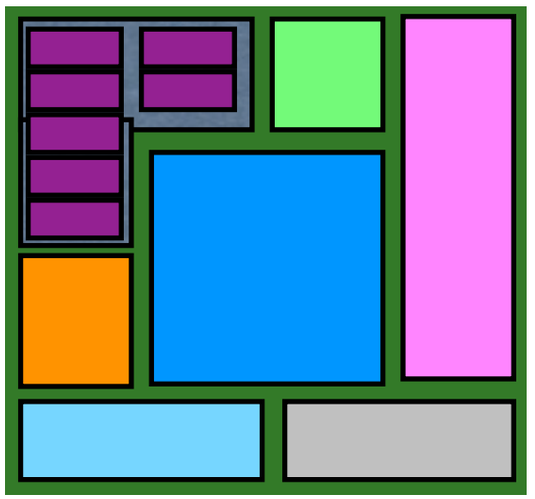
Introduction to Computational Materials Science

Simulating plasticity at the mesoscale



Richard LeSar

ICMR Summer School, UCSB
August 2013

Materials Science and Engineering
IOWA STATE UNIVERSITY
OF SCIENCE AND TECHNOLOGY

modeling talks at the Summer School

		Week 1 – Aug 19 – 23		
Date	**9:00 am – 10:30am**	**11:00am – 12:30pm**	**2:00pm – 3:30 pm**	**3:30 pm – 5:00pm**
Mon Aug 19th	Marc De Graef	Peter Voorhees	Emmanuelle Marquis	Poster Session (1001 ESB Patio)
Tues Aug 20th	Matt Miller	Stuart Wright	Mike Jackson	McLean Echlin
Wed Aug 21st	Mike Mills	Satoshi Hata	Richard LeSar	Poster Session (1001 ESB Patio)
Thurs Aug 22nd	Samantha Daly	Dan Gianola	Dave Rowenhorst	Joann Kuchera-Morin Matt Wright
Fri Aug 23rd	Yunzhi Wang	Marc DeGraef	Open Demo Session	Free Time
		Week 2 – Aug 26 – 30		
Date	**9:00 am – 10:30am**	**11:00am – 12:30pm**	**2:00pm – 3:30 pm**	**3:30 pm – 5:00pm**
Mon Aug 26th	Simon Philpot	Matt Begley	Michelle Johannes	Poster Session (1001 ESB Patio)
Tues Aug 27th	Simon Philpot	Mike Uchic	Frederic Gibou	*TBA*
Wed Aug 28th	Michelle Johannes	Anton Van der Ven	Baron Peters	*TBA*
Thurs Aug 29th	Jianwei (John) Miao	Jianwei (John) Miao	Anton Van der Ven	*TBA*
Fri Aug 30th	James Rondinelli	James Rondinelli	Barbecue at Goleta Beach	

DFT/atomistics

multiscale

mesoscale

Definitions: modeling and simulation

A **model** is an idealization of real behavior, i.e., an approximate description based on empirical and/or physical reasoning.

A **simulation** is a study of the dynamical response of a modeled system found by subjecting **models** to inputs and constraints that simulate real events.

A **simulation** does not mimic reality, rather it mimics a **model** of reality.

modeling and simulation

The accuracy of a **simulation** depends on many factors, some involving the **simulation** method itself (accuracy in solving sets of equations, for example).

Often, however, the biggest errors in a **simulation**, as least with respect to how well it describes a real system, are the inadequacies of the **models** upon which the **simulation** is based.

Thus, one cannot separate **simulations** from the underlying **models**.

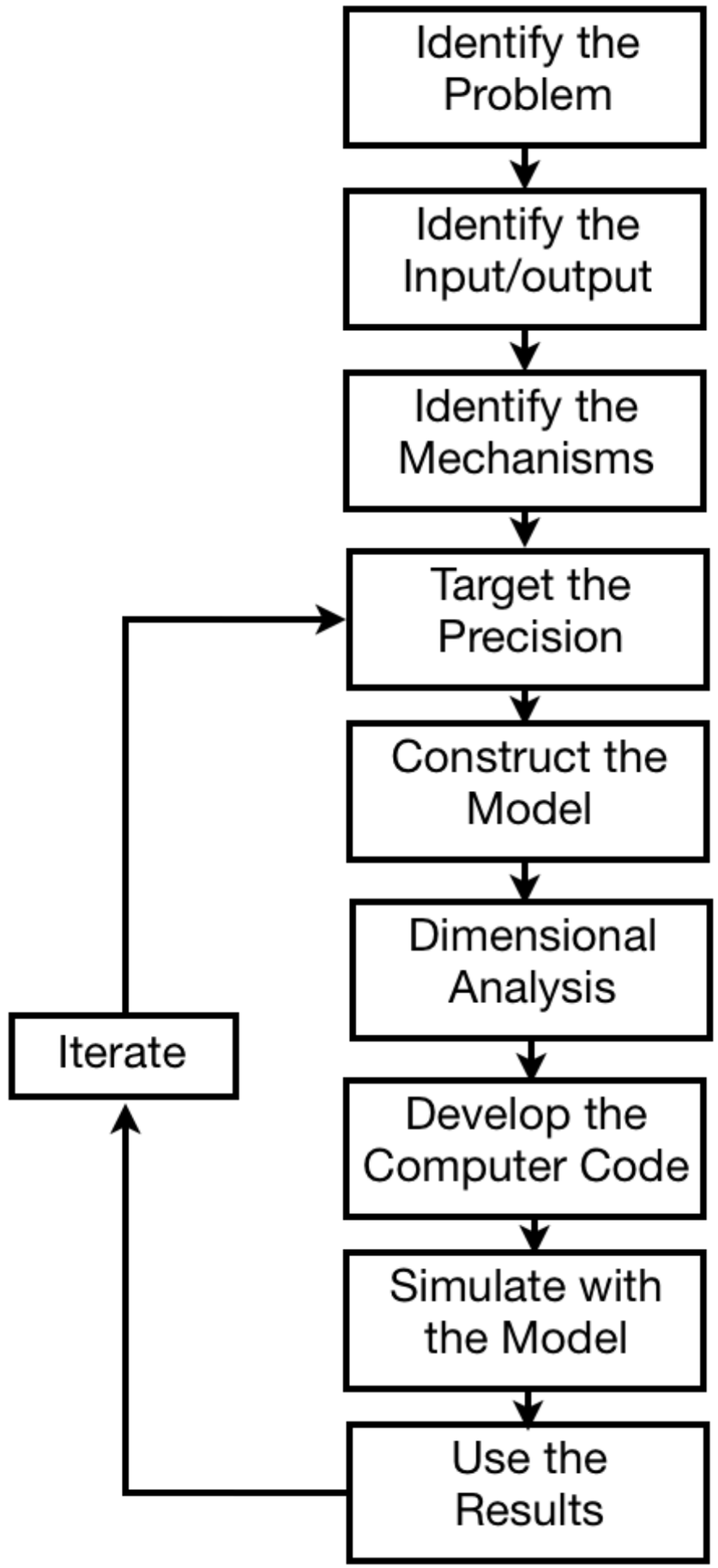
How do we create models?

Useful article by Mike Ashby (Materials Science and Technology 8, 102 (1992))

Discusses a systematic procedure that one can follow to produce models.

Many models would have been improved if this process had been followed.

Think before you compute!



scales of deformation

Table 1 Length scales and timescales used to describe the mechanics of materials, as adapted from Reference 9[a]

Unit	Length scale	Timescale	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	Micromechanics
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

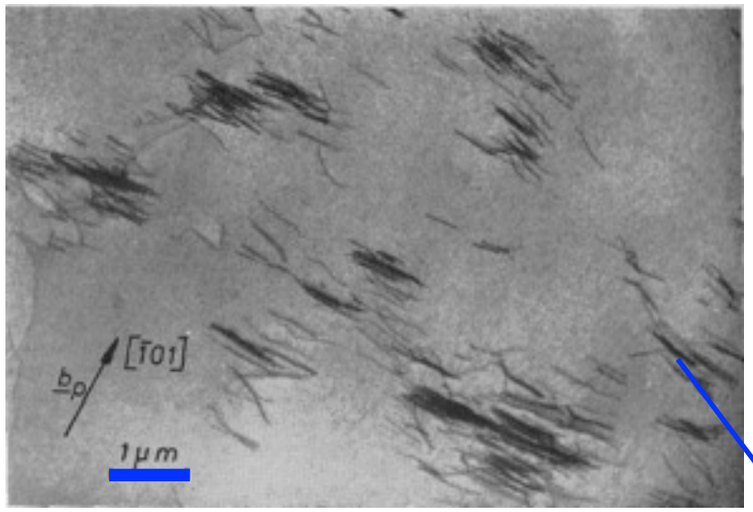
we typically have methods and models for individual scales of behavior - the coupling across scales is referred to as ***multiscale***

based on Ashby, *Physical modelling of materials problems*. Mater. Sci. Tech. 8, 102–111 (1992).

