Theory, Modeling and Simulation of the Collective Behavior of Dislocations

Richard LeSar
Iowa State University

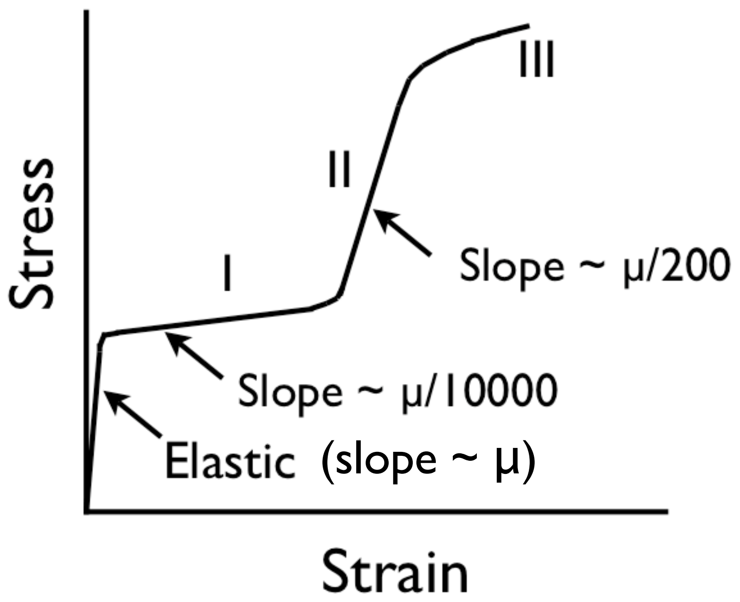
(1) Introduction to dislocations and plasticity
(2) Simulation strategies
- discrete dislocation dynamics in 2D and 3D
- phase-field simulations

(3) Coarse-graining strategies
- temporal
- spatial

(4) Scaling and intermittency

A disclaimer: no quantum mechanics (today)!

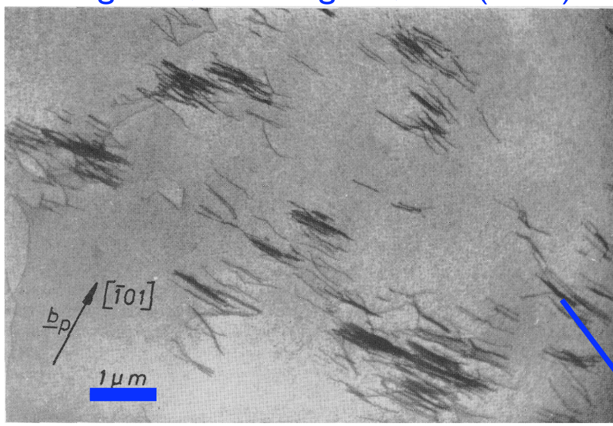
Macroscopic deformation in *fcc* metals



single crystal under single slip
μ is the shear modulus

Macroscopic deformation in *fcc* metals

Mughrabi, Phil. Mag. **23**, 869 (1971)

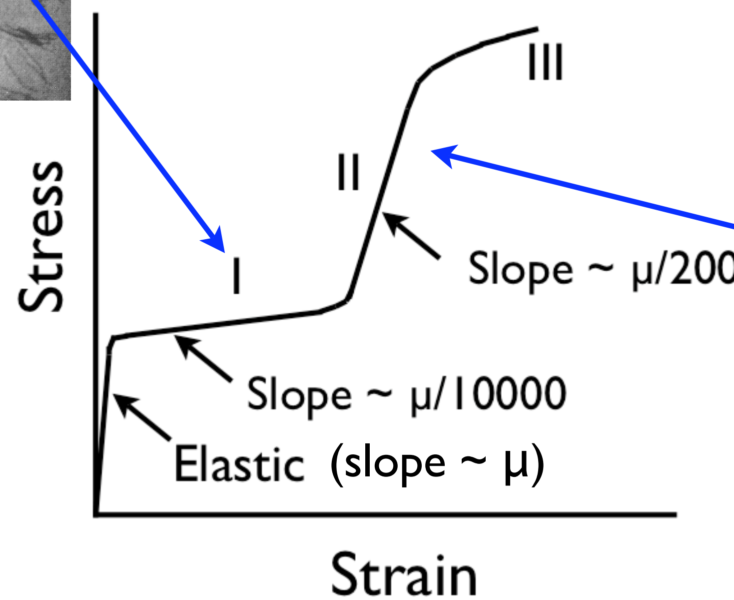


1 μm

$$\varepsilon^p = b\,\rho\,\langle x \rangle$$

dark lines in micrographs are dislocations

All micrographs from a Cu single crystal



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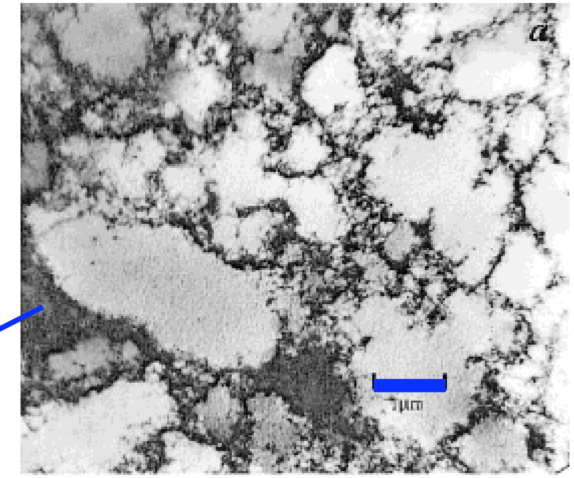

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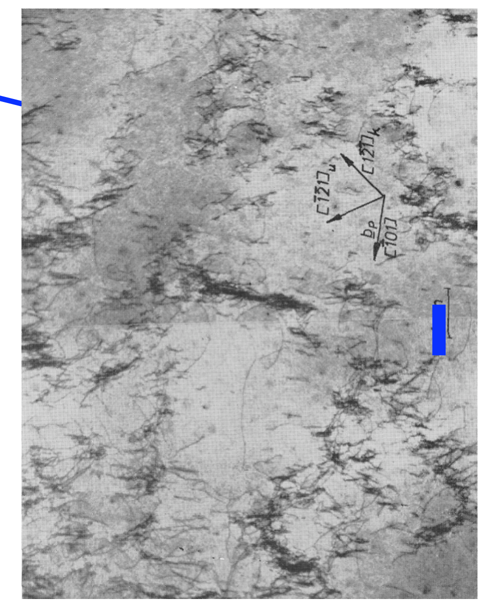
Szekely, Groma, Lendvai, Mat. Sci. Engin. A **324**, 179 (2002)



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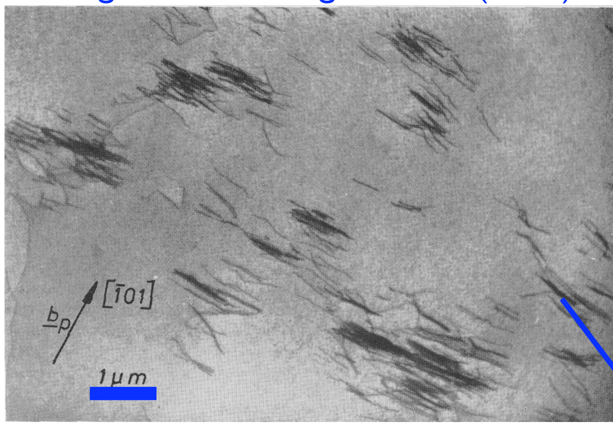

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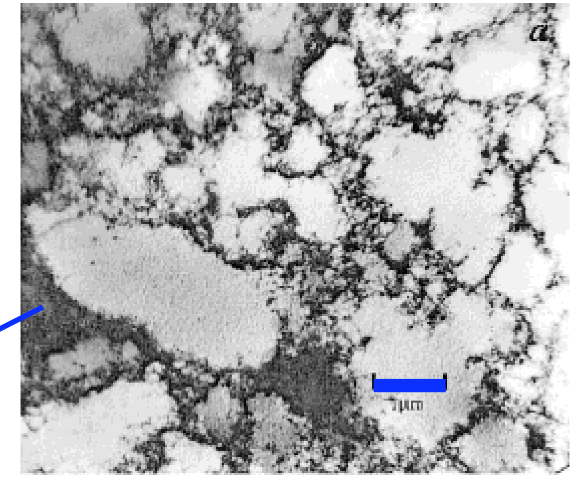

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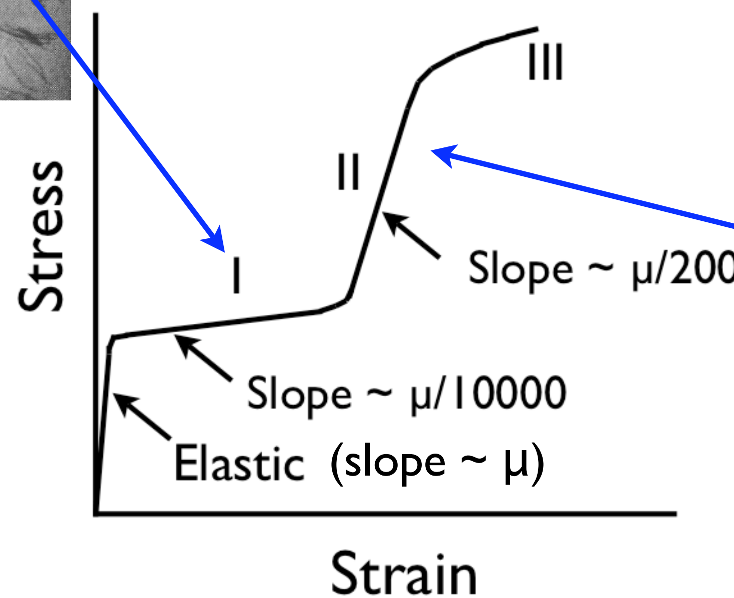

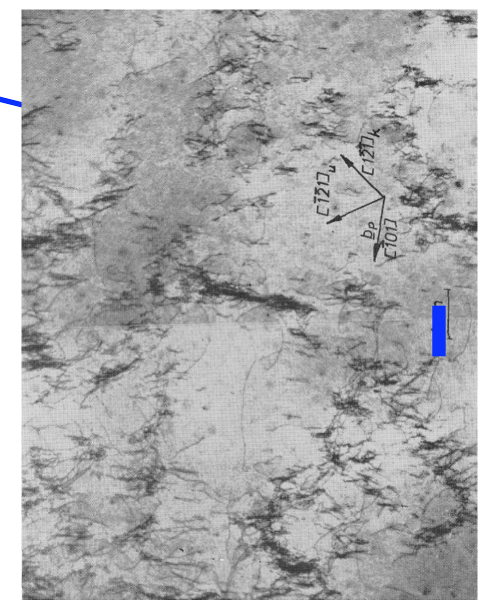

1 μm

- only a few macrovariables are relevant

→ suggestive of inherent spatial coarse graining

single crystal under single slip
μ is the shear modulus

Mughrabi, Phil. Mag. **23**, 869 (1971)

Multiscale landscape

Unit	Length Scale	Time Scale	Mechanics
Complex Structure	10^{3} m	10^{6} s	Structural Mechanics
Simple Structure	10^{1} m	10^{3} s	Fracture Mechanics
Component	10^{-1} m	10^{0} s	Continuum mechanics
Grain Microstructure	10^{-3} m	10^{-3} s	Crystal plasticity
Dislocation Microstructure	10^{-5} m	10^{-6} s	Micro-mechanics
Single Dislocation	10^{-7} m	10^{-9} s	Dislocation Dynamics
Atomic	10^{-9} m	10^{-12} s	Molecular Dynamics
Electron Orbitals	10^{-11} m	10^{-15} s	Quantum Mechanics

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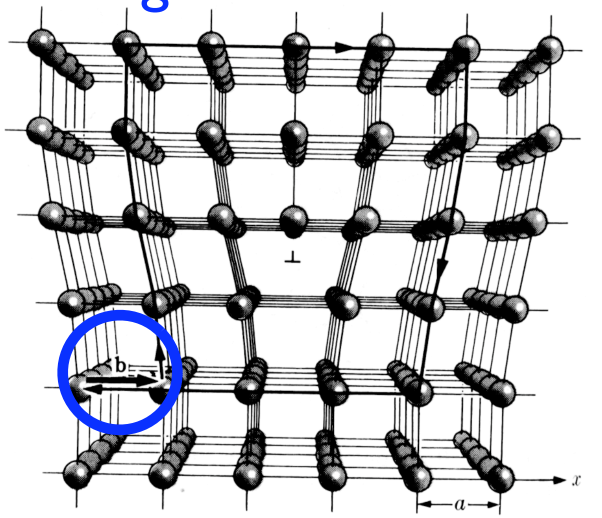
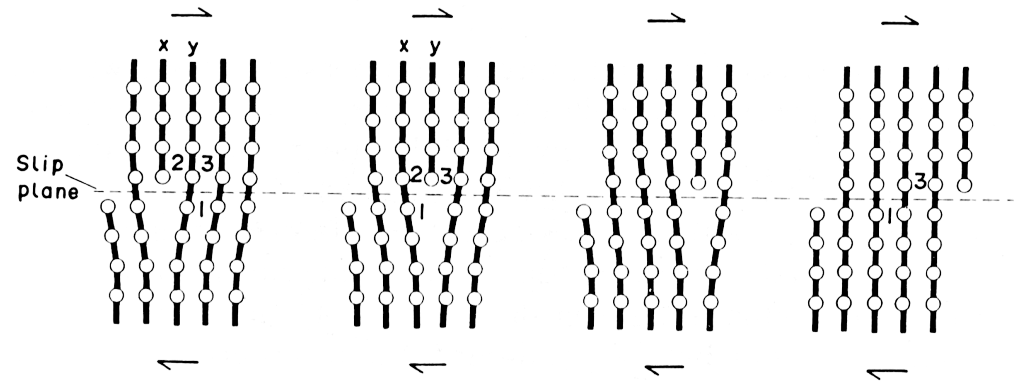
each level is based on different methods and often done by different groups

How do we link these together?

Dislocations are curvilinear topological defects that "carry" deformation

edge dislocation





edges move along slip direction

Burgers vector ($\vec{b}$) measures displacement.

Edges defined by $\vec{b} \perp \hat{\xi}$. Note: dislocations are "signed."

Concept connecting flow of dislocations to deformation dates to 1934.

