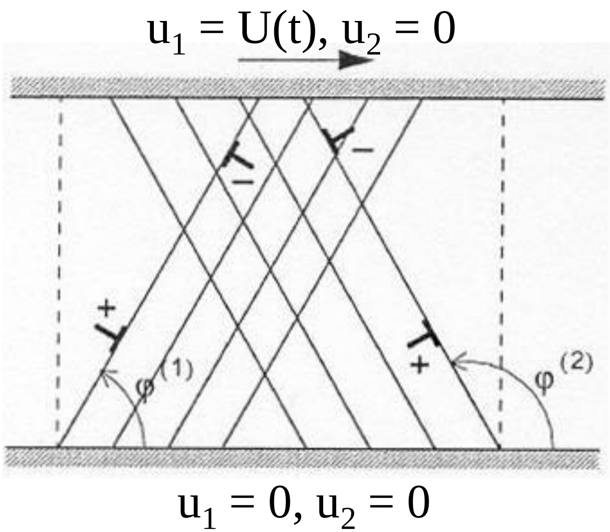


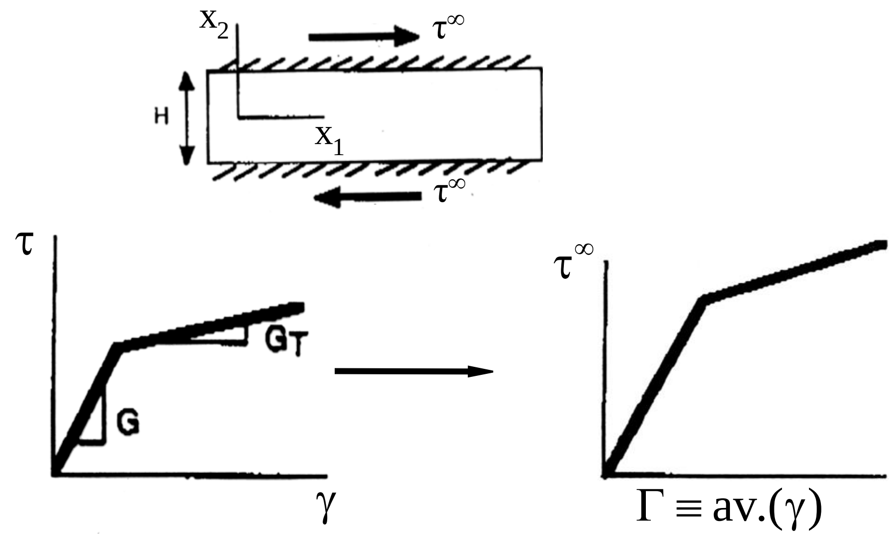


■ A Note on Plastic Boundary Layers

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

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



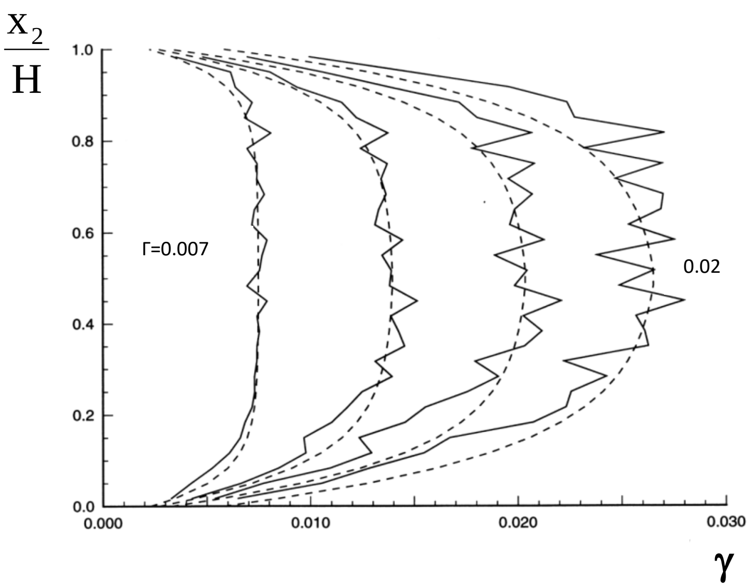


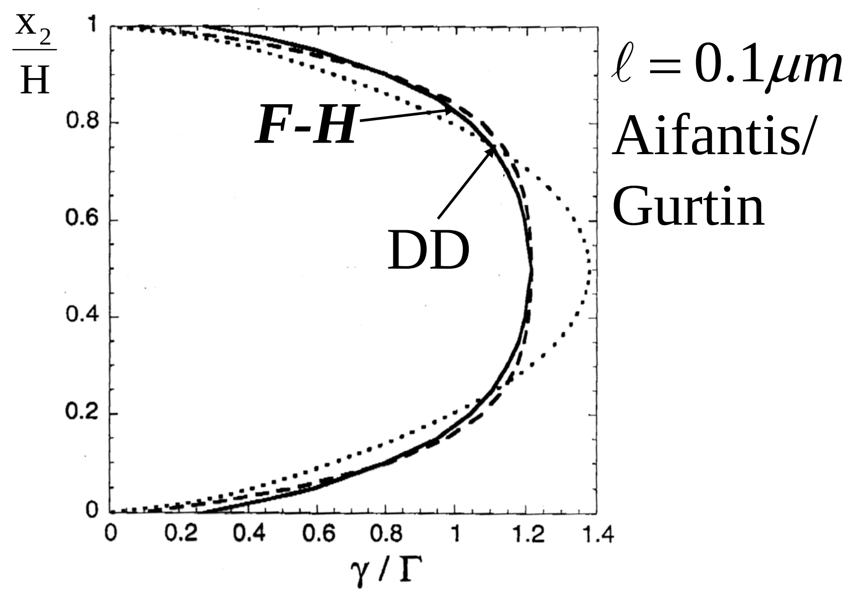
- ***Aifantis (1984) / Gurtin (2000)***

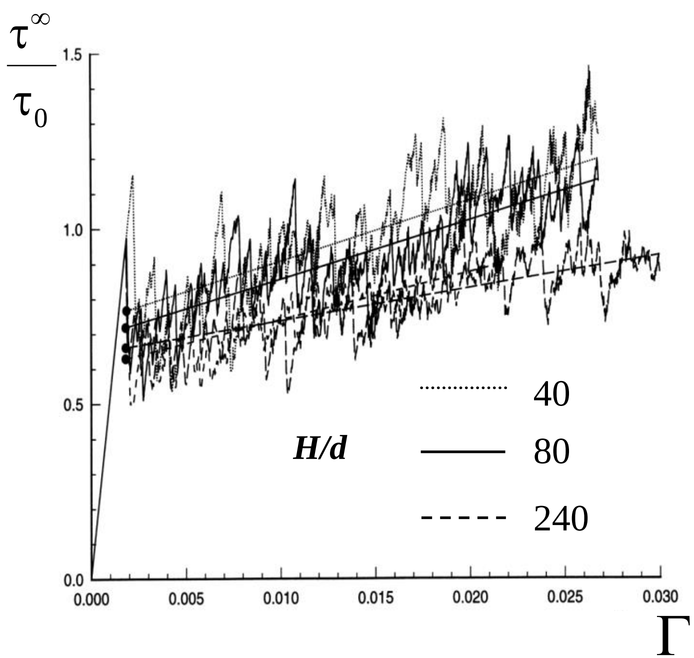
$$\tau = \tau_0 + G_T \gamma - G_T \ell^2 \nabla^2 \gamma = \tau^\infty \quad \Rightarrow \quad \gamma = \frac{\tau^\infty}{G} + \frac{\tau^\infty - \tau_0}{G_T}\left[1 - \frac{\cosh(x_2/\ell)}{\cosh(H/\ell)}\right]$$

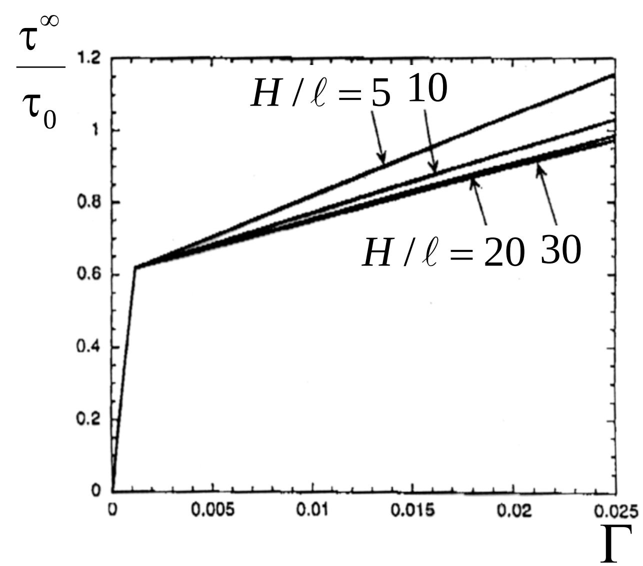
$$\Gamma = \frac{1}{H}\int_{-H/2}^{H/2} \gamma(x_2)\,dx_2 = \frac{\tau^\infty}{G} + \frac{\tau^\infty - \tau_0}{G_T}\left(1 - \frac{2\ell}{H}\tanh\frac{H}{2\ell}\right)$$

• *Plastic Strain Profiles / Size Effects*

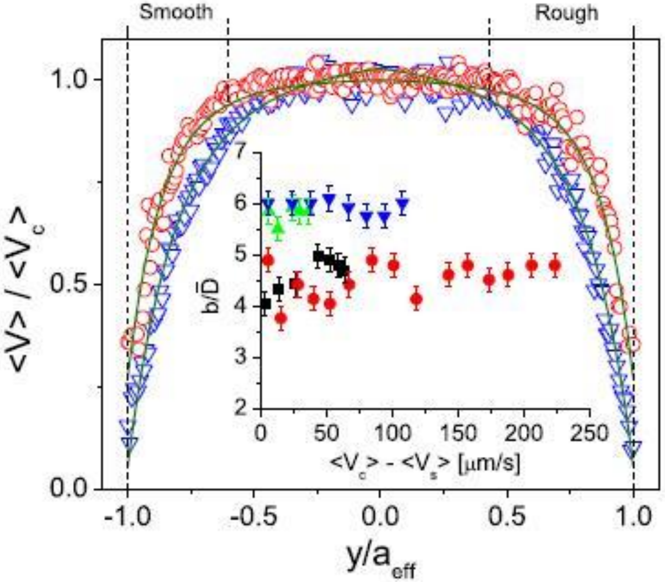






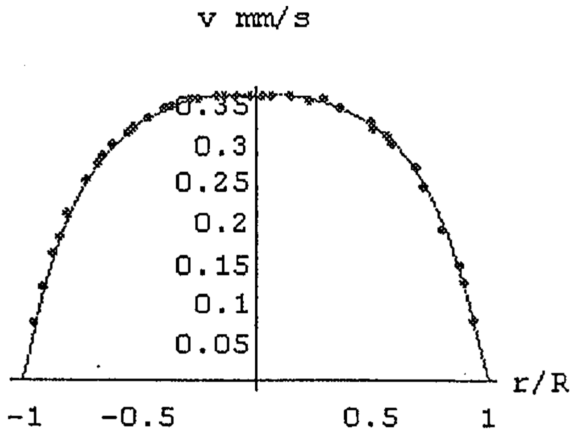


- **L. Isa, R. Besseling & W.C.K. Poon**, Shear Zones in the Capillary Flow of Colloidal Suspensions [*Phys. Rev. Lett.* **98**, 198305 (2007)]



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

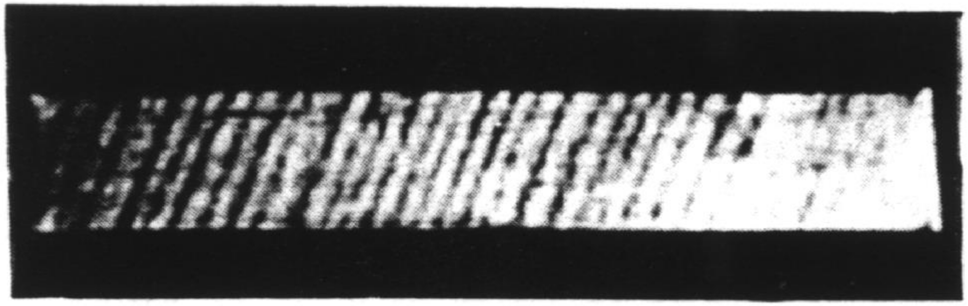
- **Silber et al / Goldsmith & Turitto Experiments on Blood Flow**

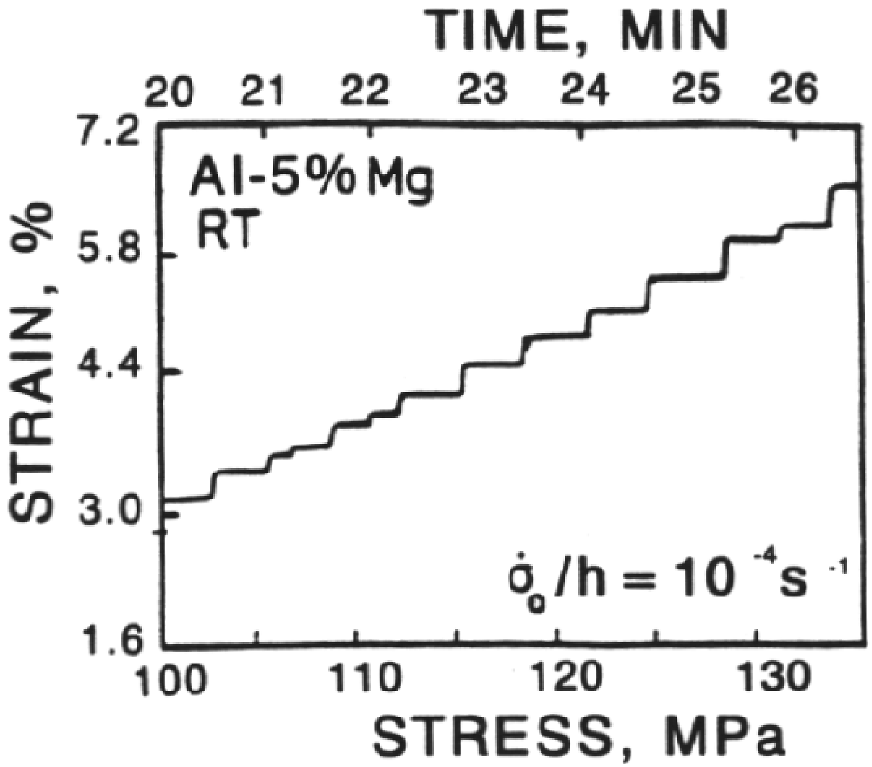


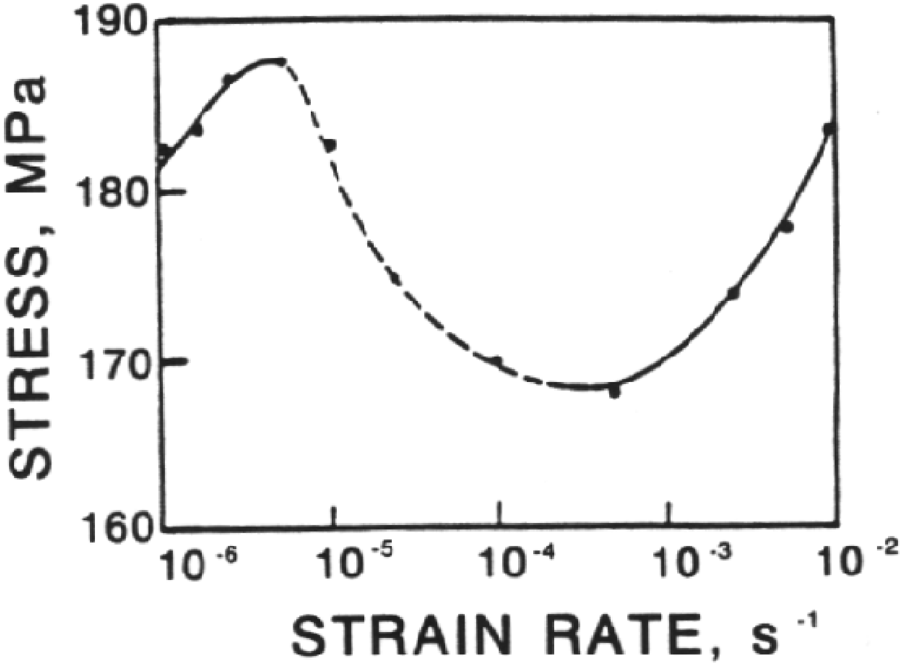
Poiseuille flow of a transparent suspension through circular glass capillaries of R = 51.8 μm Ghost cells and tracer red cells; Hematocrit H = 52%

■ A Note on Portevin-Le Chatelier bands (PLC)

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







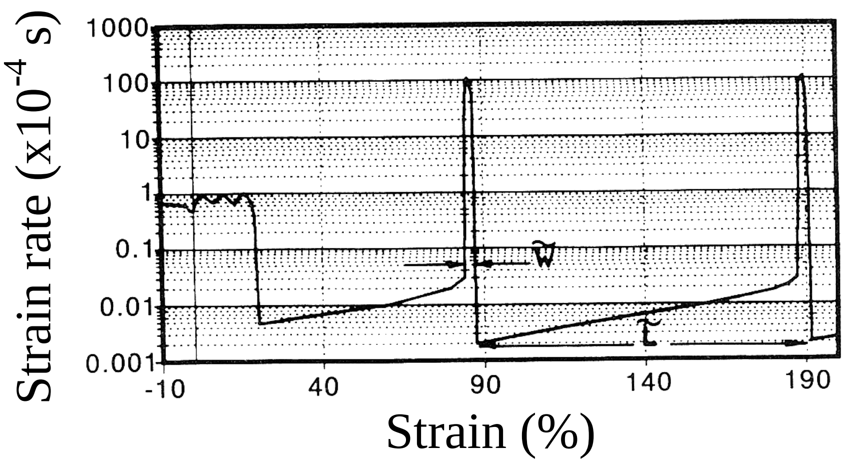
- ***PLC (Preliminary) Modeling (Zbib and ECA 1987)***

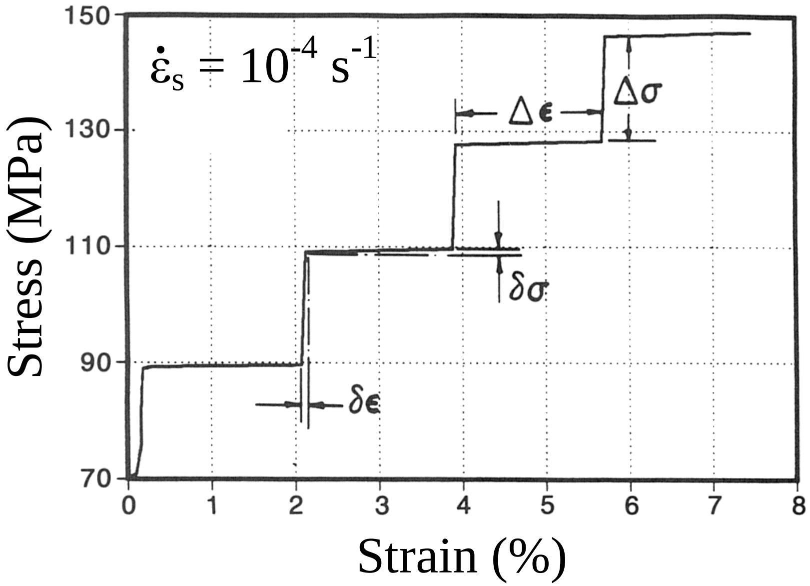
$$\sigma = h\varepsilon + f(\dot{\varepsilon}) + c\varepsilon_{xx}$$

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

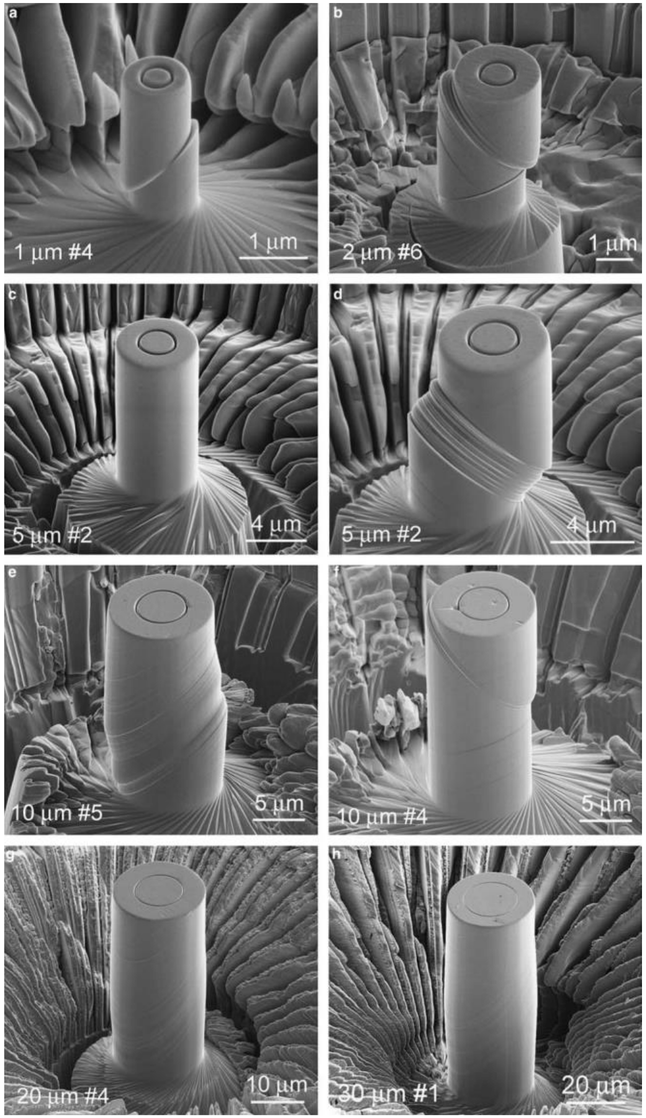
$$\dot{\varepsilon} = z(Vt - x) \quad ; \qquad \eta = \sqrt{\frac{h}{c}}(Vt - x)\,;$$