experiments

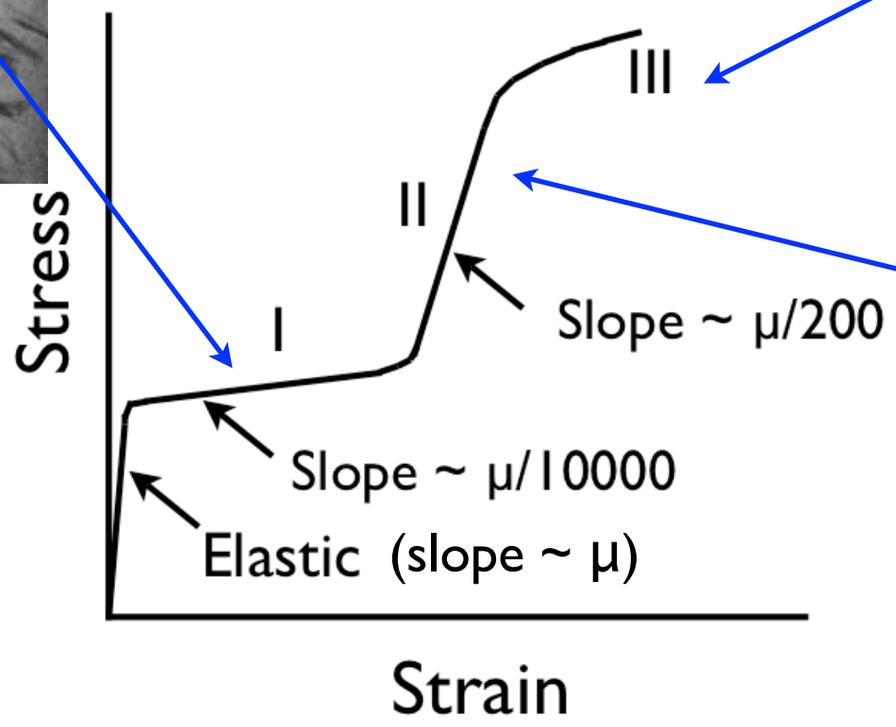
strain hardening in single *fcc* crystals

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



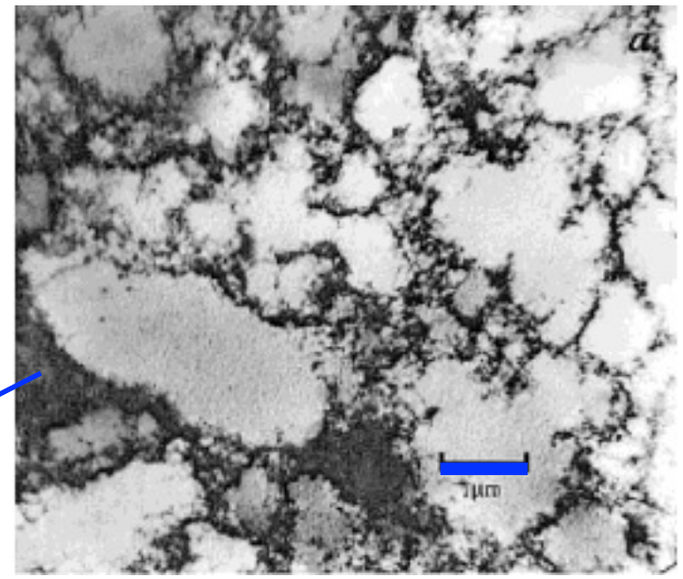
1 μm

despite 80 years of dislocations, we have no good theories for this fundamental structure-property relation



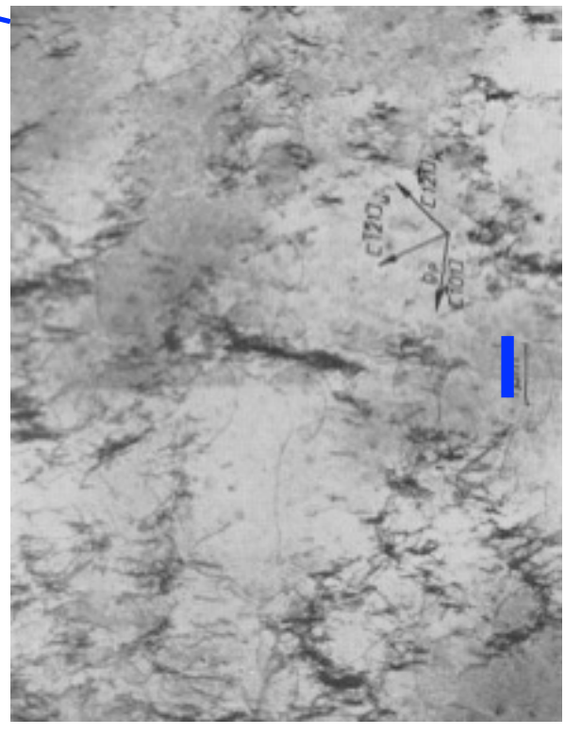
single crystal under single slip
μ is the shear modulus

Taylor law: $\rho^{1/2} \propto \tau$



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

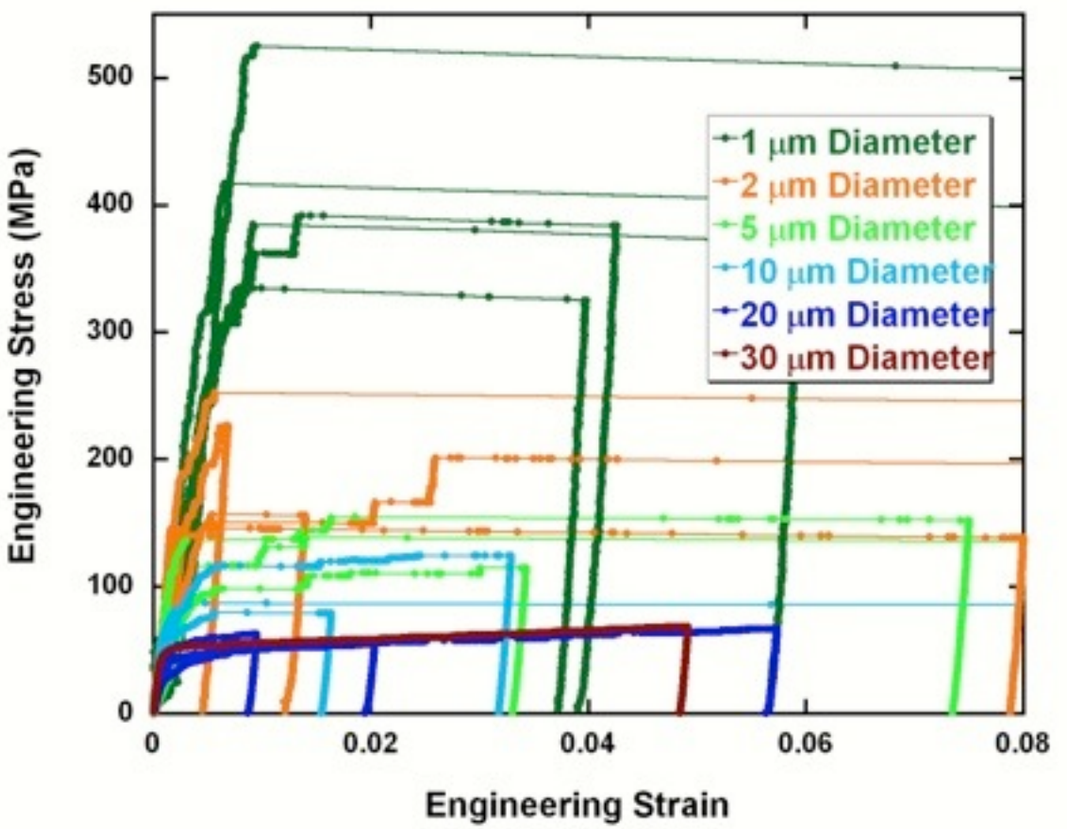
1 μm



1 μm

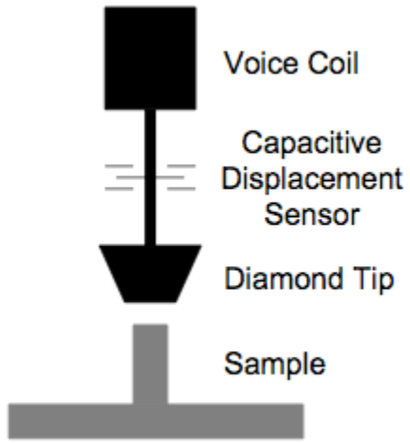
Mughrabi, Phil. Mag. **23**, 869 (1971)

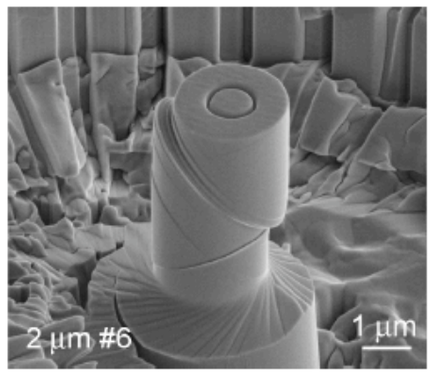
pure Ni at small scales



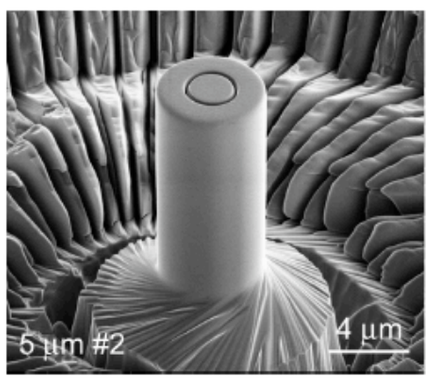
strong size effects, stochastic variation, intermittent flow, stresses sufficient to activate most slip systems.