- E. Orowan, Z. Physik, **84**, 605 (1934)
- G. I. Taylor, Proc. Roy. Soc. London Serial A **145**, 362 (1934)

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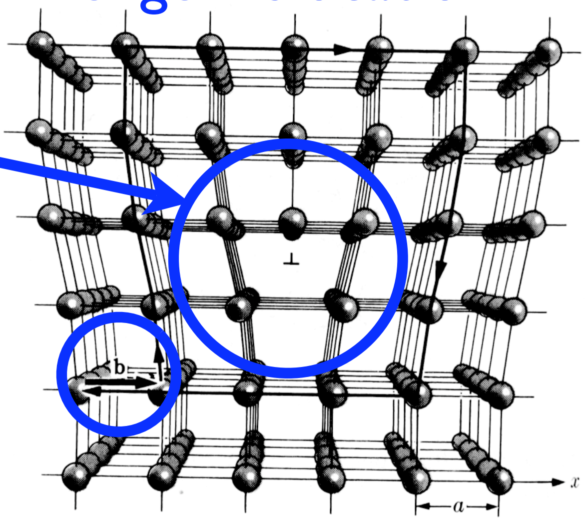
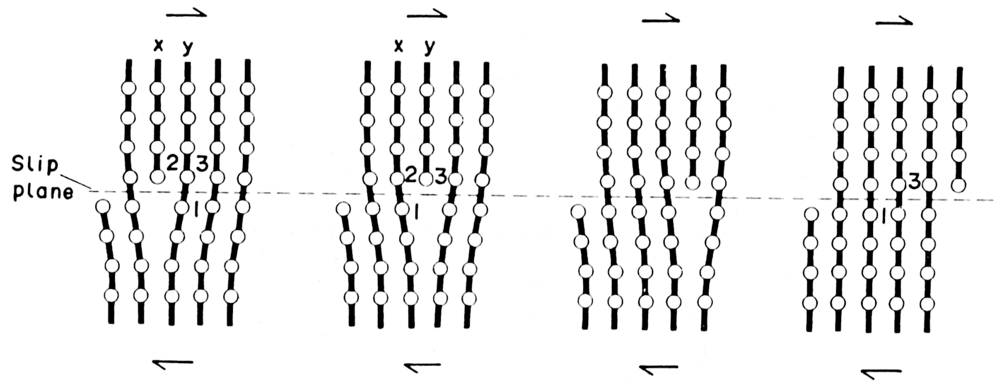
core





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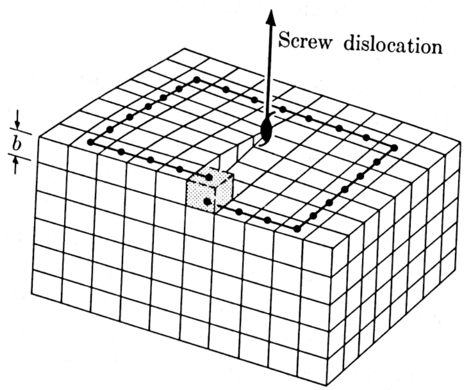
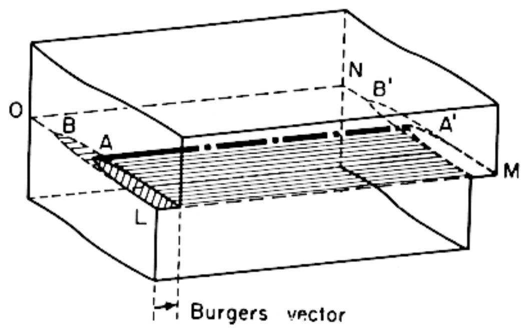
Other types of dislocations

screw dislocation has $\vec{b} \,||\, \hat{\xi}$

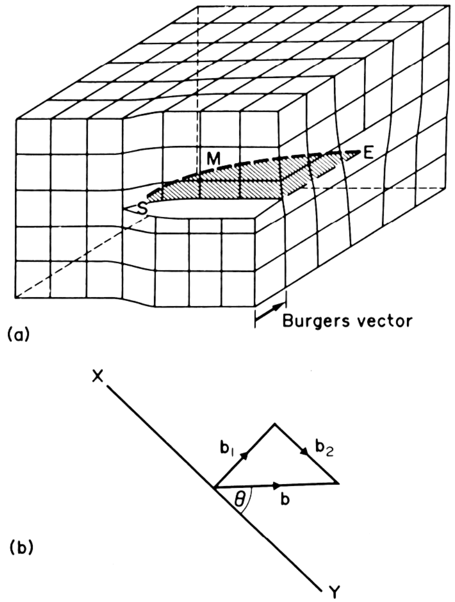




Screw dislocation structure and movement.

In general, dislocations are of mixed character:

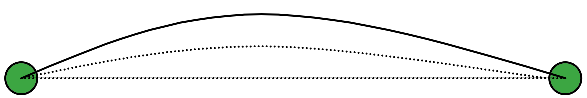
- dislocations cannot end in a crystal
  - must exist as loops or end at surfaces or other defects
- the Burgers vector is constant for each dislocation loop
- must obey crystallographic constraints



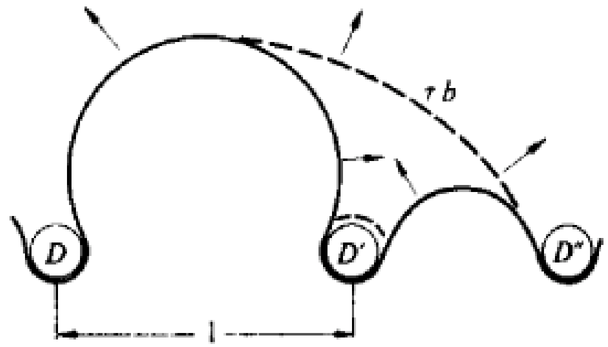
"Mixed" dislocation

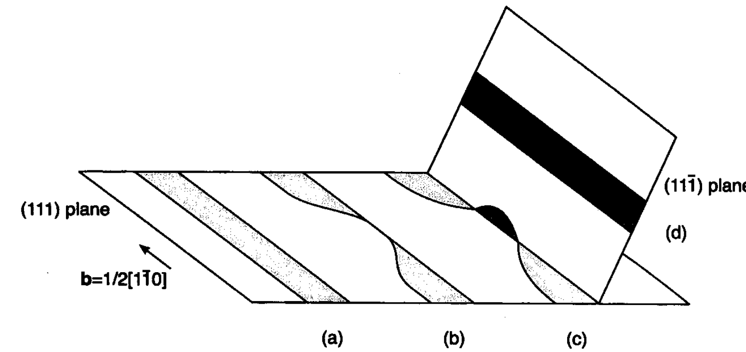
Crystallographic constraints

Owing to constraints of edge components, most dislocation movement is planar.



stress balanced
by "line tension"

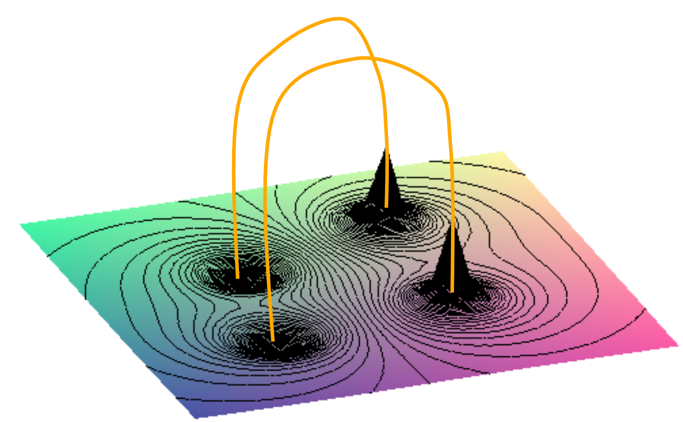




cross slip

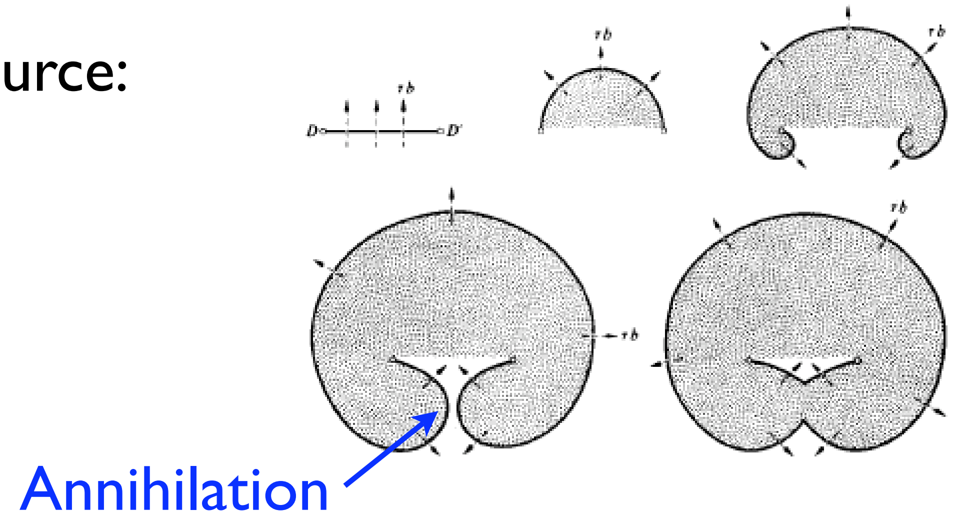
Movement off plane is atomic-level activated process.

In 3D, dislocations on other slip planes act as barriers to dislocation motion:

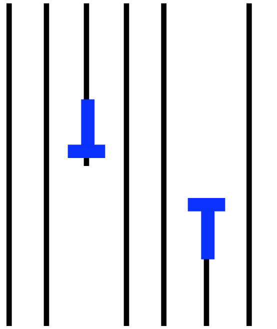


Dislocations are not conserved

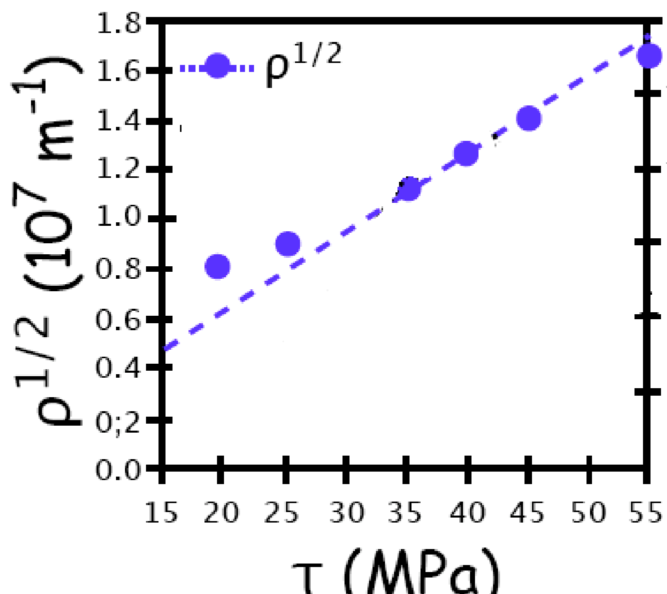
Frank-Read source:



Dislocations of opposite sense can annihilate each other:



Dislocation density increases with deformation:



$$= \frac{\tau^2}{(\alpha \mu b)^2}$$

Dislocations are not conserved

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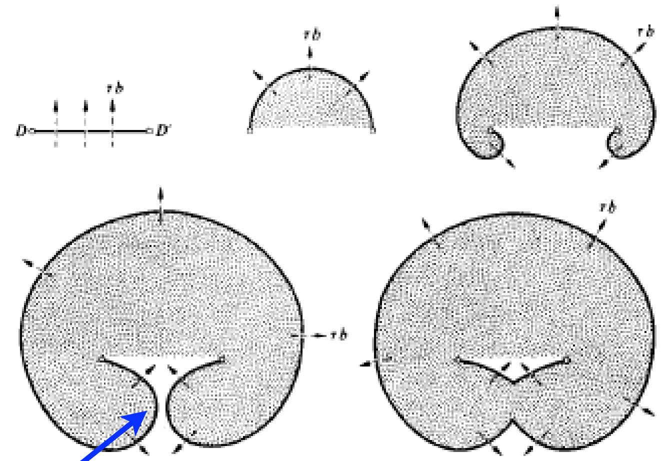
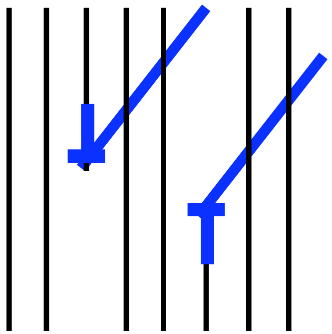


Annihilation

Dislocations of opposite sense can annihilate each other:



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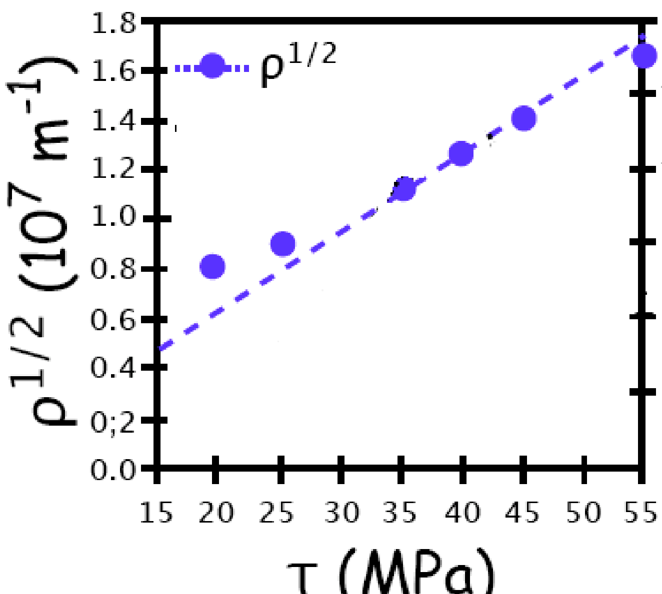


$$= \frac{\tau^2}{(\alpha \mu b)^2}$$

Isotropic linear elasticity

Strain is derivative of displacement (**u**):

$$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) = \frac{1}{2}(u_{i,j} + u_{j,i}) \qquad \left(f_{,i} = \frac{\partial f}{\partial x_i} \right)$$

Relation between stress and strain: $\sigma_{kl} = c_{klij}\varepsilon_{ij}$

$$c_{ijkl} = \lambda\delta_{ij}\delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$$

We assume isotropic, linear elasticity:

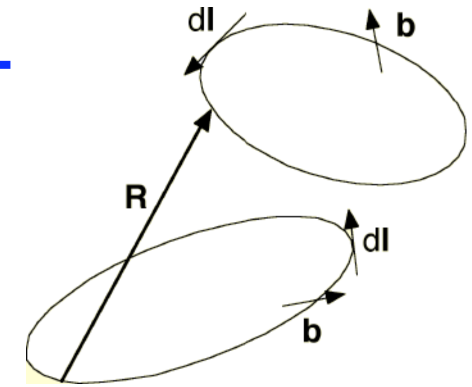
- elastic properties independent of direction

$$\sigma_{11} = (\lambda + 2\mu)\varepsilon_{11} + \lambda\varepsilon_{22} + \lambda\varepsilon_{23}$$
$$\sigma_{12} = 2\mu\varepsilon_{12}$$

Elastic constants: $\mu = c_{44} \quad \lambda = c_{12} \quad \nu = \dfrac{\lambda}{2(\lambda + \mu)}$

Have formalism for anisotropic elasticity.

