האוניברסיטה העברית בירושלים
THE HEBREW UNIVERSITY OF JERUSALEM

Simulations of dislocations and plastic processes in ductile materials -

outsider perspectives for outsiders

Yinon Ashkenazy
Racah Institute of Physics,
Hebrew University, Jerusalem, Israel

contents

- introduction to dislocations induced plasticity
- Constitutive equations from dislocations reactions
- Critical properties in dislocation reactions:

  Glide, dissociation, pileup, cross-slip, climb, sources and sinks,
- Linking atomistic – DDD – continuum

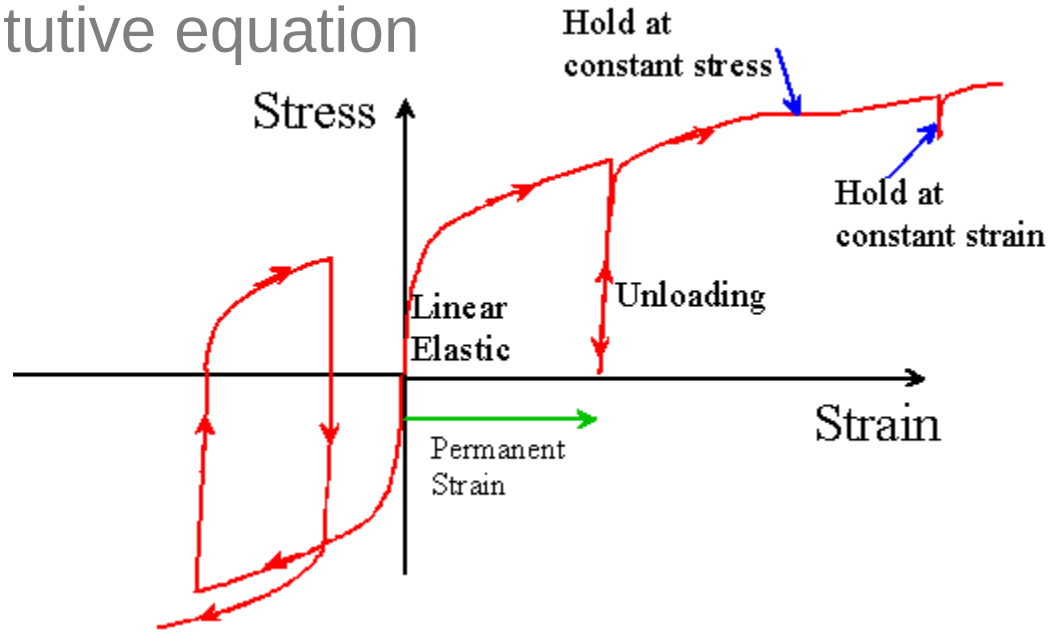
  Need for reactions, effects of solute, grain boundaries.
- Mean field models - Linking dislocations and critical processes - stochastic processes and models
- Some experimental observations

plasticity

- Materials response to external drive formulated through macroscopic equations:

Three main rules:

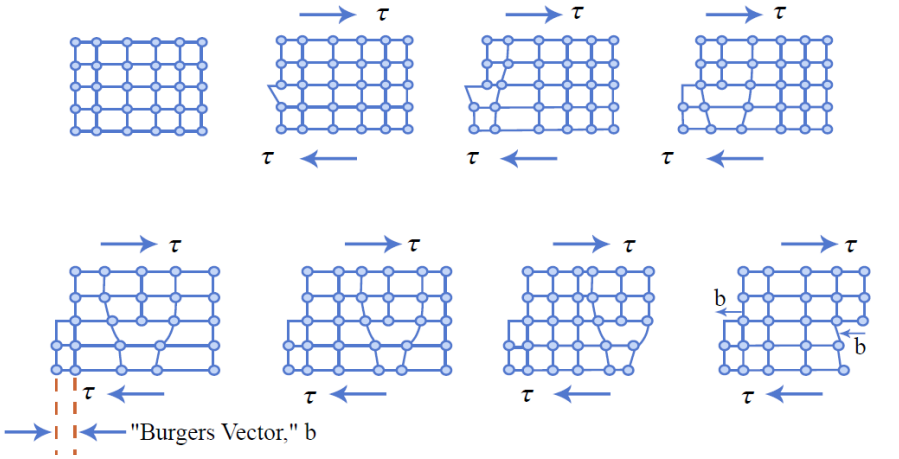
a. Yield criterion
b. strain hardening
c. Plastic flow constitutive equation

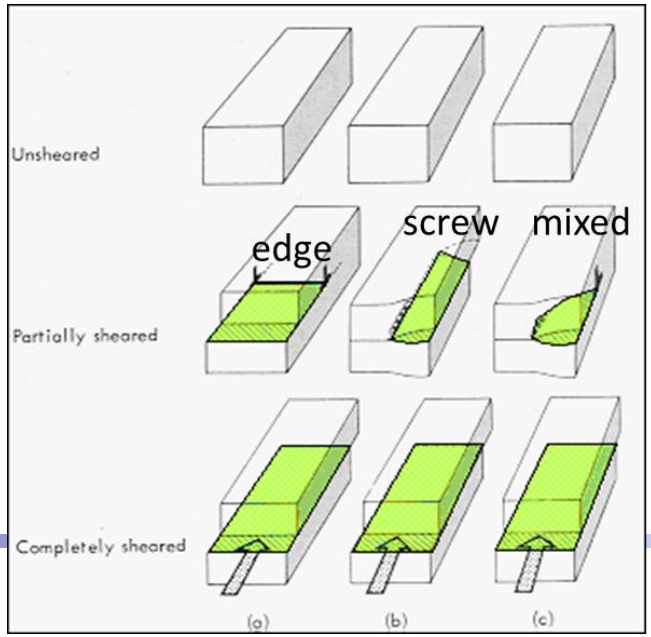


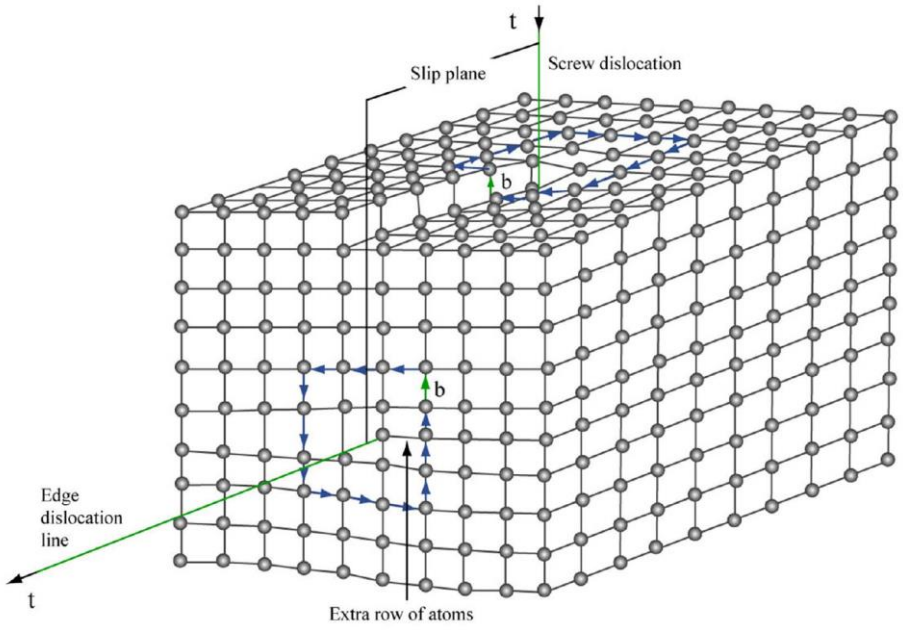
Dislocations and plastic deformation

- Yield through dislocation motion

- Edge / screw dislocations
  - Each displacement field can be decomposed to a combination of dislocations.

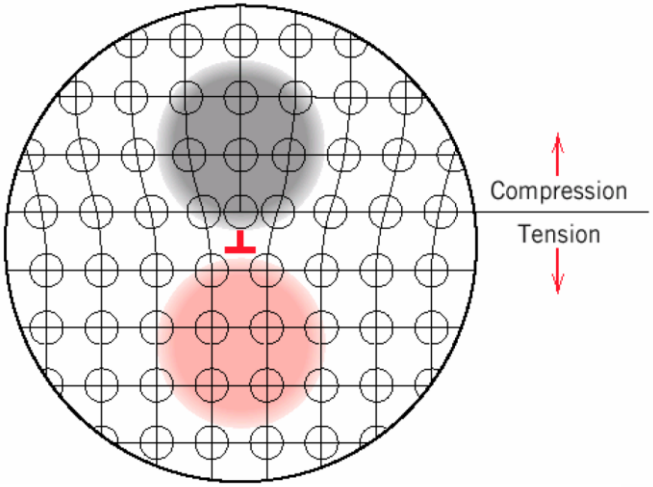


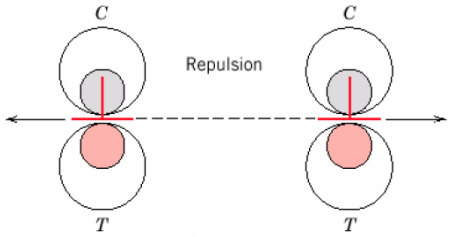


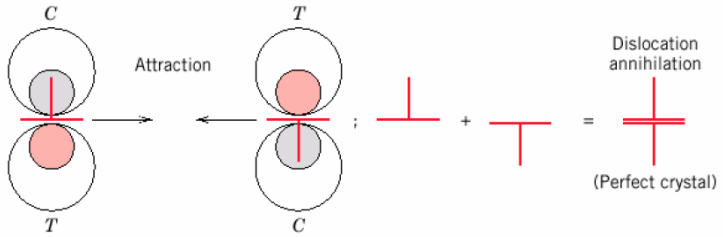


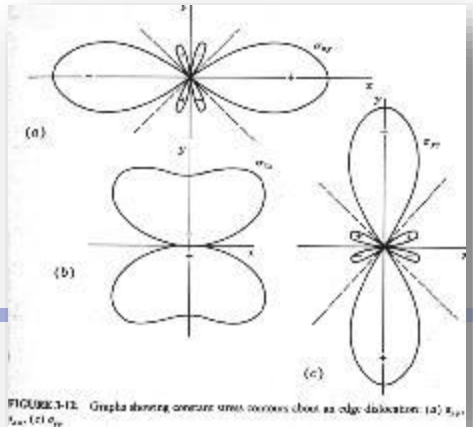
Anisotropic strain field of a dislocation

- Dislocations create a strain/stress field around them.
- Usually assumed to obey expression derived from continuity…
  screw – create pure shear strain
  edge – compressive, tensile and shear strains
- Spatial variation -> effective interaction:
  same sign – repel, opposite sign attract









Forces on dislocations – Peach Koehler

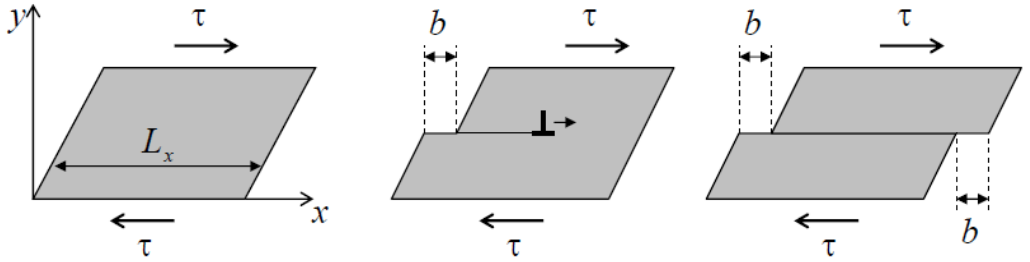
PHYSICAL REVIEW VOLUME 80, NUMBER 3 NOVEMBER 1, 1950

The Forces Exerted on Dislocations and the Stress Fields Produced by Them

M. PEACH AND J. S. KOEHLER*
Carnegie Institute of Technology, Pittsburgh, Pennsylvania
(Received May 4, 1950)

It is shown that the force $d\mathbf{F}$ exerted on a line element $\mathbf{v}d\sigma$ of a dislocation with Burgers vector f by a stress τ is given by $d\mathbf{F}=-\mathbf{v}\times(\mathbf{f}\cdot\tau)d\sigma$. An analogy is drawn between the behavior of a closed line dislocation in a

Application of external stresses and stresses generated by other crystal defects may cause movement of a dislocation on its glide plane. As a result, work may be done by the applied stresses. Let's consider dislocation motion in a sample with dimensions $L_x \times L_y \times L_z$ due to the shear stress τ :



The work done by the shear stress τ in changing the system from the initial to the final state is equal to $\tau Sb = \tau L_x L_z b$. If we consider the process as movement of a dislocation under the action of force F acting on a unit length of the dislocation, the same work can also be written as $(\textit{force}\ FL_z) \times (\textit{distance}\ L_x) = FL_zL_x$

Thus $F = \tau b$

The force acting on a dislocation line is not a physical force (like mechanical force of a spring or electrostatic force acting on a charged particle) but a way to describe the tendency of dislocation to move through the crystal when external or internal stresses are present.