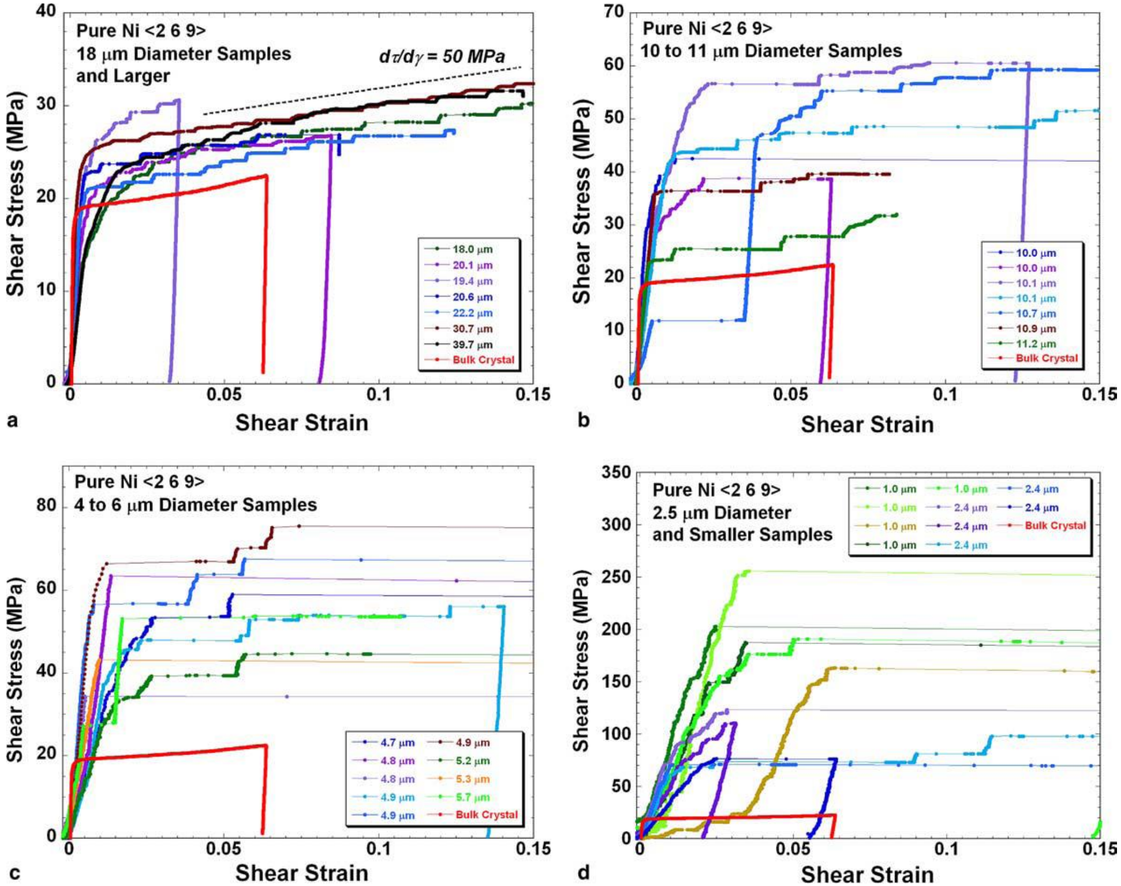
$$z_{\eta\eta} + \mu f'(z) z_\eta + (z - z_s) = 0 \quad \text{.......... Lienard's Eq.}$$





#4. Incipient/Intermittent Plasticity/Gradient-Stochastic Models





Nix et al, *Science* 2004;

Dimiduk et al, *Acta Mater.* 2005;

Dimiduk et al, *Science* 2006

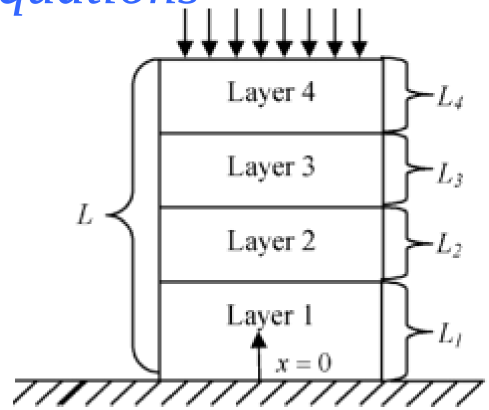
- ***Serrated Plastic Flow: The Gradient-Stochastic Model***

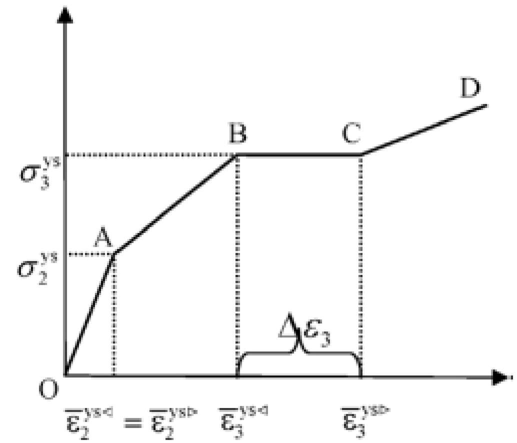
- *Governing Deterministic Equations*

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

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

(Zhang and K.E. Aifantis, 2011)





- *Serrations*

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

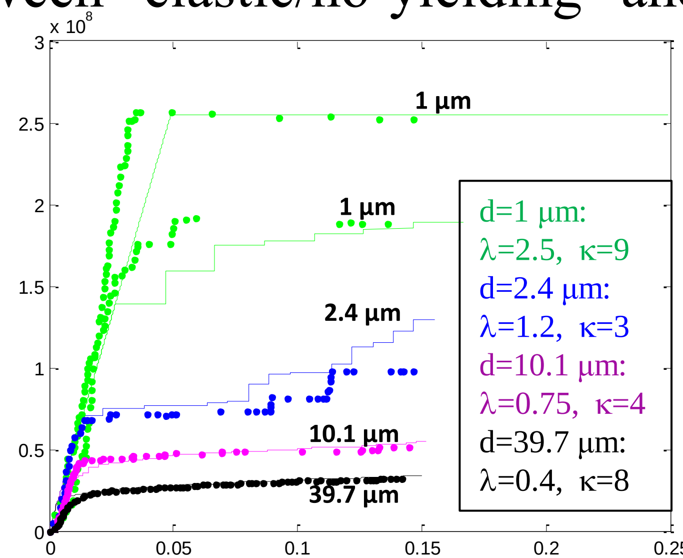
- *Introducing Stochasticity*

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

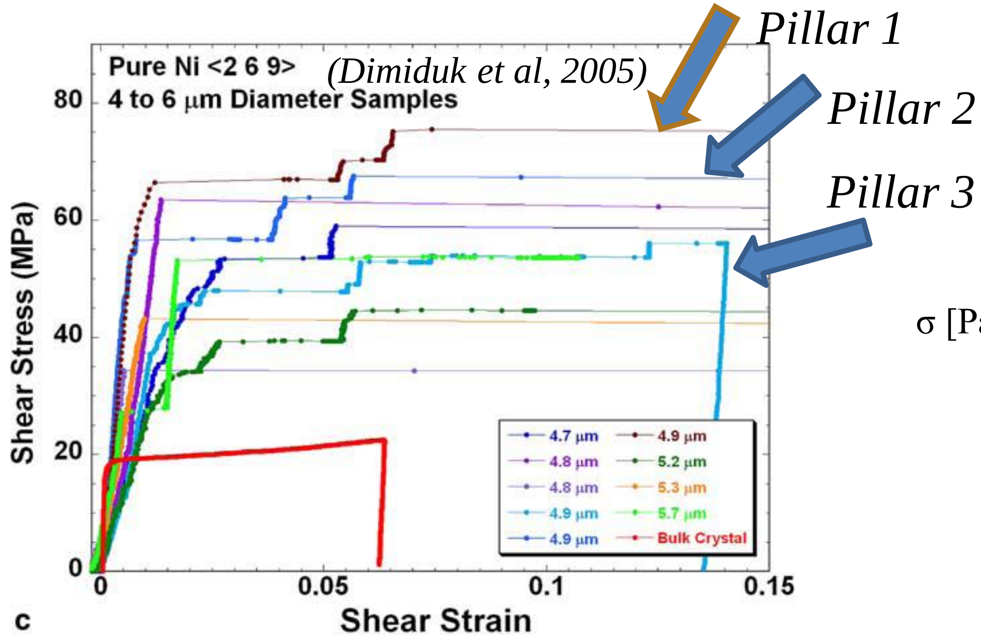
$$PDF(\delta) = \frac{k}{\lambda}\left(\frac{\delta}{\lambda}\right)^{k-1} e^{-(\delta/\lambda)^k};$$

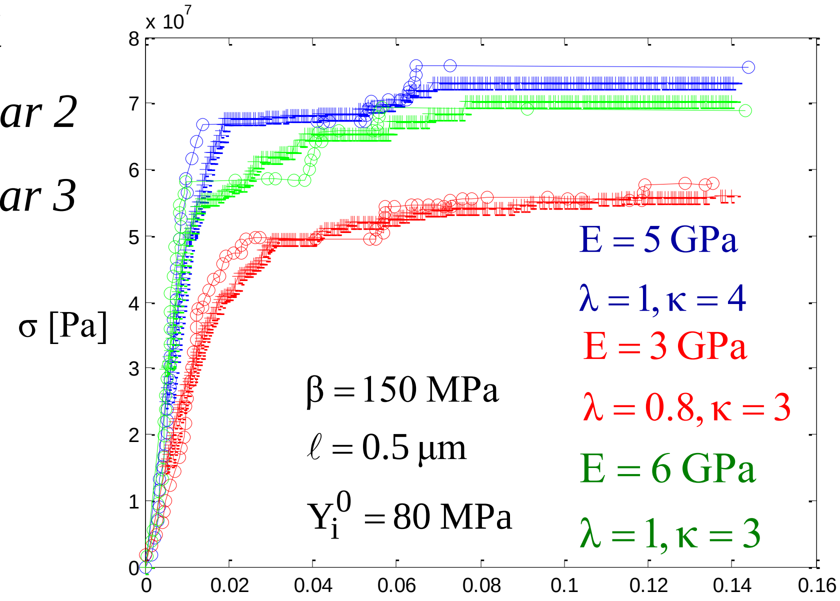
$$\bar{\delta} = \lambda \Gamma\left[1 + (1/k)\right], \quad \left\langle \delta^2 \right\rangle = \lambda^2 \Gamma\left[1 + (k)\right] - \bar{\delta}^2$$

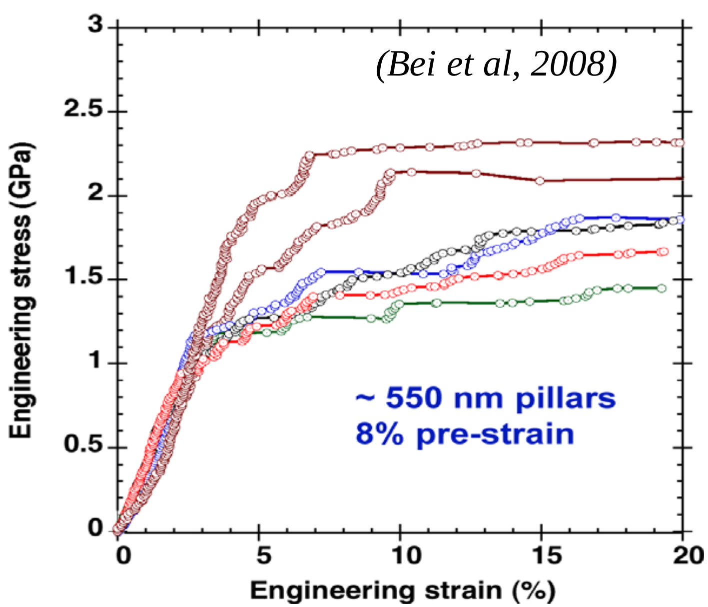
k/λ : shape/scale parameters

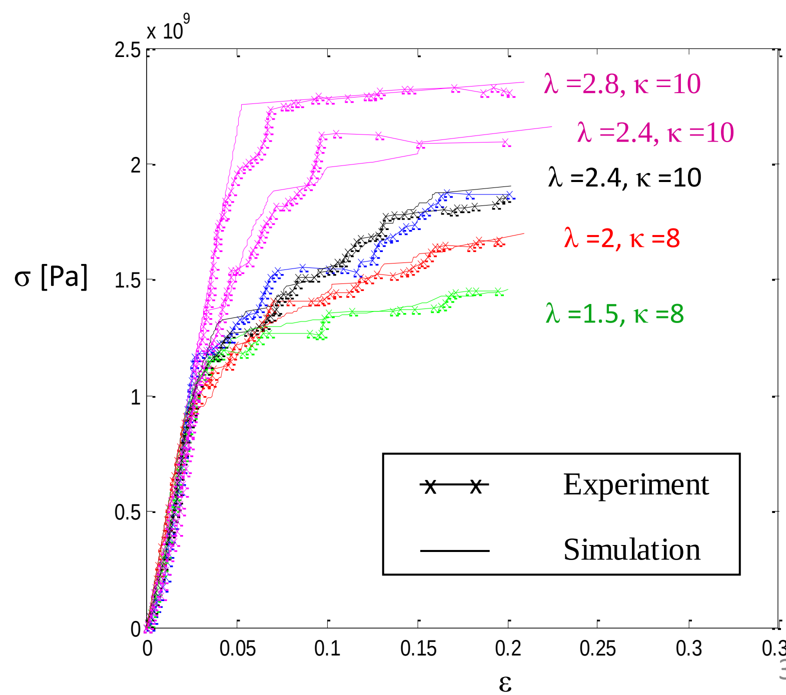


• *Random Response of Same Diameter Micropillars*









■ A Note on Stochasticity Information from Entropy

- ***Tsallis q-Entropy***

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

$$[\; q=1 \quad \Rightarrow \quad S=-k_B\sum_I P\left(I\right)lnP\left(I\right) \quad \ldots \; \textit{B-G-S Entropy} \;]$$

Maximum entropy principle leads to q-exponential distribution

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

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

- ***Extracting Information on Randomness – q PDFs***

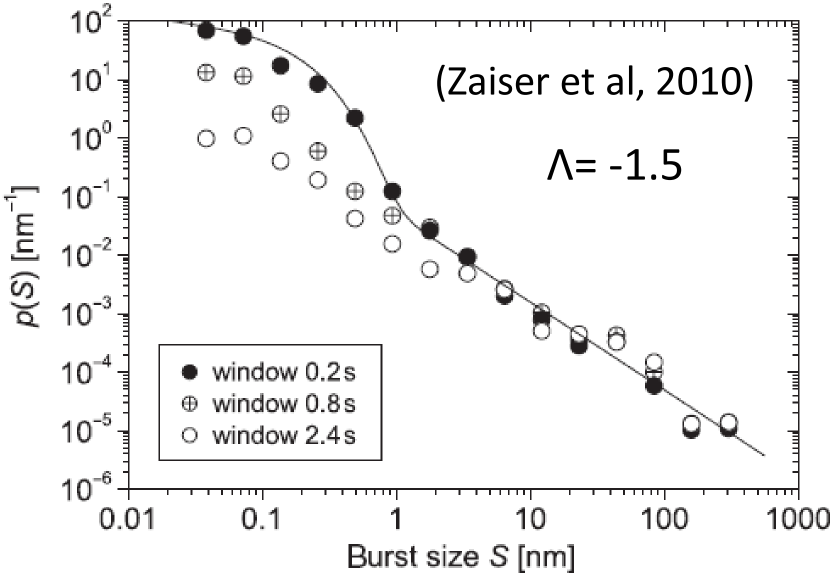
Probability of bursts of size s — *Burst size relation to local yield stress*

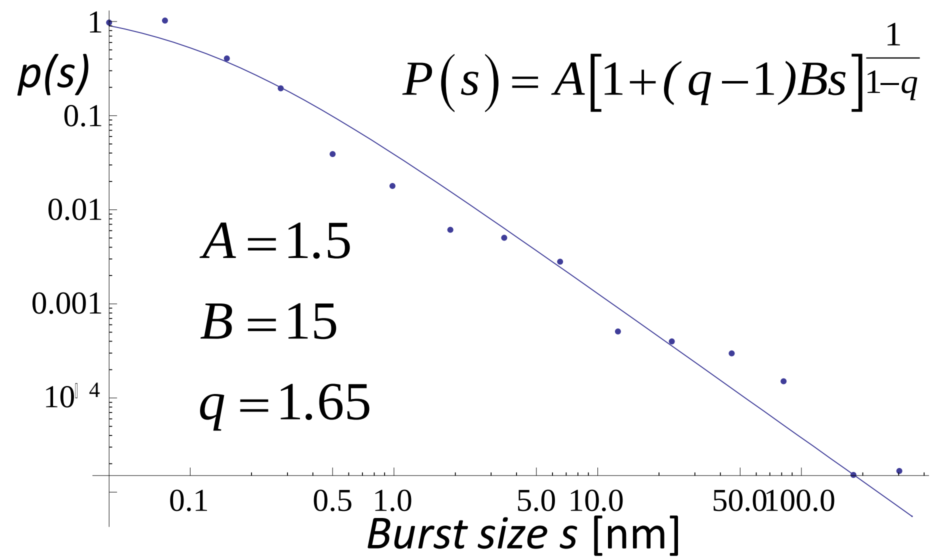
$$P\left(s\right)=A\left[1+(q-1)Bs\right]^{\frac{1}{1-q}} \qquad s=nL\varepsilon_y^{loc}=nL\frac{\sigma_y^{loc}}{E}; \quad P\left(\sigma_y^{loc}\right)\equiv P\left(\varepsilon_y^{loc}\right) \quad (L\text{: cell size})$$

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

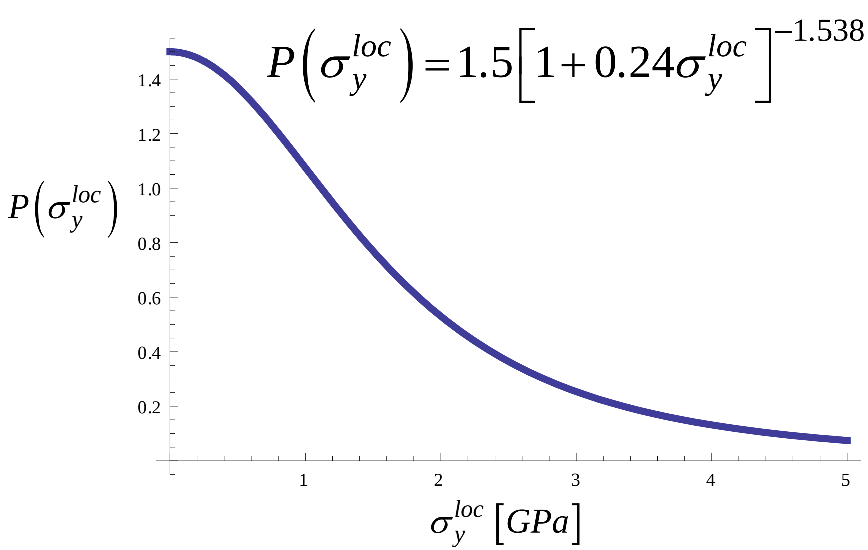
$$\therefore \quad P\left(\sigma_y^{loc}\right)=A\left[1+(q-1)Bs_b\left(\frac{\sigma_y^{loc}}{\sigma_y^b}\right)^2\right]^{1/(1-q)}$$

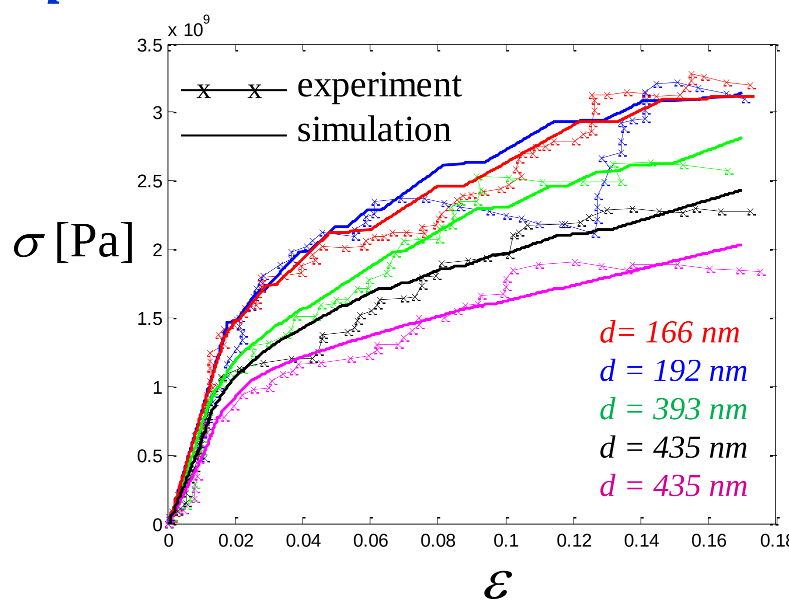
• Strain bursts in Mo micropillars under compression





• CA simulations with input from q-statistics

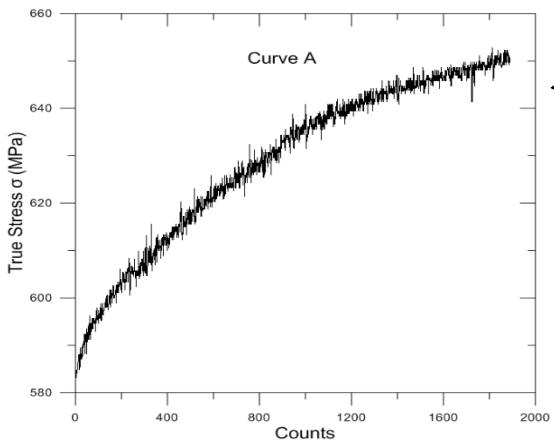




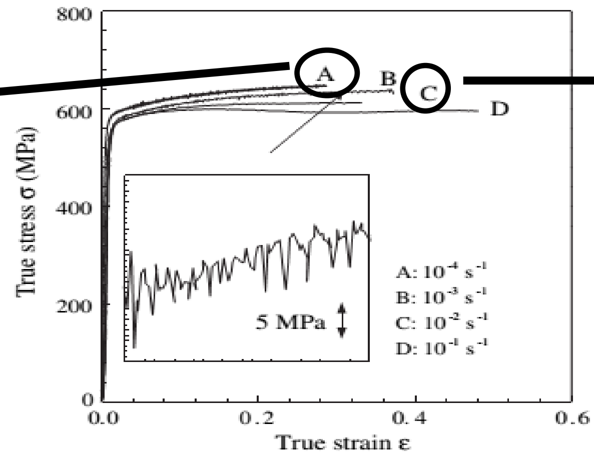
■ A Note on No Equations – q Statistics

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

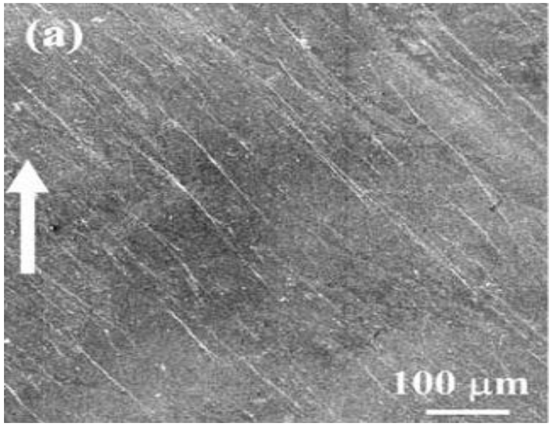
(Fan *et al*. Scripta/Acta Materialia 2005/2006)