Dimiduk, Uchic, and coworkers (many papers, including Science 2004).





b



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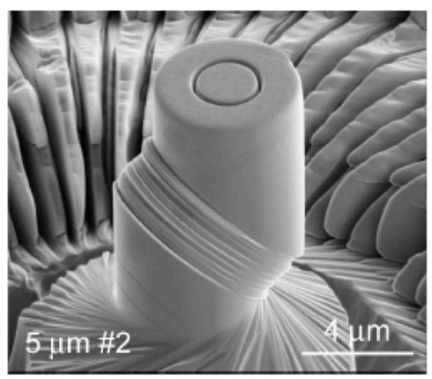
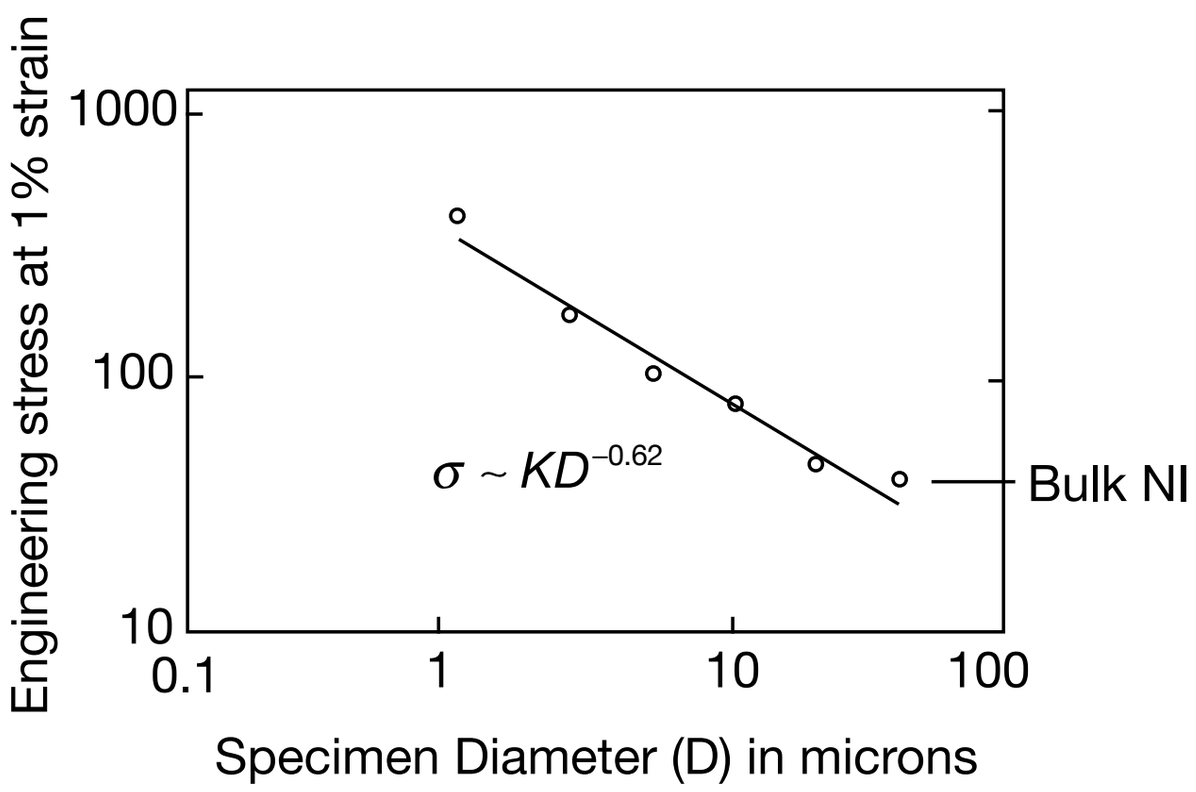
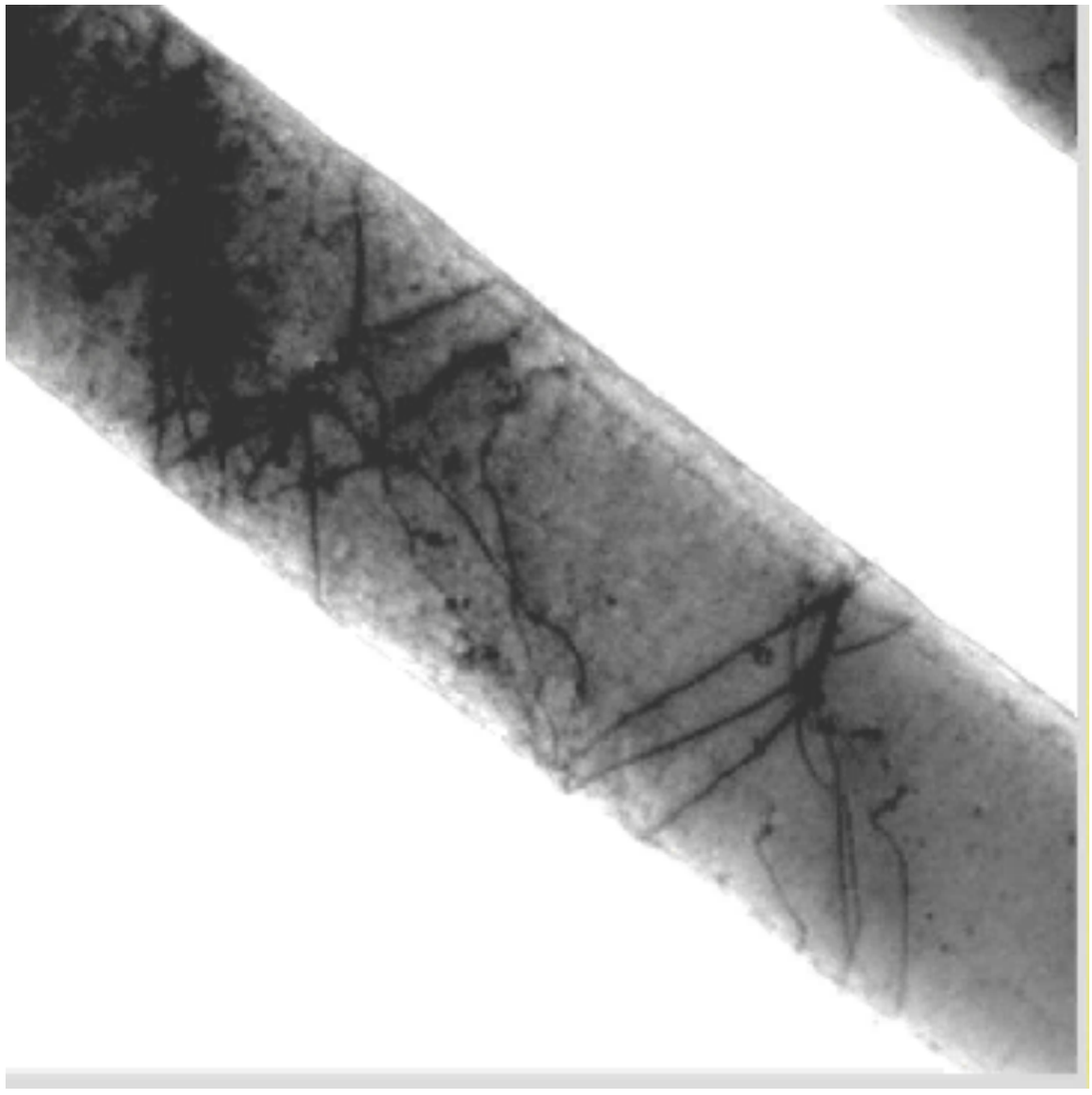


d



Diffraction Contrast STEM Tilt Series



0.6 μm Thick
Mo fiber

J. Kwon (OSU)

EFRC Center for Defect Physics (DOE-BES)