This work done at the slip plane is dissipated into heat (similar to work done by friction forcers)

Dislocation multiplication and critical resolved shear stress

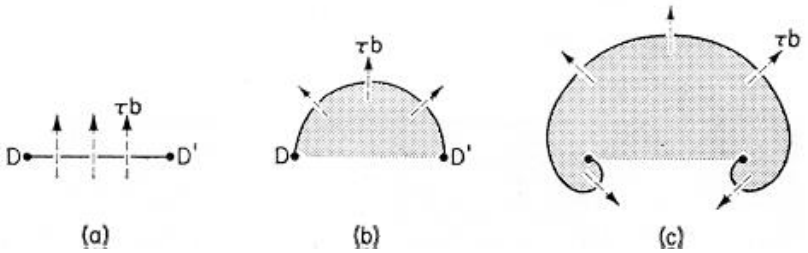
- Stress applied to a pinned dislocation can lead to bowing and generation of a new dislocation

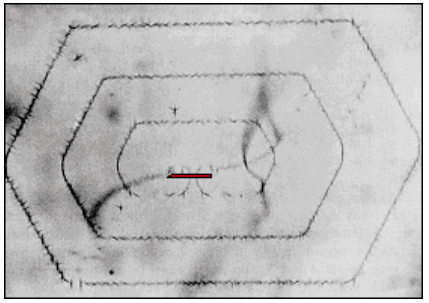
  (Frank-Reed source)
- Shear along slip planes.
- Resolved shear stress:

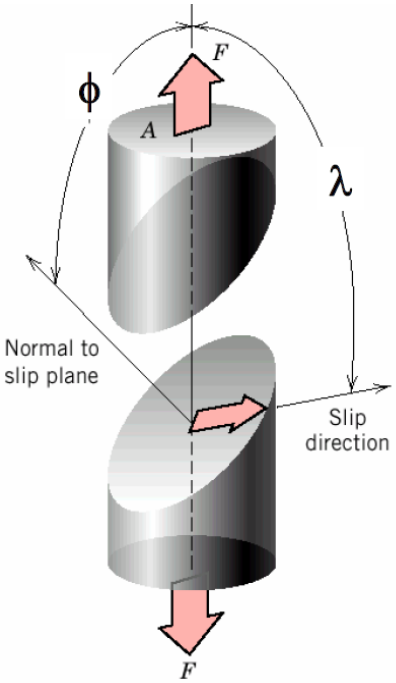
$$\tau_{res} = \sigma \cos\lambda \cdot \cos\phi$$

Projection of tensile stress on slip plane and in slip direction.

Thee critical parameter ->
Critical resolved shear stress

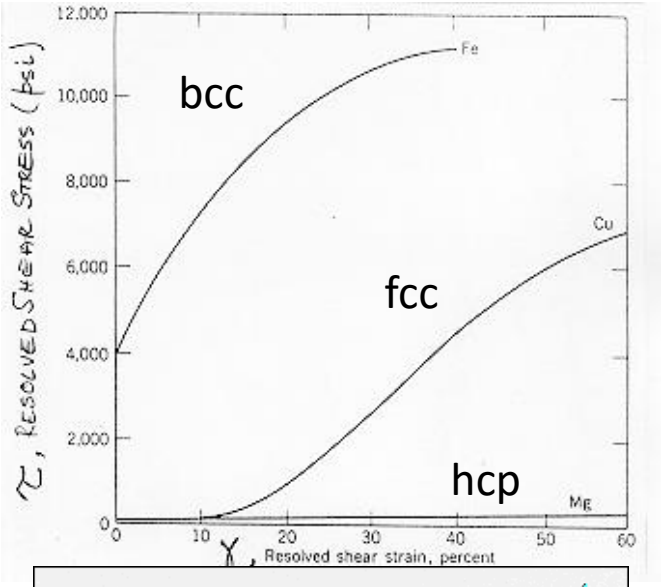






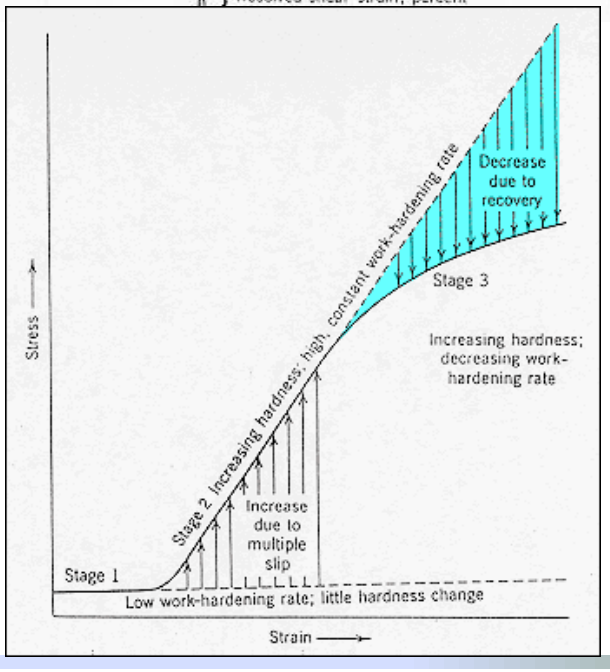
Work hardening

- Work hardening –
  - increase in stress that is required to cause in increase in strain as a material is plastically deformed.

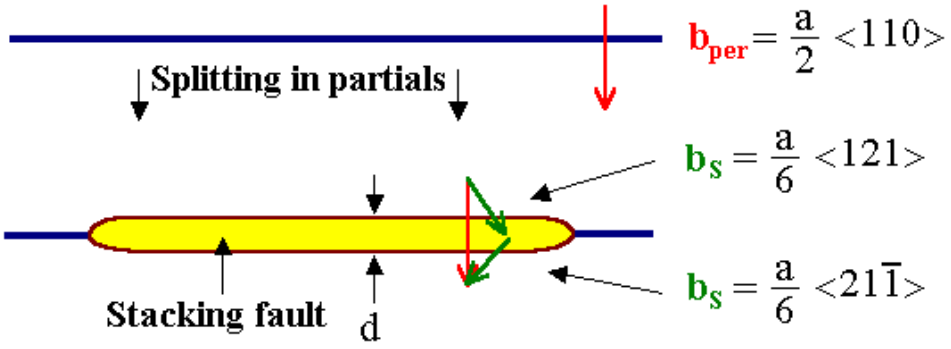


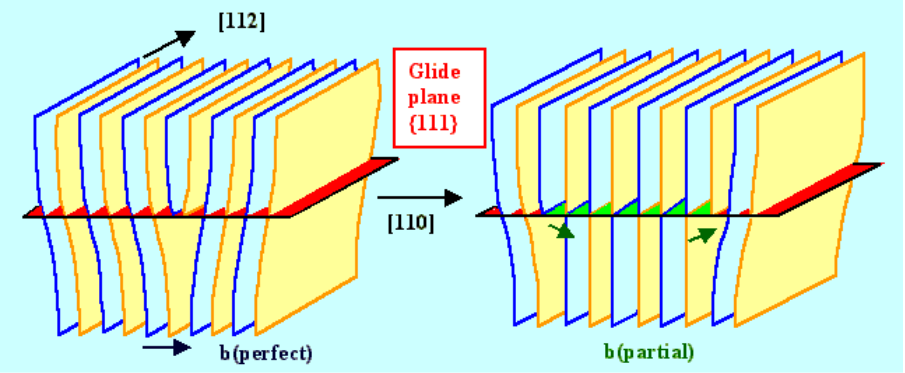
- Ductile materials – 3 stages of work hardening in an FCC single crystals are illustrated.
  1. slip is on a single active system.
  2. two active slip systems are involved and dislocation reactions and interactions increase the work hardening rate.
  3. "recovery" processes which reduce the dislocation interactions cause the work hardening rate to decrease.

  - Dislocation reactions: Jog formation - > climb. Dissociation -> cross slip.



Dislocations can split to two partials





$$E = G \cdot b^2 = G \cdot (\frac{a}{2} < 110 >)^2 = G \cdot \frac{a^2}{2}$$

Perfect dislocation dissociates into two partials an a stacking fault

$$E = G \cdot (\frac{a}{6} < 112 >)^2 + \gamma A_{sf} = G \cdot \frac{a^2}{3} + \gamma A_{sf}$$

But…

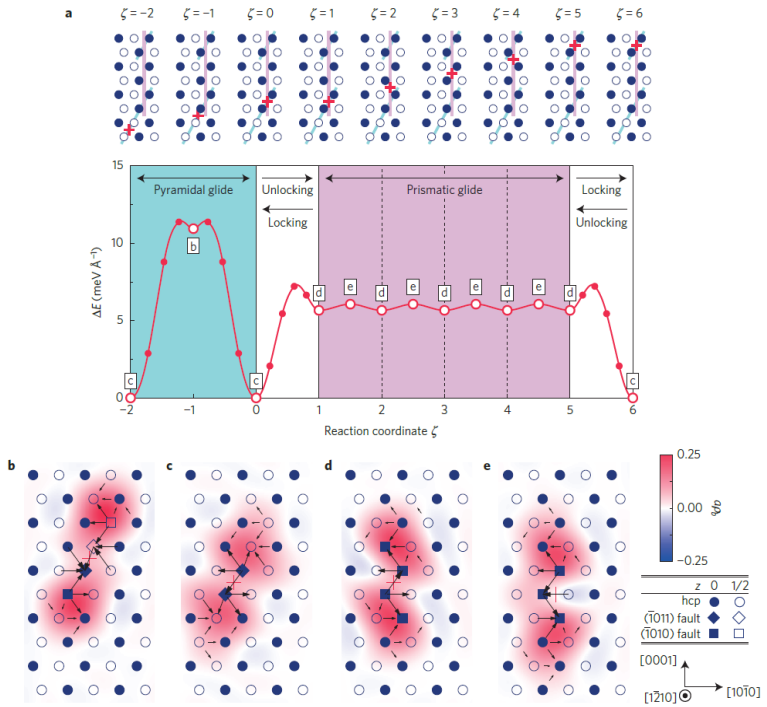
nature materials

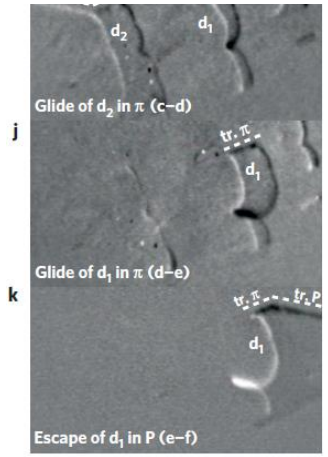
ARTICLES

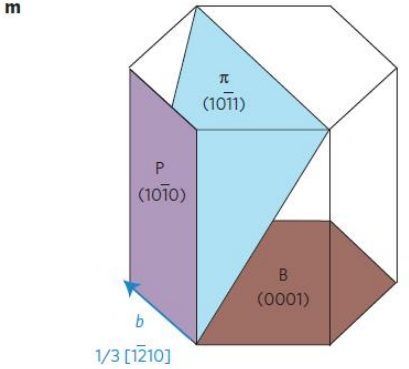
PUBLISHED ONLINE: 6 JULY 2015 | DOI: 10.1038/NMAT4340

Dislocation locking versus easy glide in titanium and zirconium

Emmanuel Clouet[1]*, Daniel Caillard[2], Nermine Chaari[1], Fabien Onimus[3] and David Rodney[4]





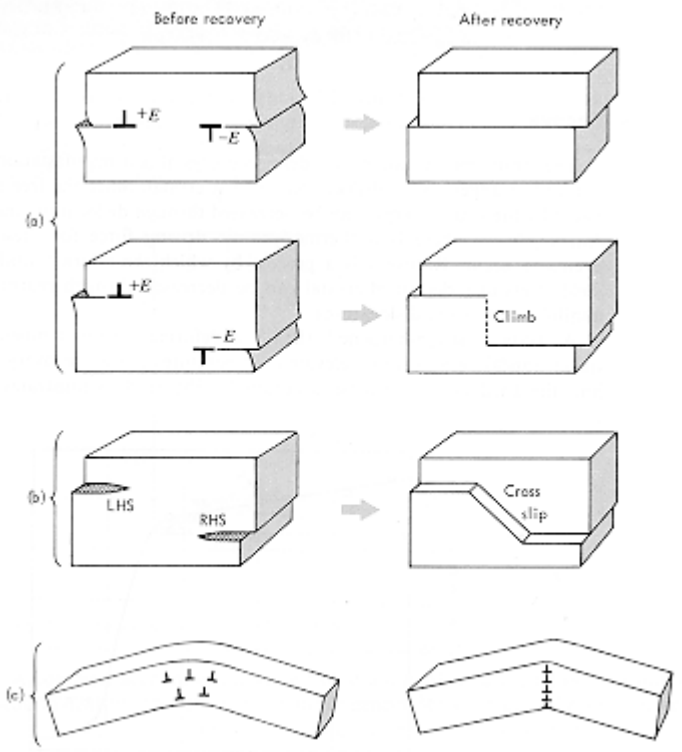


Example - even same column HCP metals show striking dis-similarity.