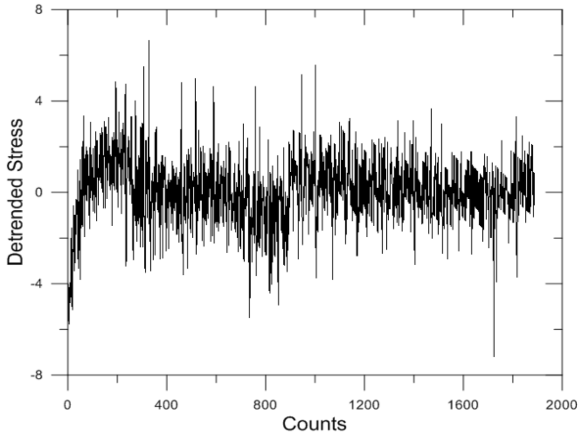
Low $\dot{\varepsilon}$ (10^{-4} s^{-1}) – Serrations



σ-ε curves (compression)



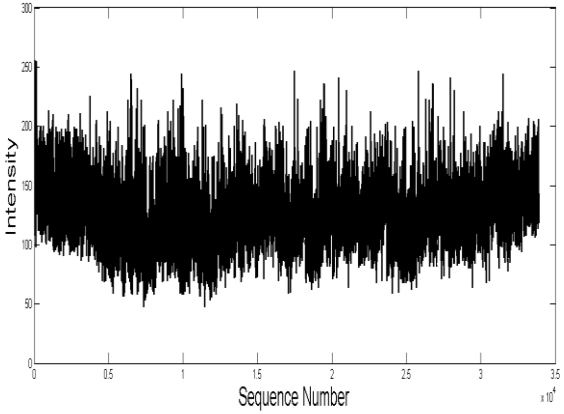
High $\dot{\varepsilon}$ (10^{-2} s^{-1})
Shear Bands (SEM)



Stress Drops time series

[Remove hardening effect (slope)]

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



Intensity series for Shear Band Distribution

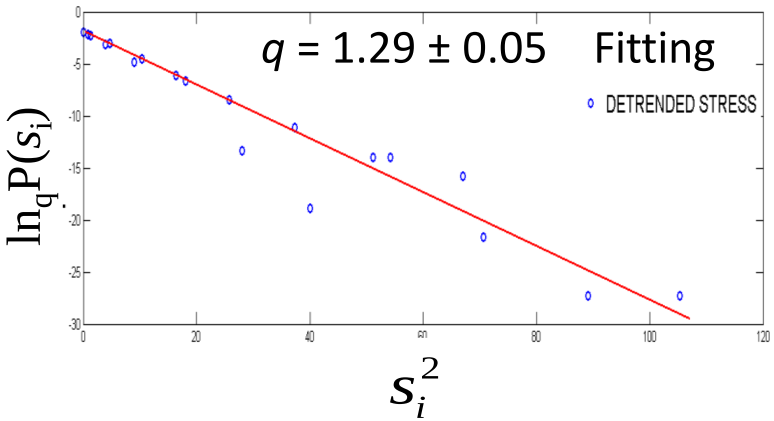
[2D → 1D: Space Filling Curve Method (Morton, 1966)]

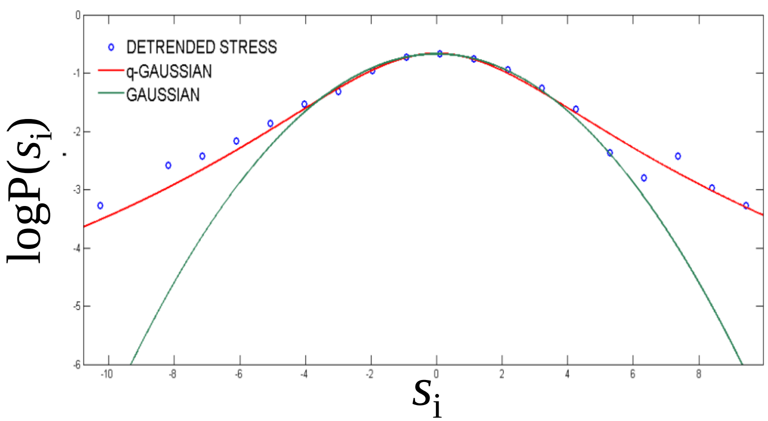
■ Serrations: q-PDFs /no Power Laws

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

•*Fitting:* $\ln_q(P(s_i))$ vs s_i^2

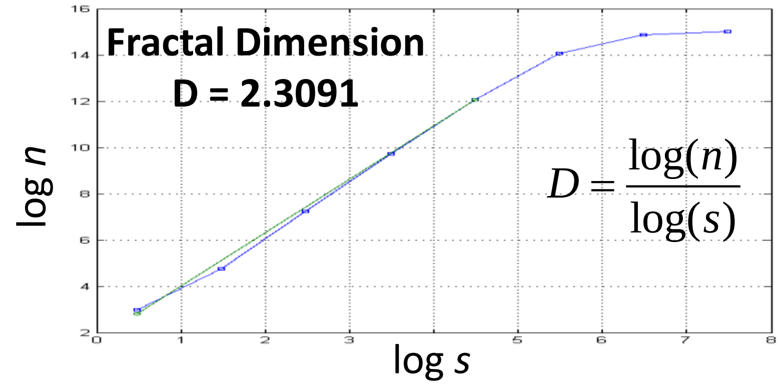
•*Power Law Tail (q>1):* $P(|s|) \sim |s|^{-2/(q-1)}$

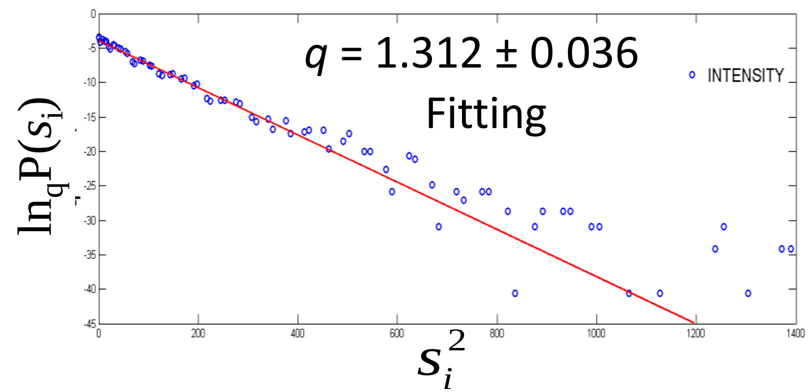


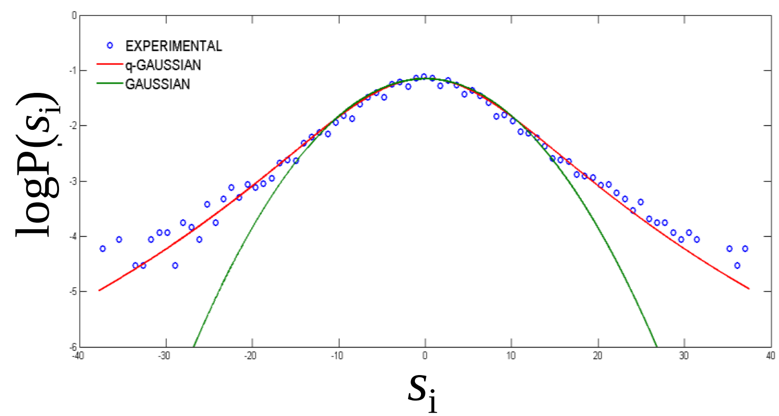


$q > 1 \longrightarrow$
- Non-Gaussian Statistics
- Tsallis Nonextensive Statistics,
- Temporal Long range correlations

■ Shear Banding: Fractality







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

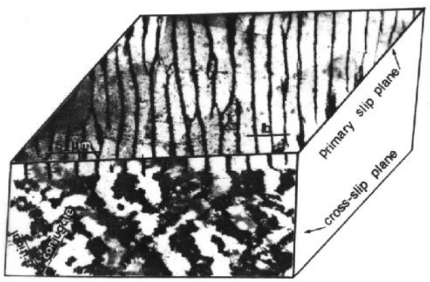
$q > 1 \longrightarrow$
- Non-Gaussian Pixels Distributions
- Spatial Long range correlations

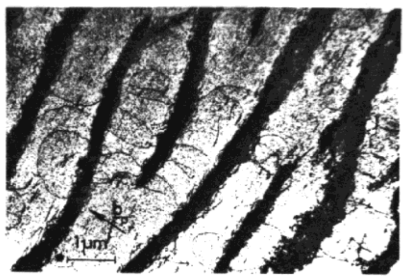
#5. Gradient Dislocation Dynamics: The W-A Model

- **Nicolis & Prigogine Book *Exploring Complexity* (1989), Chapter 5**
- **Glazov & Laird, Acta. Mater., 1986 / Xu & Zhang, Mat. Sci. Eng., 2014**
- **Ord & Hobbs, Phil. Trans., 2010**

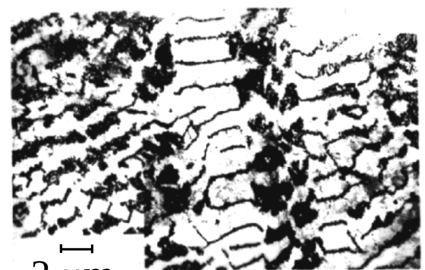
- ***PSBs Ladder/Labyrinth Structures in Cyclic Deformation***

[The Initial Motivation for Dislocation Patterning Developments]

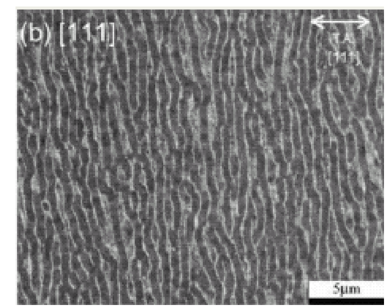




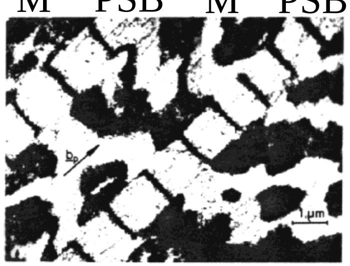
1µm



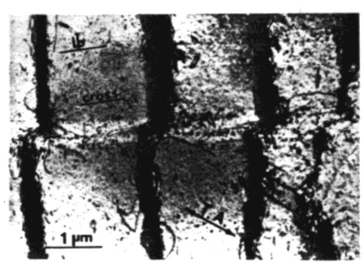
2 µm



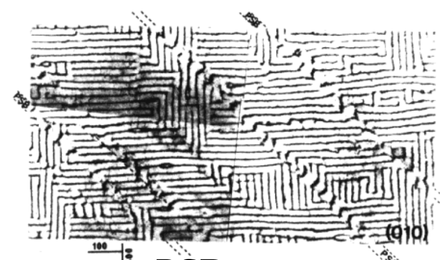
M PSB M PSB



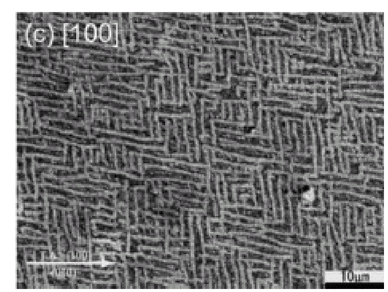
1µm



1µm

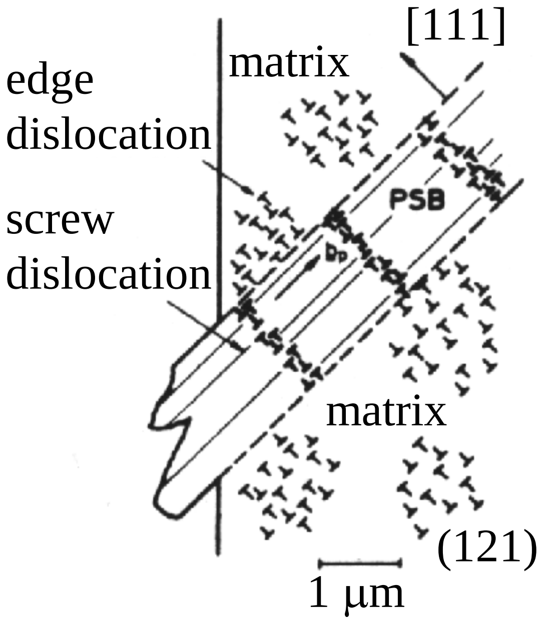


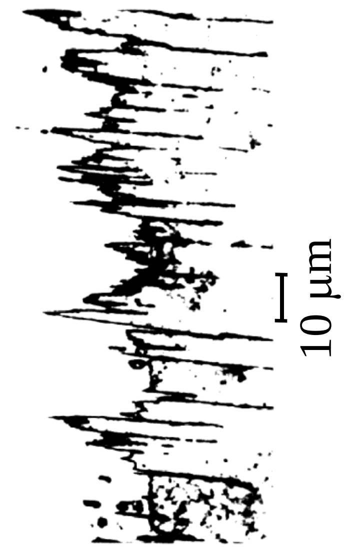
PSB PSB PSB 5 µm



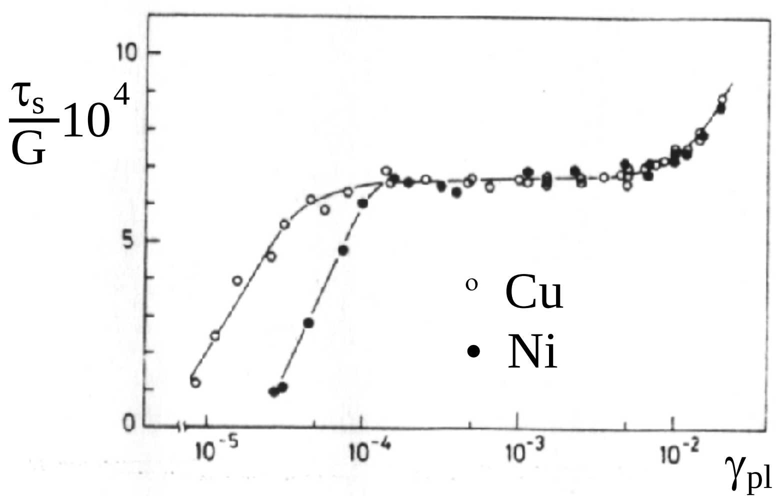
Winter-Mughrabi-Laird; Tabata et al; Kaneko-Hashimoto / TEM; SEM

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



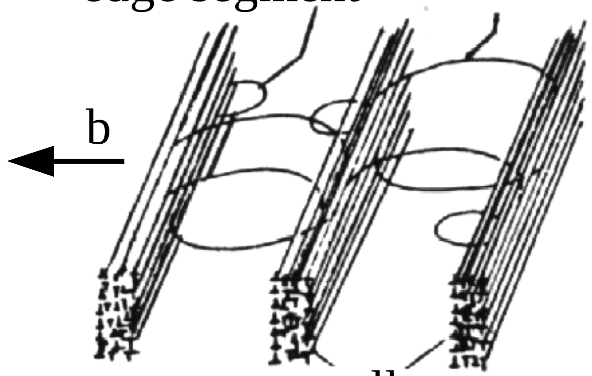


  - *Stress – strain graph*



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

- Selforganization of Dislocation on the Slip Plane



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

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

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

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

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

(α, γ) … reaction cross-section parameters

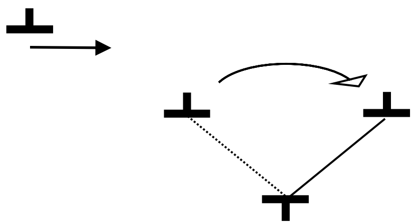
- Phenomenology of the Underlying Diffusive – Reaction Mechanisms

$(D_i, D_m) \longrightarrow$ microscopic expressions; dipole switching/sweeping

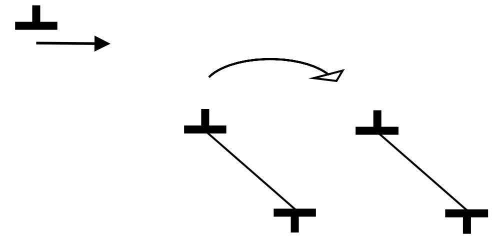
$(\alpha, \gamma) \longrightarrow$ Generalized chemical reactions; dipole dissolution/clustering

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

  - *Diffusive Mechanisms (D_i)*

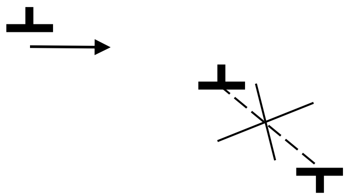


Dipole “switching“



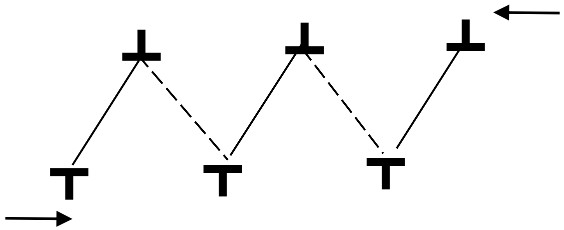
Dipole “sweeping“

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



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

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

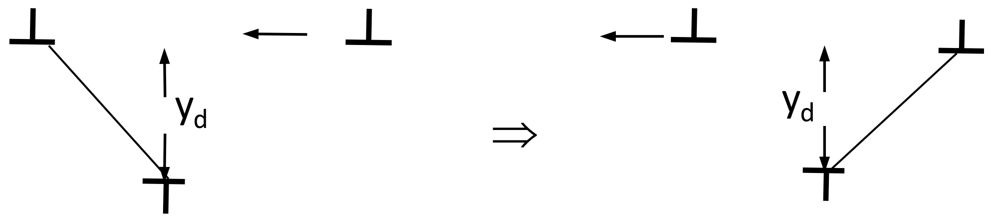


$$\left(\frac{\partial \rho_i}{\partial t}\right)^{+} \sim \gamma\, \dot{\gamma}^{pl}\, \rho_m\, \rho_i^2$$

- ***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)



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

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)

$$\begin{aligned} \rho_m &= \rho_m^+ + \rho_m^- \\ k_m &= \rho_m^+ - \rho_m^- \quad (\ldots = \rho_{GND}) \end{aligned} \quad \Rightarrow \begin{cases} \dot{\rho}_m = -\upsilon\, \partial_x k_m + \beta \rho_i - \gamma \rho_m \rho_i^2 \\ \dot{k}_m = \upsilon\, \partial_x \rho_m - \gamma k_m \rho_i^2 \end{cases}$$

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)

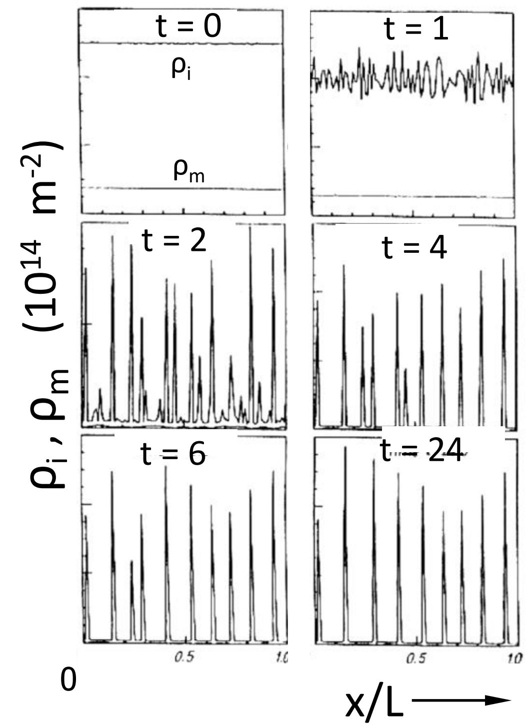
$$\therefore \; q_{critical} = q_c = \frac{2\pi}{\lambda_c} = \left(\frac{\alpha \gamma \rho_i^2}{D_i D_m} \right)^{1/4}$$

  – *Ladder Wavelength:* λ_c

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

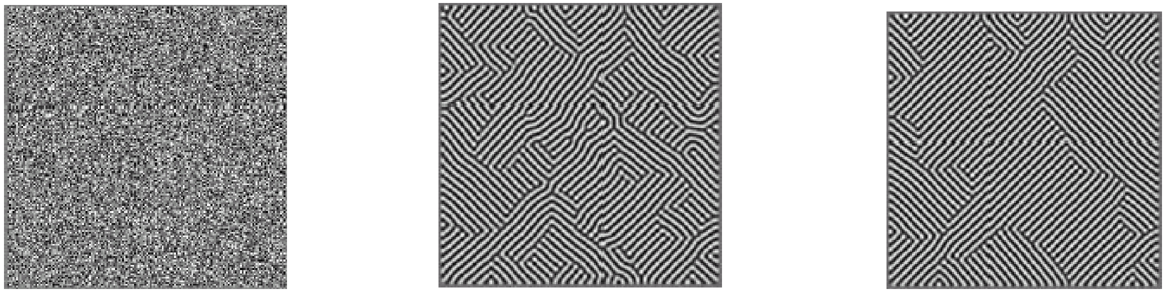
$$\therefore \; \lambda_c = d \cong \frac{16}{\sqrt{\rho_i}} \quad \Rightarrow \quad \rho_i \sim \frac{256}{d^2}$$

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)

- *Simulation Results*



t = 0 t = 100 t = 20000

7.5% anisotropy

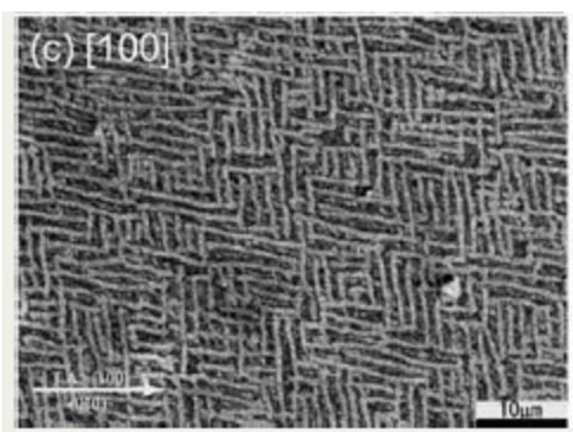
(a)

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)

■ A Note on Micro/Nano Defect Kinetics (Romanov and ECA 2010)

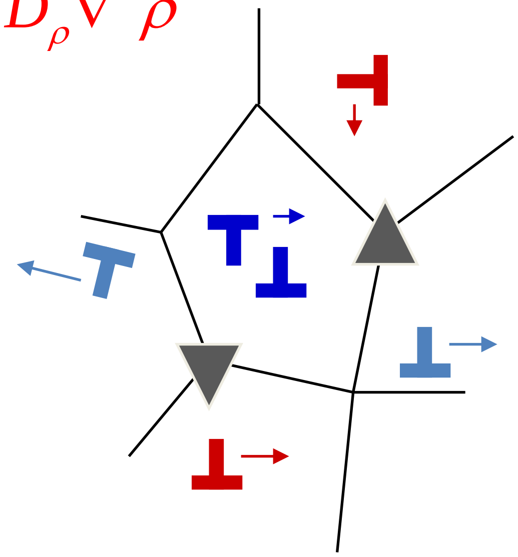
- ***Nanopolycrystals***

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

$$\varphi_t = A_\varphi \rho - B_\varphi \rho^2 - C_4 \rho\varphi - K\varphi + D_\varphi \nabla^2 \varphi$$

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

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



ρ – mobile dislocations in the grain interior

φ – low-mobility (immobile) dislocations (dipoles)

ϑ – immobile junction disclinations

ψ – grain boundary sliding dislocations

■ A Note on Earth Patterns

PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A

Phil. Trans. R. Soc. A (2010) **368**, 95–118
doi:10.1098/rsta.2009.0199

Fracture pattern formation in frictional, cohesive, granular material

BY ALISON ORD[1,2,*] AND BRUCE E. HOBBS[1,2]

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One contribution of 17 to a Theme Issue 'Patterns in our planet: applications of multi-scale non-equilibrium thermodynamics to Earth-system science'.