Dislocation interactions are long ranged and anisotropic



Peach-Koehler force: $\frac{\vec{F}}{L} = (\vec{b} \cdot \bar{\bar{\sigma}}) \times \hat{\xi} = \varepsilon_{ijk} b_l \sigma_{jl} \xi_k \hat{x}_i$

$$\sigma_{ij} = \frac{\mu b_n}{8\pi} \oint_C \left[R_{,mpp}(\varepsilon_{jmn} dl_i + \varepsilon_{imn} dl_j) \right.$$
$$\left. \frac{2}{1-\nu}(R_{,ijm} - \delta_{ij} R_{,ppm}) \varepsilon_{kmn} dl_k \right]$$

$$(R_{,ijk} = \partial^3 R / \partial x_i \partial x_j \partial x_k)$$

Total stress (linear elasticity):

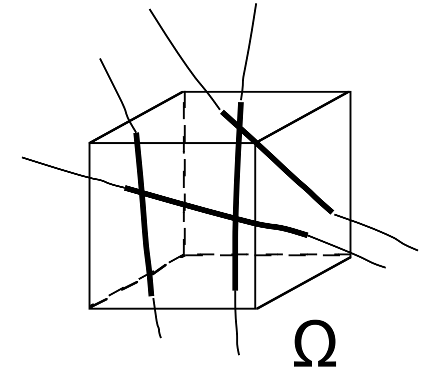
$$\bar{\bar{\sigma}}_i = \bar{\bar{\sigma}}_{app} + \bar{\bar{\sigma}}_i^{self} + \sum_{j \neq i}^{N_{dis}} \bar{\bar{\sigma}}_j$$

self force is interaction of dislocation with self - line tension

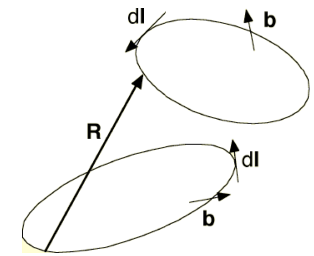
Long-ranged interactions:

$F \sim 1/R^2$, $E \sim 1/R$

Energetics



Dislocation density tensor: continuous, discrete



Kosevich:

$$E_I = \frac{\mu}{16\pi} \int \int \varepsilon_{ipl}\varepsilon_{jmn} R_{,mp}(\vec{r},\vec{r}\,') d\vec{r} d\vec{r}\,' \times \left\{ \rho_{jl}(\vec{r})\rho_{in}(\vec{r}\,') + \delta_{ij}\rho_{kl}(\vec{r})\rho_{kn}(\vec{r}\,') + \frac{2\nu}{1-\nu}\rho_{il}(\vec{r})\rho_{jn}(\vec{r}\,') \right\}$$

$$R = |\vec{r} - \vec{r}\,'|$$

$$R_{,mp} = \partial^2 R / \partial x_m \partial x_p$$

Nelson-Toner:

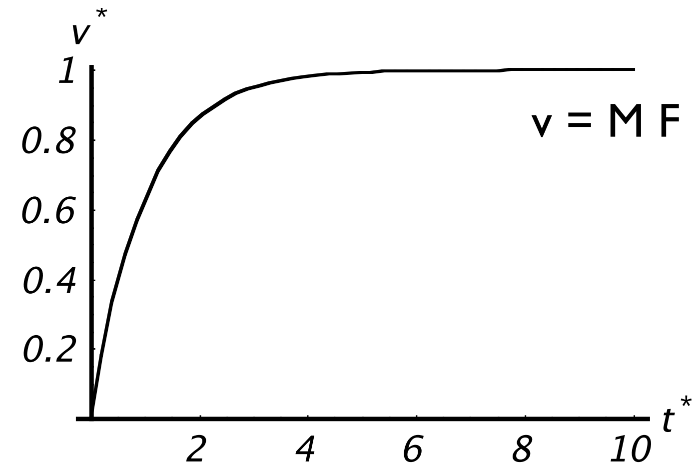
$$E[\rho(\vec{q})] = \frac{1}{2} \int d^3 q \, K_{ijkl}(\vec{q}) \rho_{ij}(\vec{q}) \rho_{kl}(-\vec{q})$$

$$K_{ijkl} = \frac{\mu}{q^2} \left[Q_{ik}Q_{jl} + C_{il}C_{kj} + \frac{2\nu}{1-\nu} C_{ij}C_{kl} \right]$$

$$Q_{ij} = \delta_{ij} - \frac{q_i q_j}{q^2} \qquad C_{ij} = \varepsilon_{ijk} \frac{q_k}{q}$$

Dynamics

Dynamics are dissipative: $m(v)\,\vec{a} = \vec{F} - \gamma\vec{v}$



If *inertial* effects are not important, assume over damped dynamics (i.e., a=0)

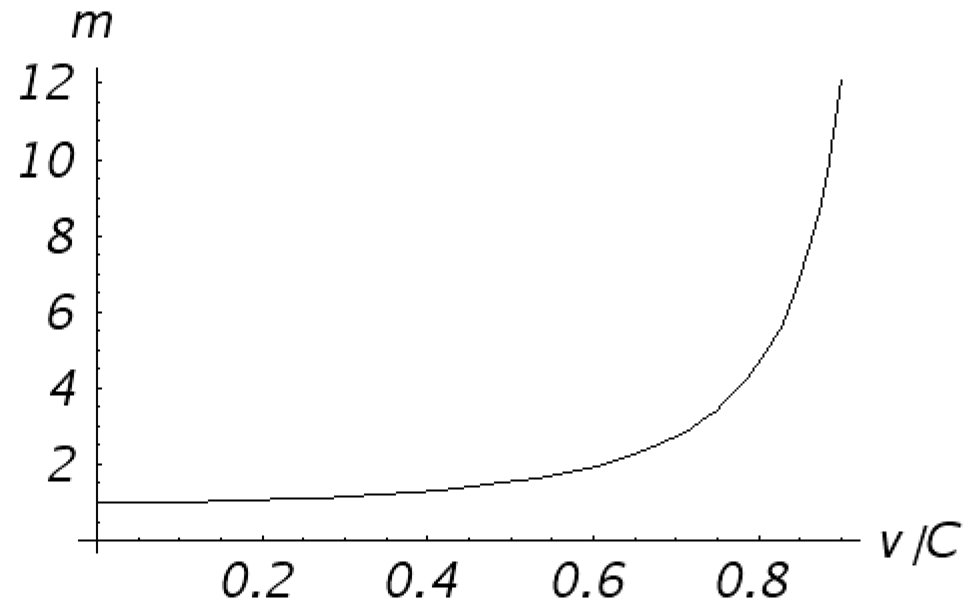
$$\vec{v} = \vec{F}/\gamma = M\vec{F}$$

Velocity-dependent mass:

$$m_s(v) = \frac{W_0}{v^2}\left(-\gamma^{-1} + \gamma^{-3}\right)$$

$$\gamma = (1 - v^2/C^2)^{1/2}$$

$$W_o = \frac{\mu b^2}{4\pi}\ln\left(\frac{R}{r_o}\right)$$



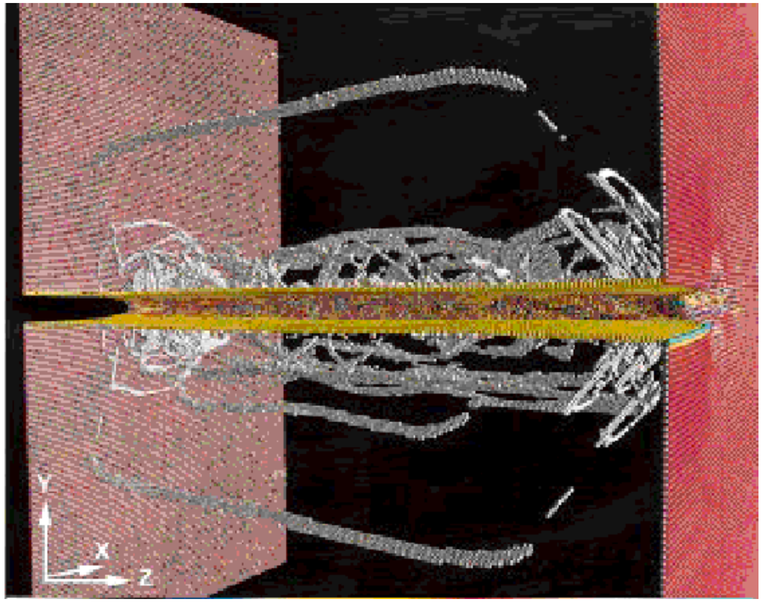
Simulation strategies

Microstructures on a scale of many microns

- 1 μm^3 of copper includes approximately 10^{11} atoms
- standard molecular dynamics methods can be used only for *small* numbers of dislocations

Mesoscale simulations:

- *dislocations are the entities of the simulations*
- atomic-level effects included as models



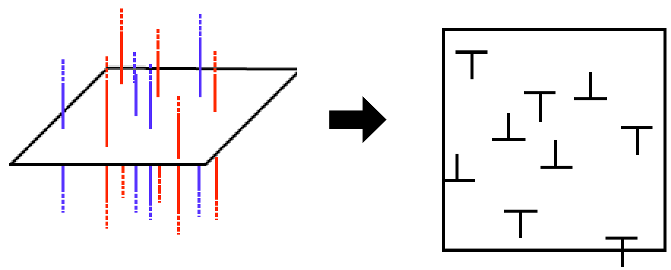
Dislocations around crack tip in shocked Cu. Example from Lomdahl, Holian, et al.

2D model

Parallel dislocations: "vector" lattice gas of charged particles in 2D.

$$\frac{F_i}{L} = \tau_{ext} b_i + \sum_j \frac{F_{ij}}{L} b_i b_j$$

$$\frac{F_{ij}}{L} = \frac{\mu}{4\pi(1-\nu)} \frac{x_{ij}(x_{ij}^2 - y_{ij}^2)}{(x_{ij}^2 + y_{ij}^2)^2}$$



Note: b can be +/-

sign change in F at 45°

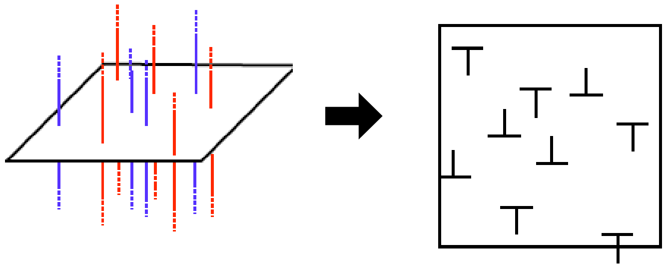
F ~ 1/R (2D), E ~ ln R

Constraints lead to frustration

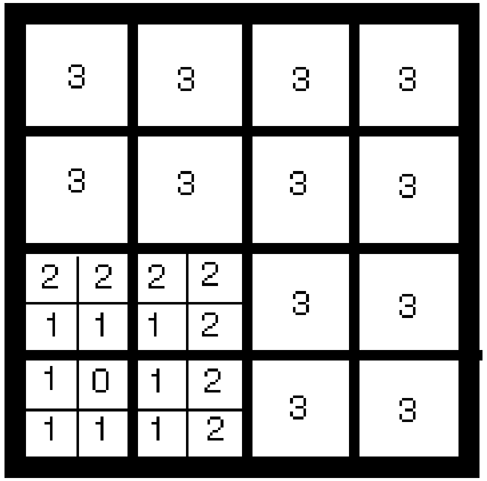
Long-range interactions - the Fast Multipole Method in 2D

$$\frac{F_i}{L} = \tau_{ext} b_i + \sum_j \frac{F_{ij}}{L} b_i b_j$$

$$\frac{F_{ij}}{L} = \frac{\mu}{4\pi(1-\nu)} \frac{x_{ij}(x_{ij}^2 - y_{ij}^2)}{(x_{ij}^2 + y_{ij}^2)^2}$$



Greengard-Rohklin method applied to dislocations:



Stress for edge interactions:

$$\phi_c(z) = \cos\theta \ln(z) \quad \phi_s(z) = \sin\theta \ln(z)$$

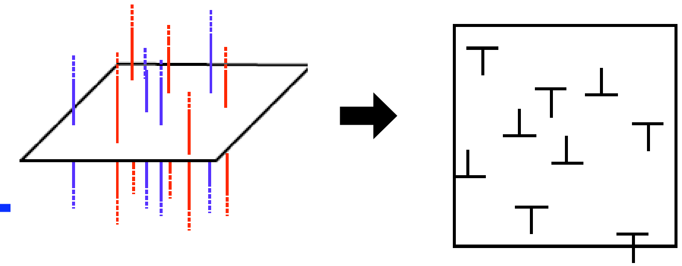
$$\phi_x(z) = x\phi_c(z) \qquad \phi_y(z) = y\phi_s(z)$$

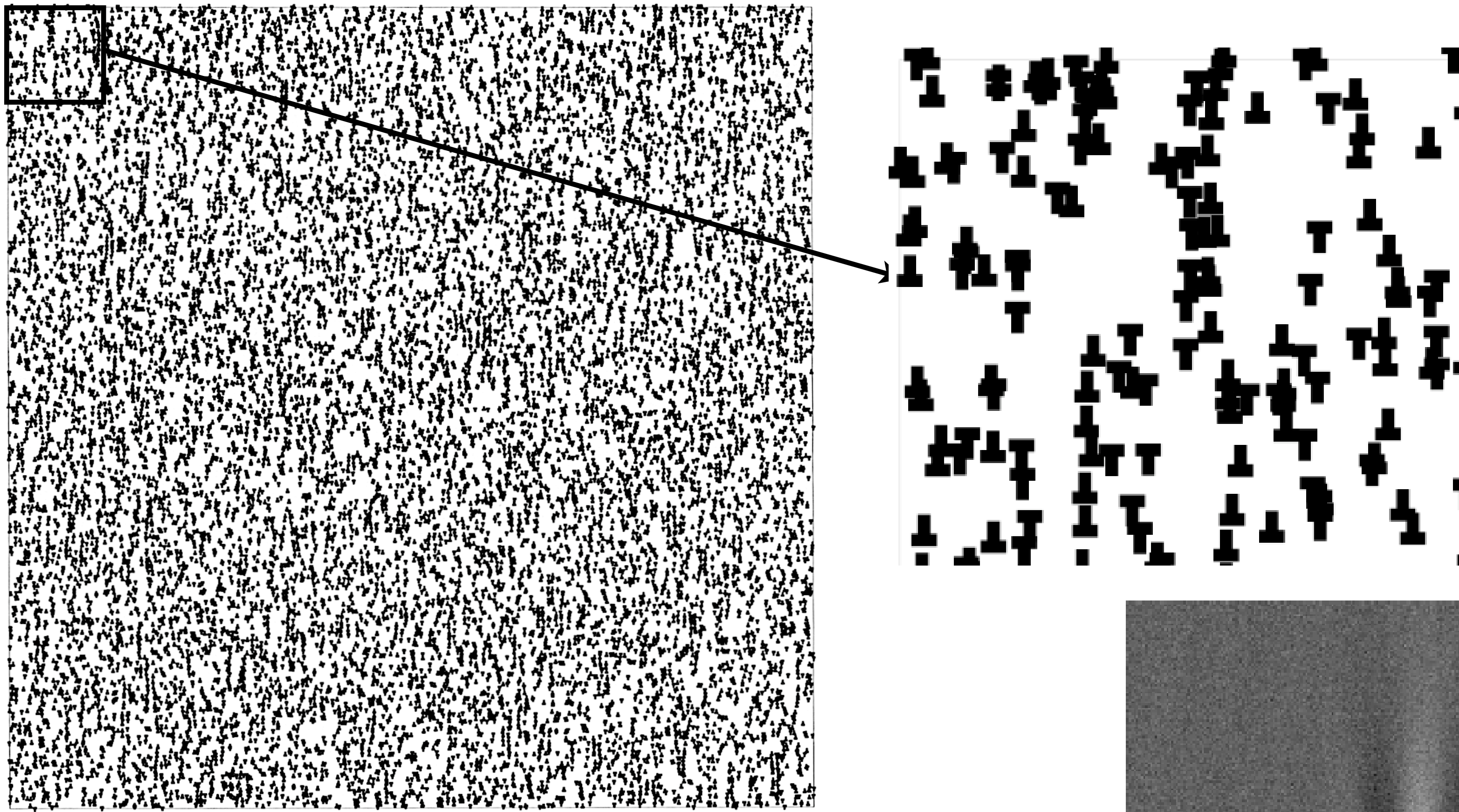
$$\sigma_{xx} = \frac{\mu b}{2\pi(1-\nu)} \left(2\,\mathrm{Im}\left(\phi_c^{'}(z)\right) - \mathrm{Re}\left(\phi_x^{''}(z)\right) + \mathrm{Re}\left(\phi_y^{''}(z)\right)\right)$$