- Dislocations dissociates in a specific habit plane. Difference between easy glide and habit plane lead to “lock-unlock” glide.

Recovery

- The diagram shows the effect of intersection on two screw dislocations on orthogonal slip planes. Each dislocation picks up a jog equal in magnitude and direction to the Burgers vector of the dislocation it intersects.
- In this case, the two jogs are of edge character and have a length of one interatomic spacing.
- The edge-type jog on the moving dislocation has a slip plane (that contains b, t) that is normal to the slip plane in which the screw dislocation is gliding.
- The jog can only follow the moving screw by the slow climb process and is essentially fixed in the crystal where it is formed.

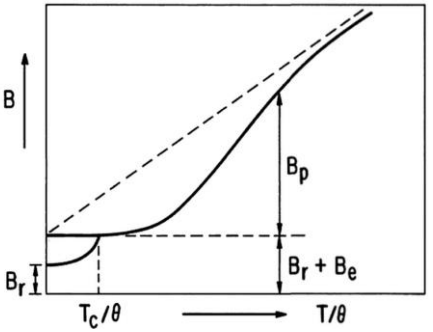


Single dislocation kinetics

PHYSICAL REVIEW VOLUME 90, NUMBER 2 APRIL 15, 1953

The Equation of Motion of a Dislocation*

J. D. ESHELBY
Department of Physics, University of Illinois, Urbana, Illinois



Granato, fund. of deformation (1984)

Dislocation as a rigid rod in an elastic media.

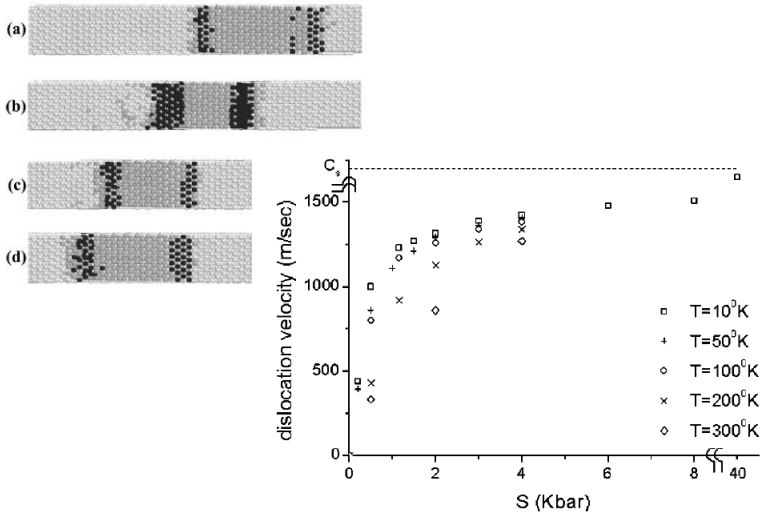
Equation of motion: $A\ddot{\gamma} + B\dot{\gamma} + C\gamma = b\sigma$

A - inertia

B - drag (phonon, point defects, dislocations)

Example-

- Isolated screw dislocation gliding in Cu
  - Pure screw is sown to dissociate.
  - Breathing, Asymptotic velocity (PRB 67(2003)24112)



From dislocations to plastic deformation

- Orowan's law for plastic deformation

$$\dot{\gamma} \propto b\rho_m v$$

b – average burgers vector

$\dot{\gamma}$ - strain rate

ρ_m - mobile dislocations density

v – average dislocations velocity

ELSEVIER Materials Science and Engineering A322 (2002) 194–216 A
www.elsevier.com/locate/msea

Plasticity of collective dislocation ensembles from microscopic to mean field

Constitutive description of dynamic deformation: physically-based mechanisms

M.A. Meyers [a,*], D.J. Benson [a], O. Vöhringer [b], B.K. Kad [a], Q. Xue [a], H.-H. Fu [a]

[a] Department of Mechanical and Aerospace Engineering, University of California, La Jolla, CA, USA
[b] Department of Mechanical Engineering, Institute for Materials Science I, University of Karlsruhe (TH), Karlsruhe, Germany

- Plastic response - controlled to a large extent by dislocations (slip, twinning)
- The stochastic nature of the underlying dislocations reactions is translated through average rates to a constitutive relation = deterministic relation between stress , strain, strain rate etc.

$$P_i = \nu_i / \nu_0 \rightarrow \nu_i \sim \nu_0 \exp\left(-\Delta G / kT\right)$$

- Using Orowan equation – dislocation motion to strain
(Δl between dislocation barriers, b -burgers vector)

$$\dot{\gamma} \propto b \rho_m v$$

- Assume V>>barrier crossing time therefor Δt between crossing is given by $1/v_1$

$$\dot{g} = \dot{g}_0 \exp\left(- \mathrm{D}G / k_B T\right) \longrightarrow \mathrm{D}G = k_B T \ln\left(\dot{g}_0 / \dot{g}\right)$$

- By assuming a functional form for ΔG one gets a constitutive link between stress, T and strain rate.

Also: Steck and Gerdes, acta mechanica, (1997)

Dislocation to constitutive models

Realistic constitutive equations hold much more ….

E.g. Zerilli Armstrong

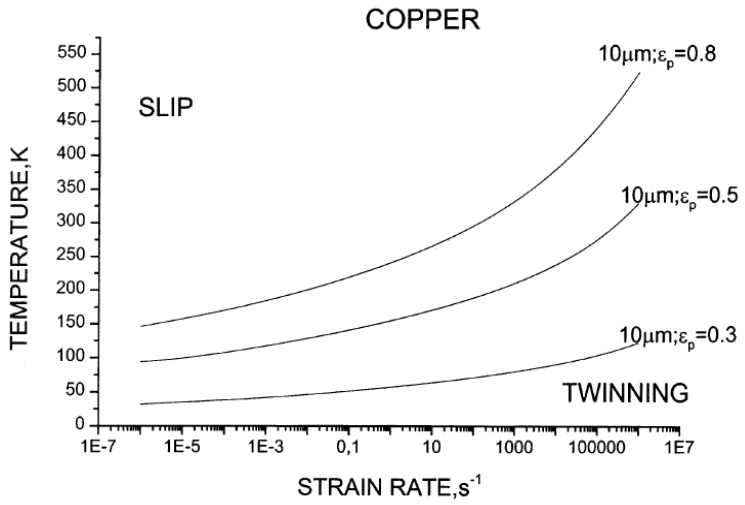
$$\sigma = \sigma_G + C_1 e^{-(C_3 - C_4 ln\dot{\gamma})T} + K\gamma^n + k/\sqrt{d}$$

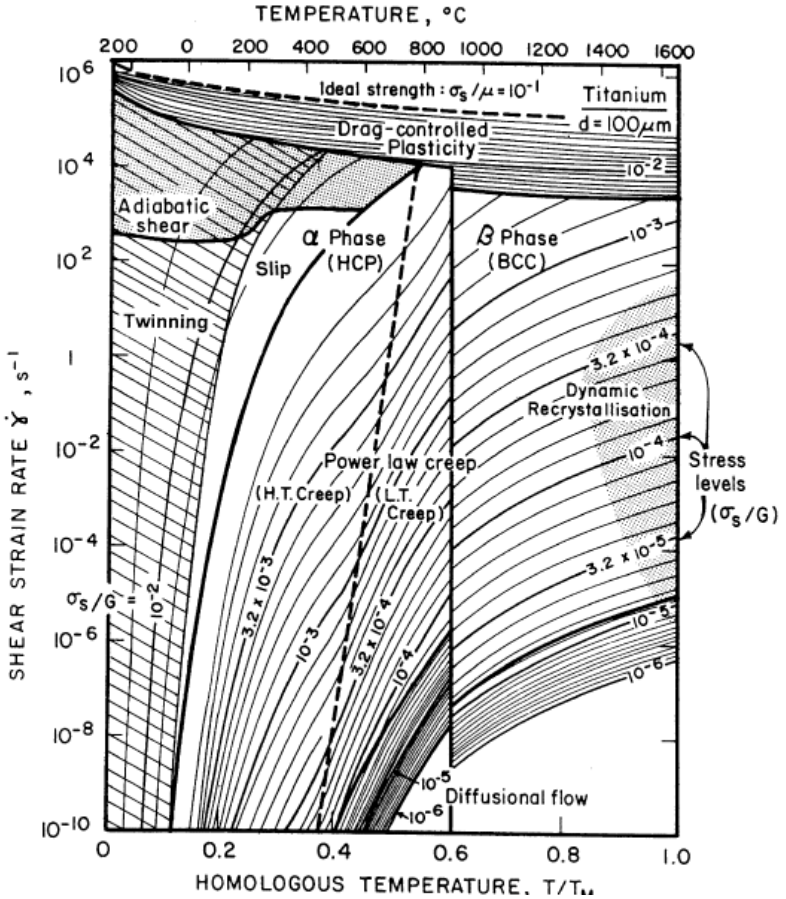
Usually assumed – only for slip.

Assuming a size dep. slip threshold

$$\sigma_{smax} = \sigma_0 + k_t/\sqrt{d}$$

-> Threshold for twin formation.

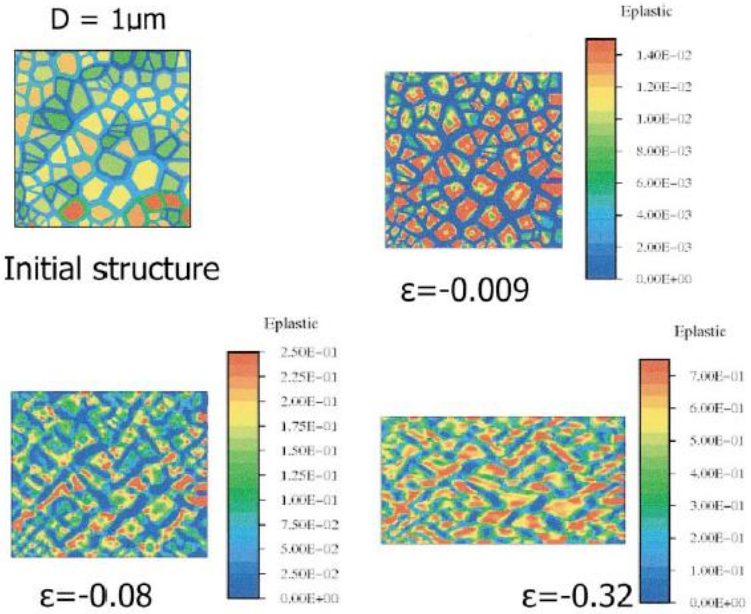




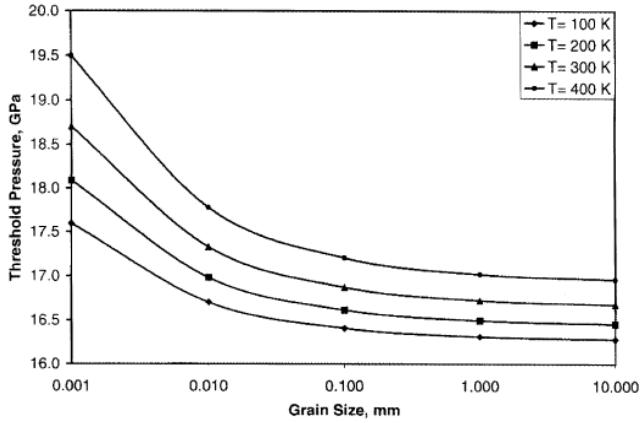
M.A. Meyers et al. / Materials Science and Engineering A322 (2002) 194–216

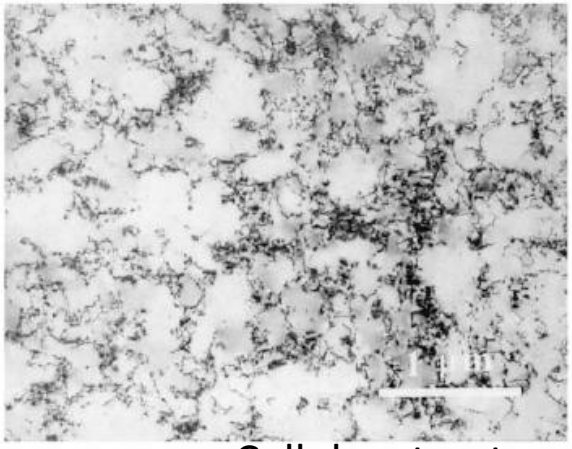
implications

Onset of shear localization

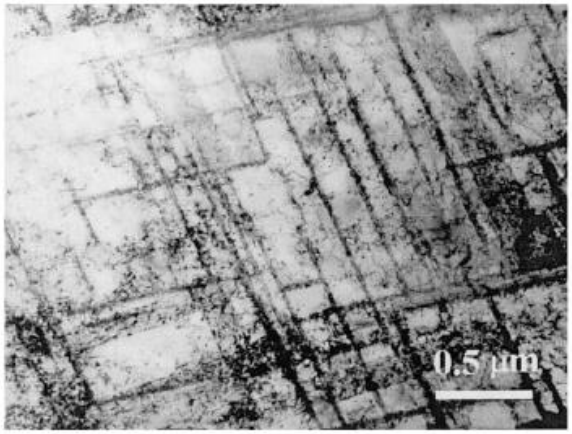


Threshold shock pressure for twinning (Cu)





Cellular structure



Twins and SF

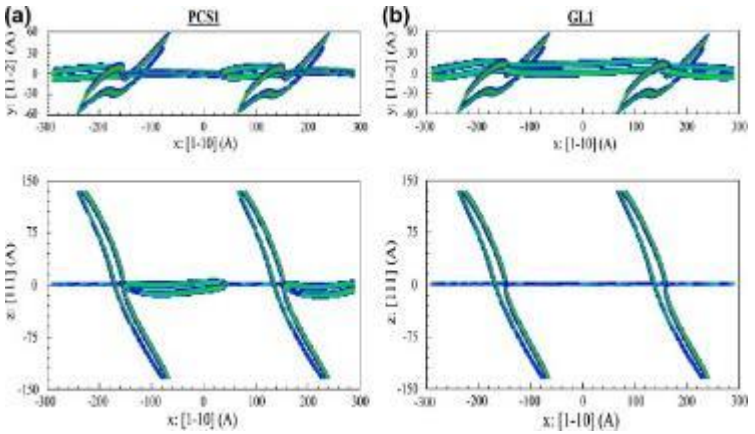
Fig. 19. Defect structures observed in copper monocrystal ([100] orientation) after laser-induced shock compression at (a) 10 GPa and (b) 40 GPa. Notice dislocation cell structure in (a) and twins/stacking faults in (b).