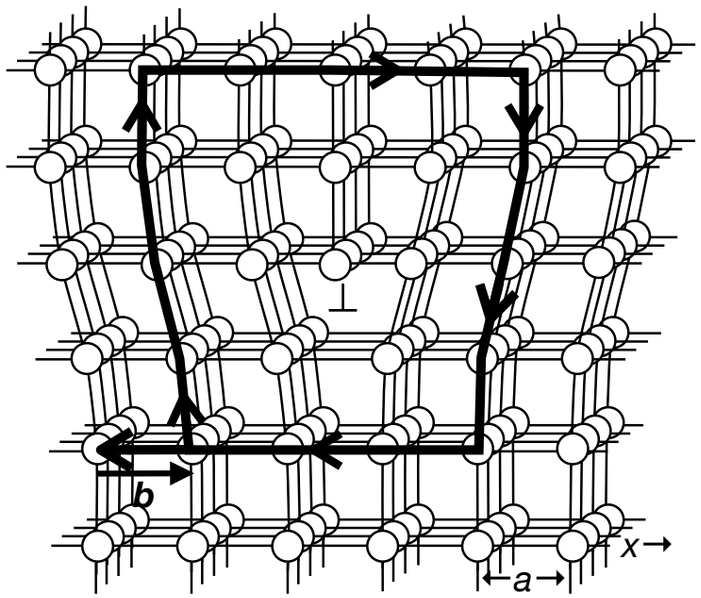
courtesy of Mike Mills

Plasticity

edge dislocations

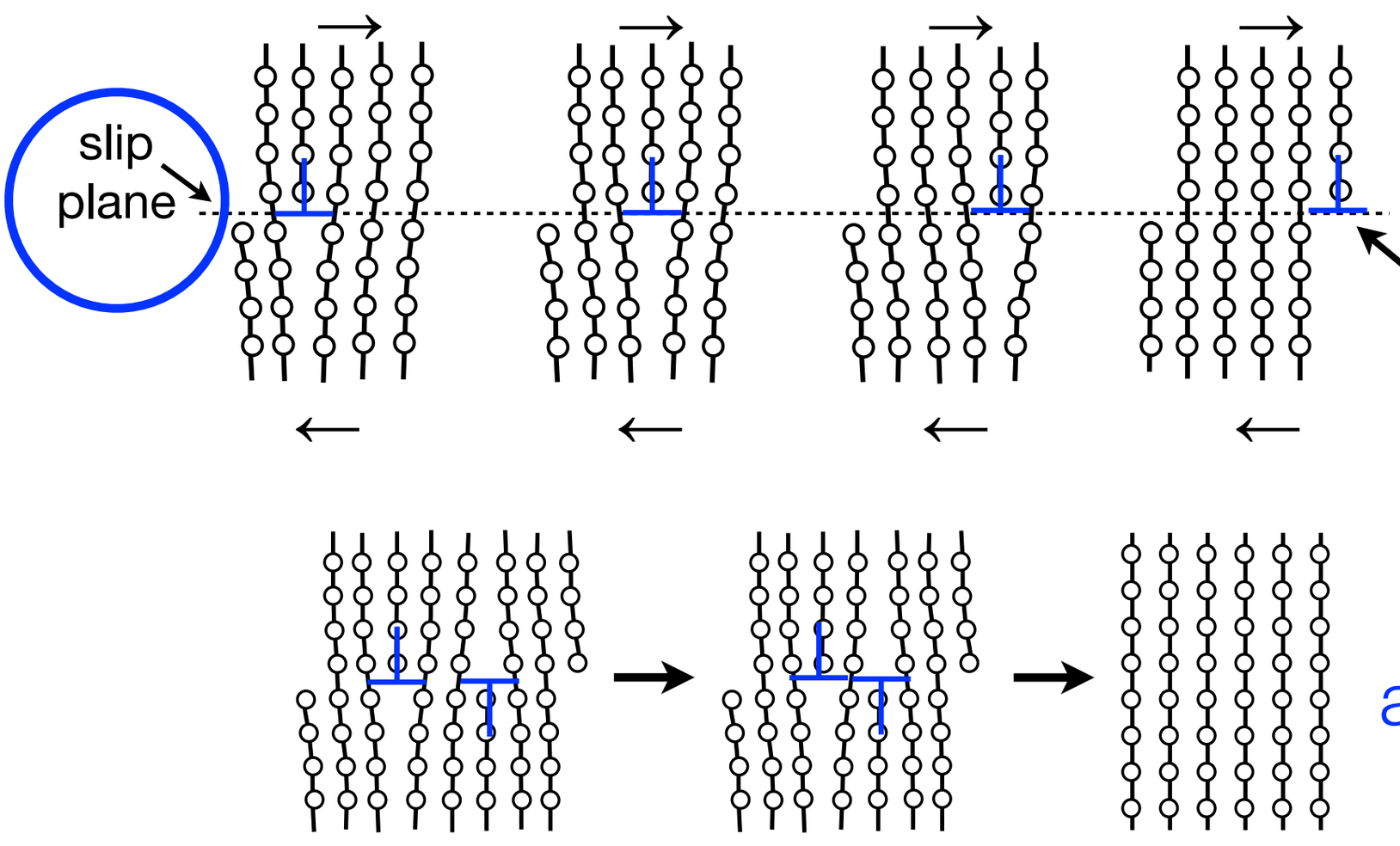
*the Burgers vector **b** is a measure of the displacement of the lattice*

distortion of lattice leads to strain field and, thus, a stress



$\vec{b} \perp \hat{\xi}$

1934
(Taylor, Polanyi, Orowan)

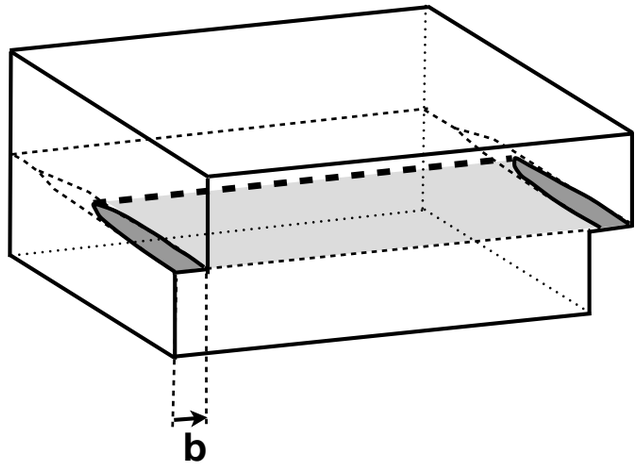


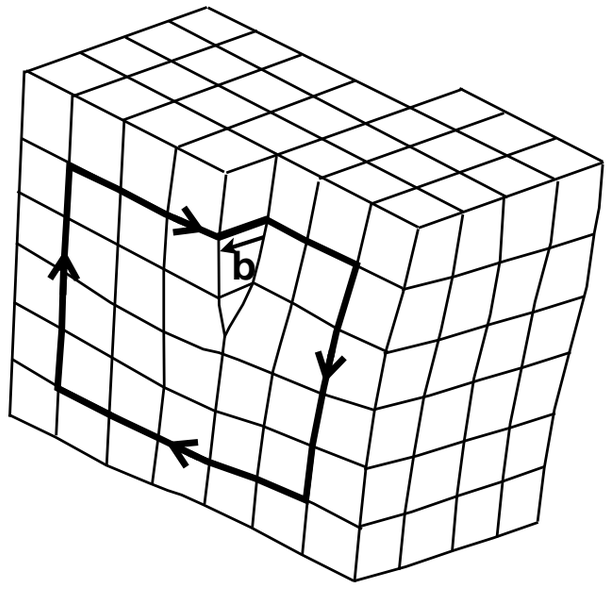
movement of an edge dislocation

note the deformation that arises from the movement of the dislocation

annihilation

screw dislocations



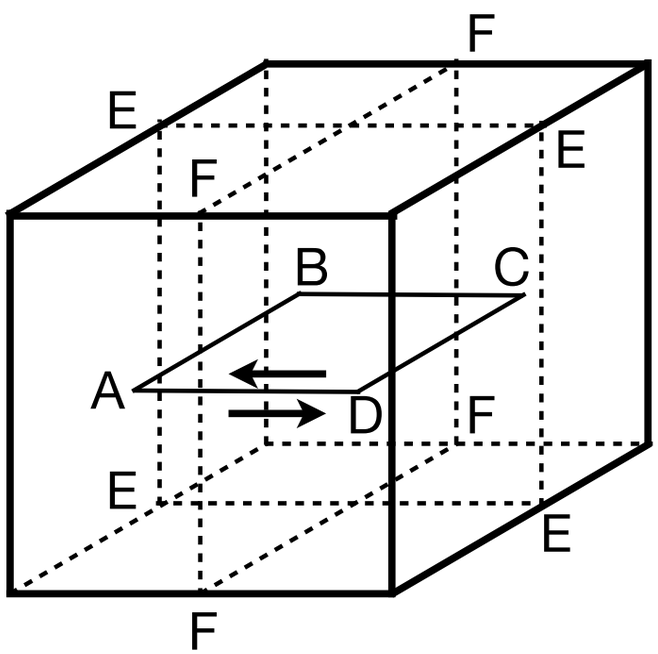


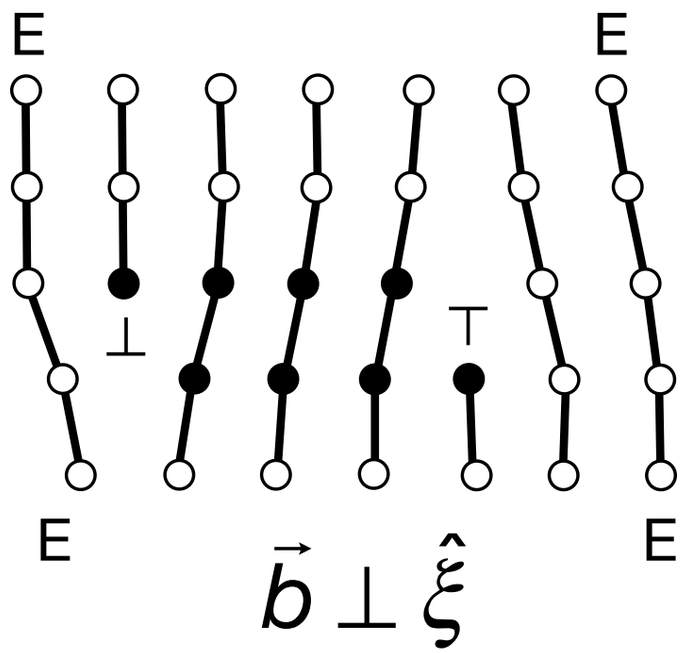
$\vec{b} \parallel \hat{\xi}$

1939
(Burgers)