Perform all expansions on generating functions

Wang and LeSar, Phil. Mag. 71, 151 (1995)

Microstructure formation

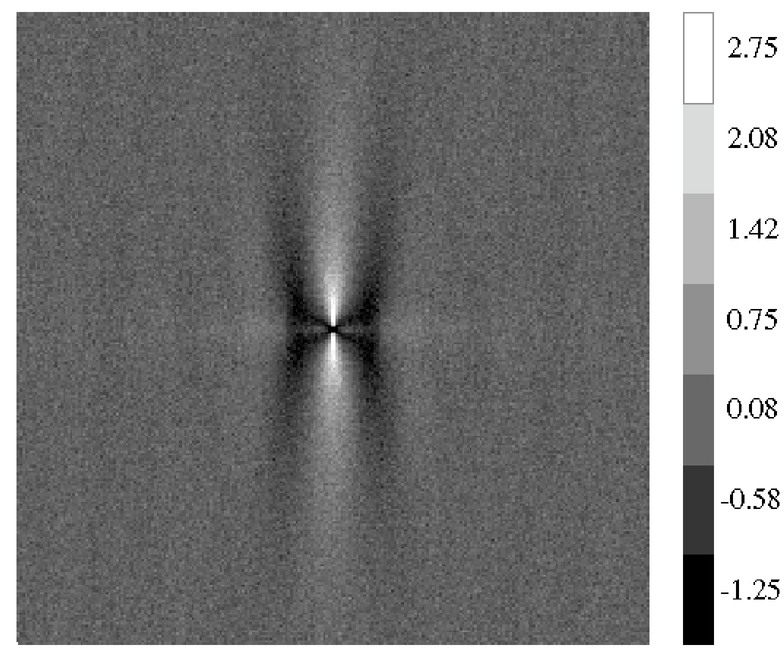




Gulluoglu, Srolovitz, LeSar, Lomdahl, Scripta Metallurgica 23, 1347-1352 (1989)

Wang, LeSar, and Rickman, Phil. Mag. A 78, 1195 (1998)

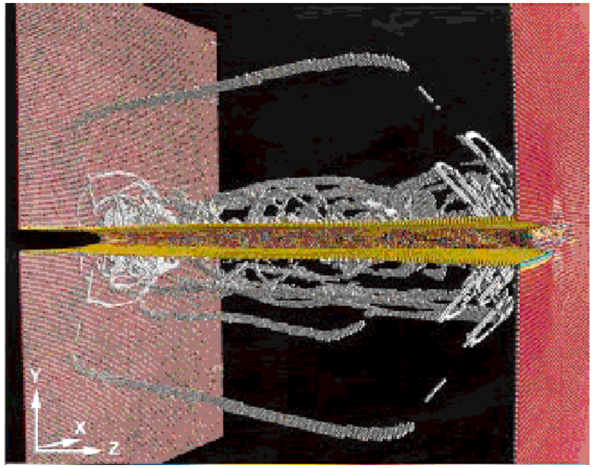
correlation functions:



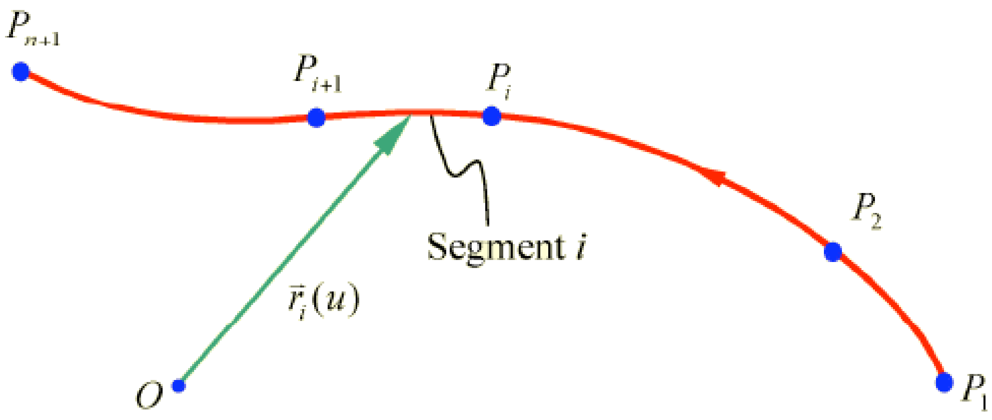
Representation of dislocations in 3D.

We represent dislocation loops with splines:‡

$$\vec{r}_i = (1 - 3u^2 + 2u^3)\vec{P}_i + (3u^2 - 2u^3)\vec{P}_{i+1}$$
$$+(u - 2u^2 + u^3)\vec{T}_i + (-u^2 + u^3)\vec{T}_{i+1}$$



Node points are $\vec{P}_i$ and tangent vectors at each node are $\vec{T}_i$.



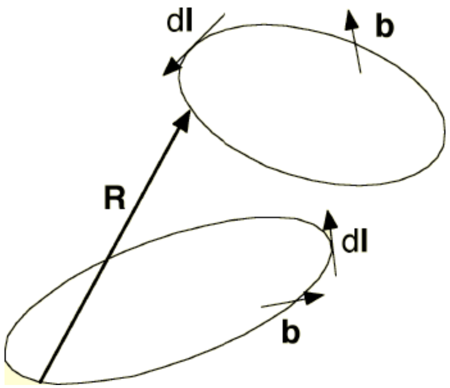
$\vec{T}_i$ are completely determined by continuous curvature at nodes.

Most other groups employ straight dislocation segments

- Kubin and coworkers, LLNL

Ghoniem and Sun, Phys Rev B **60**, 128 (1999)

Dislocation dynamics



$$\frac{\vec{F}}{L} = (\vec{b}\cdot\bar{\bar{\sigma}}) \times \hat{\xi} = \varepsilon_{ijk} b_l \sigma_{jl} \xi_k \hat{x}_i$$

$$\sigma_{ij} = \frac{\mu b_n}{8\pi} \oint_C \Big[R_{,mpp}(\varepsilon_{jmn} dl_i + \varepsilon_{imn} dl_j) \\ \frac{2}{1-\nu}(R_{,ijm} - \delta_{ij} R_{,ppm}) \varepsilon_{kmn} dl_k \Big]$$

$$\left(R_{,ijk} = \partial^3 R / \partial x_i \partial x_j \partial x_k\right)$$

$$\bar{\bar{\sigma}}_i = \bar{\bar{\sigma}}_{app} + \bar{\bar{\sigma}}_i^{self} + \sum_{j\neq i}^{N_{dis}} \bar{\bar{\sigma}}_j$$

Numerical integration along lines gives force on the nodes.

Equation of motion for nodes: $\vec{x}(t+\delta t) = \vec{v}(t)\delta t$

$$\vec{v} = \vec{F}/\gamma = M\vec{F}$$

Basic dislocation motion and interactions

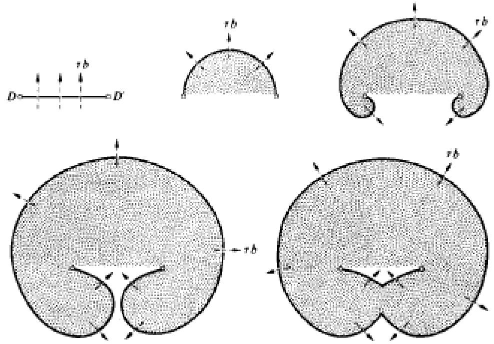
Time sequences of configurations:

(a) F-R source;

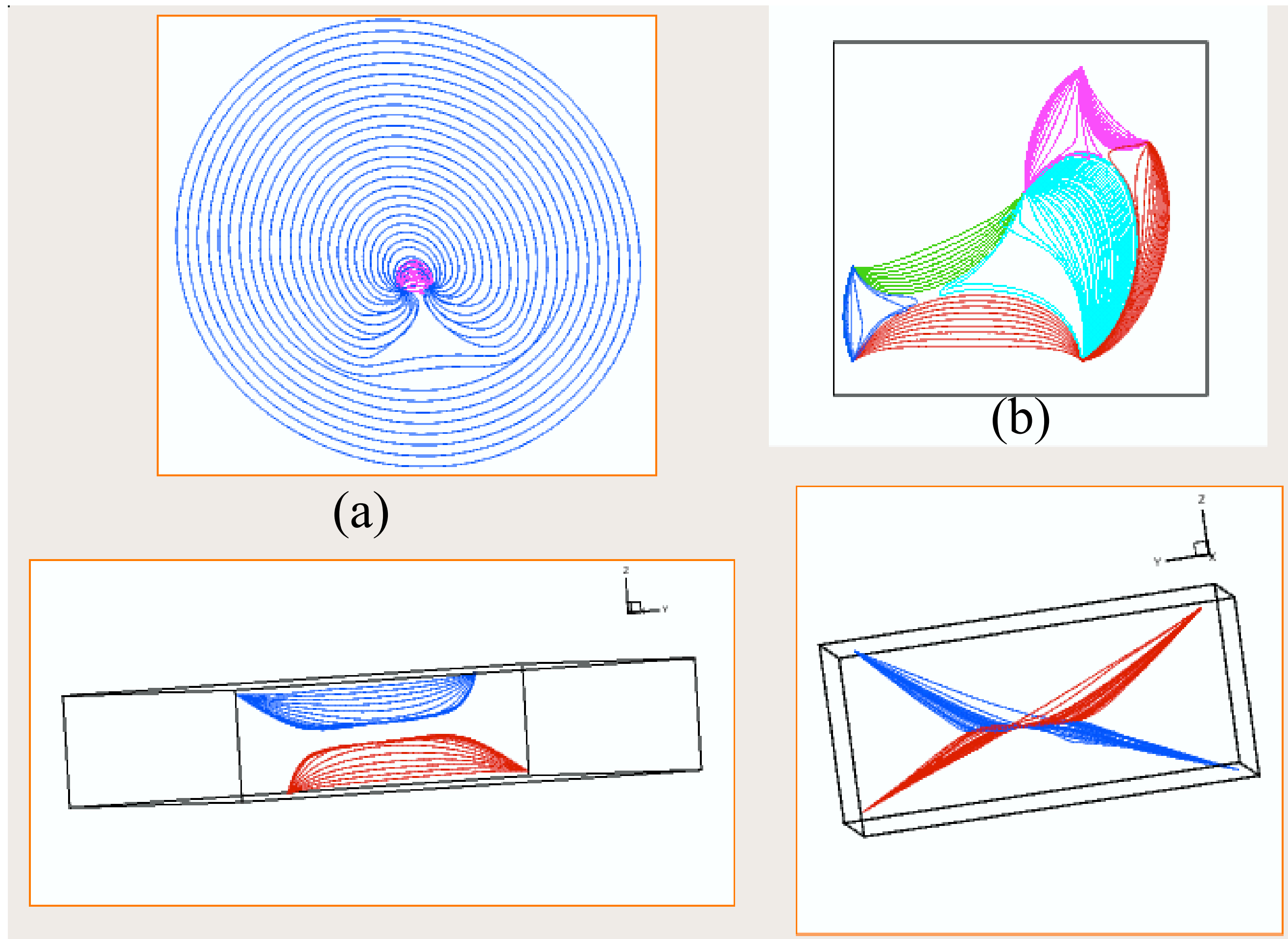
(b) Annihilation;

(c) Dipole;

(d) Junction.

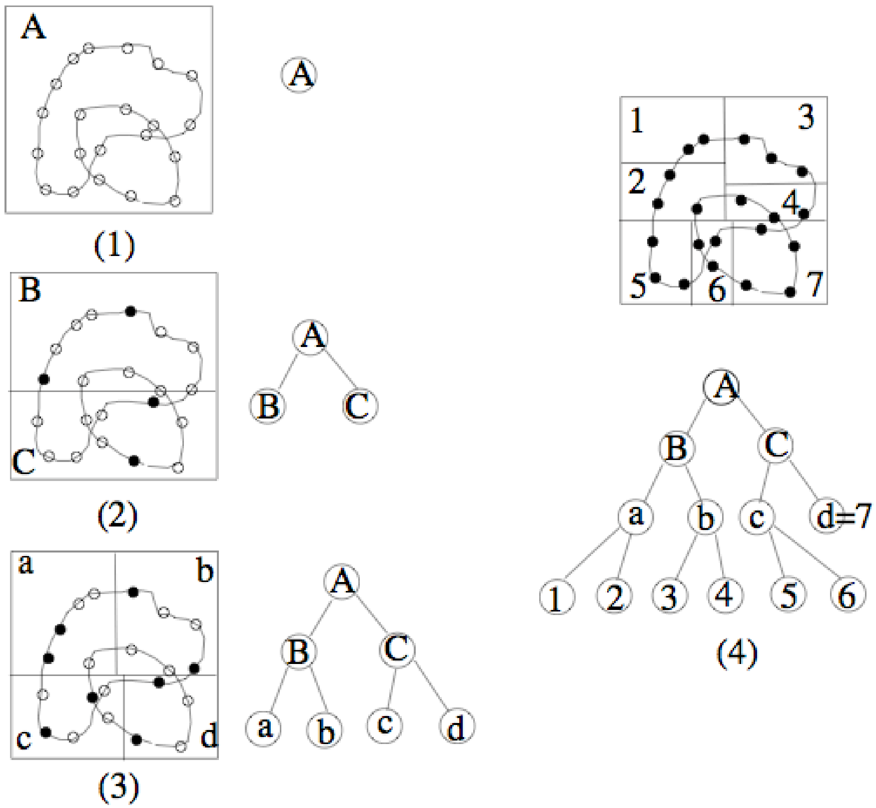


(a)