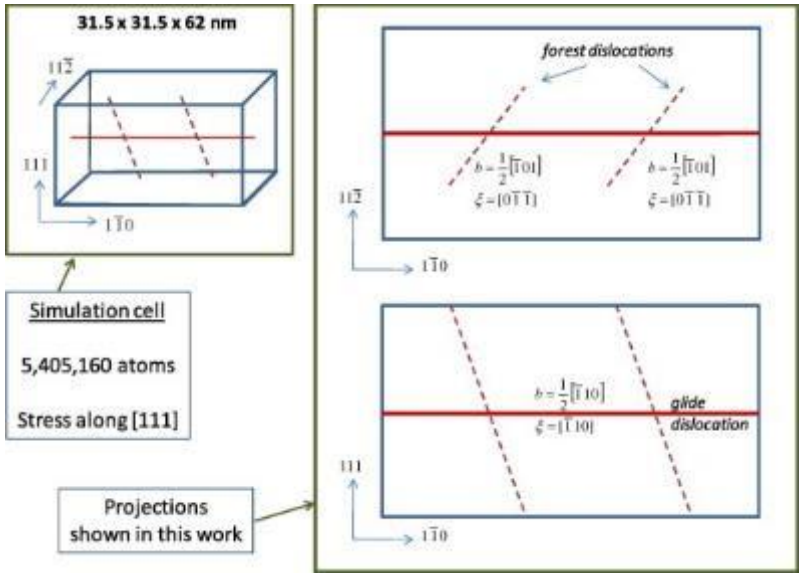
Dislocations related simulations

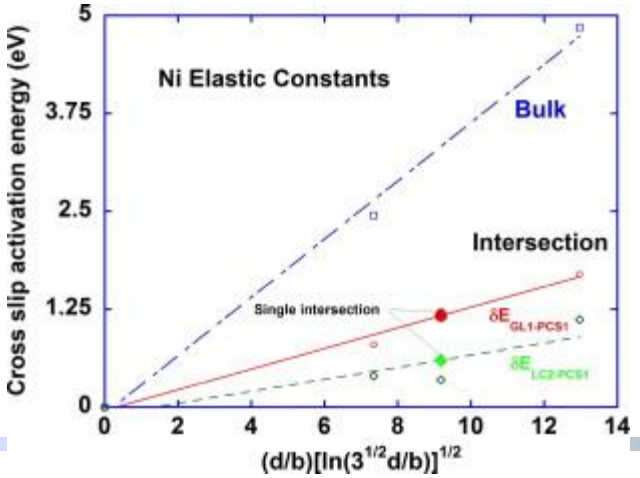
- Atomistic (MD / ab initio) of specific mechanisms:
  - Climb
  - Cross slip
  - Glide
  - Nucleation
  - Limitations – size, isolated system, strain rates
- MD of small ensembles:
  - Grain boundary response
  - Pile up
  - Impurities, interactions - limited strain rate, thermal processes
- Dislocation dynamics
  - Large ensembles response, realistic strain rates.
  - Need an external library of reactions, interactions and properties.
  - Limited size and time scales. Dependnace
- Phase field models
  - Elastoplastic macroscopic simulations. Dislocations effect through a constitutive relation. Dislocations/local damage as a phase filed.

Example… Simulating barriers

- Using MD it was shown that core structures change as screw dislocations collide. In fact the stable configuration is a partially cross slipped leading to reduction in activation energies
- Changes also due to surfaces and in habit vs slip plane stresses







DDD

- “elastic” fields - ~90% of the energy + inelastic cores .
- Long-range (1/r) interactions, complex boundary conditions

- Calculate the evolution of dislocation population using

$$m_0 \frac{\partial v}{\partial t} + Bv = \tau_{glide} b$$

$$\tau_{glide} = \mathbf{b} \cdot \bar{\boldsymbol{\sigma}}_{tot} \cdot \mathbf{n}$$

- Local variation of matrix properties
- Library of reactions

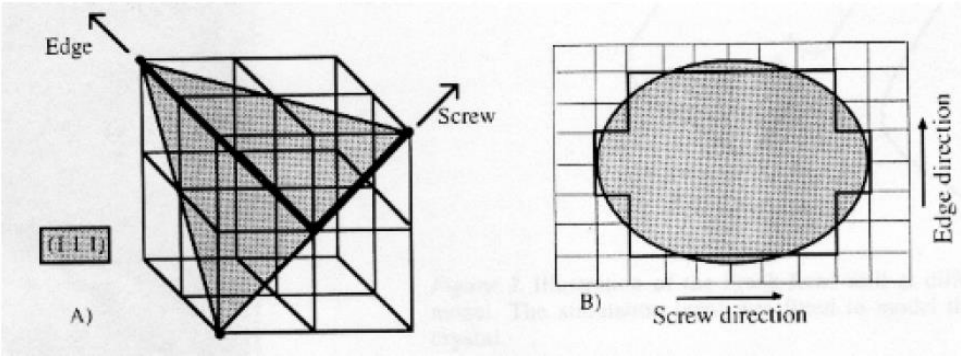
For example – cross slip is done per element based on

$$P_{cs} \propto \delta t \cdot \exp((\tau_{rs} - \tau_{III}) V / k_B T)$$

(V – activation volume, τ_{III} resolved shear stress at onset of stage 3 hardening.)

DDD

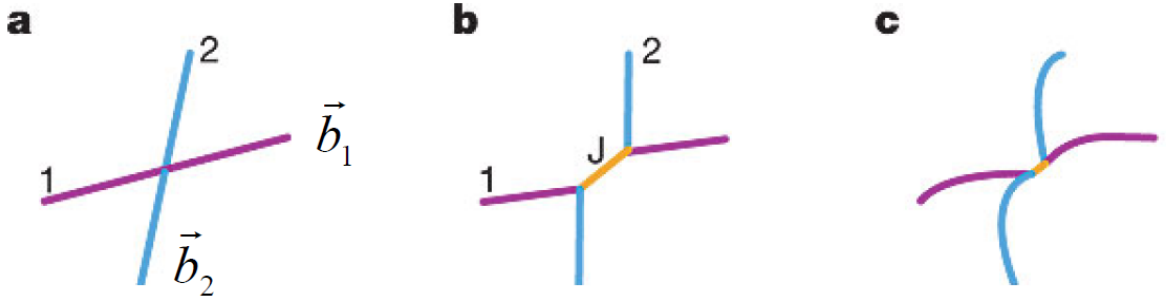
- **Space discretization** -
- Minimal grid parameter > distance of spontaneous annihilation of two edge dislocations (e.g. ~1.6 nm for Cu).
- Dislocation lines are divided to screw and edge components (Brown, Phil. Mag. 10, 441 (1964))



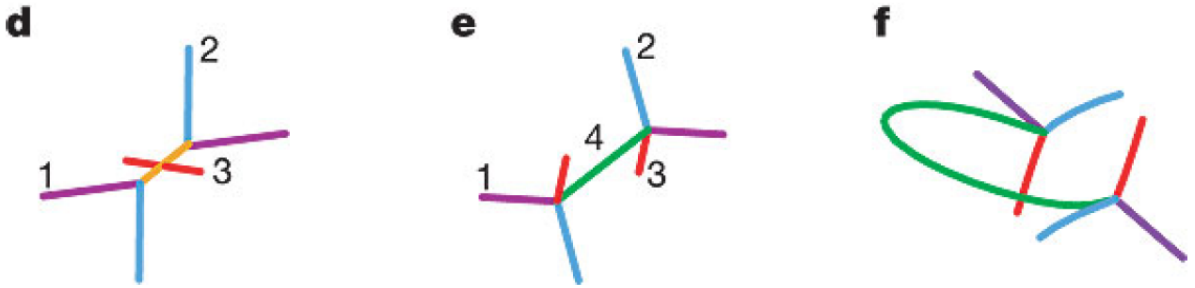
- **Interactions-**
  - Dis-dis
  - Internal (tension)
  - Peierls (resisting motion in glide)
  - Image
  - Misfit / defects / obstacles
  - External (applied stress / thermal / etc.)
- **Library of processes**
  - Pinning (at obstacles, GB), point sources, Cross slip … using MC.

Dislocation Dynamics: Example - dislocation multi-junctions and strain hardening

Bulatov et al., *Nature* **440**, 1174, 2006



Intersection of two dislocations leads to the formation of dislocation junction (a, b), which can unzip under stress (c). $\frac{1}{2}[\bar{1}\,11]+\frac{1}{2}[1\,\bar{1}\,1]=[001]$ $\quad \vec{b}_1^{\,2}+\vec{b}_2^{\,2}\Big/\left(\vec{b}_1+\vec{b}_2\right)^2=1.5$



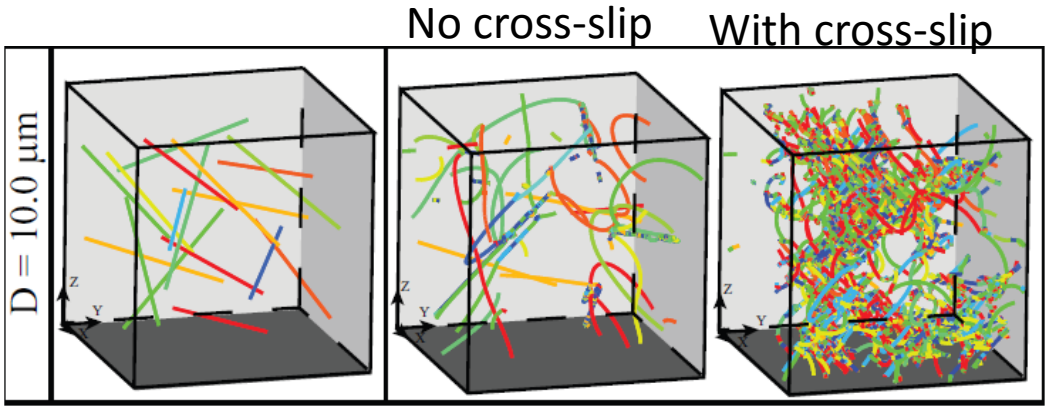
The interaction among three dislocations can form a long multi-junction (d, e), which can act as a Frank–Read source.