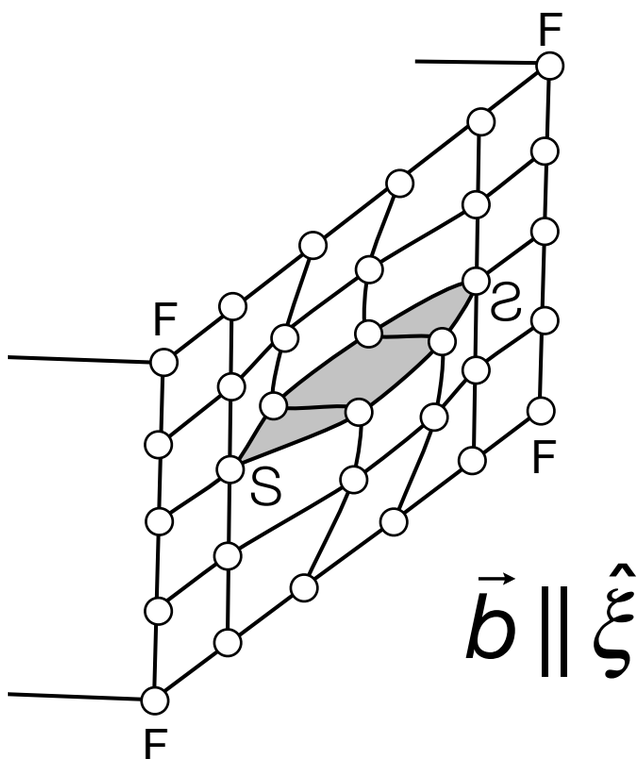
mixed dislocations

the Burgers vector is constant for a dislocation loop



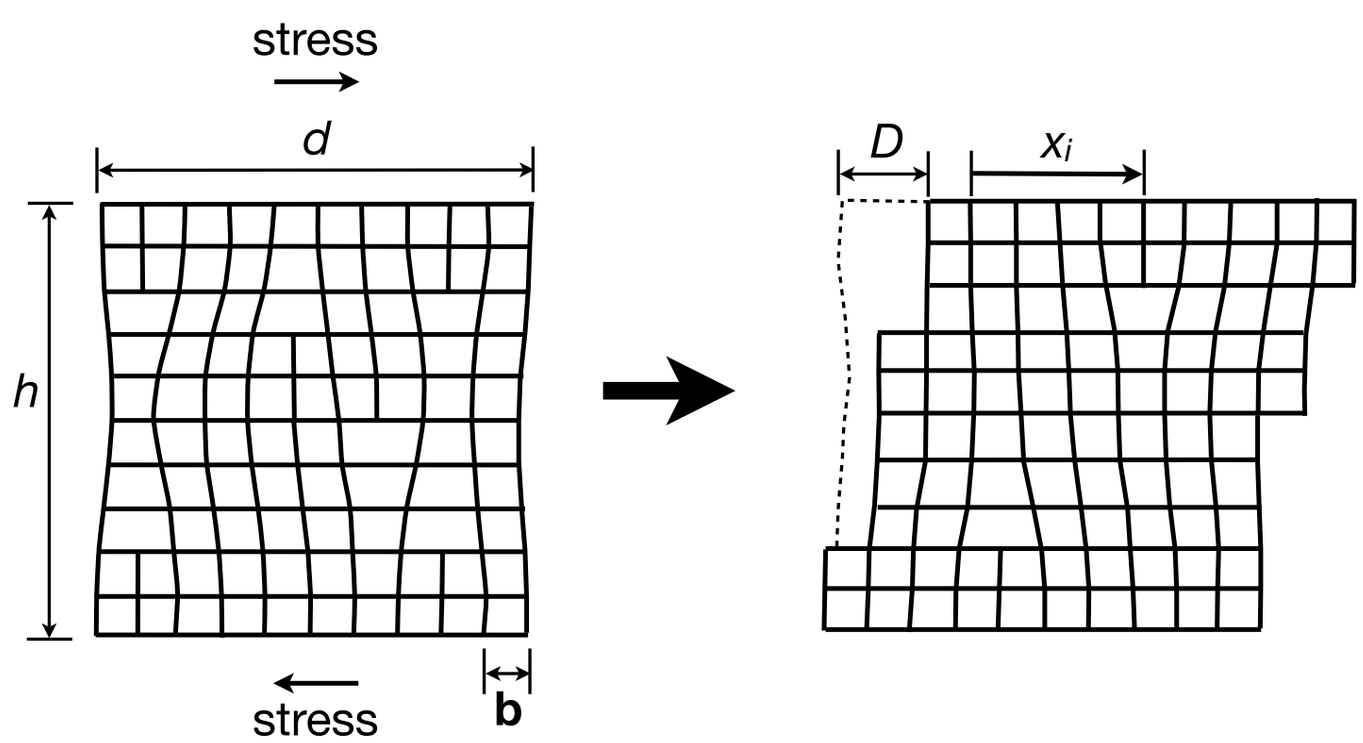


$\vec{b} \perp \hat{\xi}$



$\vec{b} \parallel \hat{\xi}$

plastic strain



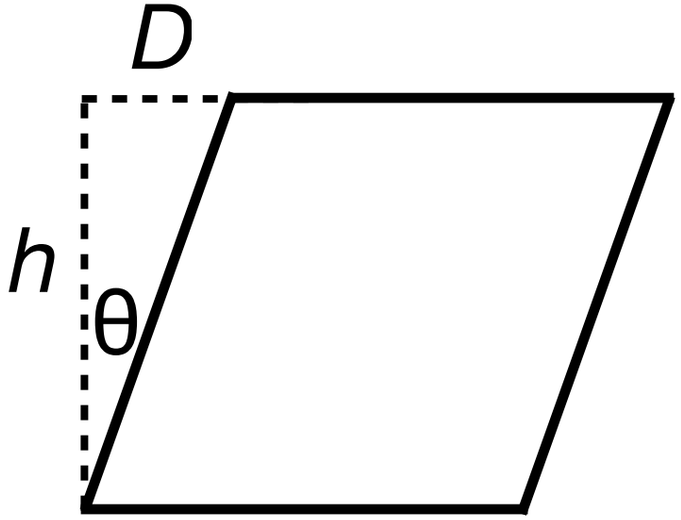
macroscopic displacement: $D = \frac{b}{d}\sum_{i=1}^{N} x_i$

plastic strain:

$$\varepsilon_p = \frac{D}{h} = \frac{b}{dh}\sum_{i=1}^{N} x_i = b\frac{N}{dh}\langle x \rangle$$

$$\varepsilon_p = b\rho\langle x \rangle$$

ρ = dislocation density = m/m^3 = 1/m^2



$$\varepsilon_p = \theta$$

$$\theta = \tan^{-1}\left(\frac{D}{h}\right) \approx \frac{D}{h}$$

Hull and Bacon, *Introduction to Dislocations* (2001)

plasticity

total strain: $\varepsilon_{kl} = \varepsilon^e_{kl} + \varepsilon^p_{kl}$

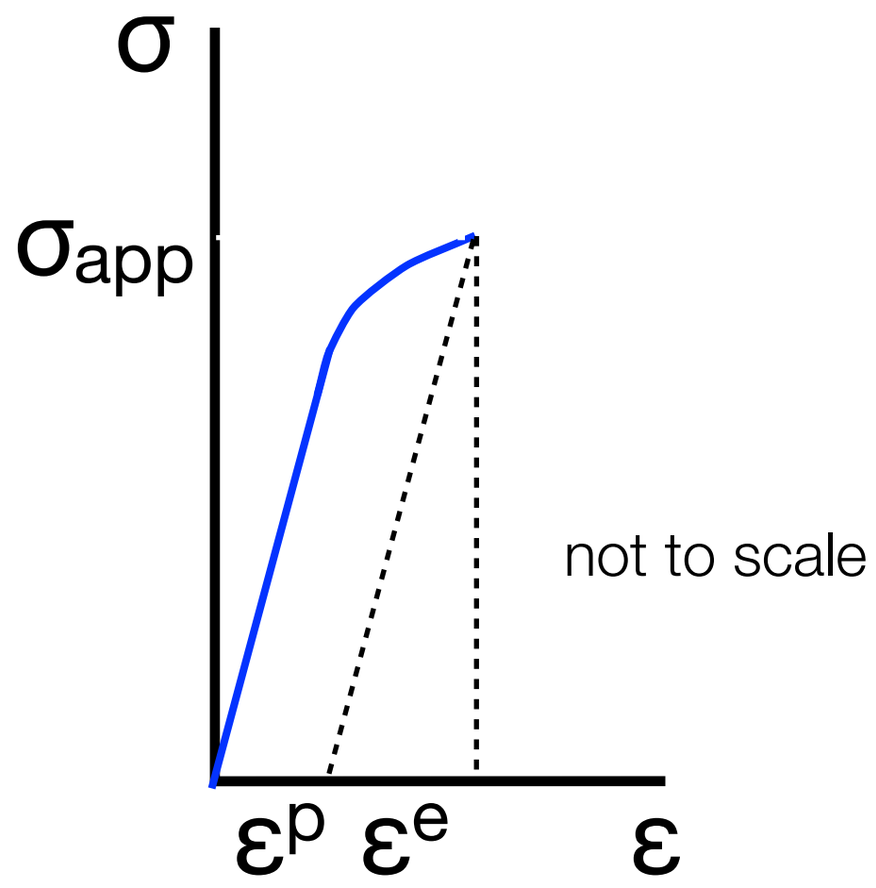
stress/strain:

$$\sigma_{ij} = C_{ijkl}\varepsilon^e_{kl} = C_{ijkl}\left(\varepsilon_{kl} - \varepsilon^p_{kl}\right)$$

for an applied stress of σ:

elastic strain from: $\sigma_{ij} = C_{ijkl}\varepsilon^e_{kl}$

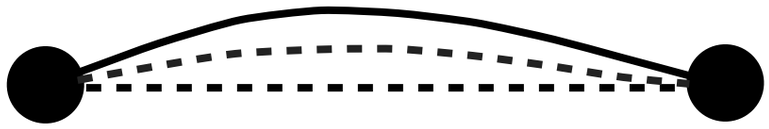
plastic strain from: $\varepsilon_p = \frac{b}{dh}\sum_{i=1}^{N} x_i$



goal of simulations:
calculate plastic strain

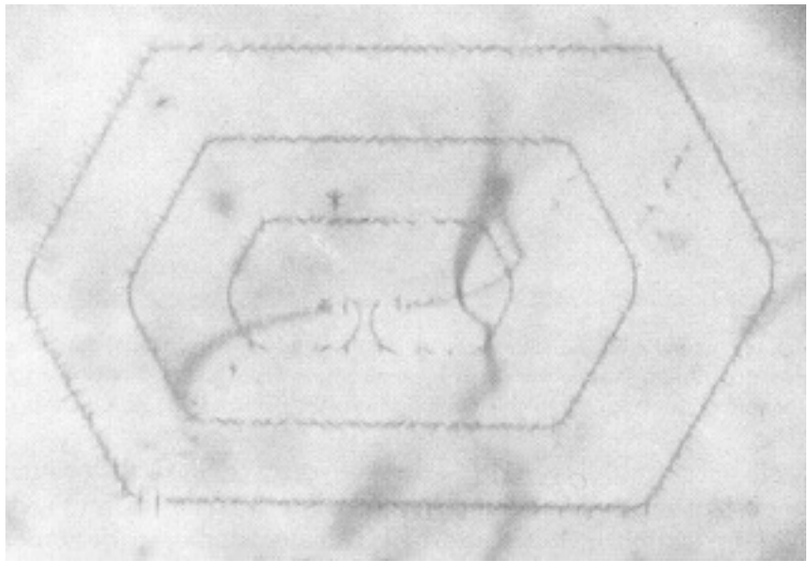
dislocation generation and motion

dislocations primarily move on slip (glide) planes:



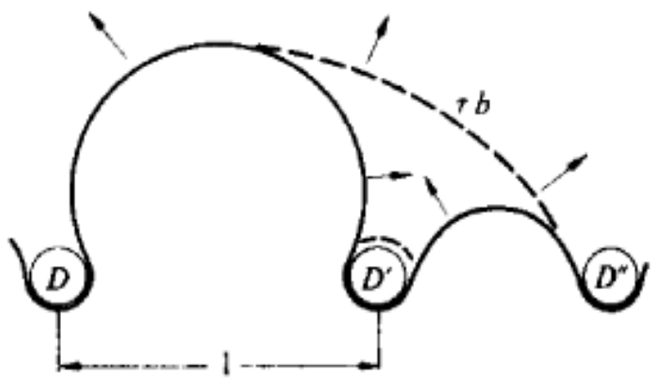
bowing from pinned sites

dislocations "grow"



Frank-Read source

serves to generate new dislocations

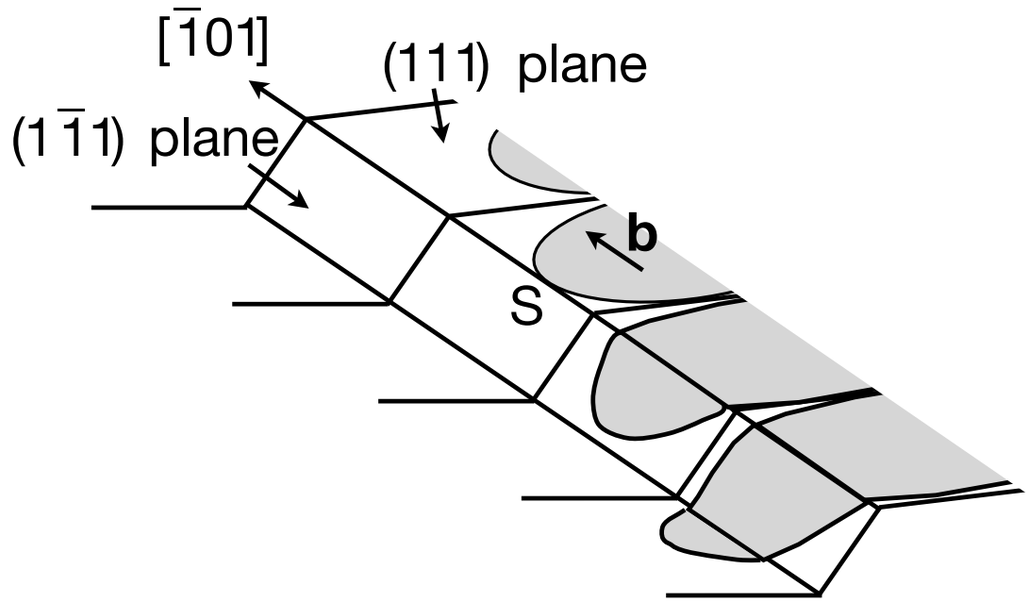


bowing around obstacles

basis for first dislocation simulation by Foreman and Makin (1967)

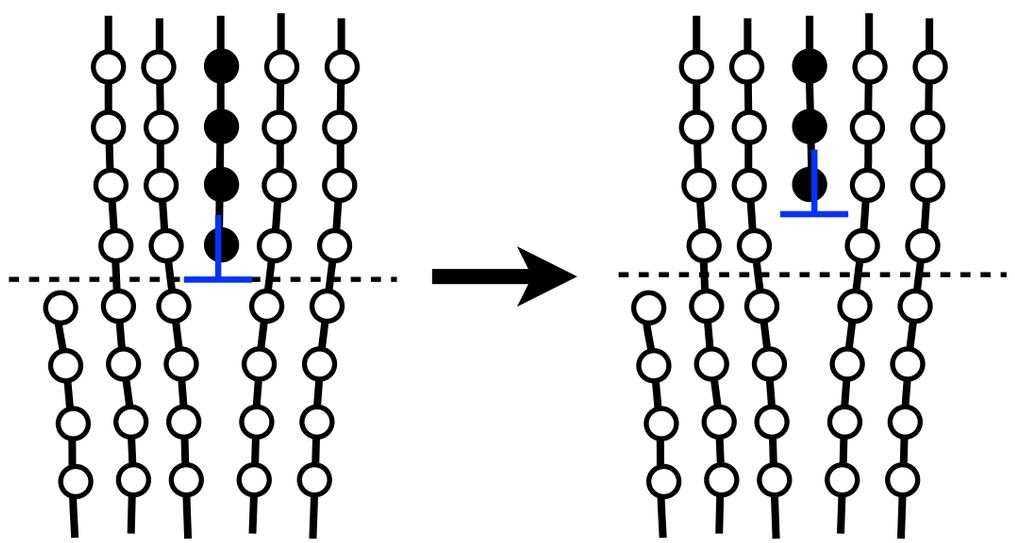
dislocation processes that move edges off their slip plane

out of plane motion (activated processes):



cross slip:
screw dislocation can move off slip plane

stress and temperature activated



climb:
a diffusive process

Simulations

scales of deformation

Table 1 Length scales and timescales used to describe the mechanics of materials, as adapted from Reference 9[a]

Unit	Length scale	Timescale	Mechanics
Complex structure	10^{3} m	10^{6} s	Structural mechanics
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Dislocation microstructure	10^{-5} m	10^{-6} s	Micromechanics
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

What computational methods we use depends on what our questions are and the limitations of the methods.

We start by identifying the "entities" in the model.

based on Ashby, *Physical modelling of materials problems*. Mater. Sci. Tech. 8, 102–111 (1992).

“density functional theory” (DFT)

entities

- electrons
- solve Schrödinger’s equation: $H\Psi\left(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N\right)=E\Psi\left(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N\right)$
- too hard to solve directly, so make numerous approximations

approximations and limitations

- convert *N*-electron problem to *N* 1-electron problems and solve those for ψ and find the electron density, ρ (the Kohn-Sham method)
- solve equations self-consistently in potential field arising from ρ
- use approximate functionals (E_{xc}) for potential field (LDA/GGA/...)
- limited (generally) to 1000s of atoms
- good for dislocation core structures and small numbers of dislocations

molecular dynamics

entities

- atoms
- force on an atom is: $\vec{F}_i = -\nabla_i U$
- solve Newton's equations: $\vec{F}_i = m_i \vec{a}_i = m_i \frac{d^2 \vec{r}_i}{dt^2}$
- need description of U $U = \sum_{i=i}^{N-1} \sum_{j=i+1}^{N} \phi_{ij}\left(r_{ij}\right)$