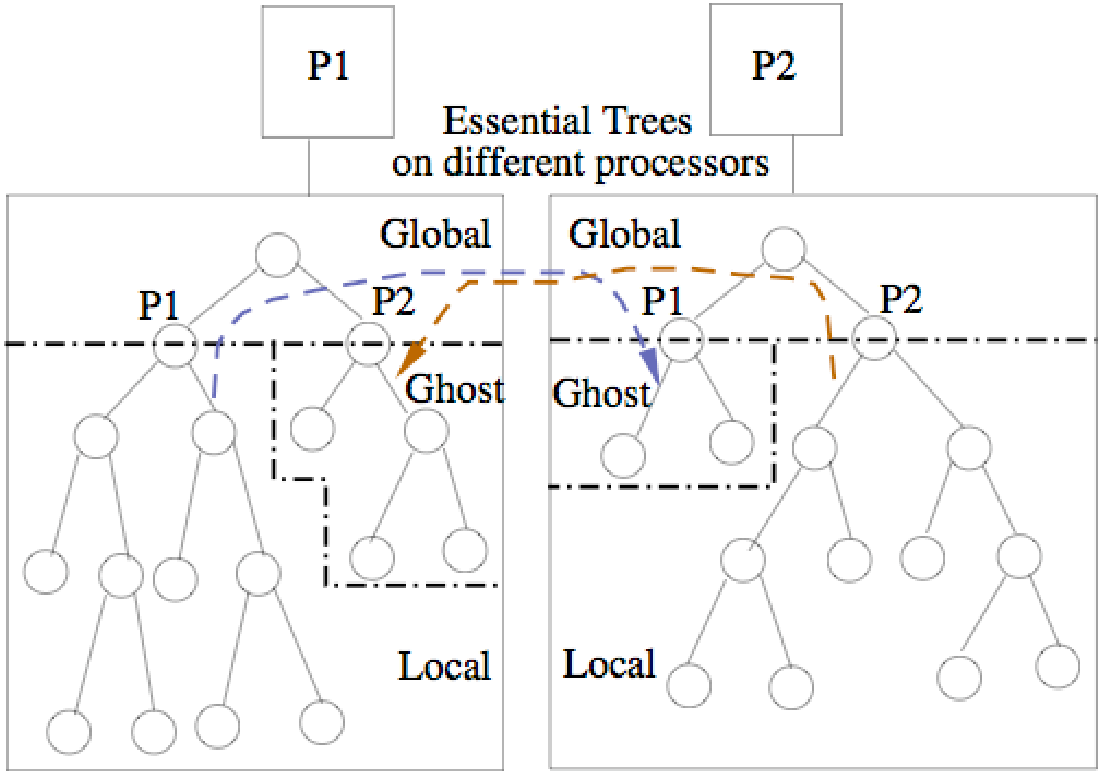
(c) (d)

Parallel algorithm



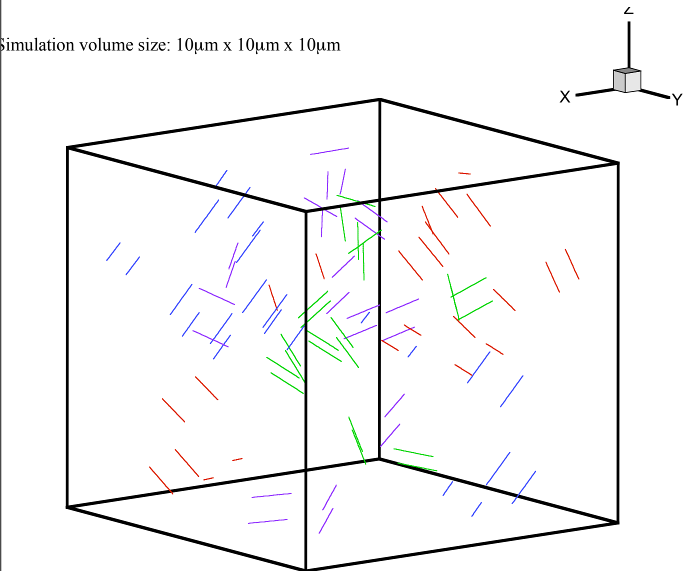
distribution of dislocations is inhomogeneous

- dislocations span regions
- long-range forces through multipole expansion

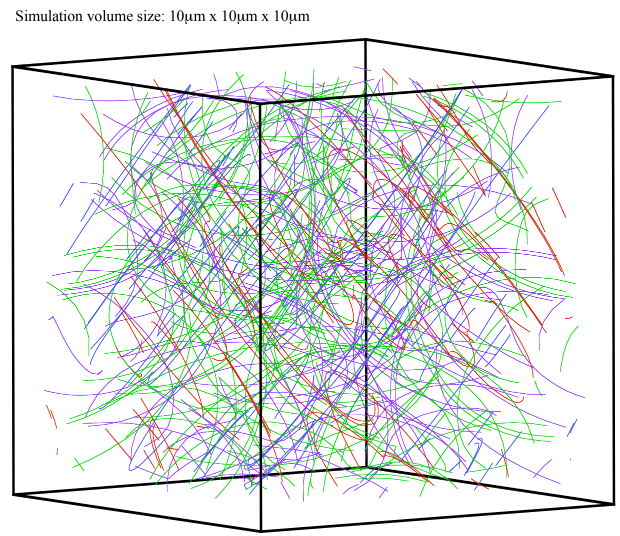


Z. Wang, N. Ghoniem, S. Swaminarayan, and R. LeSar, Journal of Computational Physics 219, 608-621 (2006)

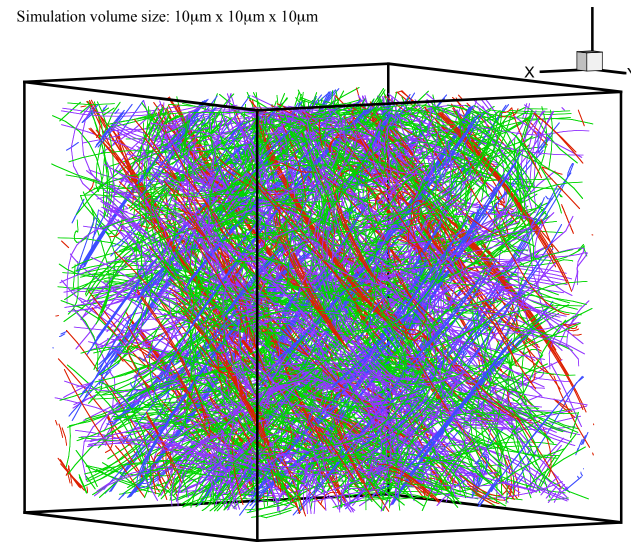
Development of dislocation microstructure



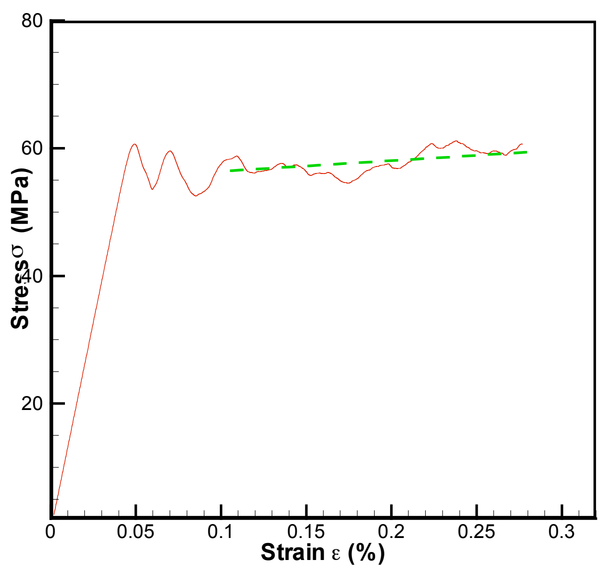
$\rho=10^7/cm^2$



$\rho=2x10^8/cm^2$



$\rho=7.5x10^8/cm^2$

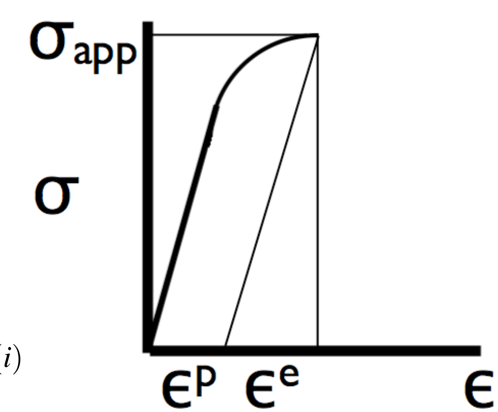


$$\varepsilon_{ij} = \varepsilon^e_{ij} + \varepsilon^p_{ij}$$

$$\sigma_{kl} = c_{klij}\varepsilon^e_{ij}$$

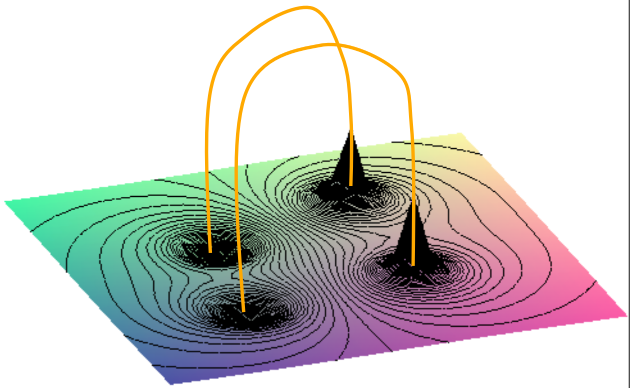
$$= c_{klij}(\varepsilon_{ij} - \varepsilon^p_{ij})$$

$$\dot{\varepsilon}^p = -\frac{1}{2V}\sum_{i=1}^{N}\oint_{l^{(i)}} v^{(i)}[\mathbf{n}^{(i)} \otimes \mathbf{b}^{(i)} + \mathbf{b}^{(i)} \otimes \mathbf{n}^{(i)}]dl^{(i)}$$



Energy-based modeling of dislocations

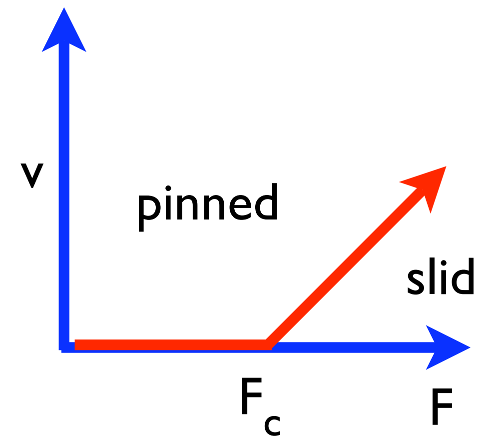
- dislocation content as order parameter
- Ginsburg-Landau dynamics
- Khachaturyan and coworkers in 3D



2D model:

- fundamental quantity is the **slip** ξ
- dislocation content is given by gradient of the slip

$$\beta^p_{ij} = \xi(y) m_j s_i \qquad u_{i,j} = \beta^e_{ij} + \beta^p_{ij} \qquad \rho_{hi} = -\varepsilon_{hlj}\beta^p_{ji,l}$$



$$E[\xi] = \int \left(\frac{\mu b^2}{4} \frac{K}{1+Kd/2} |\hat{\xi}|^2 - \frac{b \hat{s} \hat{\xi}}{1+Kd/2} \right) \frac{d^2k}{(2\pi)^2}$$

$$K = \frac{k_2^2}{\sqrt{k_1^2+k_2^2}} + \frac{1}{1-\nu}\frac{k_1^2}{\sqrt{k_1^2+k_2^2}}$$

non-local energy

pinning potential

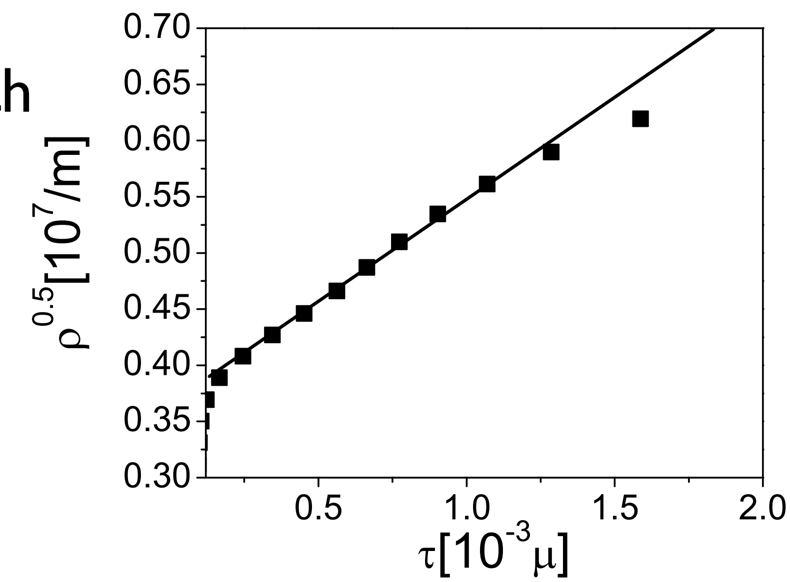
$$\frac{\partial \xi(x)}{\partial t} = \frac{\delta E[\xi(x)]}{\delta \xi(x)} + \tau - \eta(x, \xi(x))$$

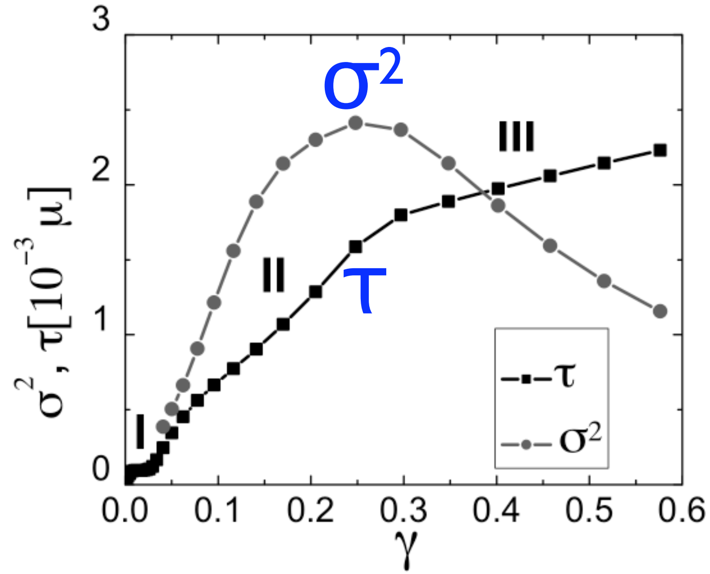
Koslowski, Cuitiño, Ortiz, J. Mech. Phys. Sol. 50, 2597 (2002)

Large-scale deformation

2D model of 3D behavior:

- stress-strain in good agreement with experiment
- variance shows peak at Stage II-III (agrees with Szekely et al.)