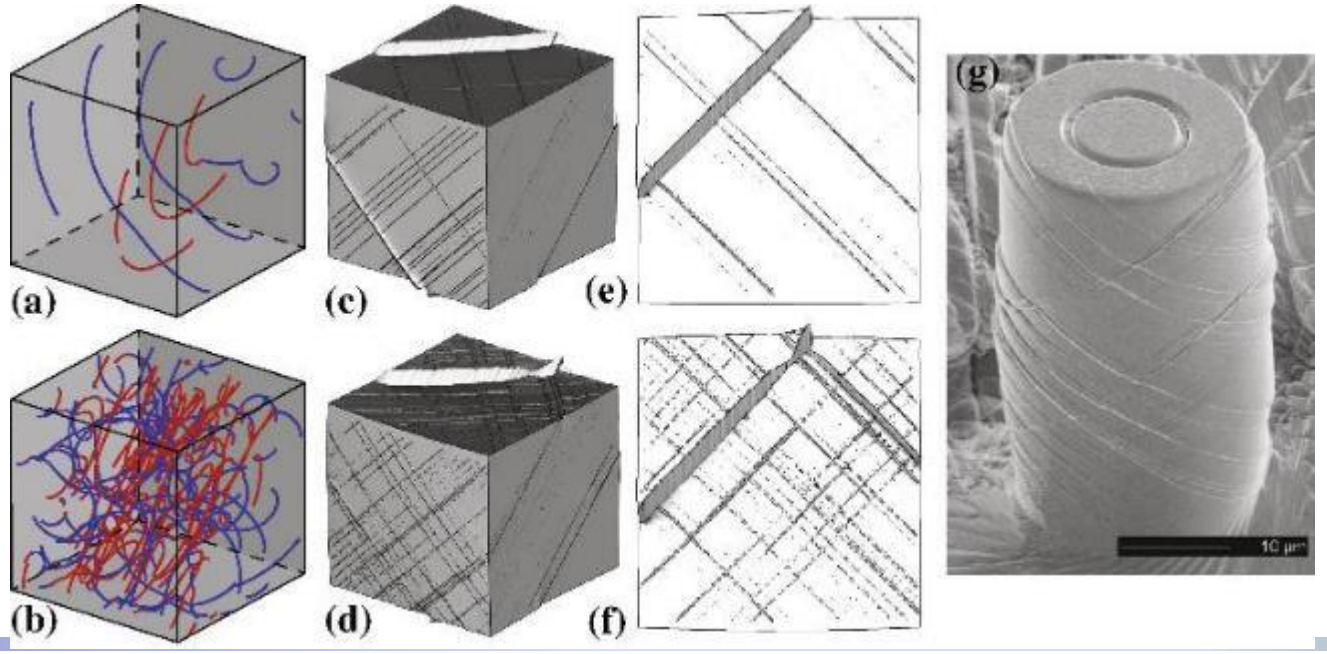
$$\vec{b}_1^{\,2}+\vec{b}_2^{\,2}+\vec{b}_3^{\,2}\Big/\left(\vec{b}_1+\vec{b}_2+\vec{b}_3\right)^2=3$$

$$\frac{1}{2}[\bar{1}\,11]+\frac{1}{2}[1\,\bar{1}\,1]+\frac{1}{2}[11\,\bar{1}]=\frac{1}{2}[111]$$

Microstructurally based cross-slip mechanisms and their effects on dislocation microstructure evolution in fcc crystals

Ahmed M. Hussein,[a,*] Satish I. Rao,[b,c] Michael D. Uchic,[d] Dennis M. Dimiduk[d] and Jaafar A. El-Awady[a]



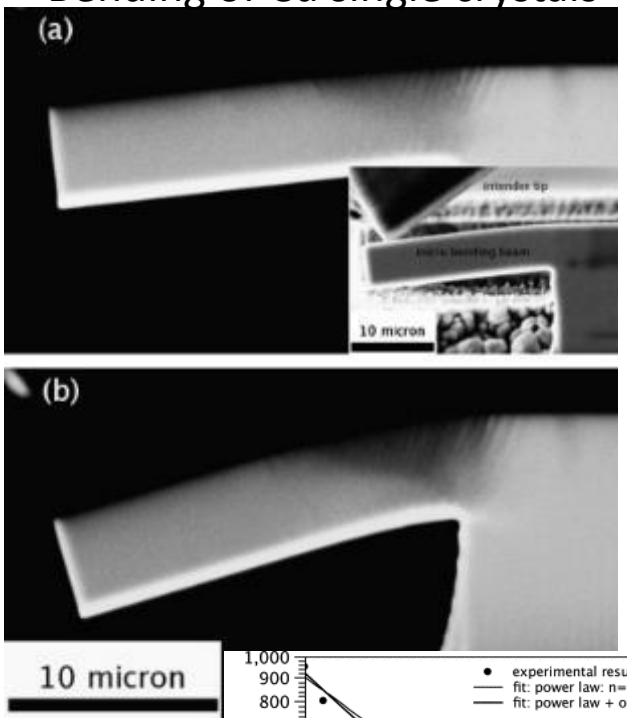


ELSEVIER
Acta Materialia 56 (2008) 1942–1955
www.elsevier.com/locate/actamat

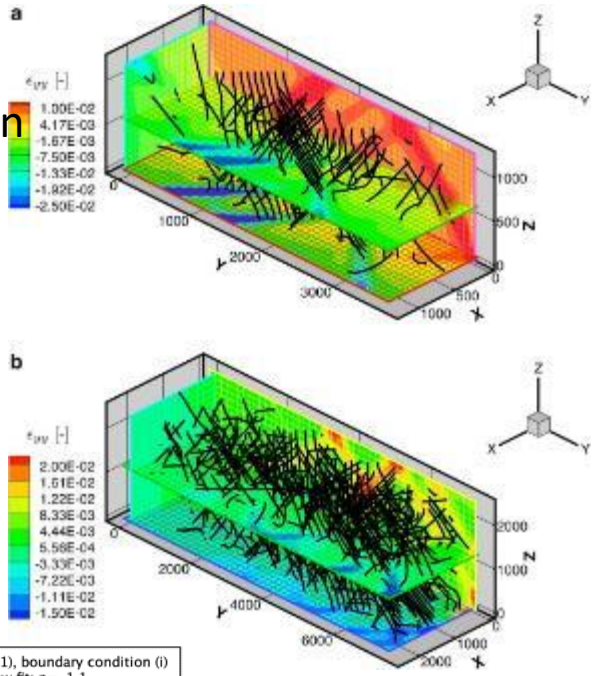
Micro-bending tests: A comparison between three-dimensional discrete dislocation dynamics simulations and experiments

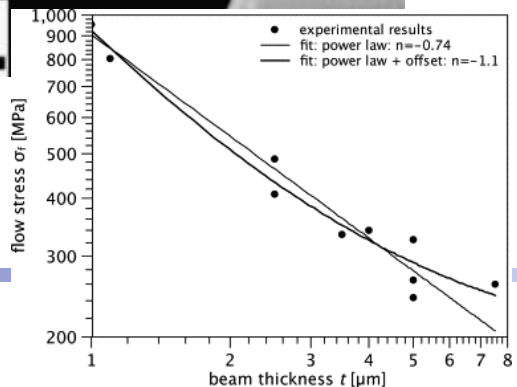
C. Motz [a,b,*], D. Weygand [a], J. Senger [a], P. Gumbsch [a]

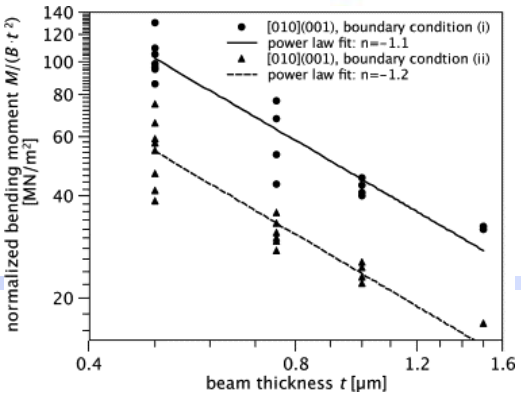
Bending of Cu single crystals



ddd simulations:
Reproduce strain localization
Dislocations near surfaces

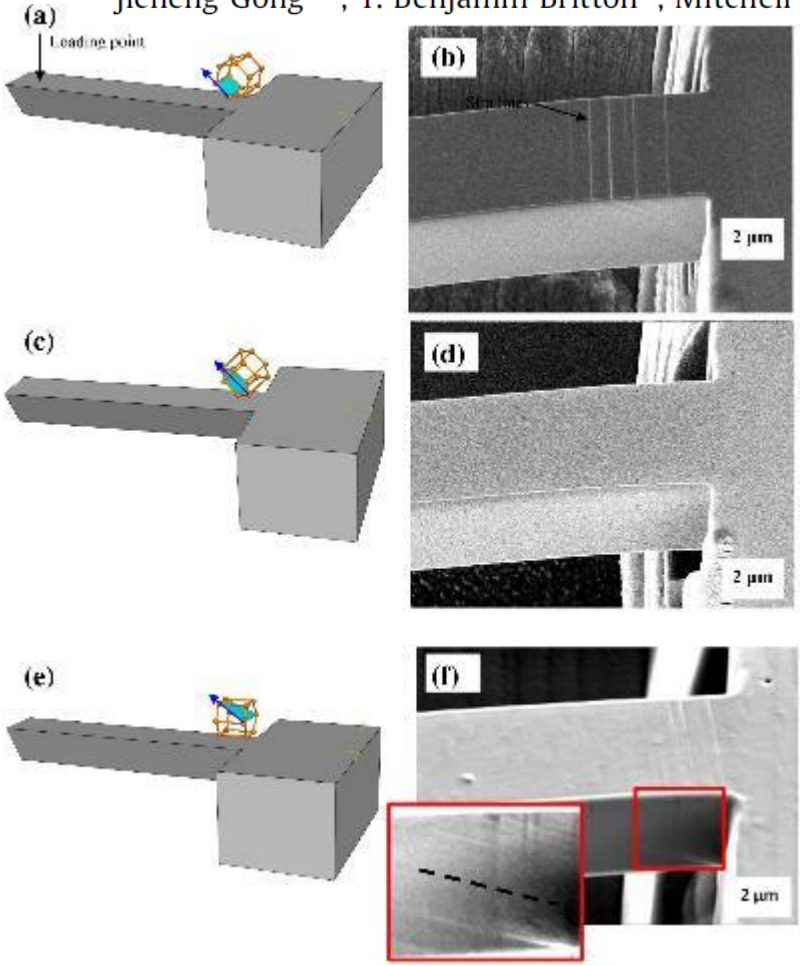






⟨a⟩ Prismatic, ⟨a⟩ basal, and ⟨c+a⟩ slip strengths of commercially pure Zr by micro-cantilever tests

Jicheng Gong [a,*], T. Benjamin Britton [b], Mitchell A. Cuddihy [b], Fionn P.E. Dunne [b], Angus J. Wilkinson [a]



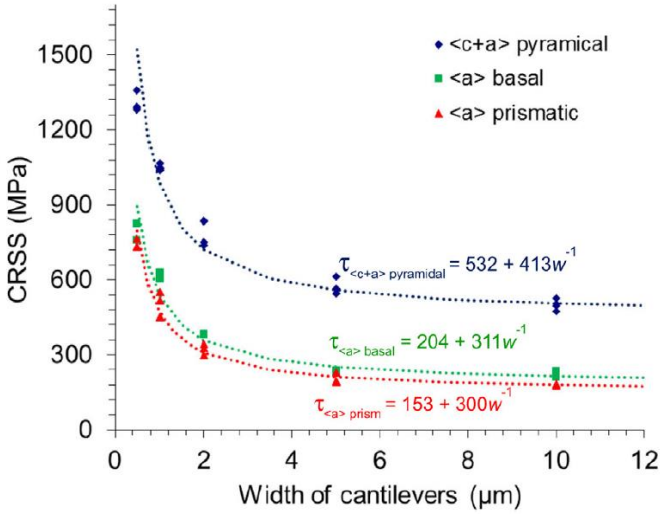
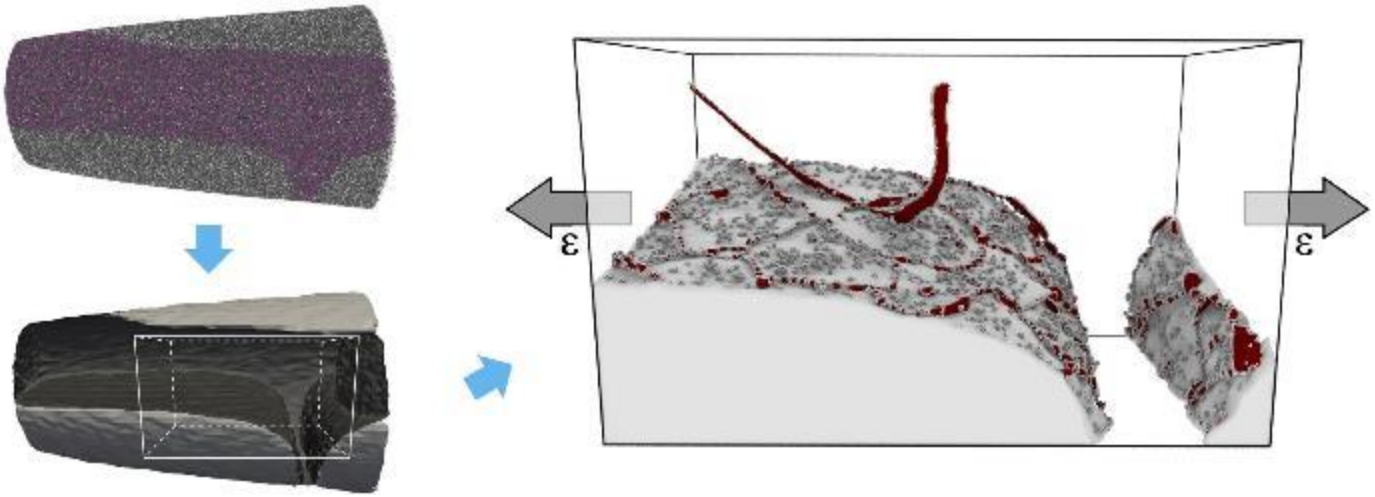


Fig. 6. CRSS vs. size (the beam width) for ⟨a⟩ prismatic, ⟨a⟩ basal and ⟨c+a⟩ commercially pure Zr cantilevers. Dash lines showing fit to $\tau_y = \tau_0 + Aw^{-1}$.