Abstract : We develop a model motivated by dislocation pattern formation in metals. The problem is formulated in one dimension in terms of coupled reaction–diffusion equations, based on computer simulations of crack development in deformed granular media with cohesion. The cracks are treated as interacting defects, and the densities of defects diffuse through the rock mass. Of particular importance is the formation of cracks at high stresses associated with force-chain buckling and variants of this configuration; these cracks play the role of 'inhibitors' in reaction–diffusion relationships. Cracks forming at lower stresses act as relatively mobile defects. Patterns of localized deformation result from (i) competition between the growth of the density of 'mobile' defects and the inhibition of these defects by crack configurations forming at high stress and (ii) the diffusion of damage arising from these two populations each characterized by a different diffusion coefficient. The extension of this work to two and three dimensions is discussed.

- Crack Patterns

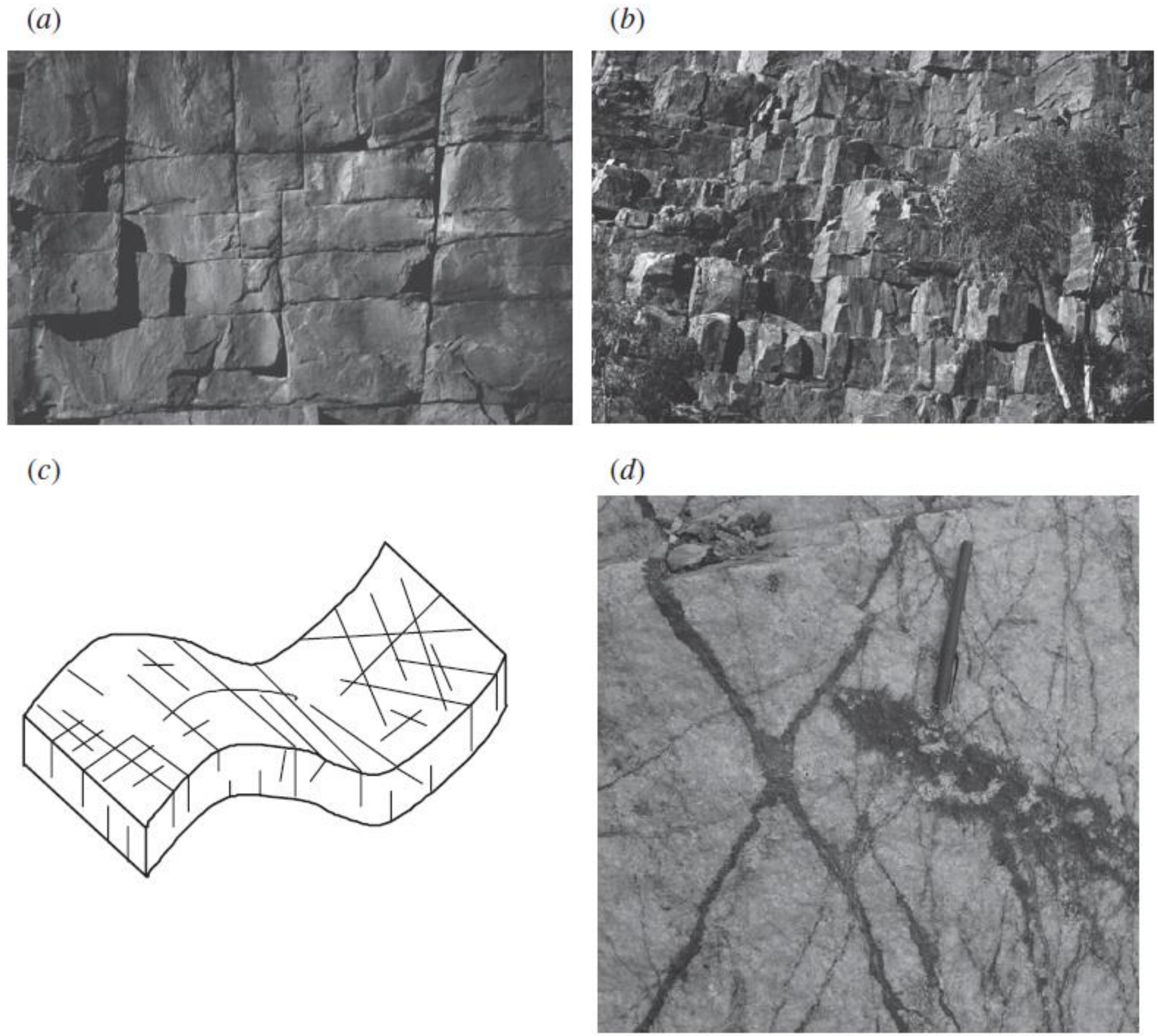


Figure 1. Patterns of fracture damage in deformed rocks. (a,b) Joint patterns in Heavitree Quartzite, Ormiston Pound, Central Australia. (c) Schematic relationships between folding and joint sets. (d) Joint sets associated with Cu mineralization in the Shi-Lu copper deposit, China. Photograph by Y. Zhang.

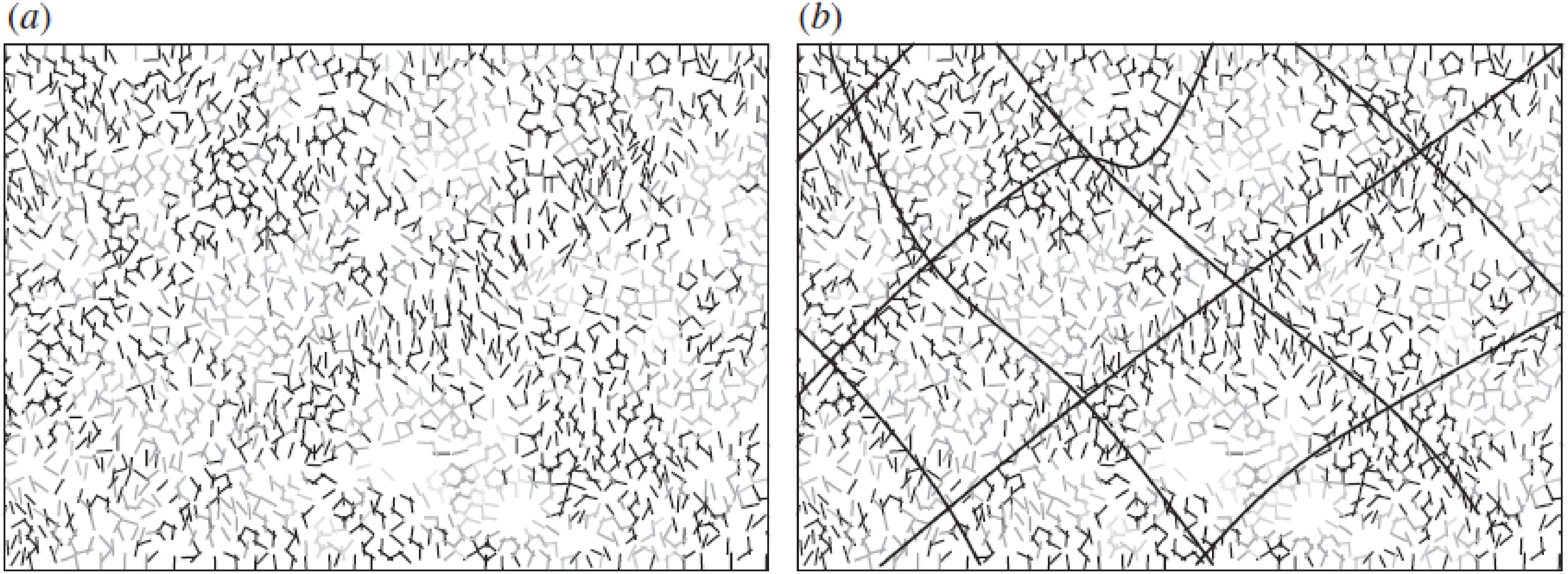


Figure 2. (a,b) Cell structure developed in deformed granular aggregate. The relative ages of formation of the cracks are shown in shades of grey, with the first formed in black, and the last formed in the lightest grey. The black lines in (b) represent possible positions for cell boundaries, with the youngest cracks within the cells and the oldest within the boundaries.

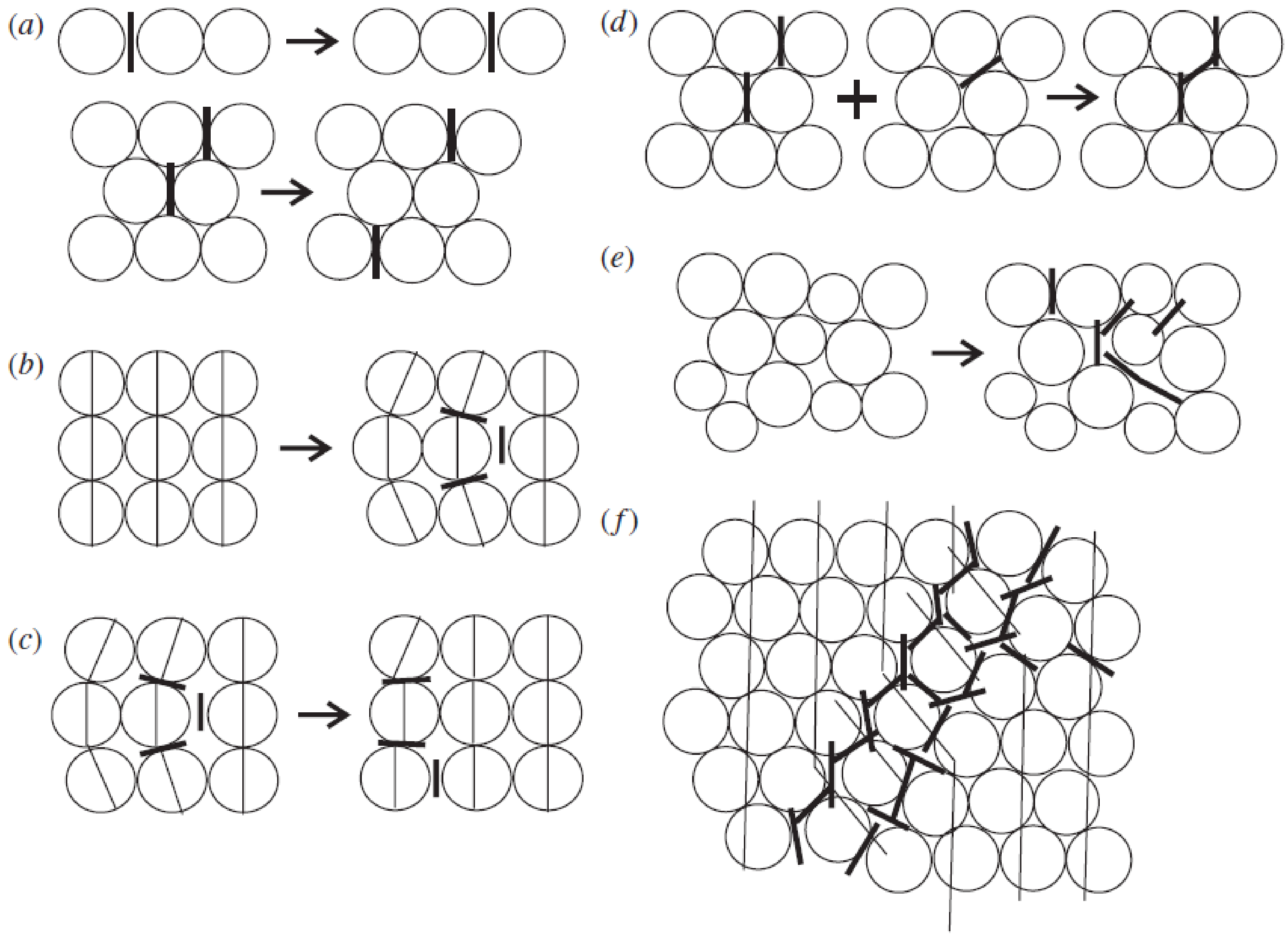


Figure 8. Crack interaction processes. (*a*) Diffusion by a 'vacancy exchange' mechanism. (*b*) Formation of crack array by a force-chain buckling mechanism. (*c*) Liberation of crack array in (*b*) by a diffusive mechanism. (*d*) Formation of wing-crack array by a combination of a mode-2 crack with two mode-1 cracks. (*e*) Generation of cracks by a local non-affine deformation. (*f*) Complicated crack arrays associated with the formation of a localized zone of shearing.

3. A model for the development of crack patterns

Motivated by the work of Walgraef & Aifantis (1985a,b,c), we propose

The above discussion indicates that the overall evolution of these crack arrays is described by two coupled reaction–diffusion equations that express the relationships and coupling between diffusion, generation, annihilation and pinning of cracks,

$$\frac{\partial \rho_{\mathrm{im}}}{\partial t} = D_{\mathrm{im}} \frac{\partial^2 \rho_{\mathrm{im}}}{\partial x^2} + g(\rho_{\mathrm{im}}) - b\rho_{\mathrm{im}} + \gamma \rho_{\mathrm{m}} \rho_{\mathrm{im}}^2 \tag{3.10a}$$

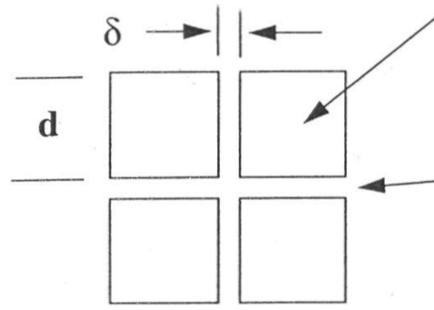
and

$$\frac{\partial \rho_{\mathrm{m}}}{\partial t} = D_{\mathrm{m}} \frac{\partial^2 \rho_{\mathrm{m}}}{\partial x^2} + b\rho_{\mathrm{im}} - \gamma \rho_{\mathrm{m}} \rho_{\mathrm{im}}^2. \tag{3.10b}$$

This is the standard set of reaction–diffusion equations introduced by Walgraef & Aifantis (1985a), and has been intensively studied over the past two decades. In particular, this coupled set of equations has the following properties:

#6. Gradient Elasticity (ECA 1992)

■ Motivation from Nanopolycrystal Elasticity



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

– ***Equilibrium***

$$div\boldsymbol{\sigma}_1 = \mathbf{f}, \quad div\boldsymbol{\sigma}_2 = -\mathbf{f} \; \text{.......}\textit{for each phase}$$
$$div\boldsymbol{\sigma} = 0, \quad \boldsymbol{\sigma} = \boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2 \; \text{.......}\textit{total}$$

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

$$\boldsymbol{\sigma}_\mathbf{k} = \mathbf{L}_\mathbf{k}\mathbf{u}_\mathbf{k}, \quad k = 1,2; \quad \mathbf{L}_\mathbf{k} = \lambda_k \mathbf{G} + \mu_k \hat{\nabla}; \quad \mathbf{G} = \mathbf{I}\, div \;; \quad \hat{\nabla} = \nabla + \nabla^T$$

$$\mathbf{f} = \alpha(\mathbf{u}_1 - \mathbf{u}_2)$$

– ***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 (Gradela)***

The above implies the following gradient-elasticity relation

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

i.e.

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

- ***Ru-Aifantis Theorem***

$$\boldsymbol{u} - c\nabla^2\boldsymbol{u} = \boldsymbol{u}_0$$

$\boldsymbol{u}$*...Gradela solution ;* $\boldsymbol{u_0}$ *...classical elasticity solution*

i.e. Inhomogeneous Helmholtz Equation: Solutions known

- ***Nanocomposites & Interfaces***

Another possible configuration to be treated with Gradela

■ A Note on Gradela Dislocation Nanomechanics

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

- ***Screw Dislocation***

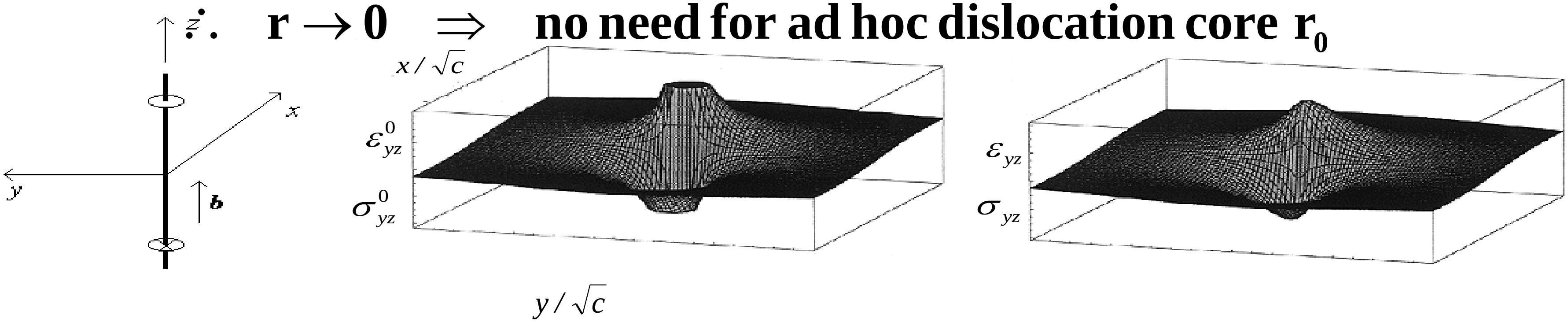
  - Stress / Strain :

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

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

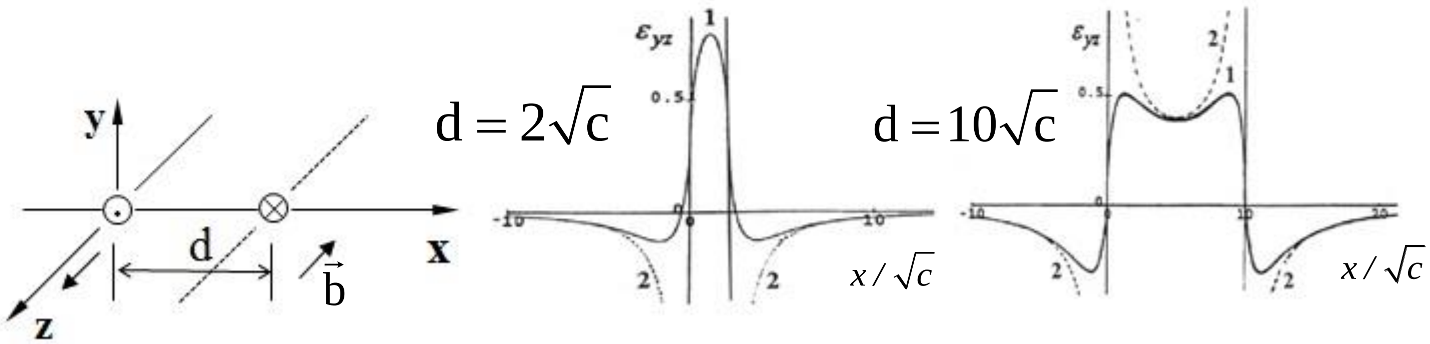
- Self – energy : $W_s=\dfrac{\mu b_z^2}{4\pi}\left\{\gamma^E+\ln\dfrac{R}{2\sqrt{c}}\right\}$ ... $\gamma^E=0.577;$ Euler constant