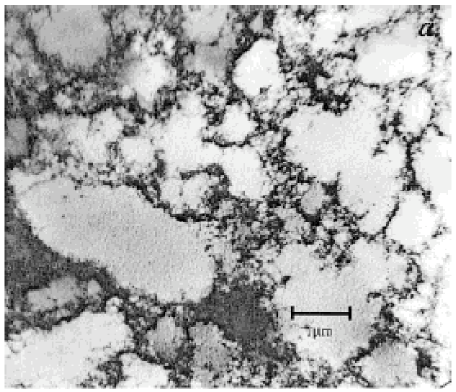
Once number of obstacles "saturates"

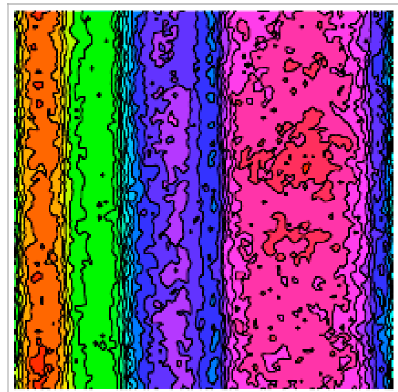
- Stage III behavior

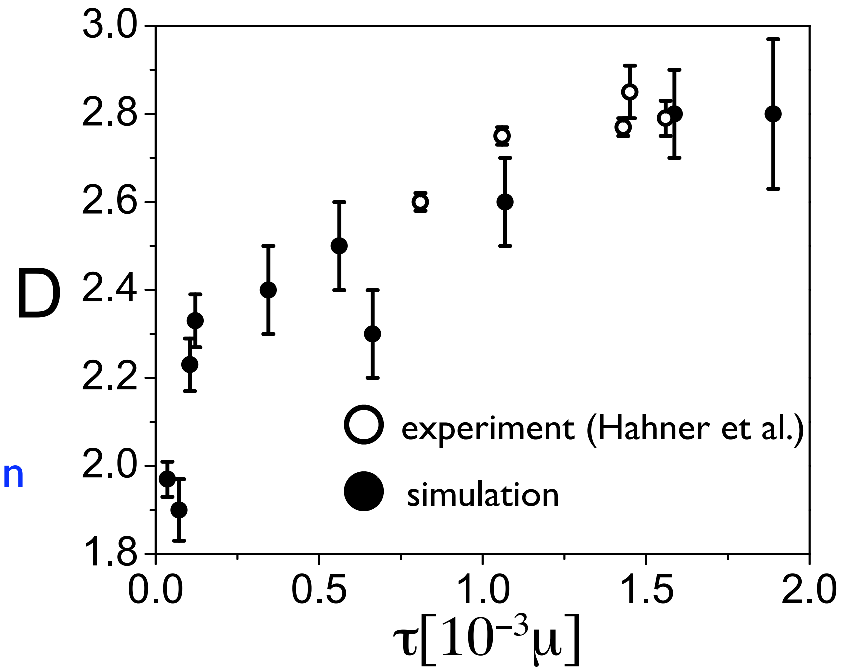
Mimics removal of LC locks (obstacles) that pin cell walls to reach steady-state.

M. Koslowski, R. LeSar, and R. Thomson, Phys. Rev. Lett. 93, 125502 (2004).

Simulations and experiment indicate structures are fractal







number of "cells" of area A

fractal dimension

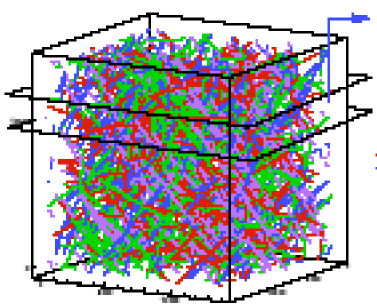
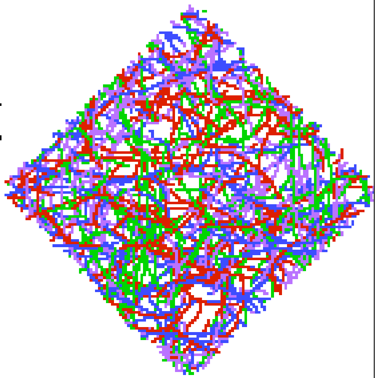
$$n(A) = CA^{-D}$$

From 2D phase field, we find same fractal dimension as experiment

- implies self-similarity extends from our structures to full cellular structure.
- we measure "cell" sizes as areas with no dislocations, extending scaling to smaller scales

M. Koslowski, R. LeSar, and R. Thomson, Phys. Rev. Lett. 93, 125502 (2004).

Direct simulations are computationally challenging

Time per force calculation $t \sim L^2$ (length of dislocation), but $L \propto \rho \propto \tau^2$

- time $t \sim \tau^4$
- calculations slow down considerably as system is deformed
- too slow to include directly in continuum calculations
- we have formalism for O(N) simulation (FMM)
- some issues with boundary conditions

We are developing a *coarse-graining* approach that enables inclusion of dislocation content without resolving dislocation content.

Spatial coarse graining

Quest in coarse graining:

- identify a relatively small set of coarse-grained variables, selected from among a myriad of degrees of freedom
- describe system on larger length/time scales than practical (or possible) at scales associated with microscopic simulations

Coarse graining in other systems:

- systems exhibiting coupling on multiple scales, including turbulent fluids, critical magnets, mesoscale mechanics of solids, ...
- there has been some success for some systems

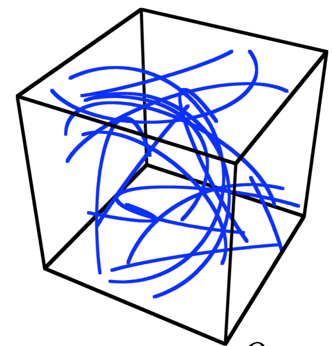
A critical question:

- Is the development of a CG for dislocations even possible?

Dislocation density tensor

Average dislocations over volume Ω to obtain the dislocation density **tensor**, ρ_{ij}

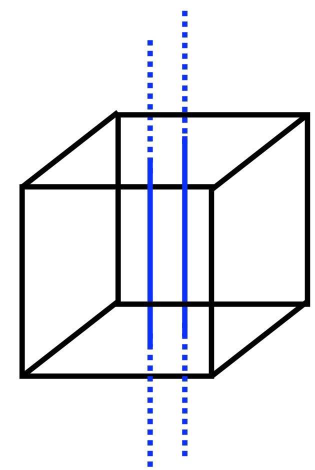
- first index is the line direction
- the second is the Burgers vector.



$$\rho_{\alpha\beta} = \sum_i b_\beta(i) \oint_{C_i} dl_\alpha(i)$$

Limitations:‡

- ρ_{ij} is an average
- no information about structure and energy within Ω
- no information about crystallography
- no differentiation between stored and "geometrically necessary" dislocations
- unclear what sets optimal length scale for Ω
- need evolution equations

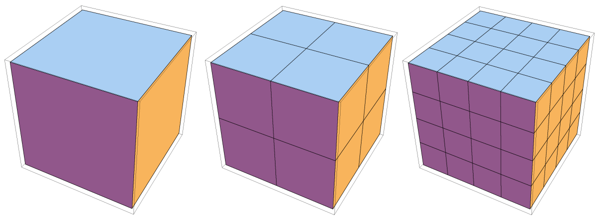


‡E. Kröner, Inter. J. Solids and Structures **38**, 1115-1134 (2001).

Development of a density functional

$$E_I = \frac{\mu}{16\pi}\int\int \varepsilon_{ipl}\varepsilon_{jmn}R_{,mp}(\vec{r},\vec{r}')d\vec{r}d\vec{r}'$$
$$\times\left\{\rho_{jl}(\vec{r})\rho_{in}(\vec{r}')+\delta_{ij}\rho_{kl}(\vec{r})\rho_{kn}(\vec{r}')+\frac{2\nu}{1-\nu}\rho_{il}(\vec{r})\rho_{jn}(\vec{r}')\right\}$$

$$R = |\vec{r}-\vec{r}'|$$
$$R_{,mp} = \partial^2 R/\partial x_m \partial x_p$$



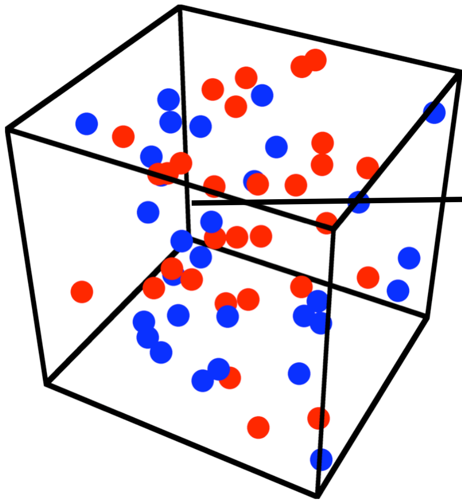
We divide space into regions with volume Ω.

Moment expansion of E_I
- find good convergence with gradient expansion (first order)
- does not provide information on structures smaller than Ω

LeSar and Rickman, PRB (2004)

Multipole expansion of dislocation interactions.

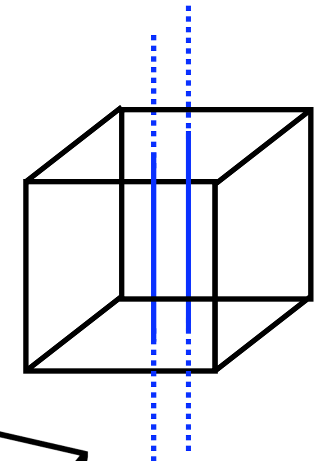
Volume of point charges.



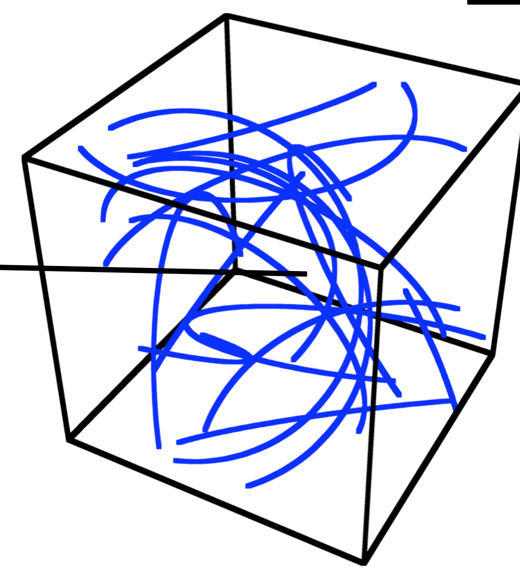
$$\Phi(\vec{r}) = \sum_j \frac{q_j}{|\vec{r}-\vec{r}_j|} \approx \frac{Q}{R} + \frac{\vec{\mu}\cdot\vec{R}}{R^3} + \ldots$$

$$Q = \sum_j q_j$$

$$\vec{\mu} = \sum_j q_j \vec{r}_j$$



$$\sigma_{ij} = \frac{\mu b_n}{8\pi} \oint \left[R_{,mpp}(\epsilon_{jmn} dl_i + \epsilon_{imn} dl_j) + \frac{2}{1-\nu}\epsilon_{kmn}(R_{,ijm} - \delta_{ij} R_{,ppm}) dl_k\right]$$



Volume of dislocation loops.

$$\rho_{\alpha\beta} = \sum_i b_\beta(i) \oint_{C_i} dl_\alpha(i)$$

$$\rho_{\alpha\beta\gamma} = \sum_i b_\beta(i) \oint_{C_i} r_\gamma(i) dl_\alpha(i)$$

$$\sim \nabla_\gamma \rho_{\alpha\beta}$$

LeSar and Rickman, PRB **65**, 144110 (2002)

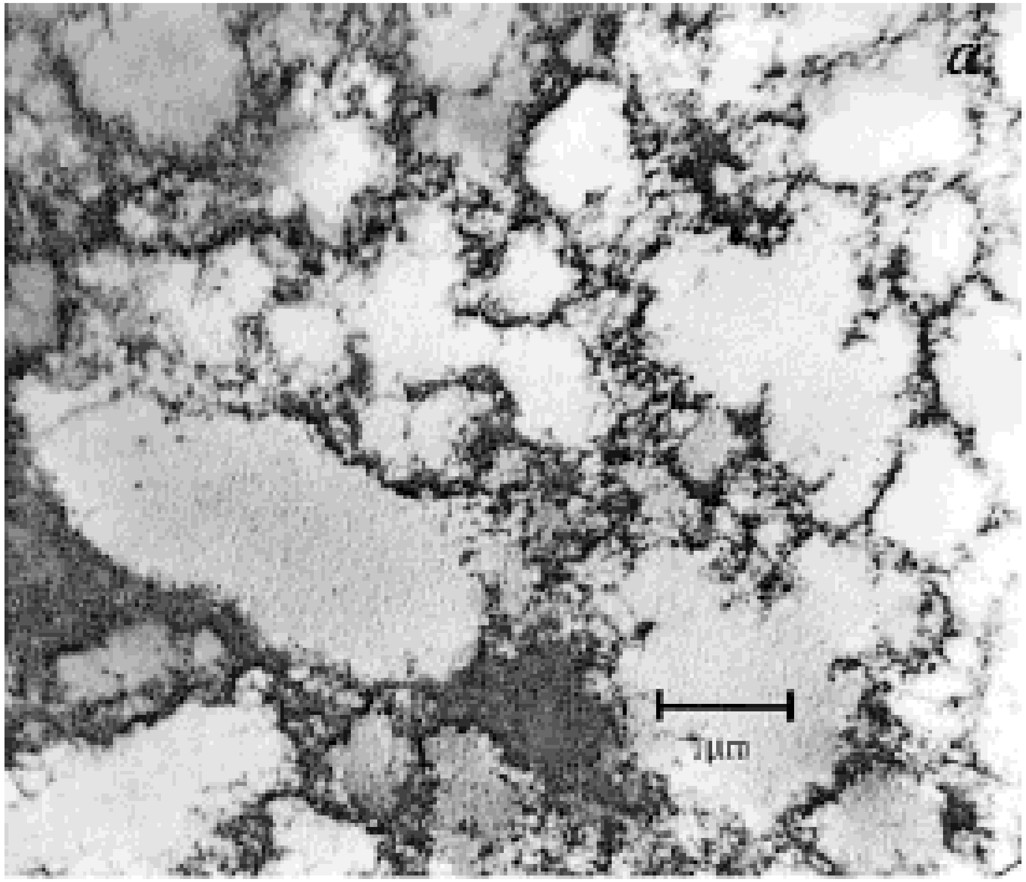
Multiple length scales

Polygonization:

- dislocations form walls
- structures within walls

Are there scaling laws that connect across scales?

What is the impact of substructure on mechanical properties?



We are developing local governing equations for substructure energetics and dynamics

- *define coarse-graining length*

Temporal coarse graining

Phenomenological approach (Holt, Rickman and Viñals):

$$\frac{\partial}{\partial t}\rho_{ij} + \varepsilon_{ilm}\frac{\partial}{\partial x_l} j_{mj} = 0$$

conservation of Burgers vector

$$\vec{j} \propto \nabla \frac{\delta E}{\delta \overleftrightarrow{\rho}}$$

flux law

Connection to mesoscale simulation:

$$\left\langle \rho_{ij}(\vec{q},t)\,\rho_{mn}(-\vec{q},t) \right\rangle$$

dynamical structure factor

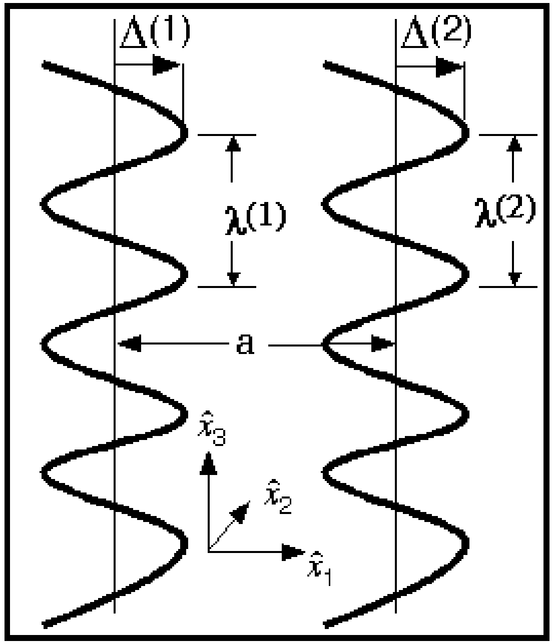
$$S_{loop} \propto \int\int ds\,ds' \left\langle \exp\left[i\vec{q}\cdot\left(\vec{R}(s,t) - \vec{R}(s',t') \right) \right] \right\rangle$$

polymer loop structure factor

Finite temperature effects

Thermally-induced kinks and jogs lead to *entropic* interactions between dislocations.