Atom probe informed simulations of dislocation–precipitate interactions reveal the importance of local interface curvature

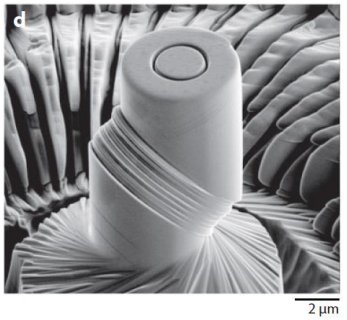
A. Prakash,[a] J. Guénolé,[a] J. Wang,[a] J. Müller,[b] E. Spiecker,[b] M.J. Mills,[c] I. Povstugar,[d] P. Choi,[d] D. Raabe[d] and E. Bitzek[a,*]



Dislocation mediated – self organized criticality

Plasticity of Micrometer-Scale Single Crystals in Compression

Michael D. Uchic,[1] Paul A. Shade,[2] and Dennis M. Dimiduk[1]



Single crystal micro-pillar compression:

Dislocation mediated intermittent flow - size effects, hardening.

Dislocation density inside a plane as a controlling parameter.

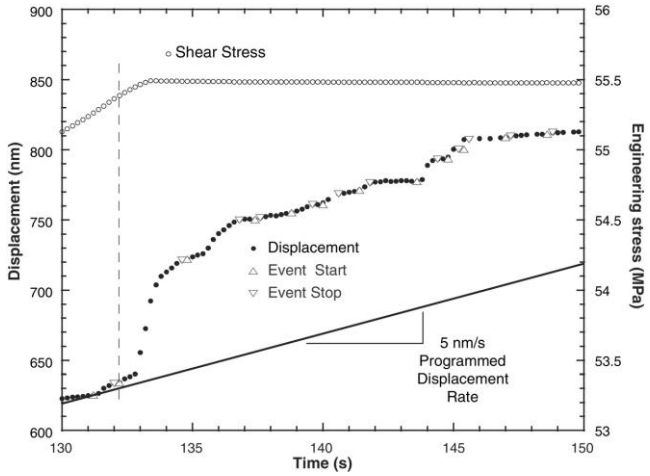
Intermittency characterized by a universal Power law burst PDF

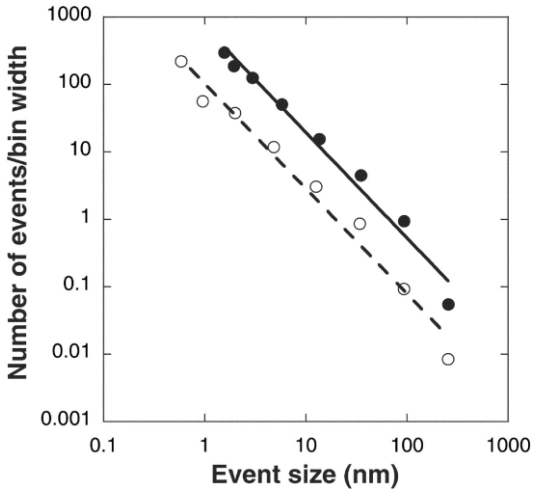
Acoustic emissions: Similar + space and time coupling between events

(Weiss & Marsan, Scjence 2003)

Earthquakes show similar PDF and spatio-temporal correlation

(Kagan, Geopgysical J. (2007)





Uchic, Shade & Dimiduk, Annual Review of Materials Research (2009).

Dimiduk, Woodward, LeSar & Uchic: “Scale-Free Intermittent Flow in Crystal Plasticity.” Science (2006) 1188.

Using dislocation dynamics to reproduce PDF

- 3D dislocation dynamics reproduce strain burst scaling

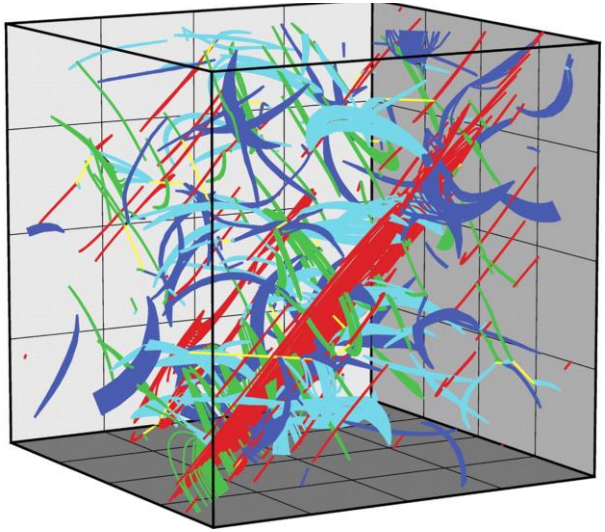
$$P(s) = Cs^{-t} \exp\left[- \left(s / s_0 \right)^2 \right]$$

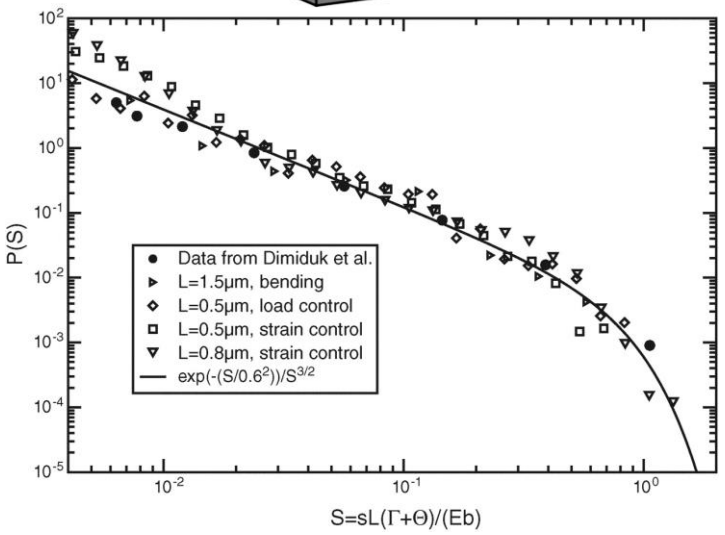
- where C is a normalization constant, τ is a scaling exponent, and s_0 is the characteristic strain of the largest avalanches.

- Intermittency – as a result of dislocation Interactions. Stochastic nature a result of varying initial conditions.

- Avalanche is a 2D event, with an upper cutoff due to structure and work-hardening. Strain is limited to about 10^-6 in a cm size sample.

- Recently (Chen, choi, papanikolaou & Sethna 2010 to 2013): scaling of structures CDD.





Csikor, Motz, Weygand, Zaiser & Zapperi, "Dislocation Avalanches, Strain Bursts, and the Problem of Plastic Forming at the Micrometer Scale" . Science (2007)

Spatial phase field modeling

- Using deterministic spatial model:
  - spatial phase filed leads to complex geometrical and topological transitions: forest hardening, multplication, slip bands
    Koslowski, Cuitino and Ortiz, J. Mech & Phys solids 2002
  - Complex governing equations. Leads to intermittent response and reproduces experimentally observed avalanche scaling laws.
  - Behavior reproduced by moving from a fully 3D system to a 1D “in slip plane” model. (Koslowski *phil. Mag.* 2003)
- Modifications
  - Modifications – such as: Introduction of Explicit fluctuations as a function of dislocations density (Zaiser & Moretti, J stat Mech 2005)
  - The main aim here is analytical tractability

Review of the various methods:

Current theoretical approaches to collective behavior of dislocations

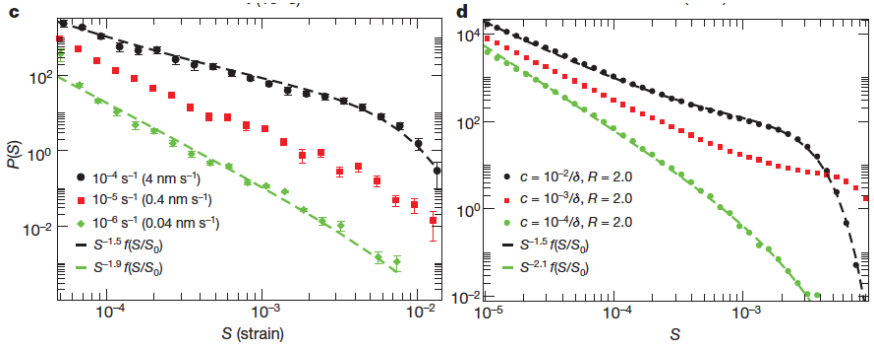
G. Ananthakrishna* Physics Rep. (2007) 113

Mean field models for critical de-pining

Quasi-periodic events in crystal plasticity and the self-organized avalanche oscillator

Stefanos Papanikolaou[1], Dennis M. Dimiduk[2], Woosong Choi[3], James P. Sethna[3], Michael D. Uchic[2], Christopher F. Woodward[2] & Stefano Zapperi[4,5]

- Reproduce strain rate variation by modifying the mean field picture to include a competing relaxation mechanism. This lead to oscillation in avalanche size. (nature, 2012)



PRL 109, 105702 (2012) PHYSICAL REVIEW LETTERS week ending 7 SEPTEMBER 2012

Distribution of Maximum Velocities in Avalanches Near the Depinning Transition

Michael LeBlanc,[1] Luiza Angheluta,[1,2] Karin Dahmen,[1] and Nigel Goldenfeld[1]

- Using a mean field model for interface depining and by solving Fokker-Planck eq. reproduced the power law decay of avalanche size and maximal velocity

$$\frac{dV}{dt} = -kV + F_c + \sqrt{V}x(t)$$

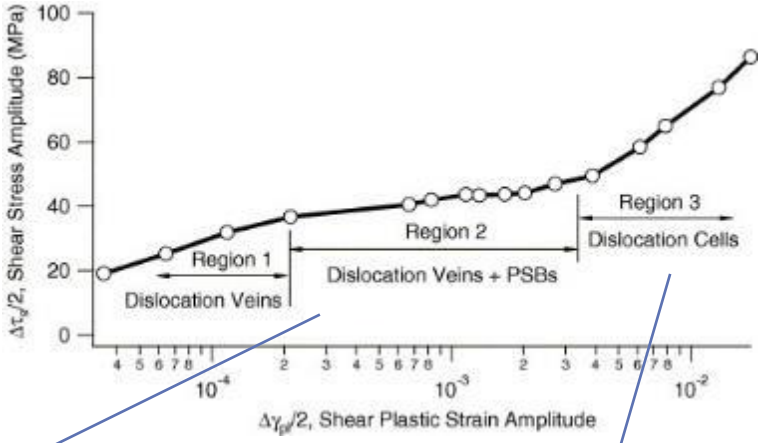
dislocations

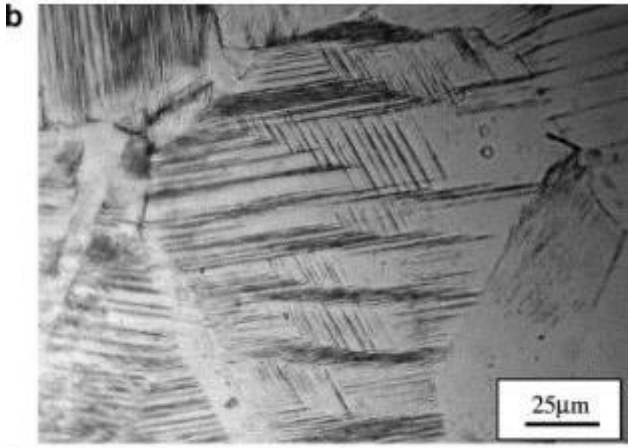
- Microscopy
  - TEM
  - STEM
  - SEM
  - Optical
- Acoustic emission

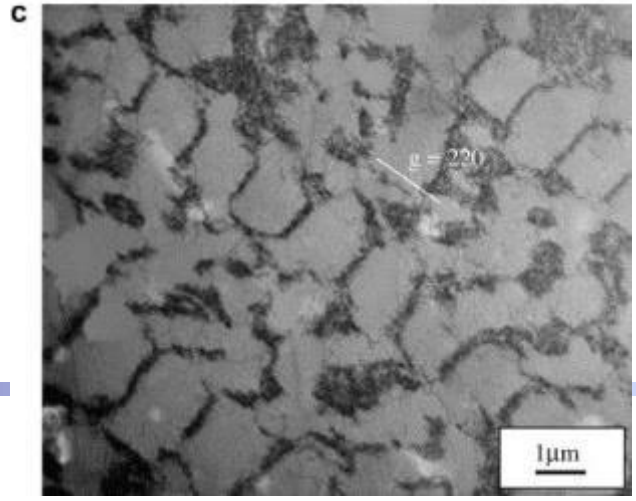
Observing dislocations

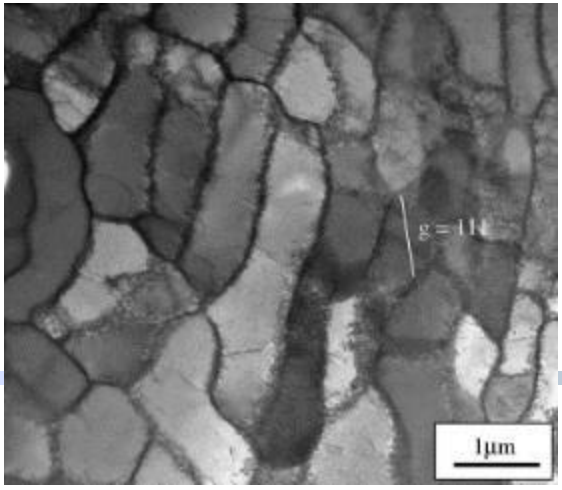
- TEM of OFHC CU
  - TEM samples ~100micron width
  - slip patterns
  - Dislocations arranged in Veins + PSB
  - Extremely large strains - cells