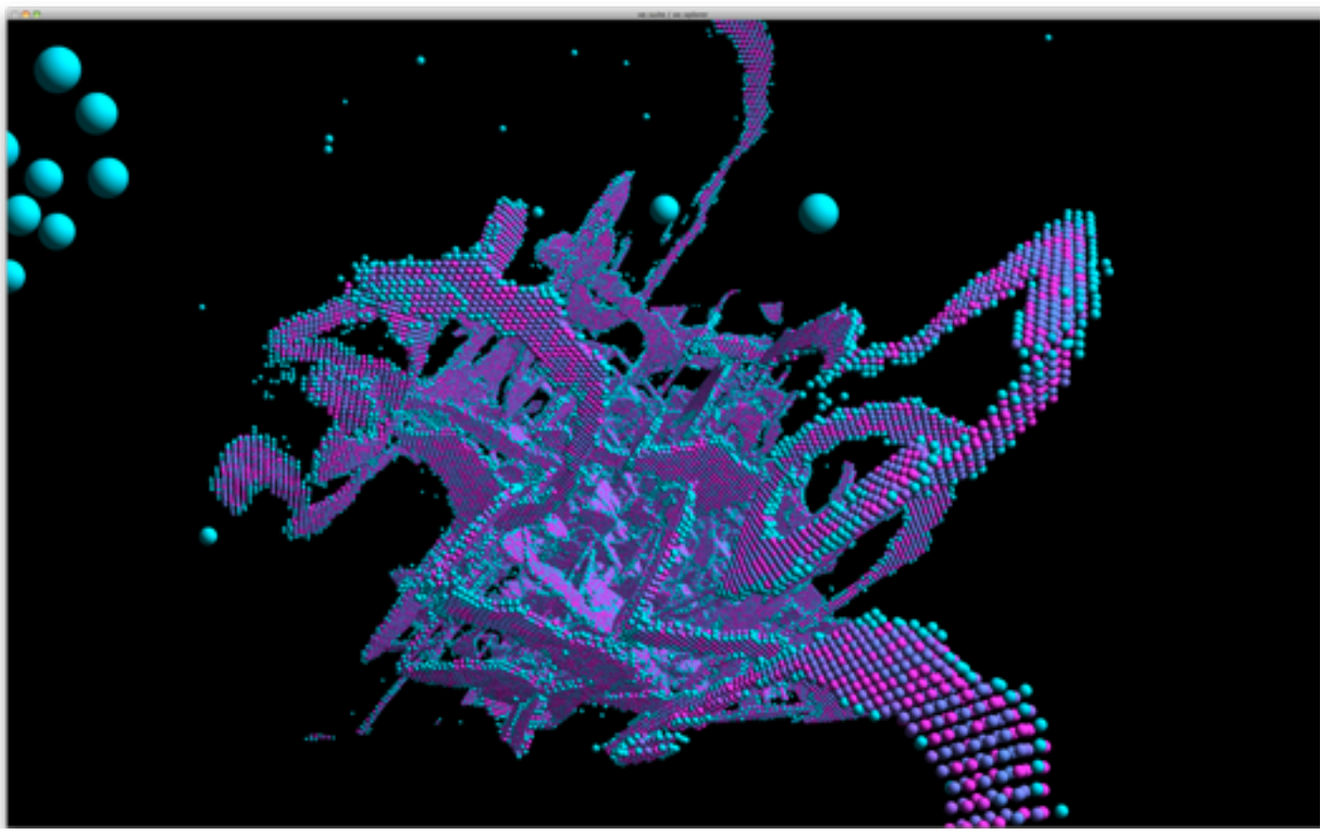
approximations and limitations

- potentials are analytic expressions with parameters fit to experiment and/or DFT (e.g., LJ, EAM)
- reasonably good potentials are available for many systems, but great potentials are not available for almost anything
- limited (generally) to 100s of millions of atoms
- time scales: typically nanoseconds

limitations of atomistics

Modeling deformation on the scale of dislocation microstructures cannot be done at an atomistic scale:

- 1 μm^3 of copper includes approximately 10^{11} atoms
- time steps in MD: ~10^{-15} sec
  - MD limited to a few hundred million atoms for a nanoseconds
- atomistic simulations can describe processes that include only small numbers of dislocations at fast rates



atomistic simulation of dislocations showing stacking fault planes between partials

courtesy of T. German, Los Alamos

modeling at the mesoscale

There are numerous methods used at the mesoscale, some force based and some energy based.

For force-based methods, one must

- define the “entities”
- determine the forces
- define the dynamics
- solve the equations of motion

These methods have similarities to molecular dynamics, but the entities are collective variables not atoms or molecules

entities

- In DFT and MD, the entities were clear: electrons and atoms.
- At the mesoscale, entities could be defects, such as dislocations or grain boundaries, or some other variables that define the physics of interest.
- These entities are ***collective*** variables, in which the actions of many smaller-scale entities are treated as one.
- We will often have flexibility in the choice of the entity, e.g., the many ways to model grain boundaries
- Most successful modeling is for cases in which there is a clear separation into collective variables

damped dynamics

Most applications of dynamical simulations at the mesoscale involve systems with damping, i.e., there are forces that dissipate the energy.

Standard equation of motion: $m_i \frac{d^2\vec{r}_i}{dt^2} = \vec{F}_i$

Force due to friction is usually velocity dependent: $\vec{F}_i^{diss} = -\gamma\vec{v}_i$

γ is the “damping coefficient”

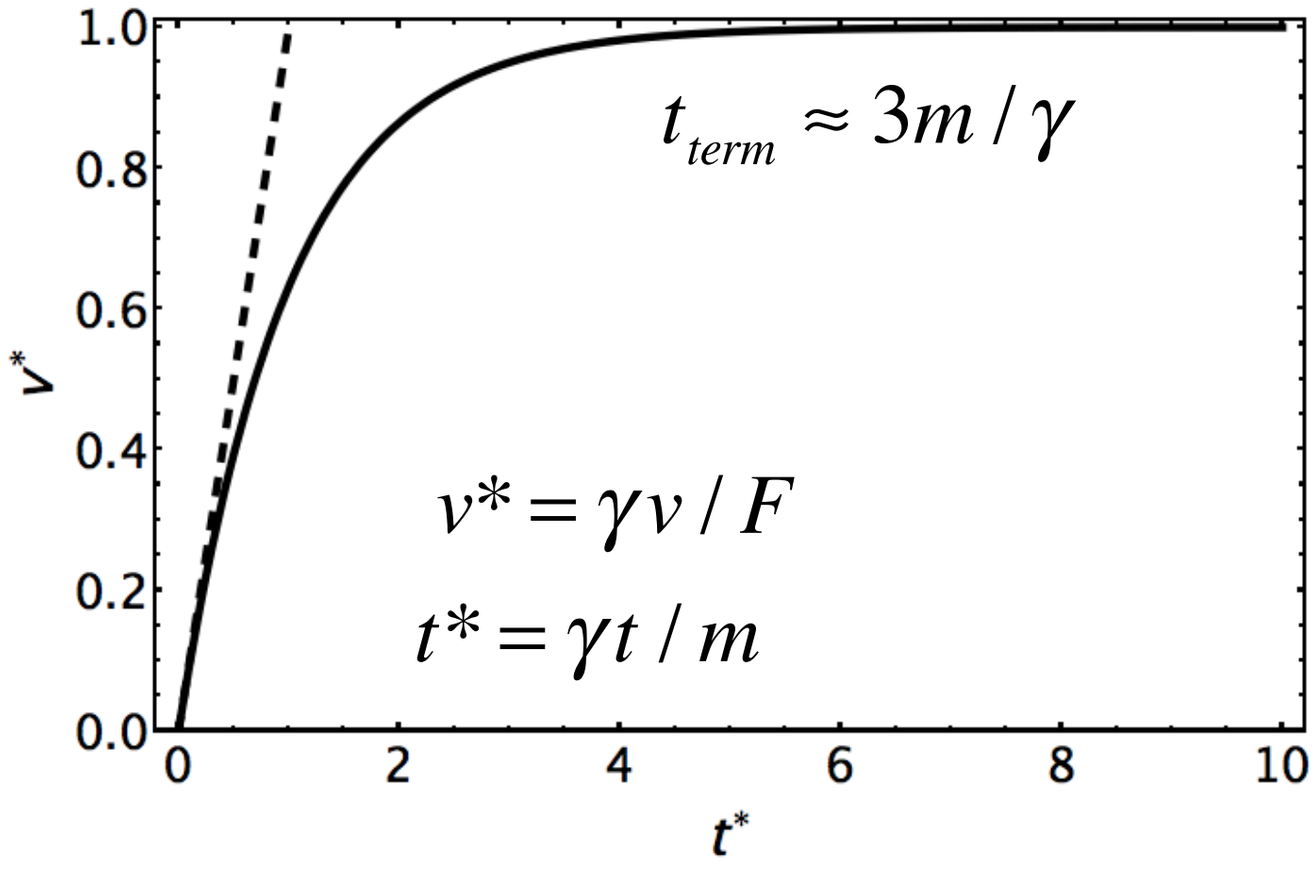
Net equation of motion is: $m_i \frac{d^2\vec{r}_i}{dt^2} = \vec{F}_i - \gamma\vec{v}_i$

solution in 1D

$$m\frac{d^2x}{dt^2} = F - \gamma v$$

For constant F (i.e., no variation with x), the solution is:

$$v(t) = \frac{F}{\gamma}\left(1 - e^{-\gamma t/m}\right)$$



For large damping (large γ), we often ignore the inertial effects and assume:

$$v = \frac{F}{\gamma} = MF$$

this is called the *over damped limit*

mesoscale simulations of dislocations

- model the behavior of only the dislocations by treating them as the entities tracked in the simulation

- three main approaches
  - force based (discrete dislocation dynamics)
  - energy based (phase field)
  - continuum methods (a “density-functional theory” - see recent work by Sanfeld, Hochrainer, Gumbsch, Zaiser, ...)

- today we discuss discrete dislocation dynamics

- on Friday, Professor Yunzhi Wang will discuss a phase-field approach

phase-field and discrete dislocation dynamics

- phase-field dislocations
  - free-energy-based
  - Ginzburg-Landau dynamics
  - advantages: links naturally to other phase-field methods, “easy” to include energy-based phenomena (e.g., partials)

- dislocation dynamics
  - force-based
  - dynamics from equations of motion
  - advantages: accurate dynamics (inertial effects), stress-driven processes (cross slip)

- the output of both methods are similar
  - dislocation substructure evolution in response to a load

outline

- simple 2D model
- basics of 3D simulations
- examples:
  1. small scale plasticity
  2. bulk plasticity
  3. strain hardening
- what is wrong with the simulations?
- connection to experiments