- analogues:
  - dipolar chains in electrorheological fluids
  - Type II superconductors (Halsey and Toor)



Energetics (Kosevich, Nelson-Toner):

$$E[\rho(\vec{q})] = \frac{1}{2}\int d^3q\, K_{ijkl}(\vec{q})\rho_{ij}(\vec{q})\,\rho_{kl}(-\vec{q})$$

$$K_{ijkl} = \frac{\mu}{q^2}\left[Q_{ik}Q_{jl} + C_{il}C_{kj} + \frac{2\nu}{1-\nu}C_{ij}C_{kl}\right]$$

$$Q_{ij} = \delta_{ij} - \frac{q_i q_j}{q^2} \qquad C_{ij} = \varepsilon_{ijk}\frac{q_k}{q}$$

Rickman and LeSar, PRB 64, 94106 (2001)

Energetics

Isolated line defects: theory of distributions

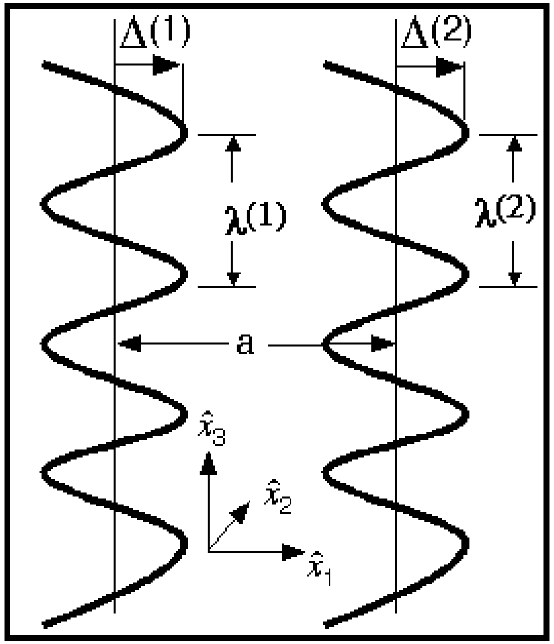
- e.g., straight screw along z

$$\rho_{ij}(\vec{r}) = b\,\delta_{i3}\delta_{j3}\,\delta(x)\delta(y)$$

- energy between straight dislocations

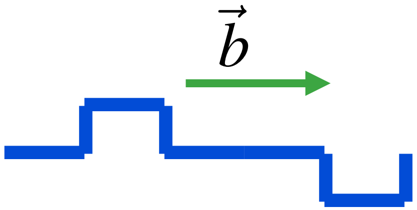
$$e_{straight}(a) = -\frac{\mu b^{(1)} b^{(2)}}{2\pi} \ln(a)$$

$$\int d^2q \, \frac{1}{q^2} \exp(-iq_x a) = -2\pi \ln(a)$$



Thermally induced kinks and jogs:

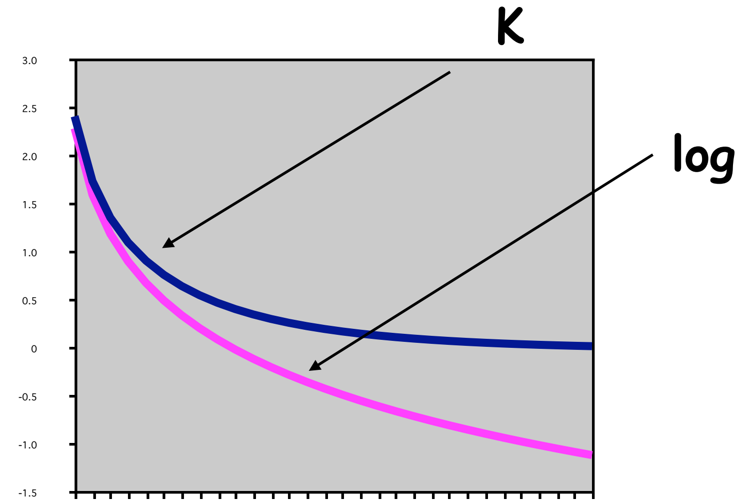
- Fourier expansion in modes



Temperature-dependent force

screened line “charge”

$$\int d^2q \, \frac{1}{q^2+k^2} \exp(-iq_x a) = 2\pi K_0(ka)$$



partition function

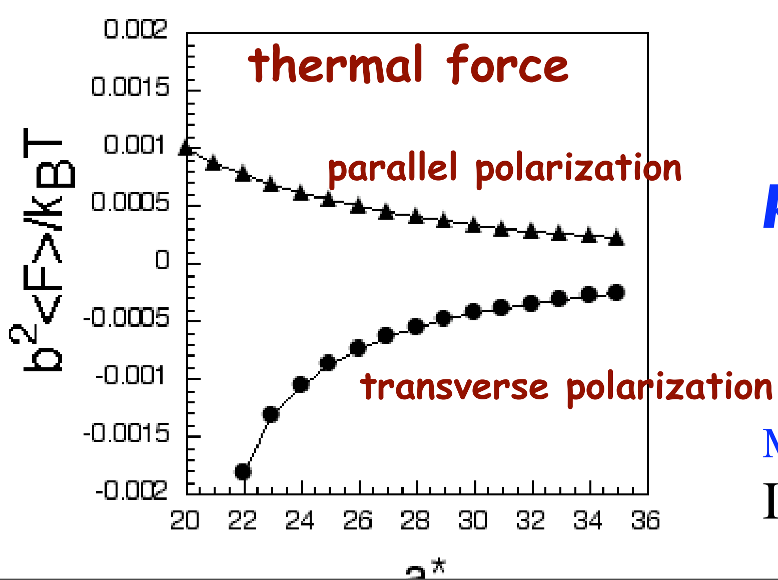
$$Z = N\left[\int d\omega_\perp \exp\left(\frac{-L\Delta e_\perp}{kT}\right)\right]\left[\int d\omega_\perp \exp\left(\frac{-L\Delta e_\perp}{kT}\right)\right]$$

free energy

$$F = -kT\ln(Z)$$

force

$$f = -\frac{\partial F}{\partial a}$$



kT << elastic force

Temperature and noise

kT << elastic energies

- effect of thermal noise mainly through atomic-level processes (cross slip, climb, jogs)

Noise arises from fluctuations in long range strain fields

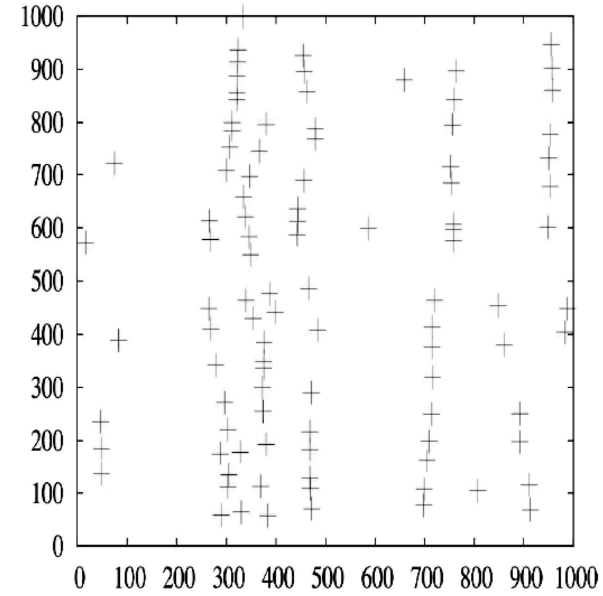
- multiplicative

Some work has been done with simple rate equations with added multiplicative noise term:

- Hahner et al: fractal structures
- our group: wall stability

Thermodynamics of local order

Find that ordering, noise, energetics all functions of dislocation density - define force for ordering



noise: $\mathcal{R} \sim \rho^{1/2}$

structural order:

$$\xi_w \propto \rho^{\alpha}$$

$$\alpha = -0.36 \pm 0.01$$

$$\xi_w \propto \mathfrak{R}^{-0.73}$$

energy:

$$E_{int} \propto -\rho^{\alpha}$$

$$\alpha = 0.998 \pm 0.001$$

force:

$$\mathfrak{F}_{\xi_w}(t,N) = -\frac{\partial E/\partial t}{\partial \xi_w/\partial t}\bigg|_N$$

$$\mathfrak{F}_{\xi_w}(2\tau) \propto \rho^{\beta} \quad \beta = 0.94 \pm 0.05$$

C(x,y) = standard correlation function

$$q(x) = \sum_y C(x,y)$$

$$\xi_w = \sum_{q(x) > q_{random}} q(x)$$

R. Thomson, M. Koslowski, and R. LeSar, Phys. Rev. B. 73, 024104 (2006).

Data provides measure of intermittent flow

Pond, 1972

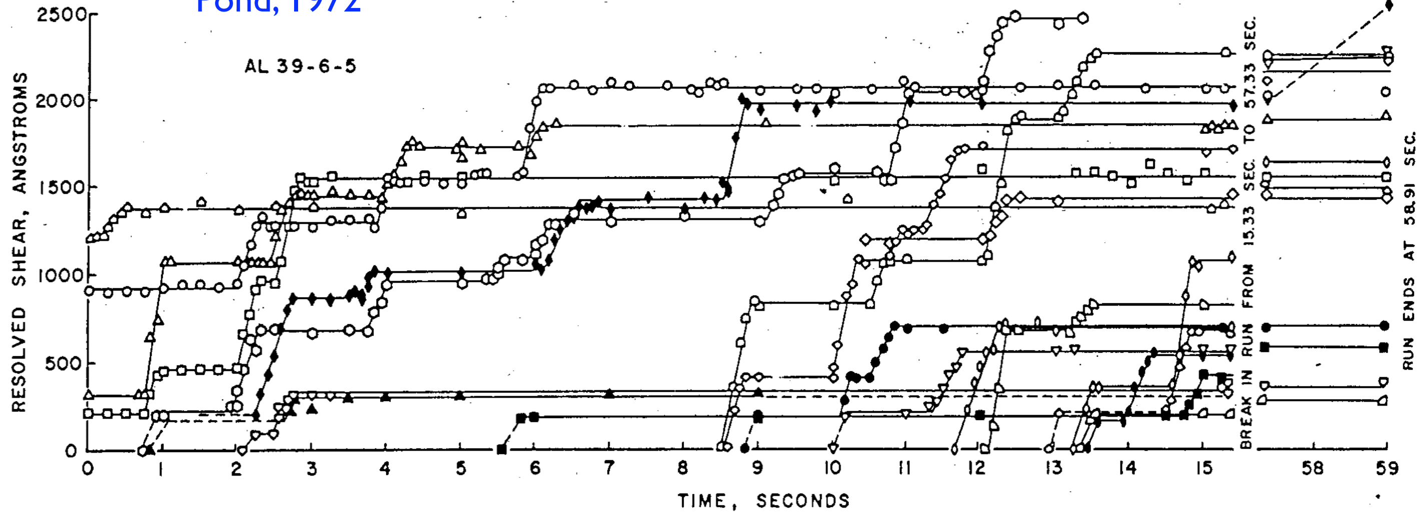
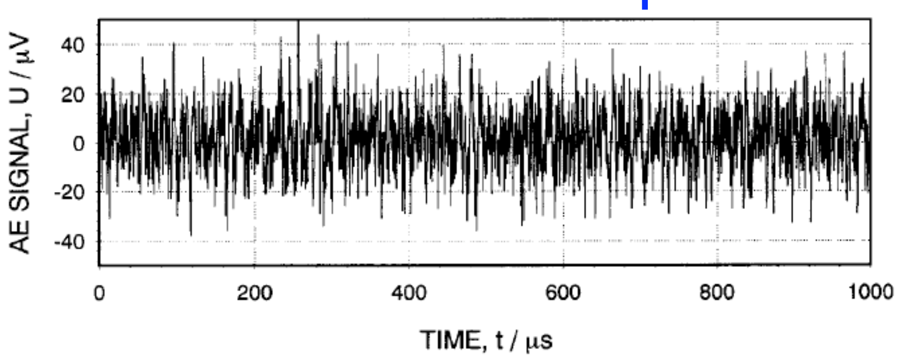
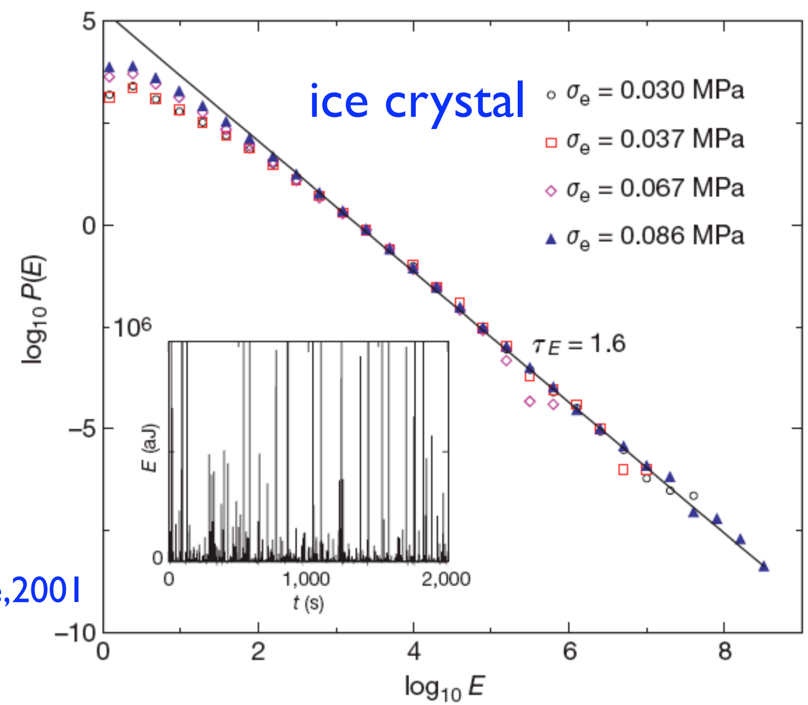


Fig. 5. Resolved shear for each slip band as a function of time for 19 slip bands is shown for an aluminum single crystal extended at 100 C

Acoustic emission experiments:





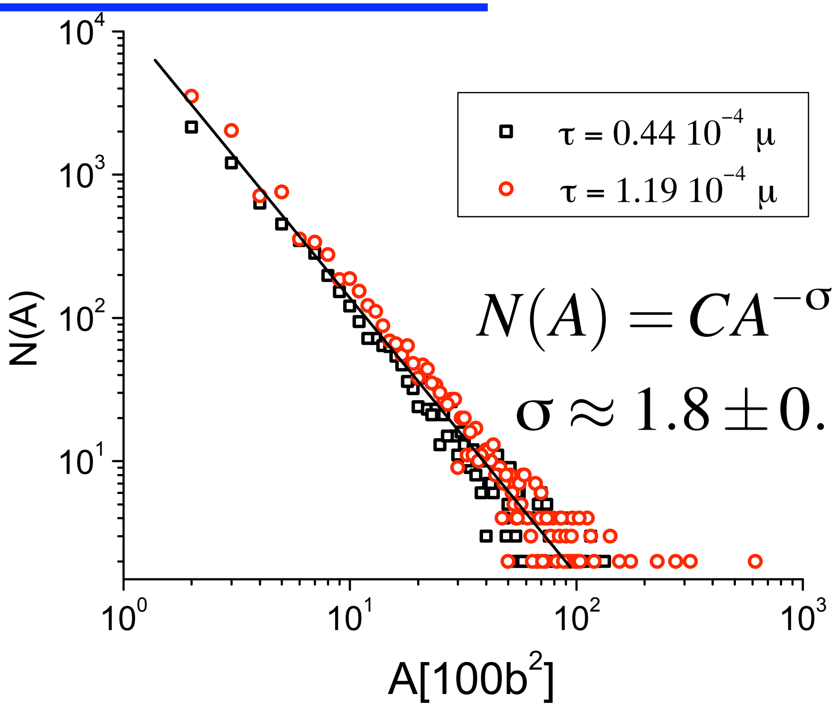
Find power law distribution of avalanche size with exponent 1.6 - 2.0.