Zhang & Jiang, Acta Mat 55, (2007), 1831









- SEM

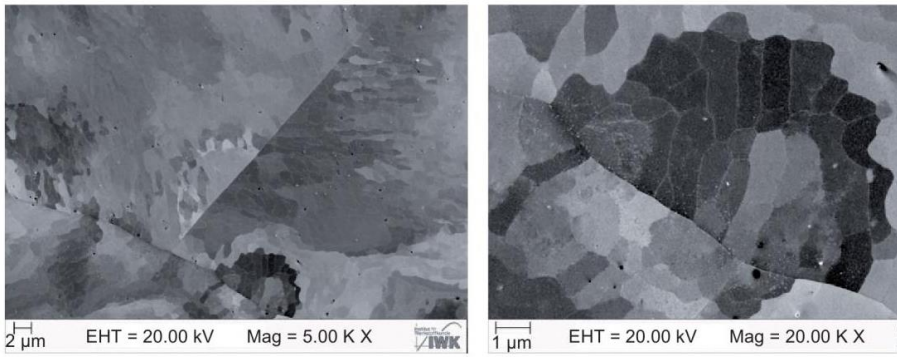
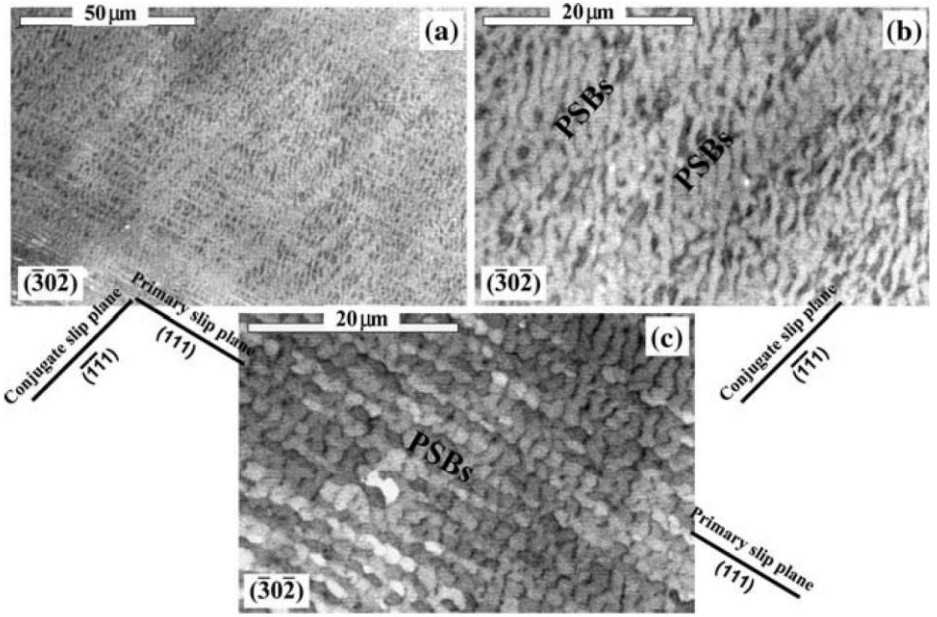


Figure 3. Cell-structure in fatigued OFHC-Copper.

Bar, J ; Proceedings of Crack Paths (CP 2012)



Li & Zhou, J Mat. Sci 42 (2007) 4716

- Optical Microscopy of surface relief

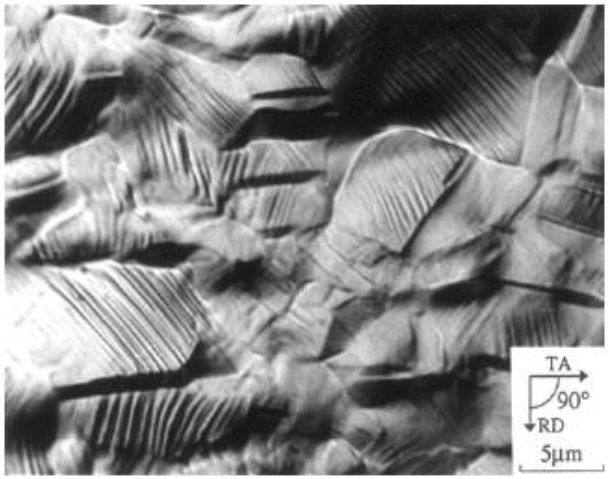
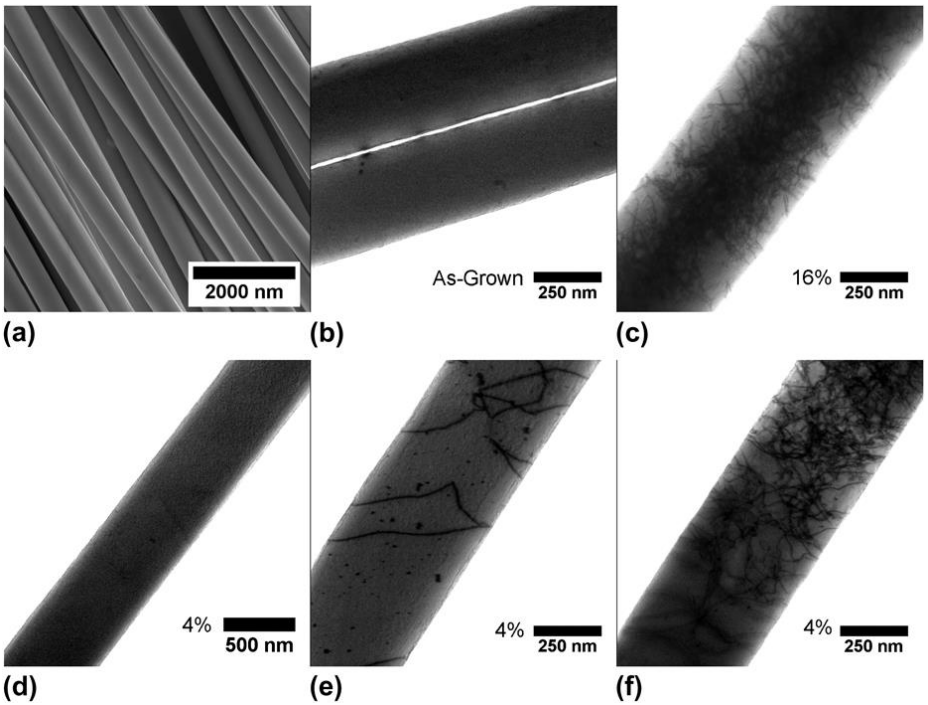


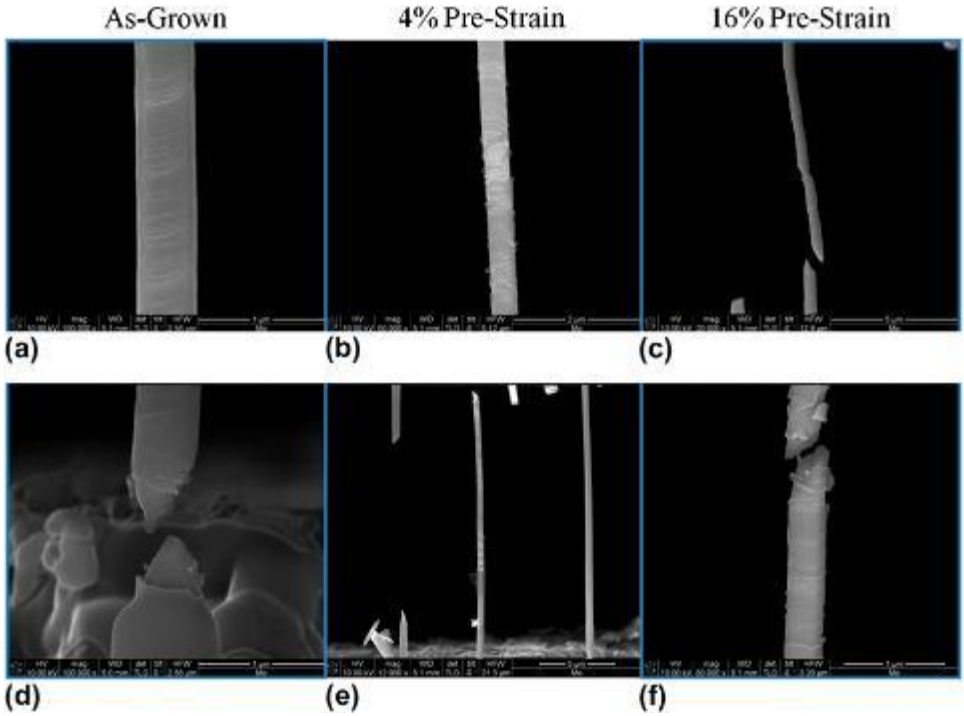
Figure 7. Optical observation of slip lines, developed during the second deformation in the macroscopic localized region (after rupture). The prestrain value is equal to 0.22.

Vieiraa M.F. & Fernandesb J.V. , Mat. Res. vol.2 n.3 (1999)
Complex Strain Paths in Polycrystalline Copper: Microstructural Aspects



Electron-microscope images of the Mo-alloy fibers tested in this study: (a) scanning electron microscope (SEM) image of as-grown Mo-alloy fibers extracted from the NiAl matrix; (b) scanning transmission electron microscopy (STEM) image of an as-grown fiber; (c) STEM image of the 16% prestrained fibers showing the high dislocation density; (d)â€(f) STEM images of the 4% prestrained fibers showing the inhomogeneous distribution of dislocation densities.

Johanns et.al. J. Mat. Research 27 (2012) 508

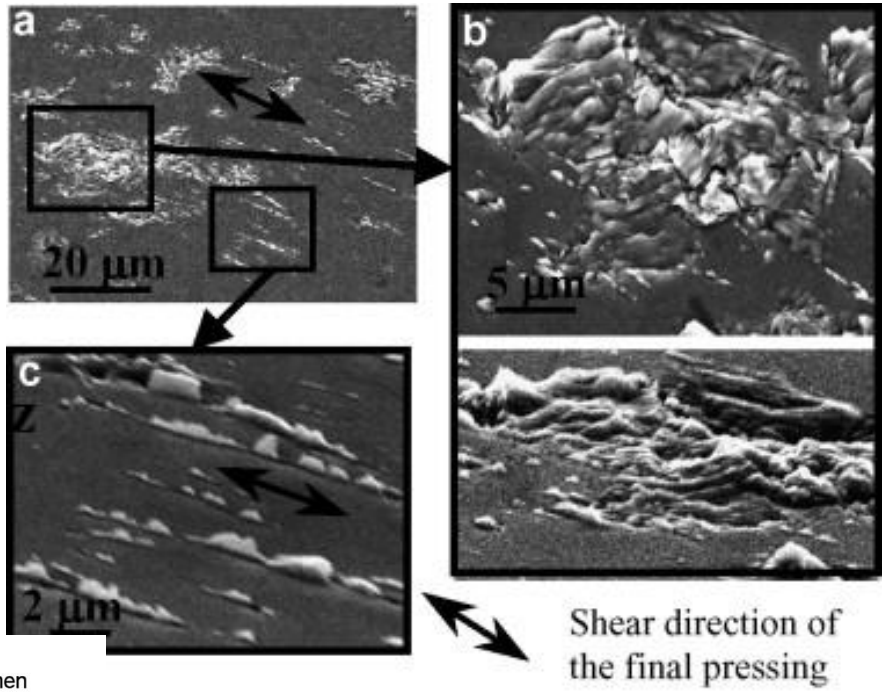


SEM images of deformation and fracture for intermittent plasticity, Type 3 behavior. (a)â€(c) show that deformation initiated locally and then propagated along the length of the fibers at all three levels of prestrain. (d)â€(f) demonstrate that failure modes were mixed between shear with limited plasticity and different types of necking.