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



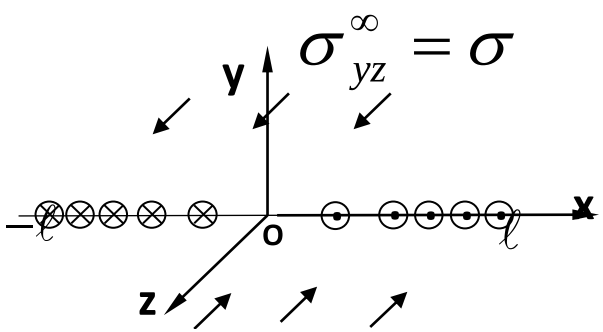
- Use these in simulations

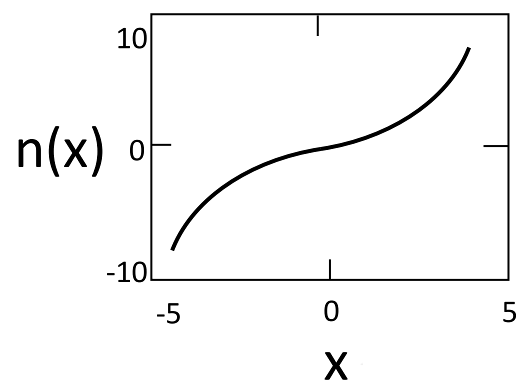
- ***Dislocation Dipoles [insight to nucleation / annihilation]***

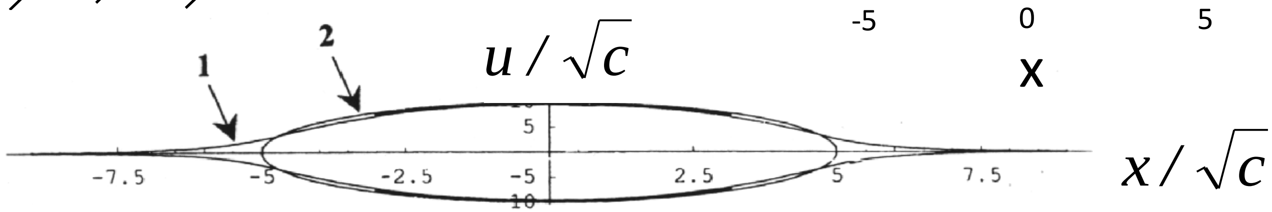


$\therefore \quad d \approx 10\sqrt{c}$.. *characteristic distance of "strong" interaction*

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





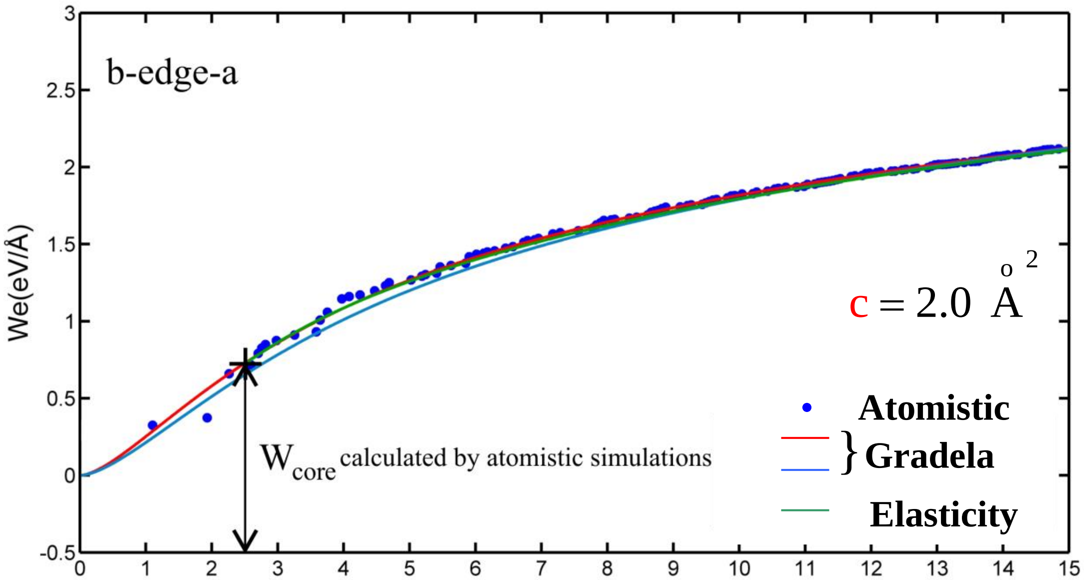


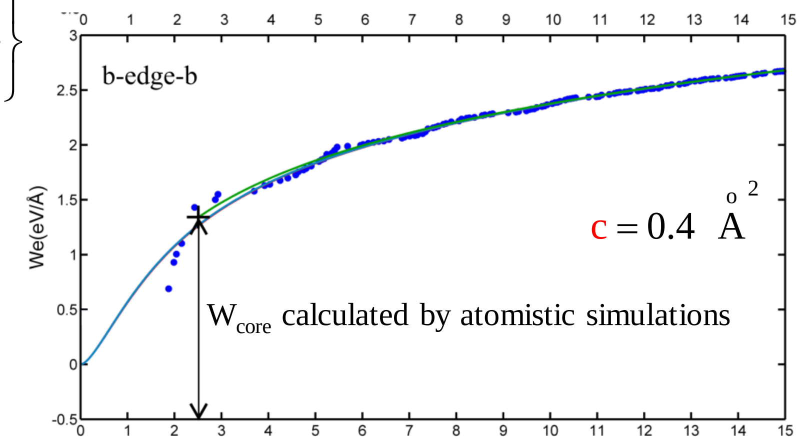
$\therefore$ *Barenblatt's "smooth closure" condition*

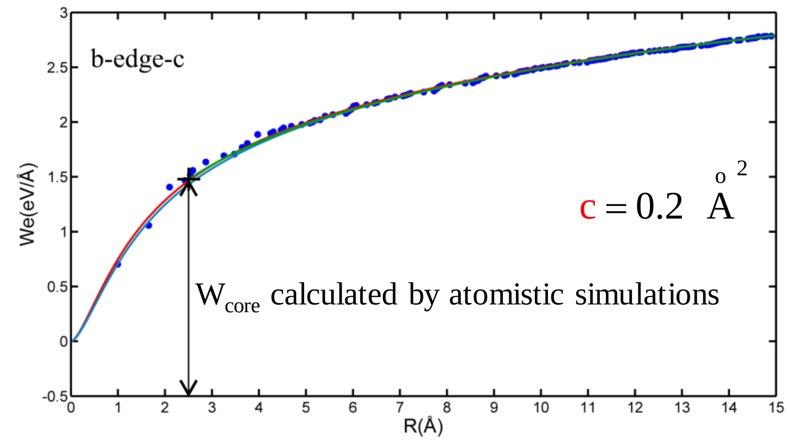
• *Comparison with MD Simulations (Stilliger – Weber Potential)*

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

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







$$c=0.2-2.2\quad \mathring{A}^2$$

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

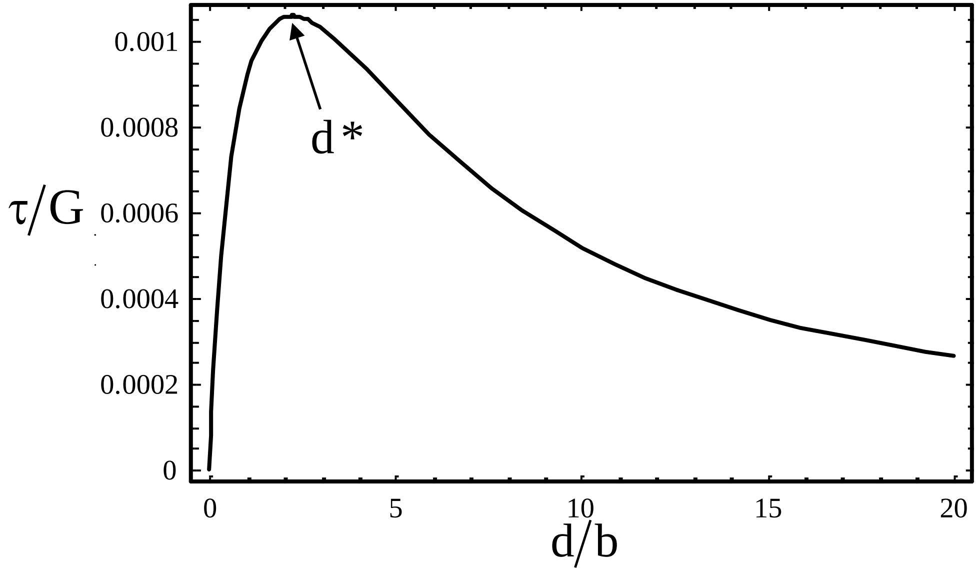
• *Image Force – Inverse Hall Petch Behavior*

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

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

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

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



$d^* \approx 9$ nm

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

■ A Note on Gradela Green's Function Dislocation Formulae

- ***Classical Elasticity Formulae***
  - Mura's Formula for the Plastic Distortion

$$\beta_{ij}^{0}(\boldsymbol{x}) = -\frac{b_k}{8\pi}\oint_L \left[\left(\varepsilon_{jkl}\delta_{ir} - \varepsilon_{rkl}\delta_{ij} + \varepsilon_{rij}\delta_{kl} \right)\partial_l \nabla^2 + \frac{1}{1-\nu}\varepsilon_{rkl}\partial_l\partial_i\partial_j \right] R\, dL_r'$$

  - Peach-Koehler's Formula for the Stress Tensor

$$\sigma_{ij}^{0}(\boldsymbol{x}) = -\frac{\mu b_k}{8\pi}\oint_L \left[\left(\varepsilon_{jkl}\delta_{ir} - \varepsilon_{ikl}\delta_{jr} \right)\partial_l \nabla^2 + \frac{2}{1-\nu}\varepsilon_{rkl}\left(\partial_i\partial_j - \delta_{ij}\nabla^2 \right)\partial_l \right] R\, dL_r'$$

  - Burger's Formula for the Displacement Vector

$$u_i^{0}(\boldsymbol{x}) = \frac{b_i}{8\pi}\int_S \nabla^2\partial_j R\, dS_j' + \frac{b_l\varepsilon_{rlj}}{8\pi}\oint_L \left[\delta_{ij}\nabla^2 - \frac{1}{1-\nu}\partial_i\partial_j \right] R\, dL_r' \; ; \quad R = \left| \boldsymbol{x} - \boldsymbol{x}' \right|$$

- ***Gradela***
  - Basic Relations

$$W = 1/2\, C_{ijkl}\beta_{ij}\beta_{kl} + 1/2\, \ell^2 C_{ijkl}\partial_m\beta_{ij}\partial_m\beta_{kl} \; ; \quad C_{ijkl} = \mu\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} + \frac{2\nu}{1-2\nu}\delta_{ij}\delta_{kl} \right)$$

  - Green Tensor for the Helmholtz-Navier Equation

$$LL_{ik}G_{kj} = -\delta_{ij}\delta\left(\boldsymbol{x} - \boldsymbol{x}' \right); \quad L = 1 - \ell^2\nabla^2, \quad L_{ik} = C_{ijkl}\partial_j\partial_l$$

$$G_{ij}(R) = \frac{1}{16\pi\mu(1-\nu)}\left[2(1-\nu)\delta_{ij}\nabla^2 - \partial_i\partial_j \right] A(R) \; ; \quad A(R) = R + \frac{2\ell^2}{R}\left(1 - e^{-R/\ell} \right)$$

  - $\left\{ \beta_{ij}, \sigma_{ij}, u_i \right\} \; : \; R \rightarrow A(R)$

■ A Note on Gradela Fracture Mechanics (Mode III)

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

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

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

  - ***Boundary Conditions***

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

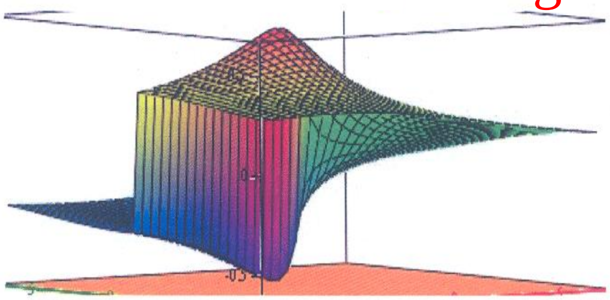
  Vanishing of stresses at the origin: $\lim_{\mathbf{r}\to 0} \boldsymbol{\sigma}_{ij} = 0$

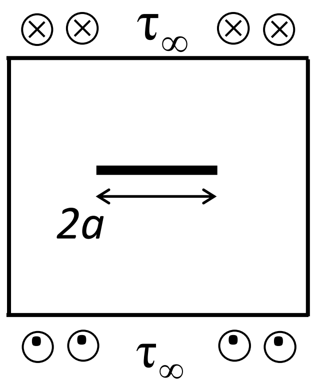
  Zero tractions on crack surfaces: $\sigma_{zy}(x,0^{\pm}) = 0 \quad ; \quad |x| \le a$

• *Nonsingular Stress Distribution in Mode III*

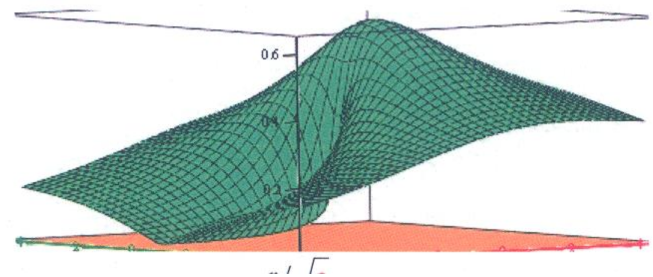
$$\sigma_{xz} = -\frac{K_{III}}{\sqrt{2\pi r}}\left[\sin\frac{\theta}{2}\left(1-\exp\left[-r/\sqrt{c}\right]\right)\right] \qquad \sigma_{yz} = \frac{K_{III}}{\sqrt{2\pi r}}\left[\cos\frac{\theta}{2}\left(1-\exp\left[-r/\sqrt{c}\right]\right)\right]$$

Gradient Stress non-singular

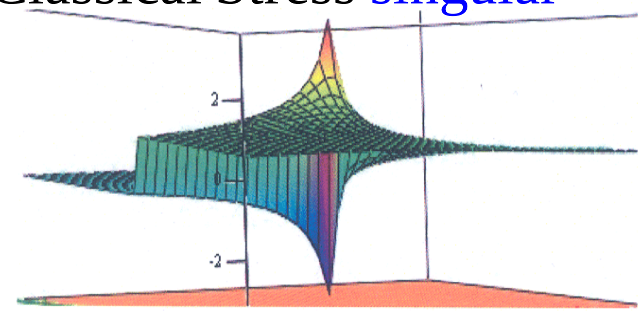




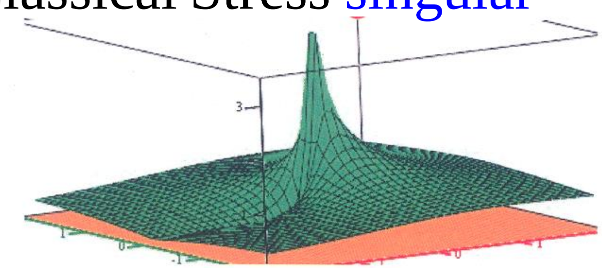
Gradient Stress non-singular



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

■ A Note on Fractional Gradela (Tarasov/ECA 2012)

- ***1D – Caputo Derivative (Translational Symmetry)***

$$\sigma(x) = E\,\varepsilon(x) \pm \ell_\beta^2 E\,{}^C D_{a+}^{\beta}\,\varepsilon(x)\ \ldots\ = E\left(1 \pm \ell_\beta^2\,{}^C D_{a+}^{\beta}\right) D_x^1 u$$

$${}^C D_{a+}^{\alpha} f(t) = I_{a+}^{n-\alpha} D_x^n f(x) = \frac{1}{\Gamma(n-\alpha)} \int_a^x \frac{D_z^n f(z)}{(x-z)^{\alpha-n+1}}\,dz$$

- ***3D – Riesz Derivative (Radial Symmetry)***

$$c_\alpha\left[(-\Delta)^{\alpha/2} u\right](\mathbf{r}) + c_\beta\left[(-\Delta)^{\beta/2} u\right](\mathbf{r}) = f(\mathbf{r}) \qquad (\alpha > \beta)$$

$$c_\alpha\left[(-\Delta)^{\alpha/2} u\right](\mathbf{r}) = \mathcal{F}^{-1}\left(|\mathbf{k}|^{\alpha}\,(\mathcal{F}u)(\mathbf{k})\right)$$

$$\text{Note:}\quad \alpha = 4, \quad \beta = 2$$

$$c_2 \Delta u(\mathbf{r}) - c_4 \Delta^2 u(\mathbf{r}) + f(\mathbf{r}) = 0\,; \quad c_2 = E,\ \ c_4 = \pm \ell^2 E$$

- ***Particular Solution***

$$u(\mathbf{r}) = \int_{\mathbb{R}^3} G^3_{\alpha,\beta}(\mathbf{r}-\mathbf{r}')\, f(\mathbf{r}')\, d^3\mathbf{r}' \;\; ; \quad G^3_{\alpha,\beta}(\mathbf{r}) = \int_{\mathbb{R}^3} \frac{1}{c_\alpha |\mathbf{k}|^\alpha + c_\beta |\mathbf{k}|^\beta}\, e^{i(\mathbf{k},\mathbf{r})}\, d^3\mathbf{k}$$

$$G^3_{\alpha,\beta}(\mathbf{r}) = \frac{1}{(2\pi)^{3/2}\sqrt{|\mathbf{r}|}} \int_0^\infty \frac{\lambda^{3/2} J_{1/2}(\lambda|\mathbf{r}|)}{c_\alpha \lambda^\alpha + c_\beta |\lambda|^\beta}\, d\lambda \;\; ; \quad J_{1/2}(z) = \sqrt{2/(\pi z)}\,\sin(z)$$

- ***Thomson's Point Load Problem***

$$f(\mathbf{r}) = f_0\, \delta(\mathbf{r}) = f_0\, \delta(x)\delta(y)\delta(z) \;\; ; \quad u(\mathbf{r}) = f_0\, G^3_{\alpha,\beta}(\mathbf{r})$$

$$\therefore \quad u(\mathbf{r}) = \frac{1}{2\pi^2} \frac{f_0}{|\mathbf{r}|} \int_0^\infty \frac{\lambda \sin(\lambda|\mathbf{r}|)}{c_\alpha \lambda^\alpha + c_\beta \lambda^\beta}\, d\lambda \qquad (\alpha > \beta)$$

- ***Super-gradient Elasticity [α > 2, β=2]***

$$c_2 \Delta u(\mathbf{r}) - c_\alpha \left[(-\Delta)^{\alpha/2} u\right](\mathbf{r}) + f(\mathbf{r}) = 0\,, \qquad (\alpha > 2)$$

$$\therefore \quad u(\mathbf{r}) = \begin{cases} \dfrac{f_0 \Gamma[(3-\alpha)/2]}{2^\alpha \pi^2 \sqrt{\pi}\, c_\alpha \Gamma(\alpha/2)} \dfrac{1}{|\mathbf{r}|^{3-\alpha}}\,, & (2 < \alpha < 3) \\[2ex] \dfrac{f_0}{2\pi\alpha c_\beta^{1-3/\alpha} c_\alpha^{3/\alpha} \sin(3\pi/\alpha)}\,, & (\alpha > 3) \end{cases} \;\; ; \qquad |\mathbf{r}| \to 0$$

• *Sub-gradient Elasticity Model* [α = 2, 0<β<2]

$$c_2 \Delta u(\mathbf{r}) - c_\beta \left[(-\Delta)^{\beta/2} u \right](\mathbf{r}) + f(\mathbf{r}) = 0\,, \qquad (0 < \beta < 2)$$

– *Soltn:*

$$u(\mathbf{r}) = \frac{1}{2\pi^2} \frac{f_0}{|\mathbf{r}|} \int_0^\infty \frac{\lambda \sin(\lambda |\mathbf{r}|)}{c_2 \lambda^2 + c_\beta \lambda^\beta} d\lambda\,, \qquad (0 < \beta < 2)$$

– *Asymptotic Form*

$$u(\mathbf{r}) = \frac{f_0}{2\pi^2 |\mathbf{r}|} \int_0^\infty \frac{\lambda \sin(\lambda |\mathbf{r}|)}{c_2 \lambda^2 + c_\beta \lambda^\beta} d\lambda \approx \frac{C_0(\beta)}{|\mathbf{r}|^{3-\beta}} + \sum_{k=1}^{\infty} \frac{C_k \beta}{|\mathbf{r}|^{(2-\beta)(k+1)+1}} \qquad (|\mathbf{r}| \to \infty)$$

$$C_0(\beta) = \frac{f_0}{2\pi^2 c_\beta} \Gamma(2-\beta) \sin(\pi\beta/2)\,; \quad C_k(\beta) = -\frac{f_0 c_2^k}{2\pi^2 c_\beta^{k+1}} \int_0^\beta z^{(2-\beta)(k+1)-1} \sin(z)\, dz$$

$$\Rightarrow u(\mathbf{r}) \approx \frac{C_0(\beta)}{|\mathbf{r}|^{3-\beta}}\,, \qquad (0 < \beta < 2)\,; \qquad |\mathbf{r}| \gg 1$$

■ A Note on Fractional/Fractal Gradela Generalizations

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

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

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

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

  Δ_W^{α}... Fractional Laplacian in **Caputo** form

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

  $({}^{R}D_t^{\beta})^2$... Fractional time derivative of non-integer order β

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

  $\Delta^{(D,d)}$... fractal Laplacian

  D... volumetric fractal dimension; d... surface fractal dimension

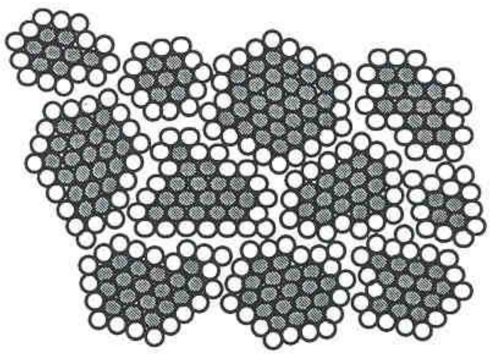
#7. Gradient Material Nanomechanics

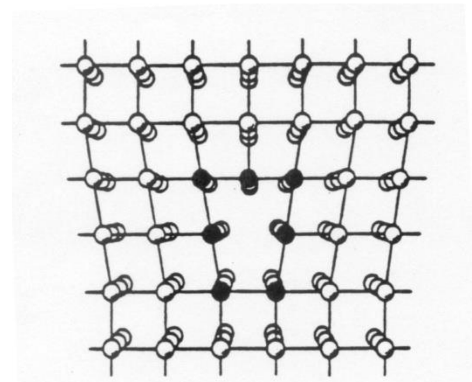
- ***Motivation from Grain Configuration at the Nanoscale***

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

Grain d

1-50 nm



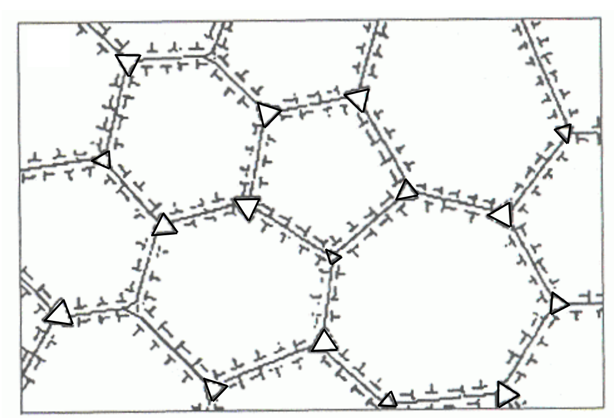


Core r_0

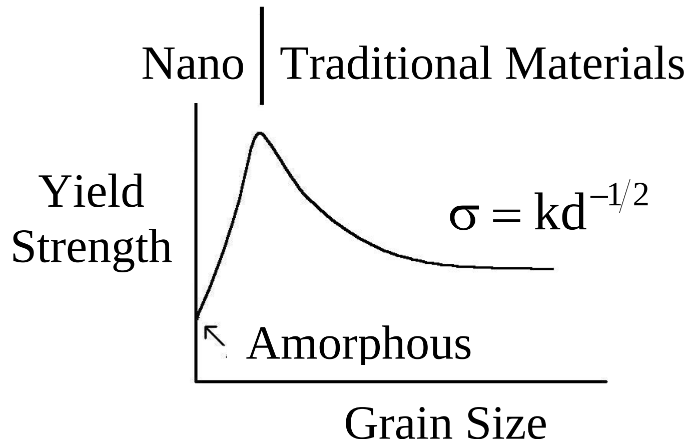
~1 nm

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

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



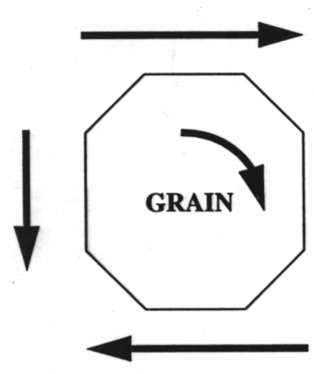
Plasticity Mechanisms ?