Miguel et al., Nature,2001

Phase-field simulations

Employed phase-field calculations as before:

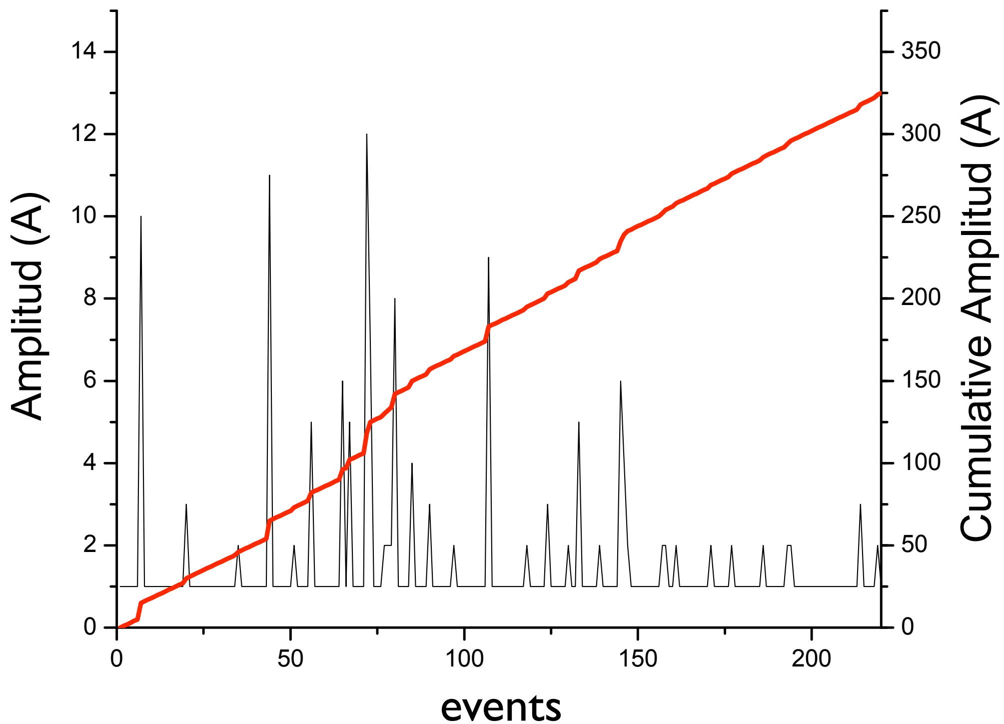
- in Stage I
- stress raised in small increments



$$N(A) = CA^{-\sigma}$$

$$\sigma \approx 1.8 \pm 0.1$$

Bursts during one loading step:

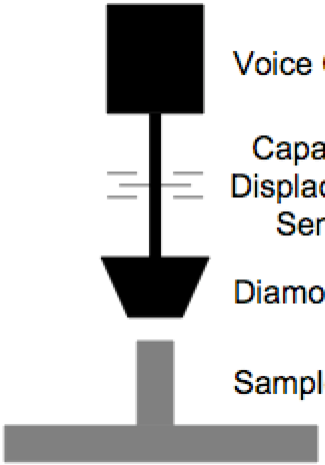


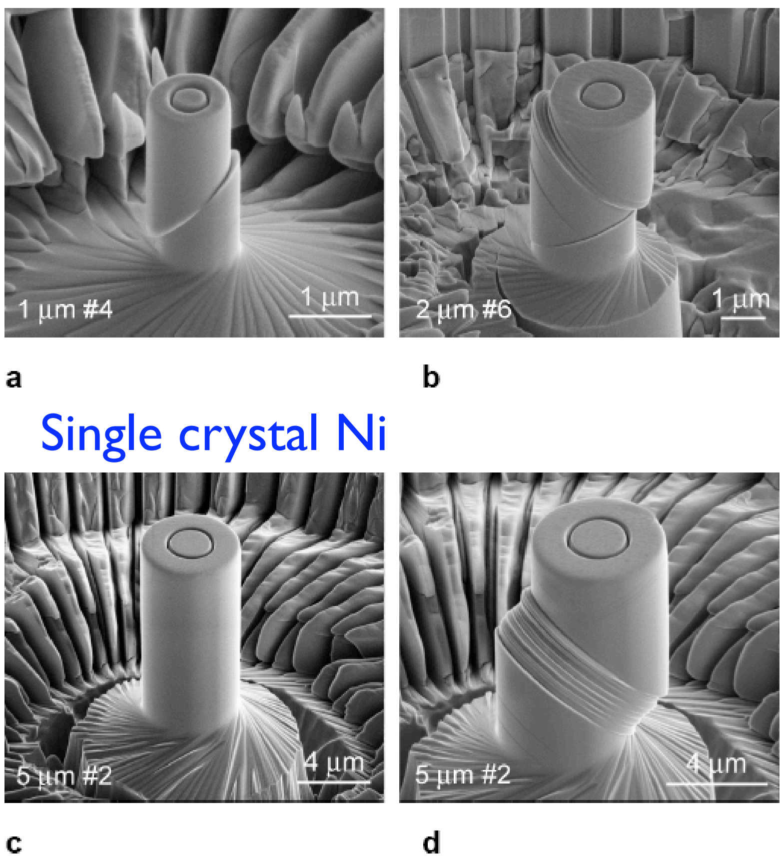
Phase-field simulations show avalanche behavior:

- power-law scaling
- same class as fracture, earthquakes, ...
- example of self-organized critical system?

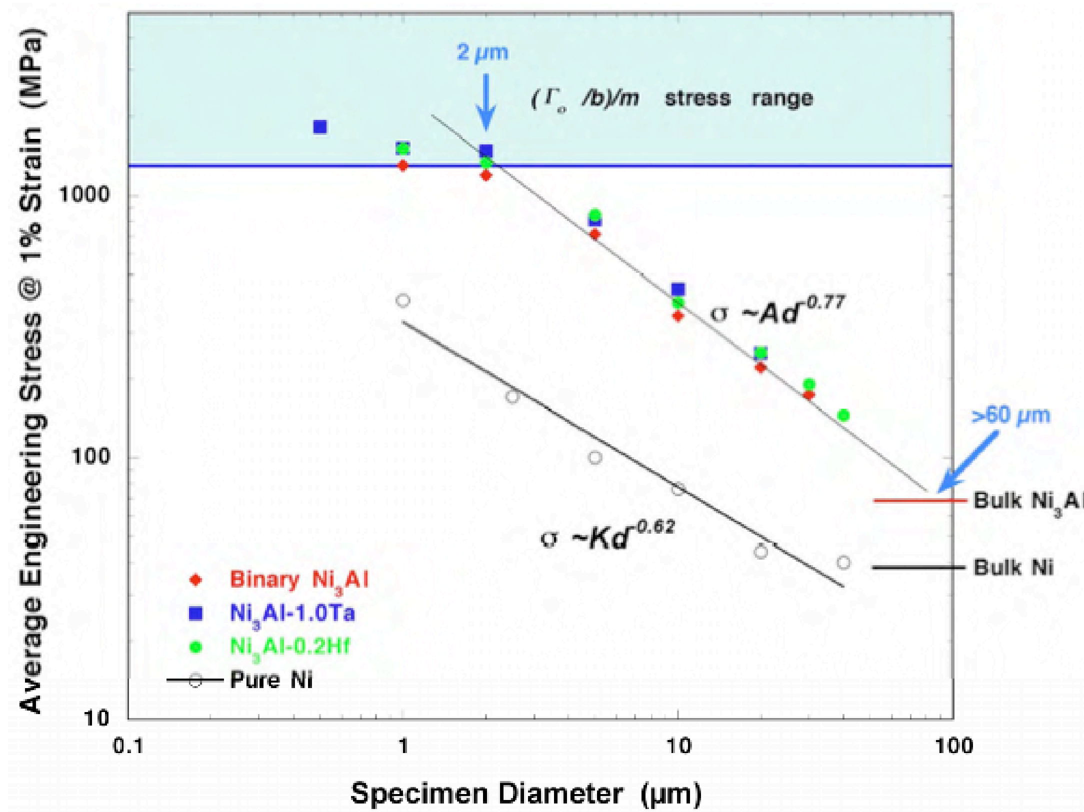
M. Koslowski, R. LeSar, and R. Thomson, Phys. Rev. Lett. 93, 265503 (2004)

Small-scale deformation



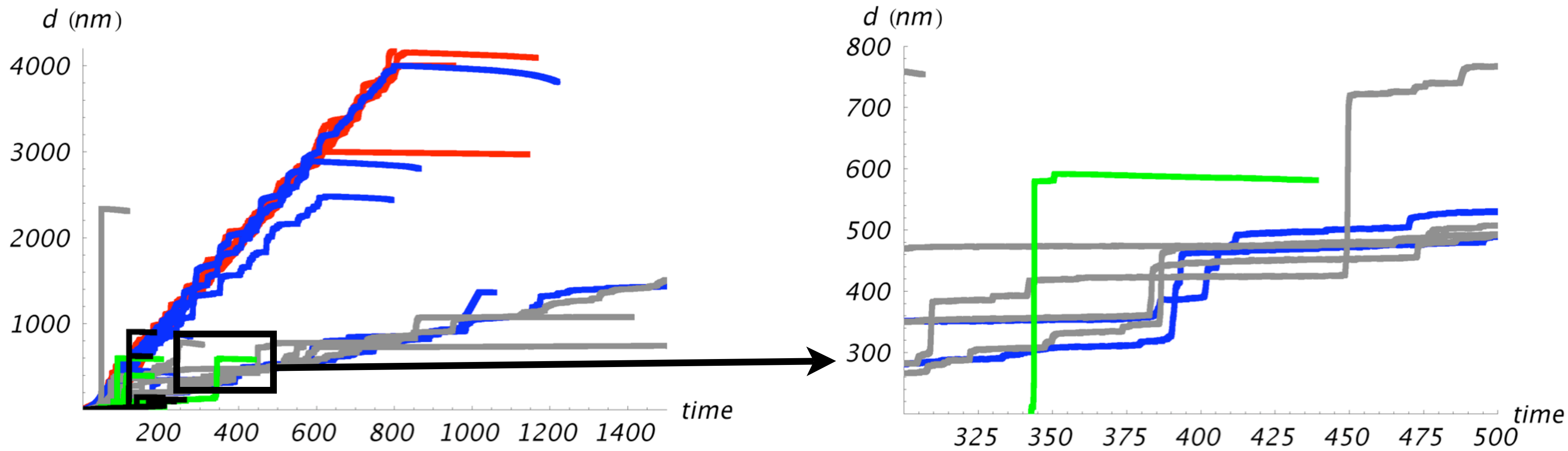


Single crystal Ni

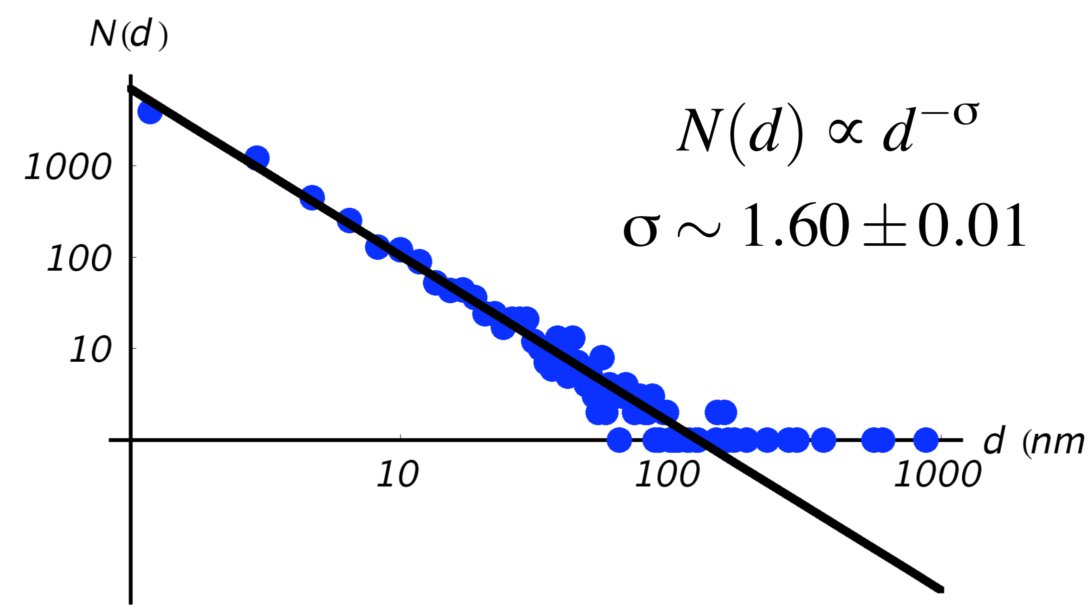


Uchic, Dimiduk et al. in Science and Acta Mater.

Direct measurement of intermittent behavior in deformation



- 30-40 μm
- 20 μm
- 10 μm
- 2 μm
- 1 μm



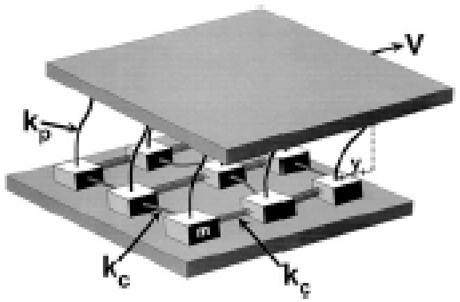
$$N(d) \propto d^{-\sigma}$$

$$\sigma \sim 1.60 \pm 0.01$$

Dimiduk, Woodward, LeSar, Uchic,
***Science** 312, 1188-1190 (2006).*

Implications

Simulations and experiment indicate that dislocations form self-organized critical systems.



Enables us to employ a new set of theories and analysis in dislocation theory.

Other recent theoretical work of note

Javier Gil Sevillano - size effects (with analogy to flow through porous media)

Michael Zaiser - scaling, statistical mechanics of dislocations

Anter El Azab - kinetic theory of dislocations

Jim Sethna - mesoscale theory based on continuous dislocation theory

Ishtvan Groma - Debye screening in dislocations

...

How far have we progressed as a field?

A. H. Cottrell:

In 1953 said of strain hardening that ``it was the first problem to be attempted by dislocation theory and may be the last that is solved"

In 2002, Cottrell summed up progress since 1953 by stating that ``It is sometimes said that the turbulent flow of fluids is the most difficult remaining problem in classical physics. Not so. Work hardening is worse"

After 50 years, still much to understand about the relation of dislocation structure and mechanical response.

QUESTIONS?