Johanns et.al. J. Mat. Research 27 (2012) 508

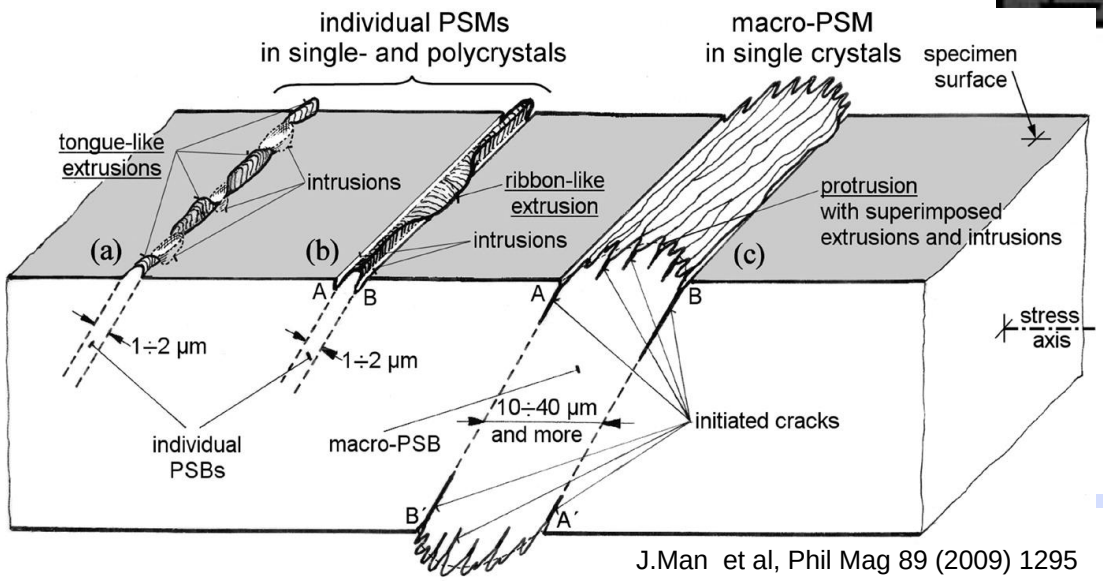
Fatigue through PSB

- Well known in fatigued surfaces
- Significant sub-surface PSB leading to these surface features -> PSM



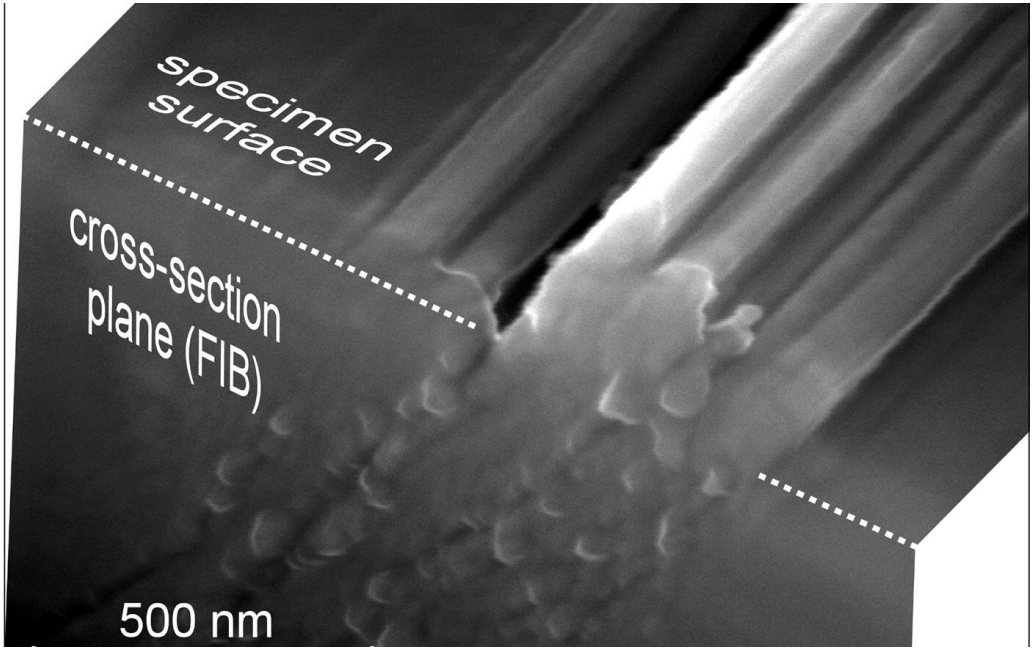
Fatigue strength and formation behavior of surface damage in ultrafine grained copper with different non-equilibrium microstructures

M. Goto et al. Int J of Fatigue. Vol 30 (2008) 1333



J.Man et al, Phil Mag 89 (2009) 1295

- FIB + ECC

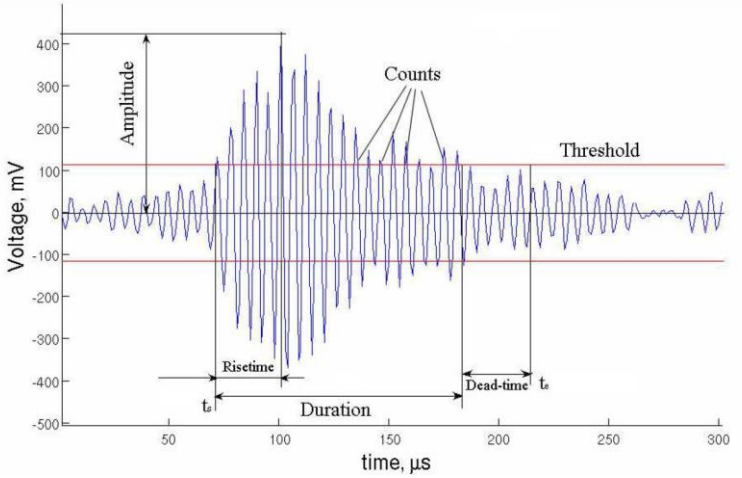


J.Man et al, Phil Mag 89 (2009) 1337

Acoustic emission

- AE – release of elastic energy (sound waves) due to localized irreversible dynamic process.
  Stress pulse -> elastic wave -> coupling to transducer

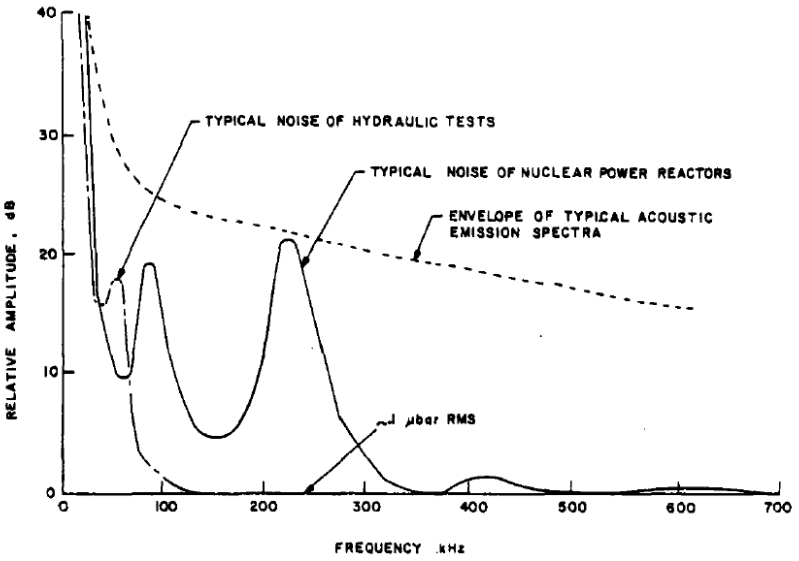
- Continuous: steady state -
  Indicative of micromechanics.
- Discrete: avalanche like.
- Measurements: counts, histogram
  Of energy, rise time, duration.

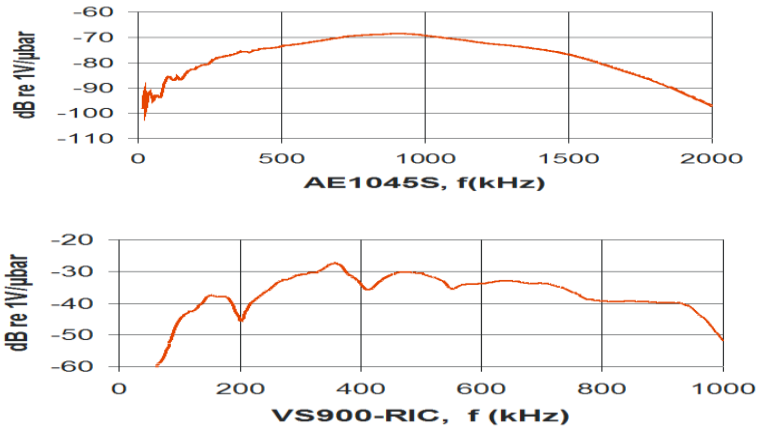


- Energy per event is estimated by elastic field change.
  Annihilation $E_{an} = \frac{\rho b^2 u^2}{8\pi}\gamma \ln\frac{d}{b} \approx 1 \cdot 10^{-10}\,\frac{J}{m}$
  motion $E_m = b\tau d \approx 10^{-7}\,\frac{J}{m}$

Acoustic emission signals

- Usual reach of AE measurements is O(1-0.01 μbar)
- Frequency range is usually above 100KHz to reduce mechanical noise and usually up to about 1MHz depending on the acoustic transducer.
- Noise sources: internal (parasitic processes), mechanical, and electronic noise (leakage / parasitic)





Examples of a transducers response curves from Vallen. Without (upper) and with (lower) an integrated preamp.

S. P. Ying (1973) Characteristics and mechanisms of acoustic emission from solids under applied stress, C R C Critical Reviews in Solid State Sciences, 4:1-4, 85-123, DOI: 10.1080/10408437308245819

Acoustic emission signals (2)

- Various type of signals:
  - Continuous (integral time behavior of population averages)
- Discrete
  - Identifying specific events

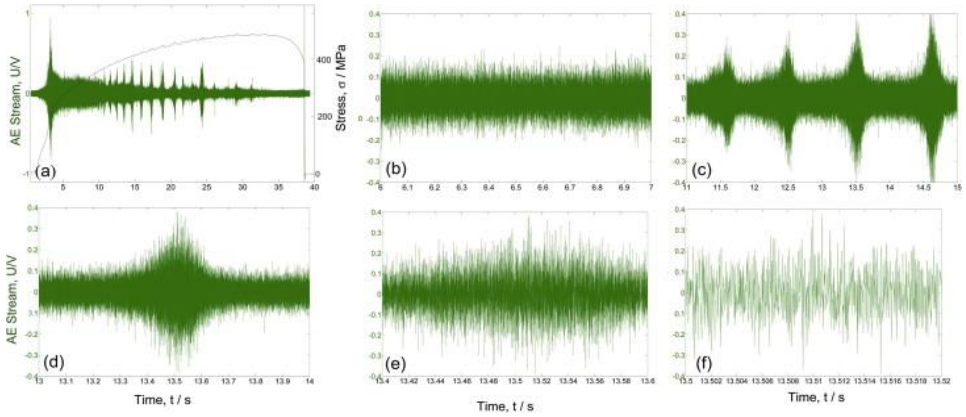


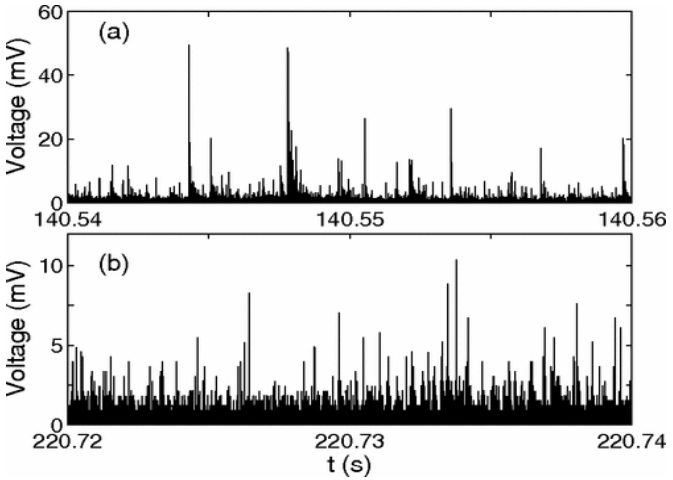
Figure 1 Continuous AE signal during intermittent plastic flow in α-brass at different temporal resolutions.

A. Vinogradov , A. Lazarev

Continuous acoustic emission during intermittent plastic flow in α-brass

Scripta Materialia, Volume 66, Issue 10, 2012, 745 - 748

http://dx.doi.org/10.1016/j.scriptamat.2012.01.053



Lebyodkin, M. A. et al. Role of superposition of dislocation avalanches in the statistics of acoustic emission during plastic deformation. Phys. Rev. E 88, 042402 (2013)

Estimated signal

Number of detectable dislocations:

nrV>0.035m2/sec... R~10^{-6}m, V~1-100m/sec ->

n_{min}~10-1000

Measurable threshold ~10^3 dislocations within measurement window.

Effected radius in the FE test ~100 microns

Distance between regions / cells ~ 10 micron

-> ~10^3 active cells

Population response time: crossing times

– are of the order of ~ 1 – 100 nsec.

-> even a single dislocation per cell would lead to a detectable signal.

Avalanche: > 10-100 increase.

Summary…

- Dislocations control microscopical mechanisms of plastic processes.
- Experimental observations - microscopy, AE.
- Linking of dislocation properties – plastic mechanism can be simulated at various scales.
  - Atomistic – specific reaction
  - DDD – interactions - external, internal
  - Macroscopic – realistic time and length scales
- Every scenario is unique….