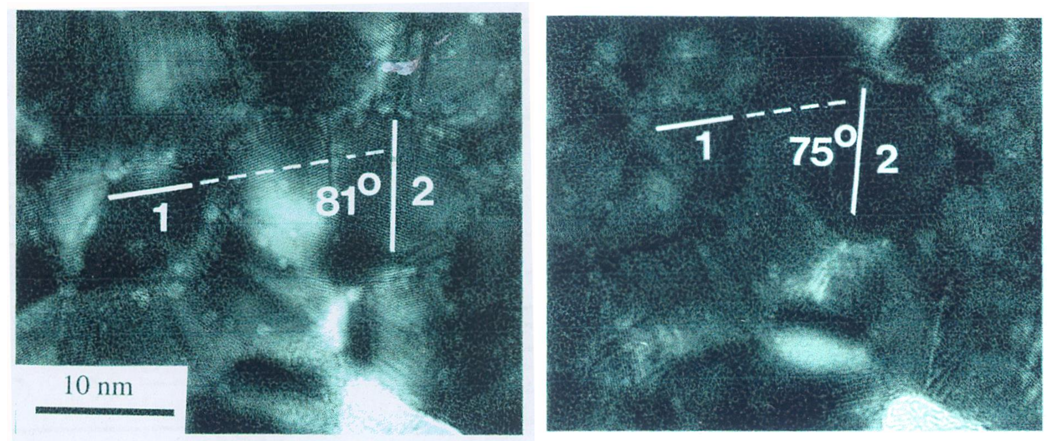


Inverse Hall-Petch (IHP) Relation ?

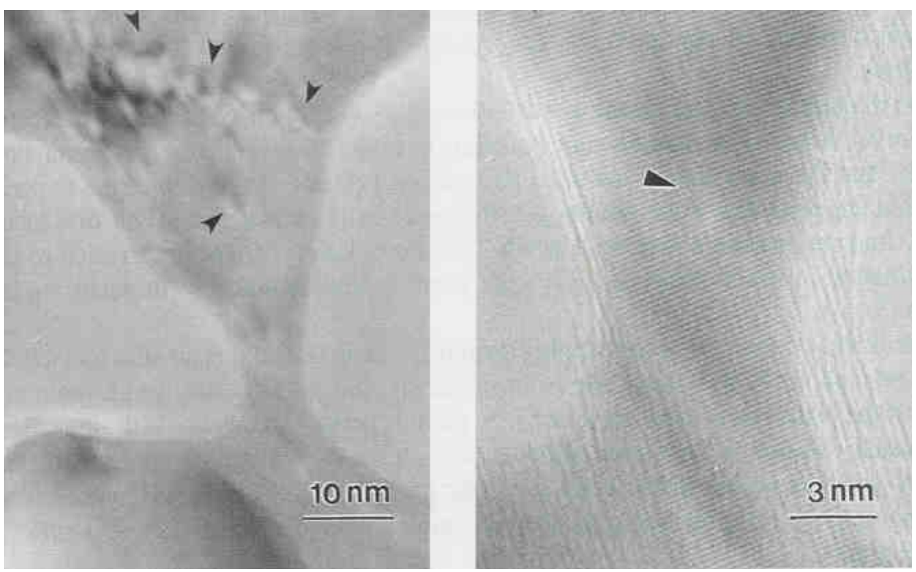
• *Motivation from Early MTU Experimental Observations*

– *Grain Boundary Sliding/ Grain Rotation*

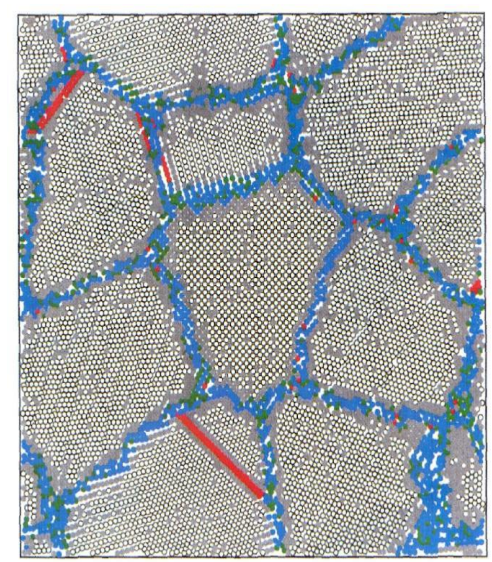




10 nm Au: 6-15 degrees relative grain rotation due to inhomogeneous GB sliding (unbalanced shear stress)



100 nm Ag film



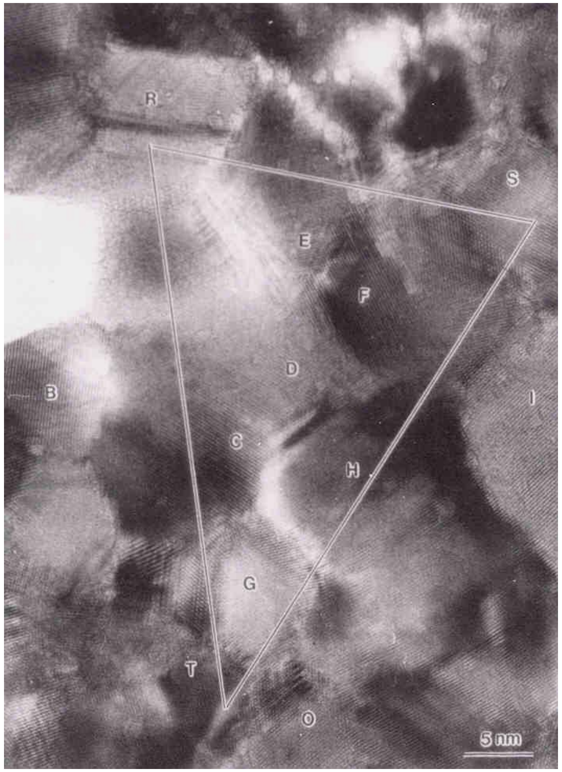
~12 nm Ni nanopolycrystals

– *Grain Rotation / Dislocation Emergence*

Elementary Rosette Analysis

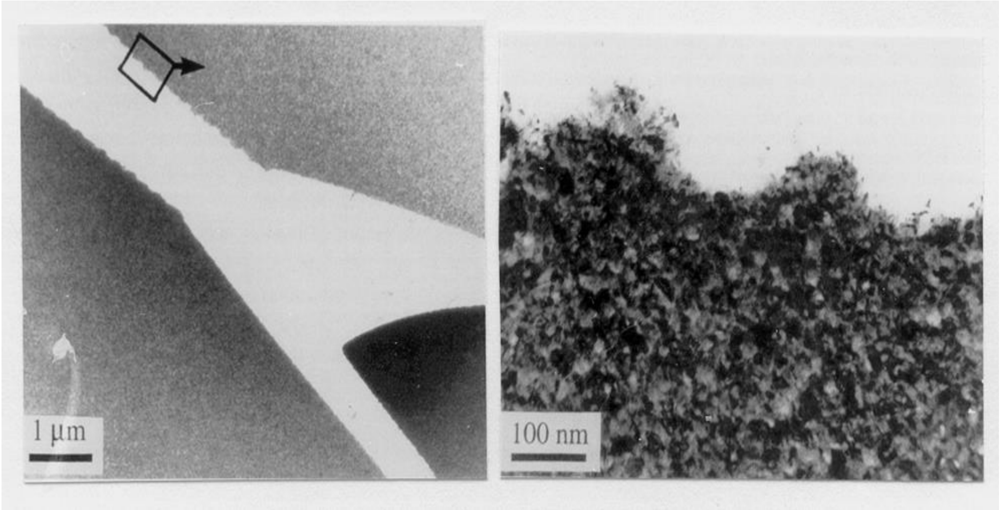
	Triangle angles (deg)			Triangle lengths (nm)		
Step	α	β	γ	a	b	c
Start	89	36	55	22.2	27.7	16.4
1	91	35	54	22.6	27.9	17.4
2	96	36	48	23.4	31.2	18.9
3	102	33	45	21.7	32.0	18.0

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



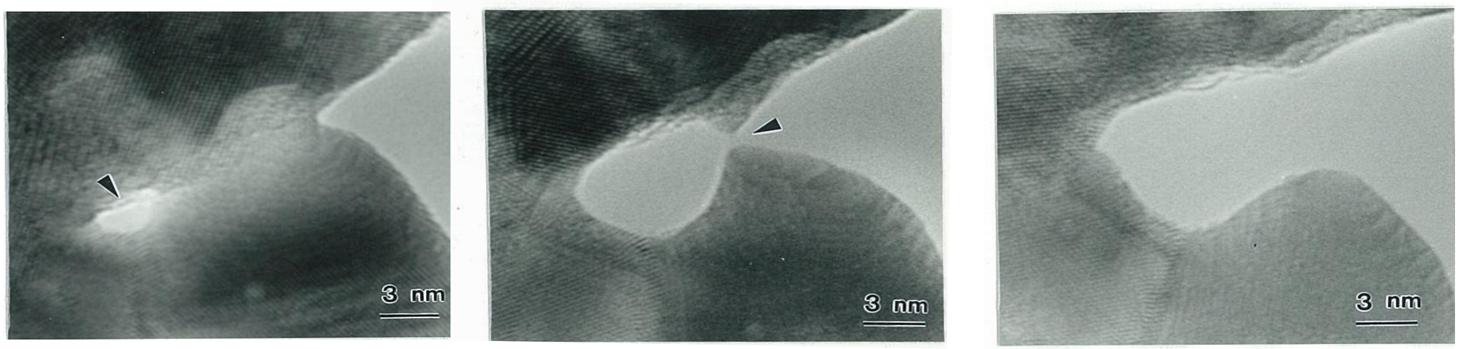
TEM Strain Rosette

– *Oscillatory Crack Propagation*

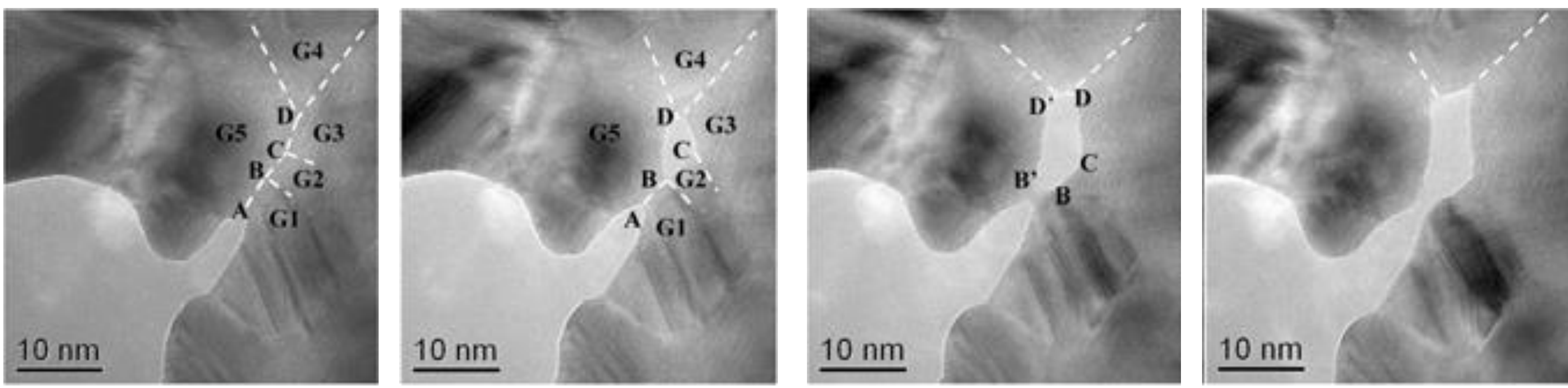


25 nm Au on C: Periodic Crack profiles and bifurcation

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

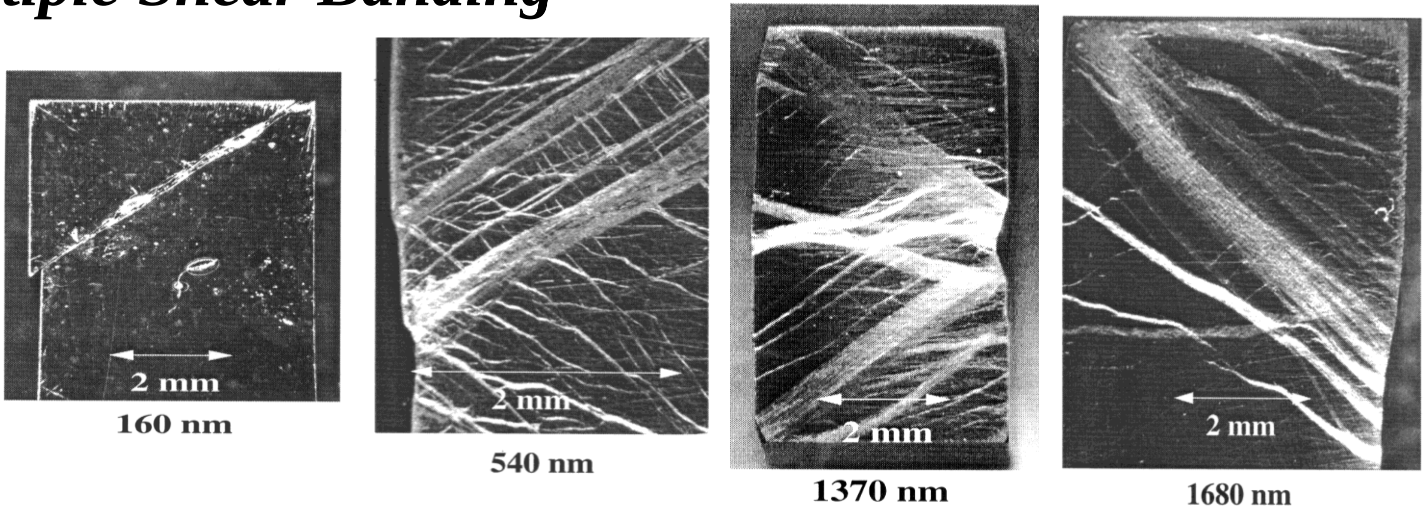


8 nm Au on C: Nanocrack growth via nanopore/nanovoid formation/nucleation at triple GB junction

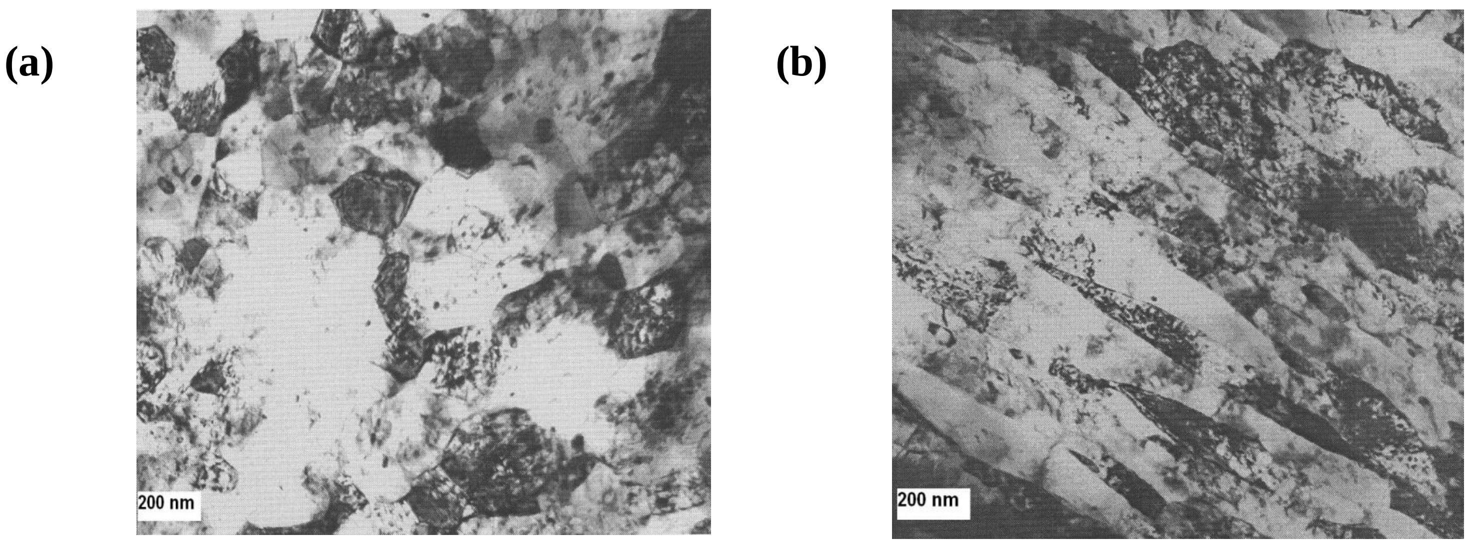


[Wei Yang et al Science / Scripta Met. 2011/2014]

– *Multiple Shear Banding*

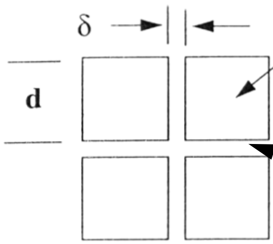


Optical micrographs showing deformation and fracture behavior under compression of nanostructured Fe-10% Cu alloy for different grain sizes



TEM micrographs of a compression-tested sample with a 100-nm grain size. **(a)** Undeformed area outside the shear band region; **(b)** heavily deformed area in the shear band region

• *Continuum Two-Phase Model for IHP Behavior*



"Bulk" Phase, Hall – Petch relation

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

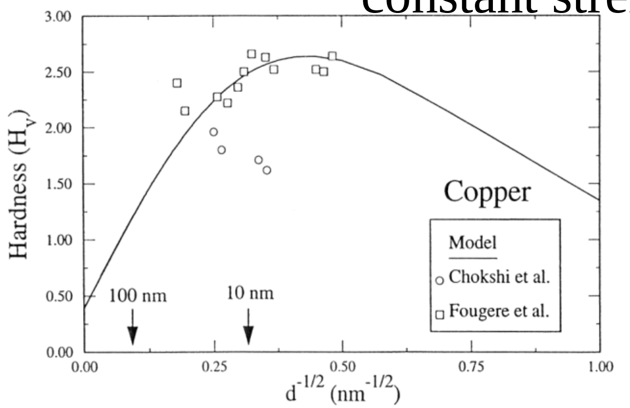
"Boundary" Phase/Amorphous constant strength (σ_{GB})

- Volume Fraction

$$f = d^3/(d+\delta)^3$$

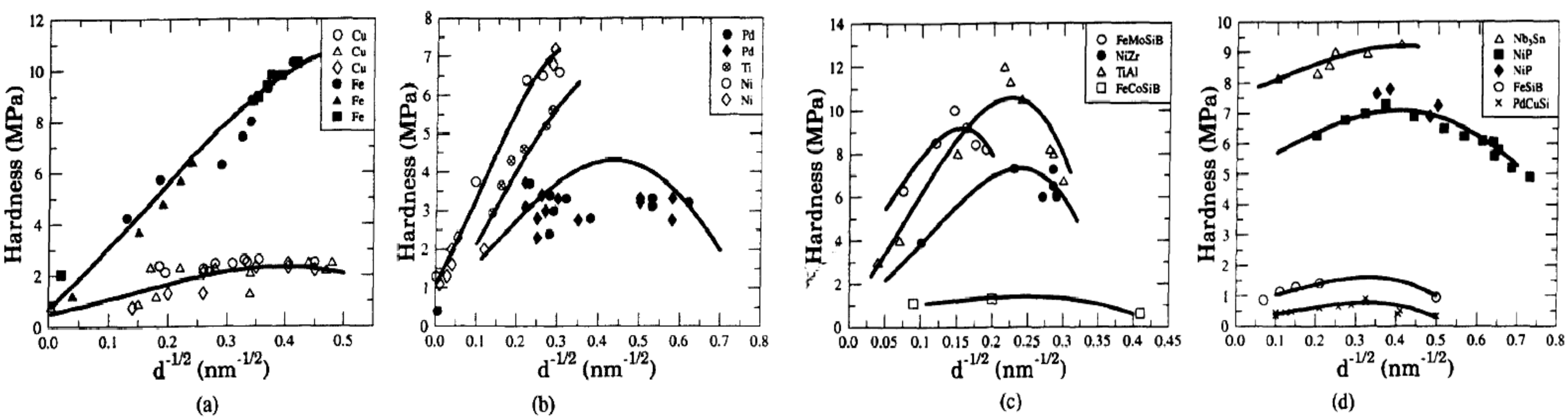
- Rule of Mixtures

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



•*Continuum Model predicts behavior of NanoCrystalline Materials*

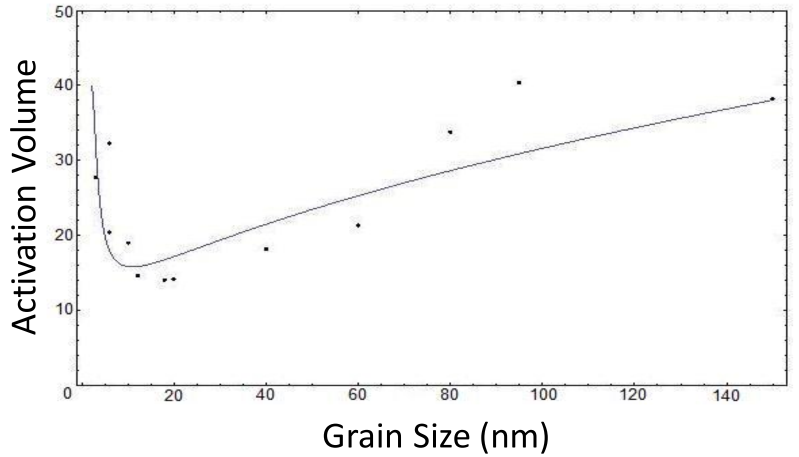
•*Continuum Model can sort out conflicting Materials Science data*

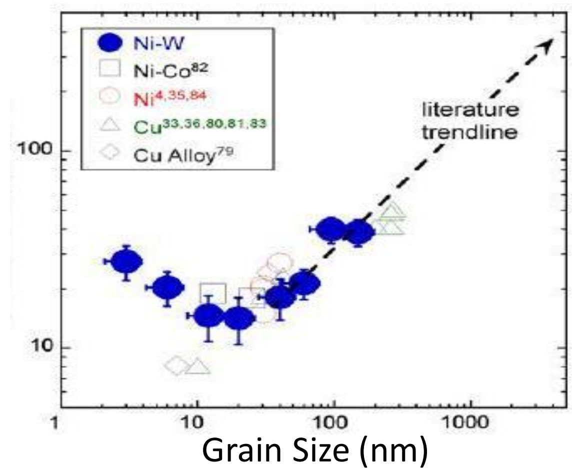


(a) & (b): nanocrystalline metals; (c) & (d): intermetallics

■ A Note on Activation Volume (υ)

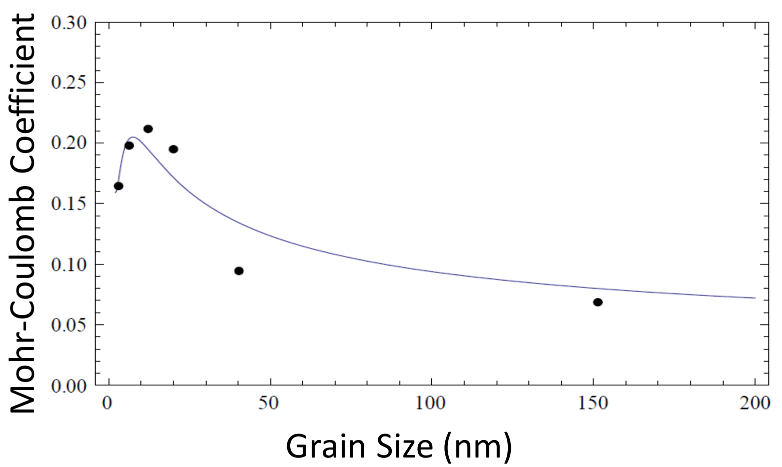
- $$\upsilon = \sqrt{3}\, kT \frac{\partial \ln \dot{\varepsilon}}{\partial \sigma} \quad ; \quad \frac{1}{\upsilon} = f \frac{1}{\upsilon_g} + (1 - f) \frac{1}{\upsilon_{gb}}$$

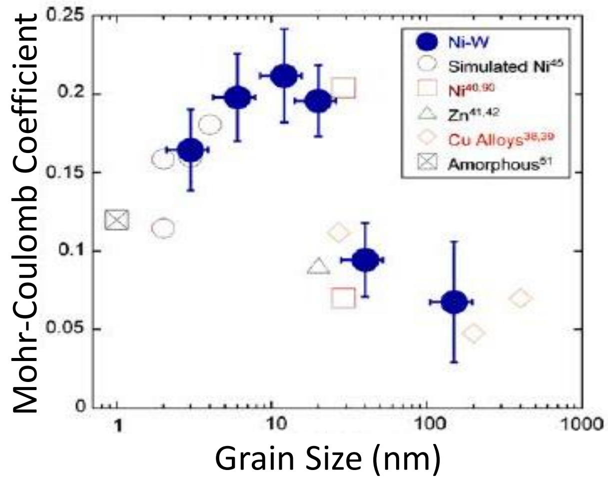




■ A Note on Pressure – Sensitivity Parameter (α)

- $$\sqrt{J} + \alpha p - \kappa = 0 \quad ; \quad \alpha = f \alpha_g + (1 - f) \alpha_{gb}$$



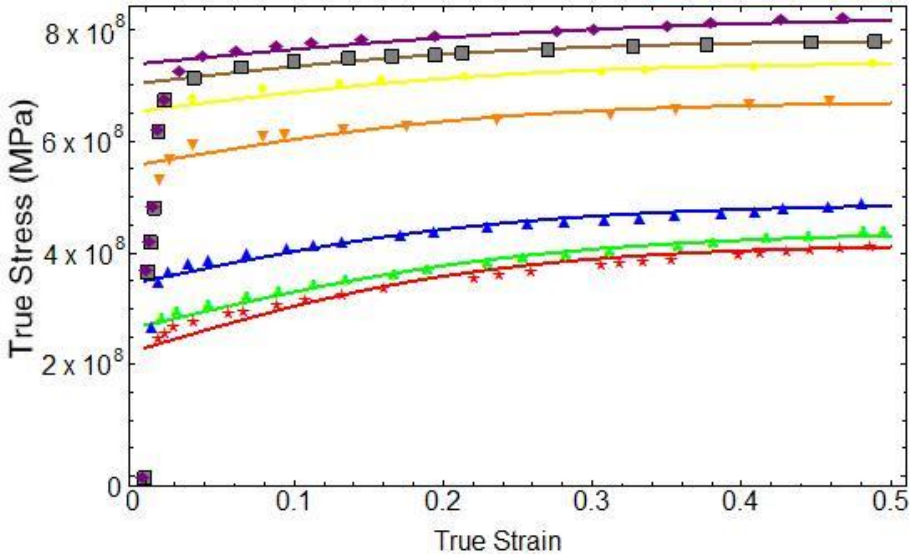


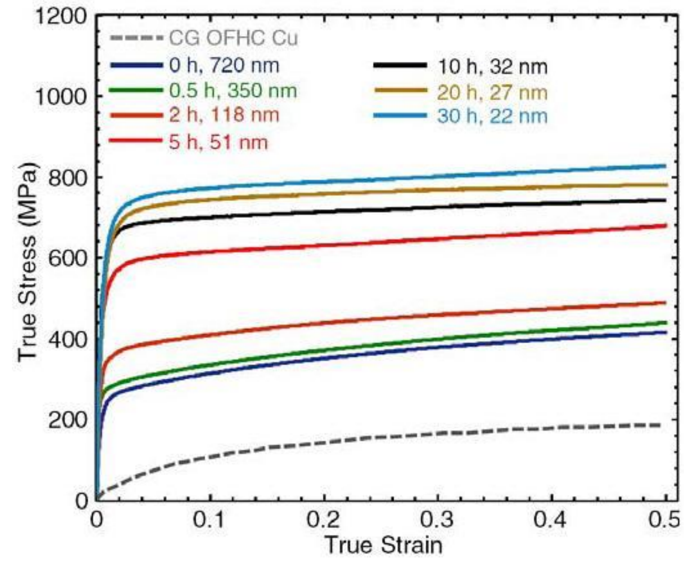
■ A Note on Extension to Size-Dependent Stress vs. Strain Curves

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

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

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





$$\sigma^0_s = 230\,\text{MPa}, \quad k_s = 92.5\,\text{kPa}\sqrt{\text{m}}, \quad \sigma^0_f = 70\,\text{MPa},$$

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

■ A Note on Nanotwinning

- ***Original Voce Relation:*** $$\sigma = \sigma_s - (\sigma_s - \sigma_y)\exp\left[-\frac{\varepsilon^p - \varepsilon_y}{\varepsilon_r^p}\right]$$

  – *Hardening* $$\sigma_y = \sigma_{y0} + k_1\lambda^{-1/2}; \qquad \sigma_s = \sigma_{s0} + k_2\lambda^{-1/2}$$

  – *Softening* $$\sigma_y = \sigma_{y1} - k_3\ln\left(\frac{d}{\lambda}\right); \quad \sigma_s = \sigma_{s1} - k_4\ln\left(\frac{d}{\lambda}\right)$$

- ***Modified Voce Relation***

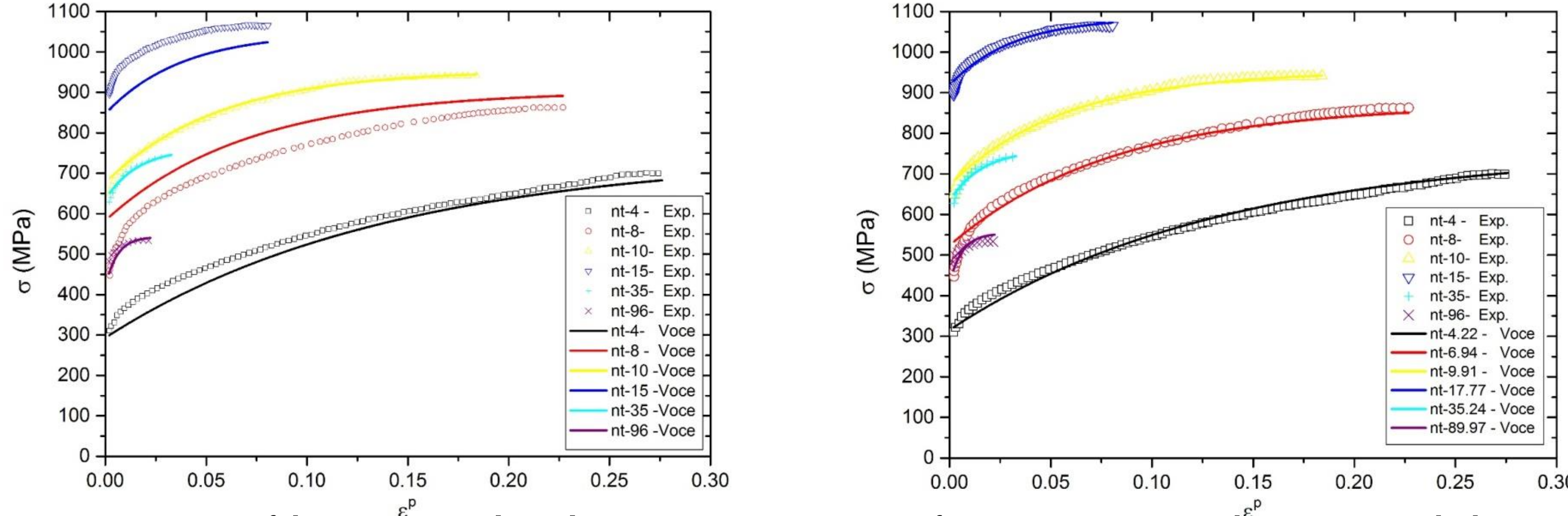
  – *Hardening* $$\sigma = \sigma_{s0} + k_2\lambda^{-1/2} - \left[\sigma_{s0} - \sigma_{y0} + (k_2 - k_1)\lambda^{-1/2}\right]\exp\left[-\frac{\varepsilon^p - \varepsilon_y}{k_5}\lambda\right]$$

  – *Softening* $$\sigma = \sigma_{s1} - k_4\ln\left(\frac{d}{\lambda}\right) - \left[\sigma_{s1} - \sigma_{y1} + (k_4 - k_3)\ln\left(\frac{d}{\lambda}\right)\right]\exp\left[-\frac{\varepsilon^p - \varepsilon_y}{k_5}\lambda\right]$$

  – *H-P & Critical Twin Thickness* $$\sigma_y = \sigma_0 + \frac{k}{\sqrt{\lambda}} + \frac{\gamma_{TB}}{2a\lambda}; \qquad \lambda_c = \left(\frac{\gamma_{TB}}{ak}\right)^2$$

- ***Note:*** $\varepsilon_r^p = k_5/\lambda$ … Kocks–Mecking–Estrin Model

• *Fitting to Experiments*



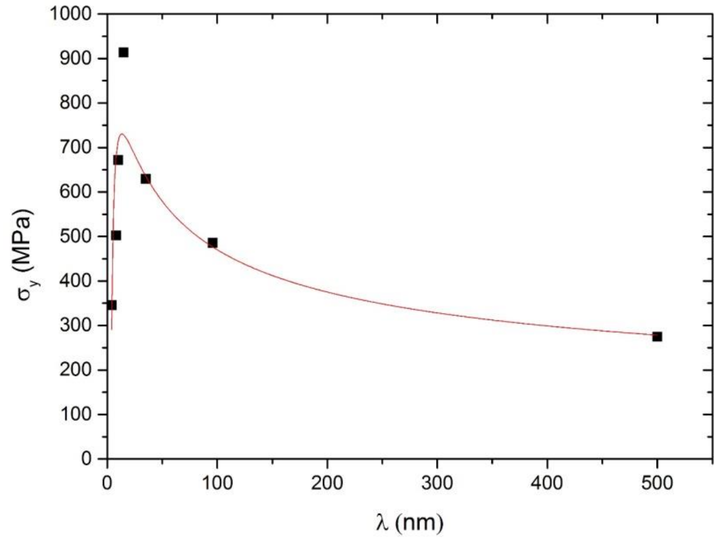
Fitting of the various size-dependent true stress-strain curves for nt-Cu specimens with varying twin thickness. **(a)** Twin thickness as reported in Lu et al, 2009 (Table 1); **(b)** Slightly modified twin thickness (Table 2).

Table 1

	σ_{y0}	k_1	σ_{s0}	k_2	σ_{y1}	k_3	σ_{s0}	k_4	k_5
	MPa	$\mathrm{kPa}\sqrt{m}$	MPa	$\mathrm{kPa}\sqrt{m}$	MPa	MPa	MPa	MPa	nm
Fitted	158	2910	210	3271	2337	422	1847	228	0.562
error	29	176	20	122	354	86	137	33	0.032
Adj. R^2	0.989		0.996		0.886		0.939		0.968

Table 2

λ (nm)	4	8	10	15	35	96
fitted (nm)	4.22	6.94	9.91	17.77	35.24	89.97
error (nm)	0.01	0.02	0.04	0.05	0.23	1.28



Comparison between theory and experiment for size-dependent initial yield stress for nt-Cu specimens with varying twin thickness.

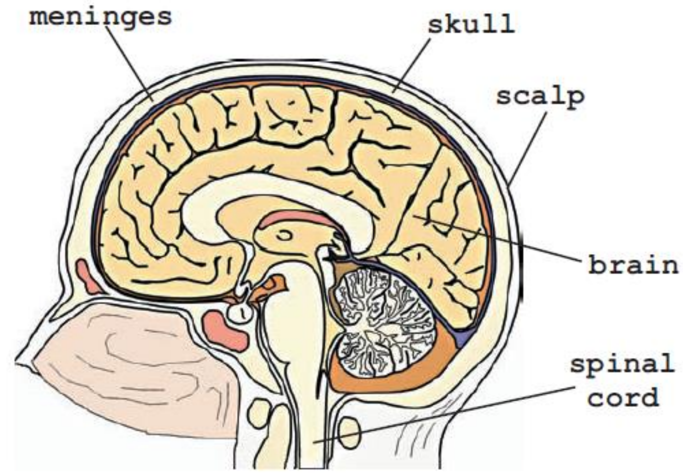
#8. Exploring Gradient Neuromechanics

■ Motivation

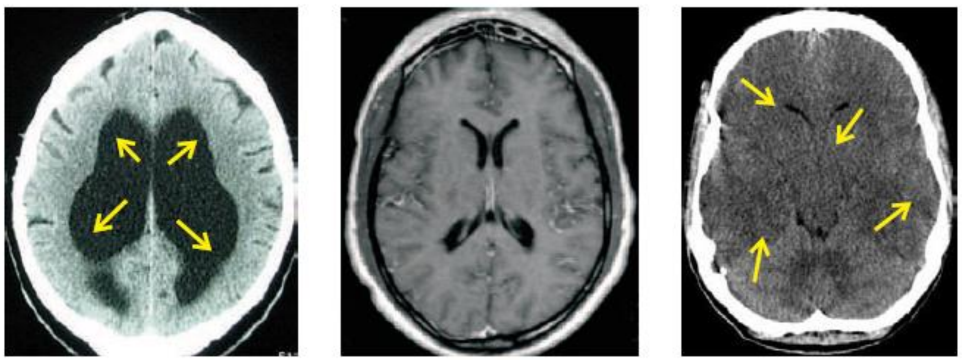
(a)

(b)

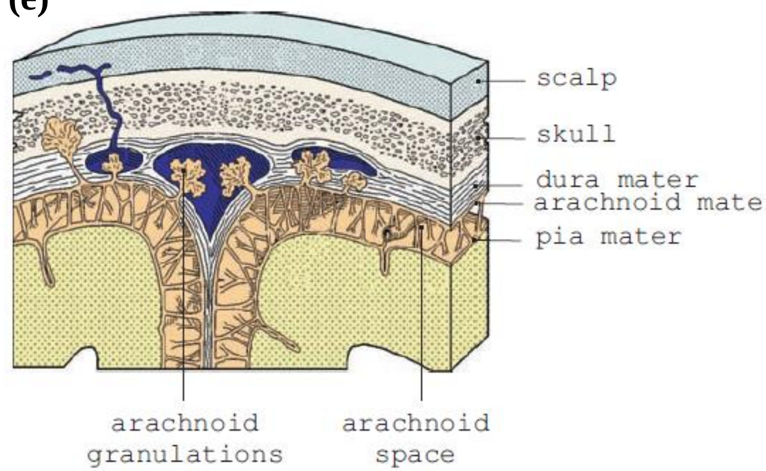
(c)



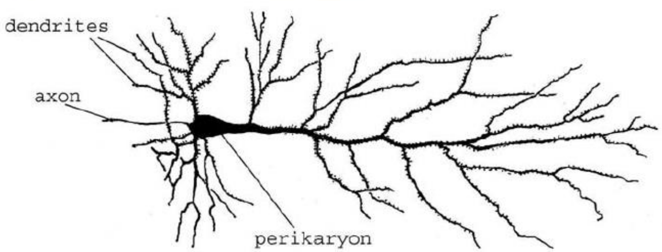
(d)



(e)



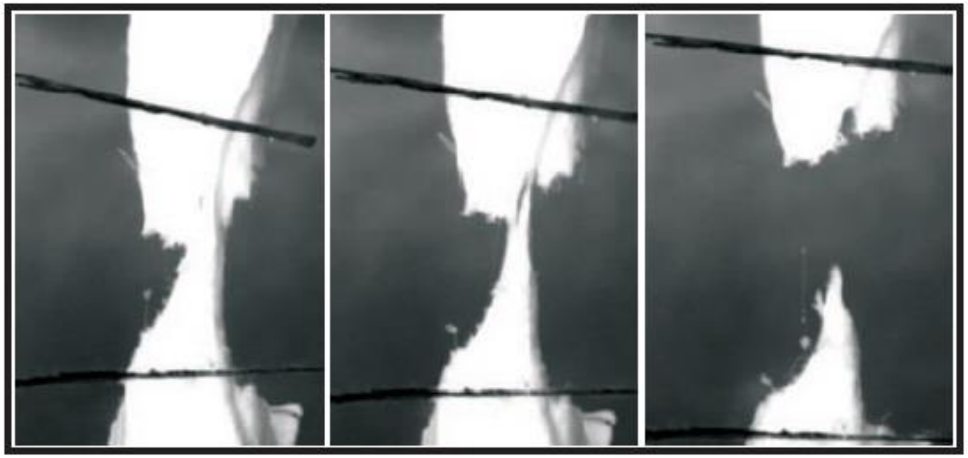
(f)



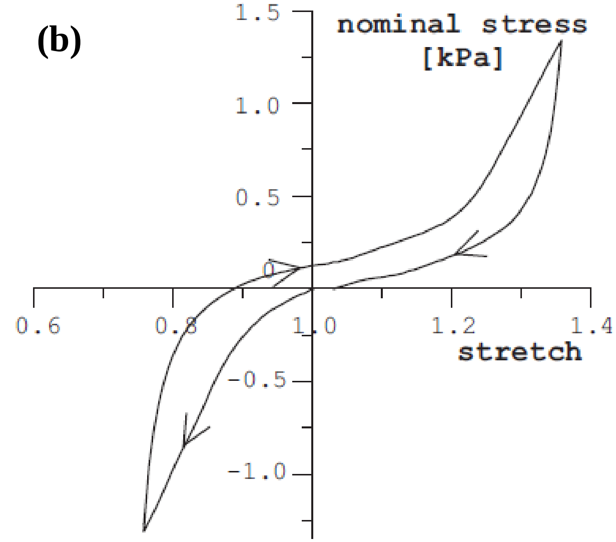
(a) An ancient skull showing artificial deformations ; **(b)** A sketch showing an apparatus adopted to impress cranial deformations. A cradle-board made up of two wood boards where child was reposed; **(c)** The human head; **(d)** Cranial tomography showing an hydrocephalus (left) and a cerebral edema (right). In the middle a cranial tomography showing a brain in normal dimension of third and lateral ventricles (black zones). However, in both pathologies, the high pressure determines a partial (left) and a total (right) disappearance of convolutions, clearly visible in the normal conditions.; **(e)** Meninges and subarachnoid space.; **(f)** A nerve cell (i.e. pyramidal cell) in the cerebral cortex.

■ Brain Tissue Tensile Test

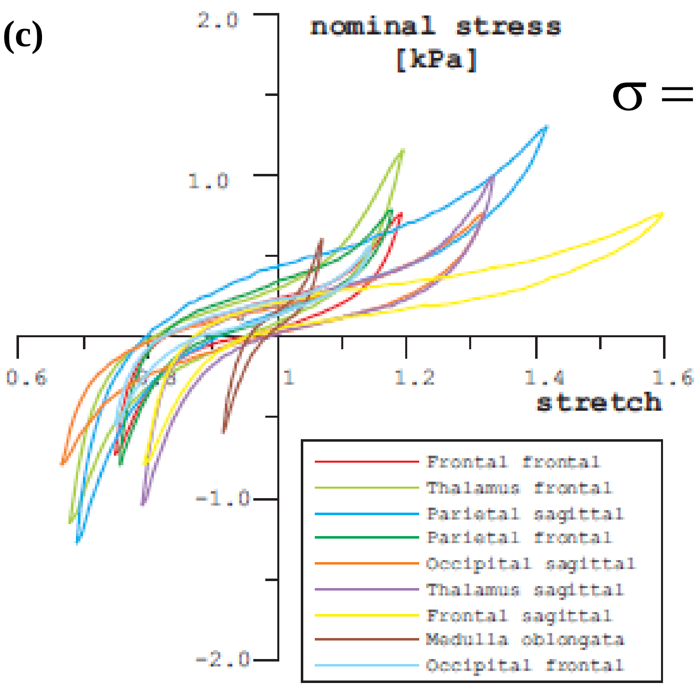
(a)



(b)

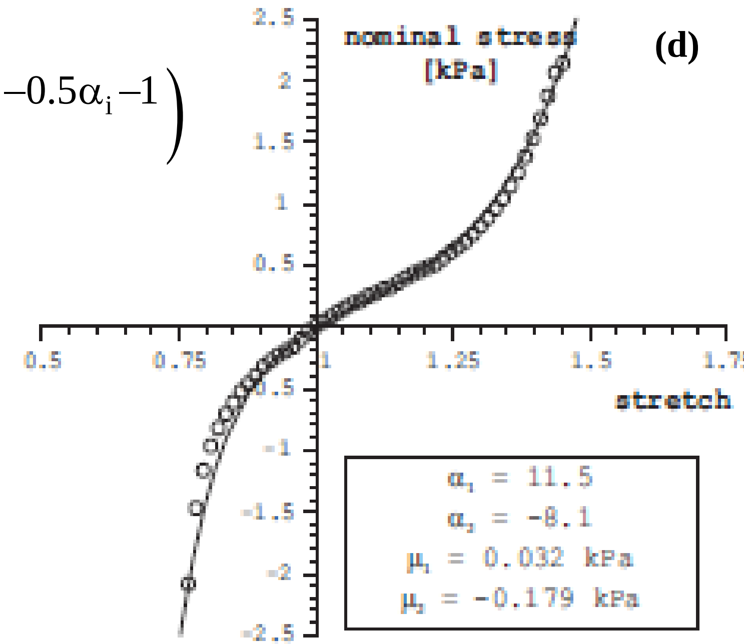


(c)



$$\sigma = \sum_{i=1}^{N} E_i \left(\varepsilon^{\alpha_i - 1} - \varepsilon^{-0.5\alpha_i - 1} \right)$$

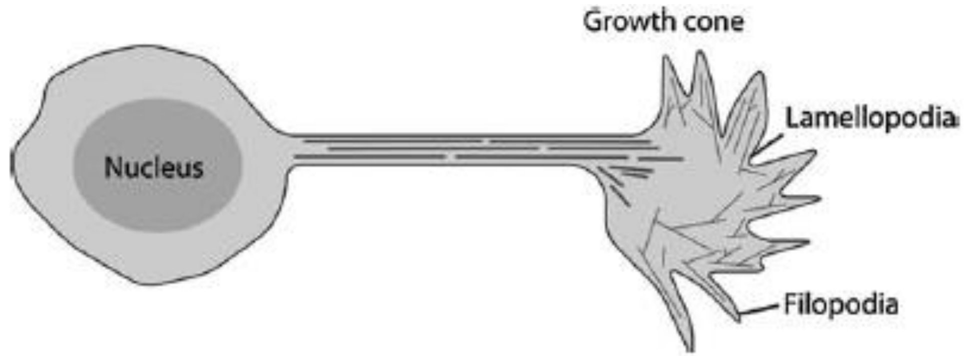
(d)



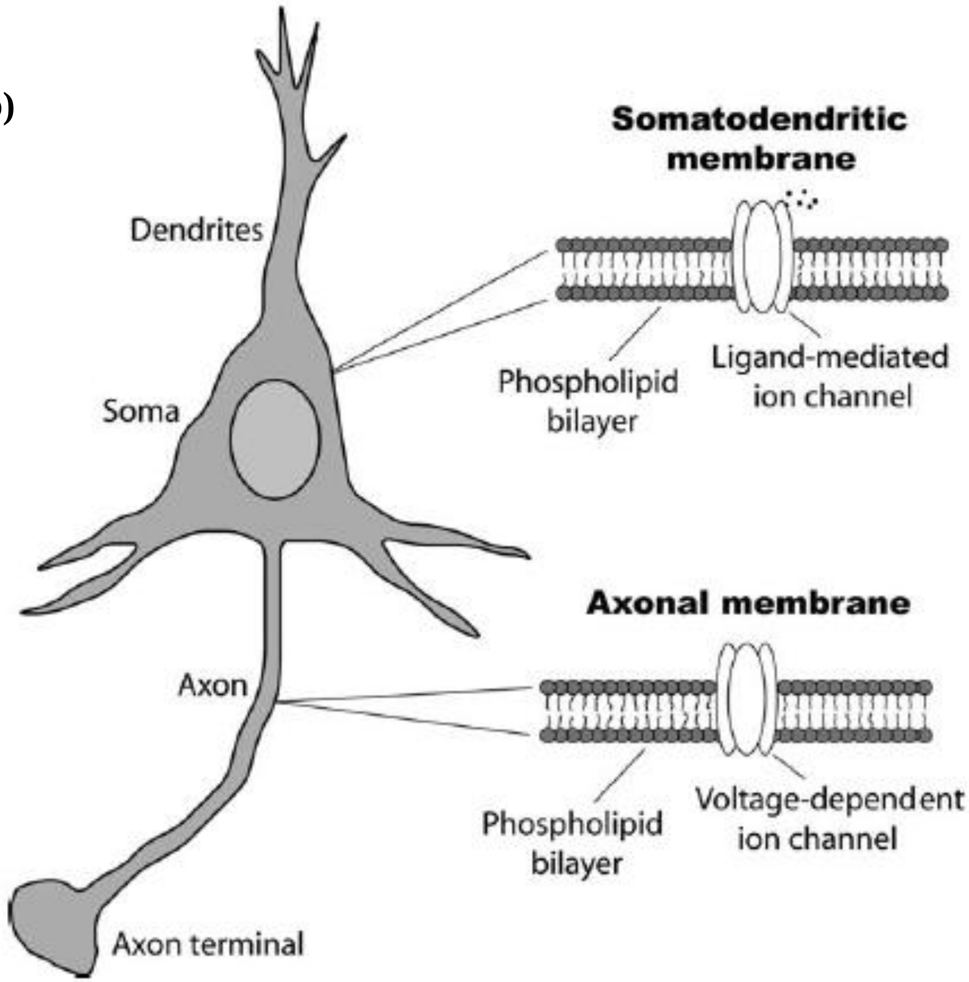
(a) The fracture process in a (11.9 mm/7 mm initial height/diameter) cylindrical specimen of brain tissue, harvested from the optical lobe in the sagittal direction; **(b)** Result of compression/tension test to a stretch well below fracture but approaching the damage threshold [14mm/9.5 mm initial height/edge] prismatic specimen of white matter, harvested from the occipital lobe in the frontal direction. Nominal stress is reported versus stretch. Arrows indicate the loading direction; © Dispersion of data of compression/tension tests to a stretch well below fracture but approaching the damage threshold on prismatic specimens of white and gray matter, harvested from the occipital lobe and from all the locations. Nominal stress is reported versus stretch; **(d)** Comparison between the Ogden theory of elasticity and a loading curve of compression/tension test performed on a specimen of white matter harvested from corpus callosum.

■ Neuron's Schematics

(a)



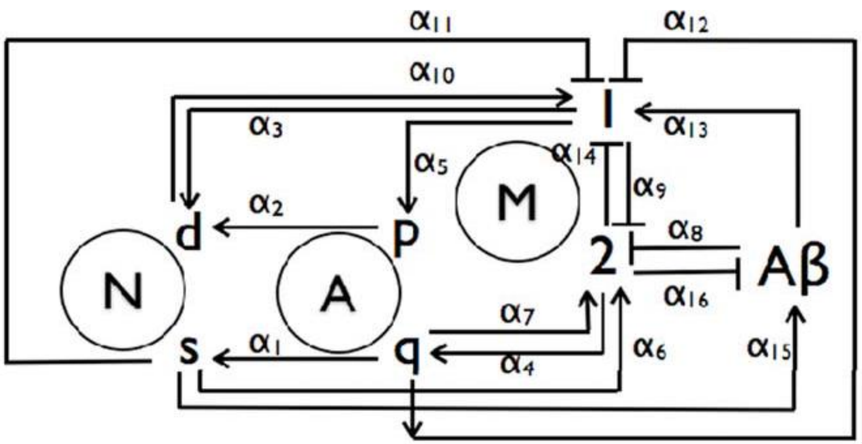
(b)



(a) The growth cone of the developing neuron. Actin filaments fill the growth cone lamellopodia and provide the structural basis of the extending filopodia. This contrasts with the main axon shaft, which is filled with microtubules; **(b)** The neuronal membrane surrounds all parts of the neuron. The somatodendritic membrane and the axonal membrane are distinguished on the basis of the types of ion channels embedded within their boundaries.

■ A Note on Alzheimer Disease Modeling

- ***Phenomenology: Extracellular Plaques vs. Intracellular Fibril Bundles***
- ***A Kinetic Model: No Gradients***



Schematic of the AD mechanism that incorporates feedback influences from surviving and dead neurons, N_s and N_d, quiescent and proliferating astroglia A_q and A_p, reactive and normal microglia, M_1 and M_2, and Aβ.

$$dN_s/dt = \alpha_1 A_q - \alpha_2 A_p - \alpha_3 M_1; \quad dN_d/dt = -dN_s/dt \quad (1,2)$$

$$dA_q/dt = \alpha_4 M_2 - \alpha_5 M_1; \quad dA_p/dt = -dA_q/dt \quad (3,4)$$

$$dM_2/dt = (\alpha_6 + \alpha_{11}) N_s - \alpha_{10} N_d + (\alpha_7 + \alpha_{12}) A_q - \alpha_9 M_1 + \alpha_{14} M_2 - (\alpha_8 + \alpha_{13}) A\beta \quad (5)$$

$$dM_1/dt = -dM_2/dt; \quad dA\beta/dt = \alpha_{15} N_s - \alpha_{16} M_2 \quad (6,7)$$

M: Microglia A: Astroglia

N: Neurons Aβ: Amyloyd-β

• *An R-D Model: The Microglia Plaque Connection*

m – activated microglia

(c_1/c_2) – attractant/repellant concentrations

$$\frac{\partial m}{\partial t} = \mu \frac{\partial^2 m}{\partial x^2} - \frac{\partial}{\partial x}\left(\chi_1 m \frac{\partial c_1}{\partial x} - \chi_2 m \frac{\partial c_2}{\partial x}\right),$$

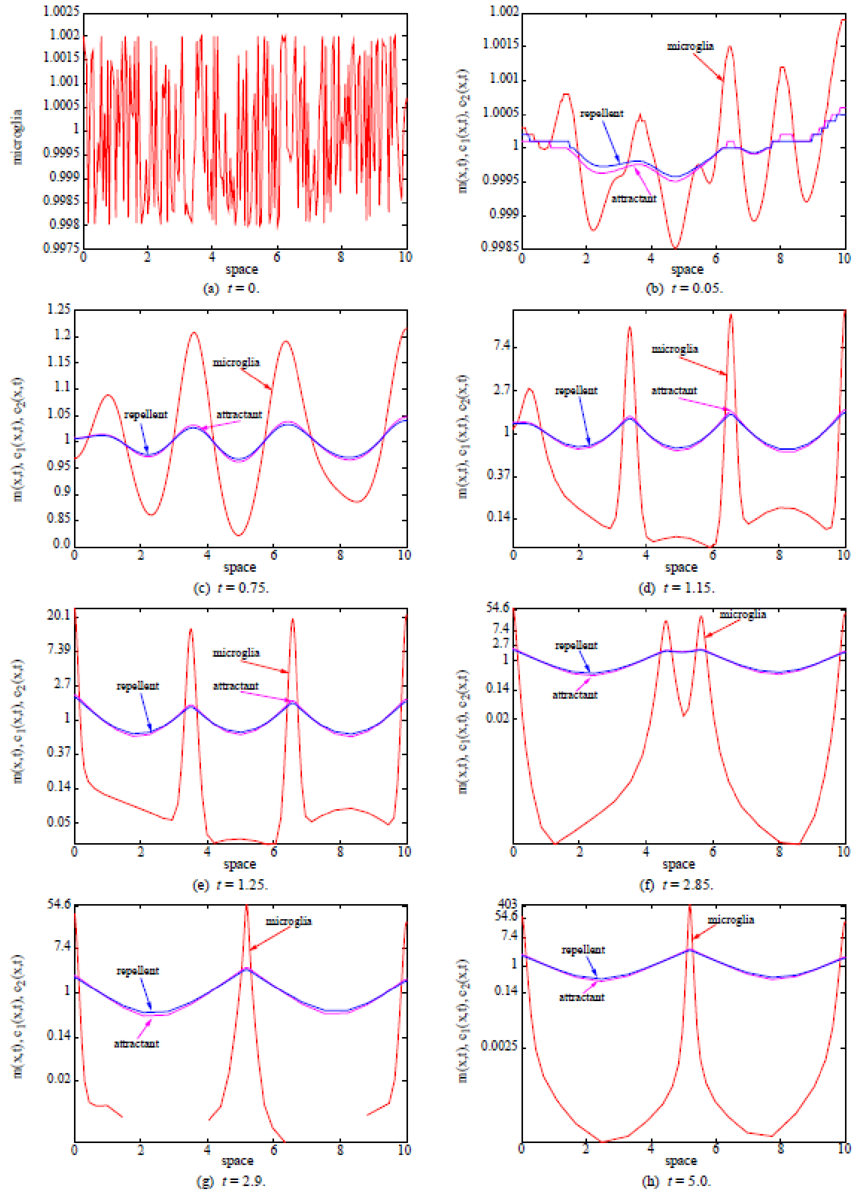
$$\frac{\partial c_i}{\partial t} = D_i \frac{\partial^2 c_i}{\partial x^2} + a_i m - b_i c_i \qquad i = 1, 2.$$

μ – microglia mobility coefficient

(χ_1/χ_2) – chemotactic attractant/repellant coeff.

(D_1/D_2) – diffusion coefficients

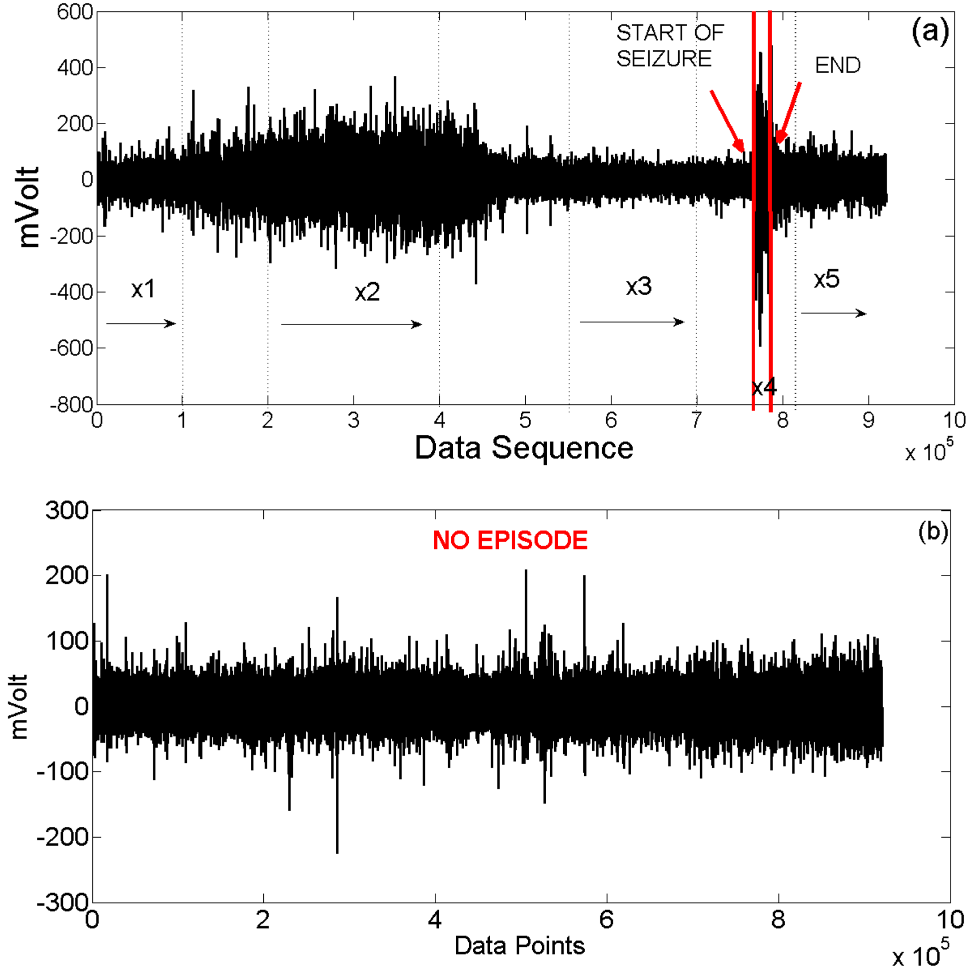
(a/b) – production/decay rates



Numerical Results – Pattern Formation

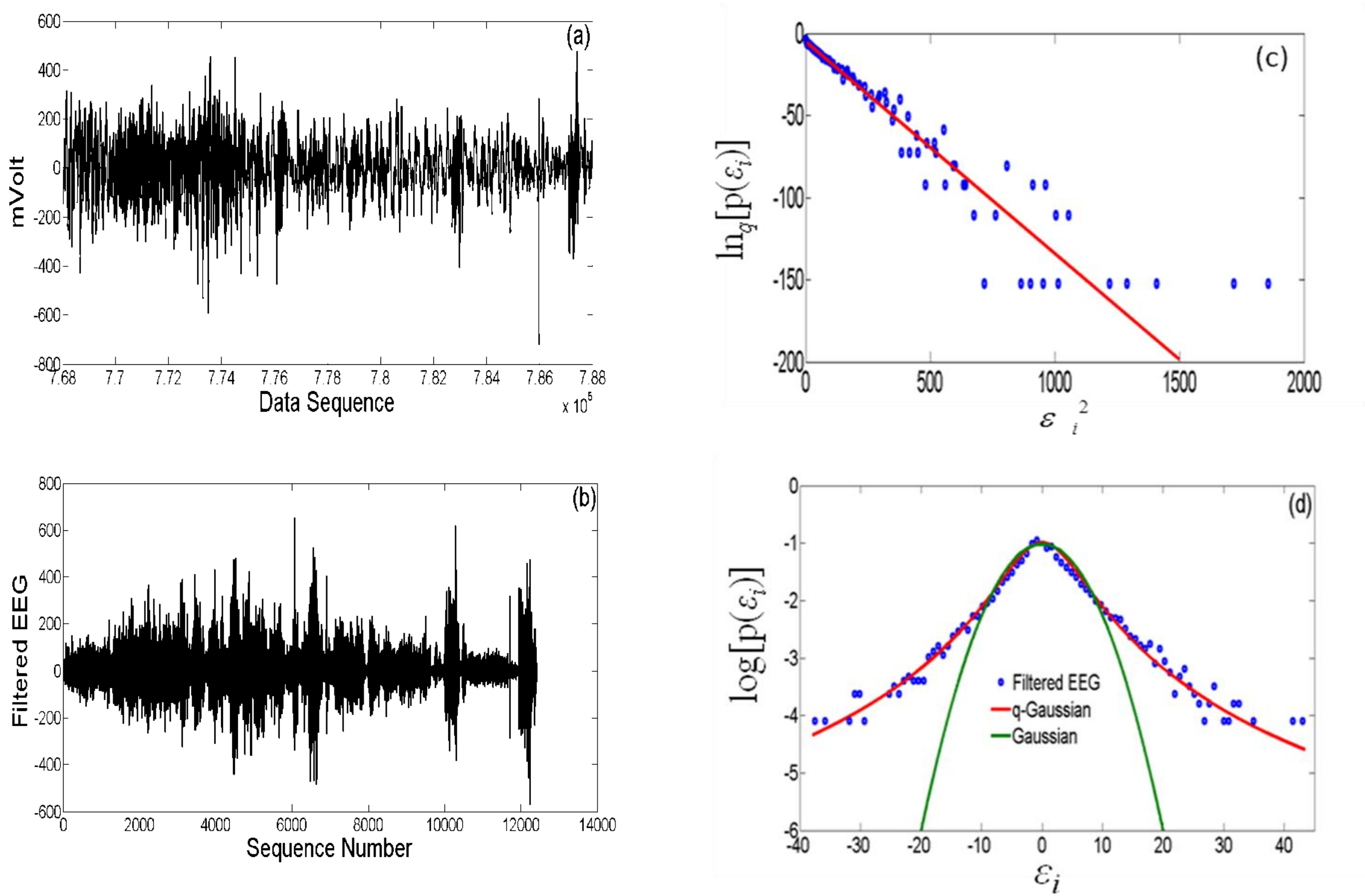
- ***Brain Signal Time Series/Tsallis q-Statistics***

Epilepsy



a) EEG time series corresponding to an epileptic episode. The initiation of the episode and its end is denoted by the red vertical lines. **b)** EEG time series without episode.

• *EEG Epileptic Regime*



a) Time series of the epileptic episode. **b)** Filtered EEG time series corresponding to Fig. 2a. **c)** Best linear correlation fitting between $\ln_q [p(\varepsilon_i)]$ and $(\varepsilon_i)^2$ for the filtered signal. **d)** $\log[(p(s_i)]$ vs s_i for the Filtered EEG time series (blue circles), the theoretical q-Gaussian (blue line) and the normal Gaussian (green line).