All simulations discussed today are based on isotropic elasticity - including anisotropy is not difficult, just very time consuming

discrete dislocation simulations in 2D

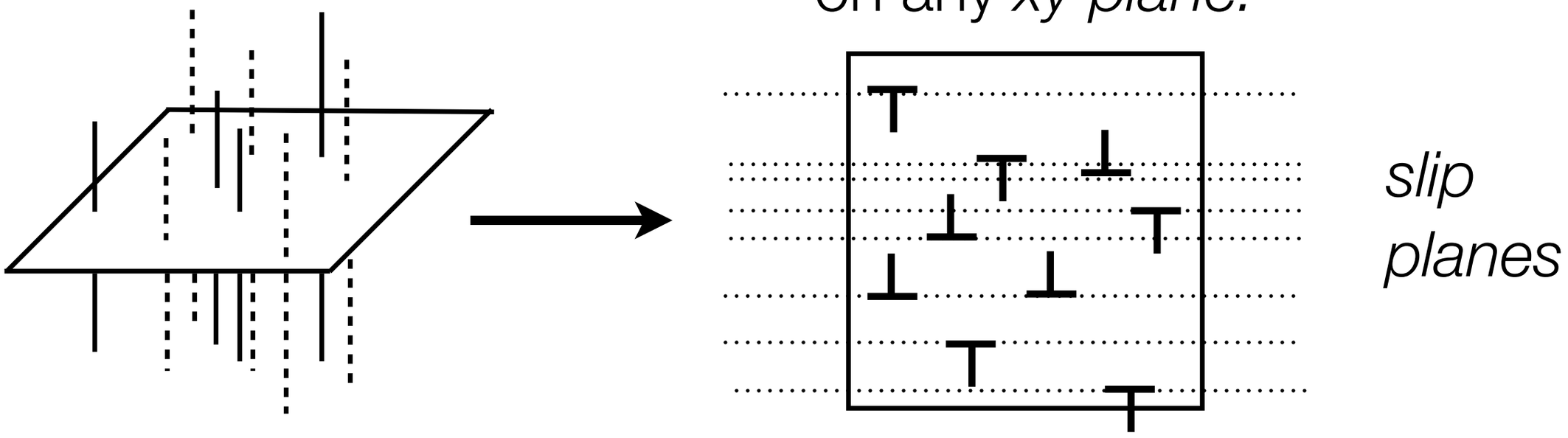
- we start with a simple 2D model that consists of parallel edge dislocations

- first “modern” dislocation dynamics simulations were based on this model (Lepinoux and Kubin, 1987; Amodeo and Ghoniem, 1988; Gulluoglu et al, 1989)

- such simulations require (a partial list):
  1. representation of dislocations in space
  2. description of interactions (forces)
  3. boundary conditions
  4. description of dynamics

Step 1: Simulation of system of straight edge dislocations: represent as points in 2D

Assume all dislocations have: $\vec{b} = b\hat{x}$ and $\hat{\xi} = \hat{z}$



at low T, no climb and dislocations can only move on their slip planes

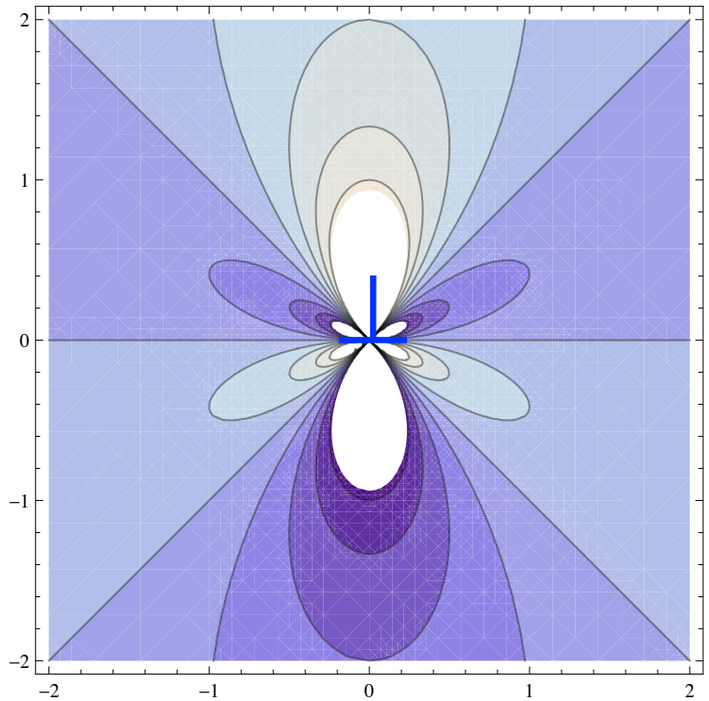
This model is sometimes referred to as 2.5 D.

Step 2a: Interactions between dislocations

Assume: $\vec{b} = b\hat{x}$ and $\hat{\xi} = \hat{z}$

Stress from dislocation:

$$\sigma_{12}(j) = \frac{\mu b_j}{2\pi(1-\upsilon)} \frac{x\left(x^2 - y^2\right)}{\left(x^2 + y^2\right)^2}$$



Force from this dislocation on another dislocation: Peach-Koehler force

$$\frac{\vec{F}(i)}{L} = \left(\vec{b}_i \cdot \sigma(j)\right) \times \hat{\xi}_i \qquad \sigma = \begin{pmatrix} \sigma_{11}\ \sigma_{12}\ \sigma_{13} \\ \sigma_{21}\ \sigma_{22}\ \sigma_{23} \\ \sigma_{31}\ \sigma_{32}\ \sigma_{33} \end{pmatrix}$$

$$\frac{F_x(i)}{L} = b_i \sigma_{12}(j) = \frac{\mu b_i b_j}{2\pi(1-\upsilon)} \frac{x_{ij}\left(x_{ij}^2 - y_{ij}^2\right)}{\left(x_{ij}^2 + y_{ij}^2\right)^2}$$

$$x_{ij} = x_j - x_i$$

NOTE: long ranged (~1/r)

Step 2b. External stress

Let τ be the applied shear stress: $\tau = \sigma_{12}^{ext}$

The force from external stress on dislocation i is: $\frac{F_x^{ext}(i)}{L} = b_i \tau$

Note: Burger's vector has sign:

- either +b or -b
- stress drives +/- dislocations in opposite directions

Net force (assuming *N* other dislocations)

$$\frac{F_x(i)}{L} = b_i \tau + \sum_{j \neq i=1}^{N} \frac{\mu b_i b_j}{2\pi(1-\upsilon)} \frac{x_{ij}\left(x_{ij}^2 - y_{ij}^2\right)}{\left(x_{ij}^2 + y_{ij}^2\right)^2}$$

Step 3. Boundary conditions

Put *N* dislocations at random positions in a 2D periodic square grid with size *D* with equal numbers of +b and -b dislocations

Dislocation density is $\rho = N / D^2$

(all important distances in this system will scale as $1/\rho^{1/2}$)

We will look at truncations of dislocation interactions:

1. short-range cutoff
2. no cutoff

Step 4. Dynamics

Assume overdamped dynamics: $v(t) = M \dfrac{F_x(t)}{L}$

Assume a simple Euler equation solution:

$$x_i(t+\delta t) = x_i(t) + v_i(t)\delta t$$

For no external stress, run the system until converged.

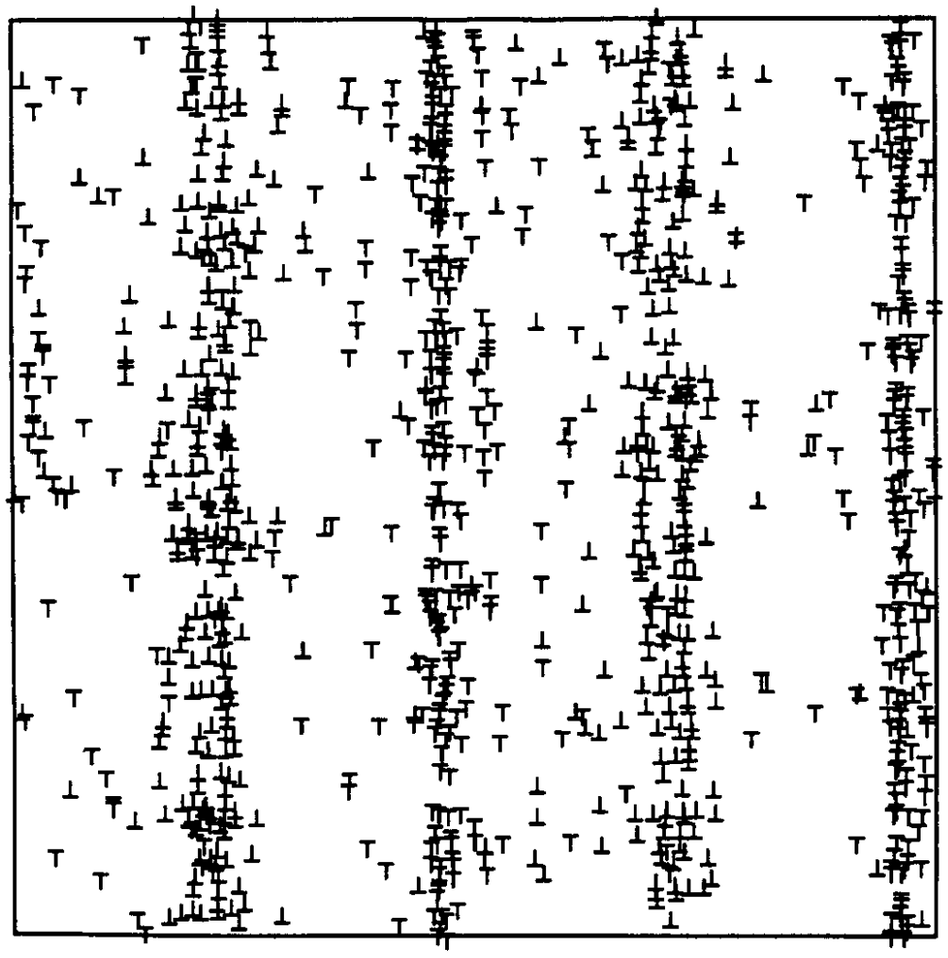
Then apply an external stress, calculate change in dislocation position, and calculate

$$\Delta\varepsilon_p = \frac{b}{D^2}\sum_{i=1}^{N}\Delta x_i = b\frac{N}{D^2}\langle\Delta x\rangle = b\rho\langle\Delta x\rangle$$

Results: truncated potential

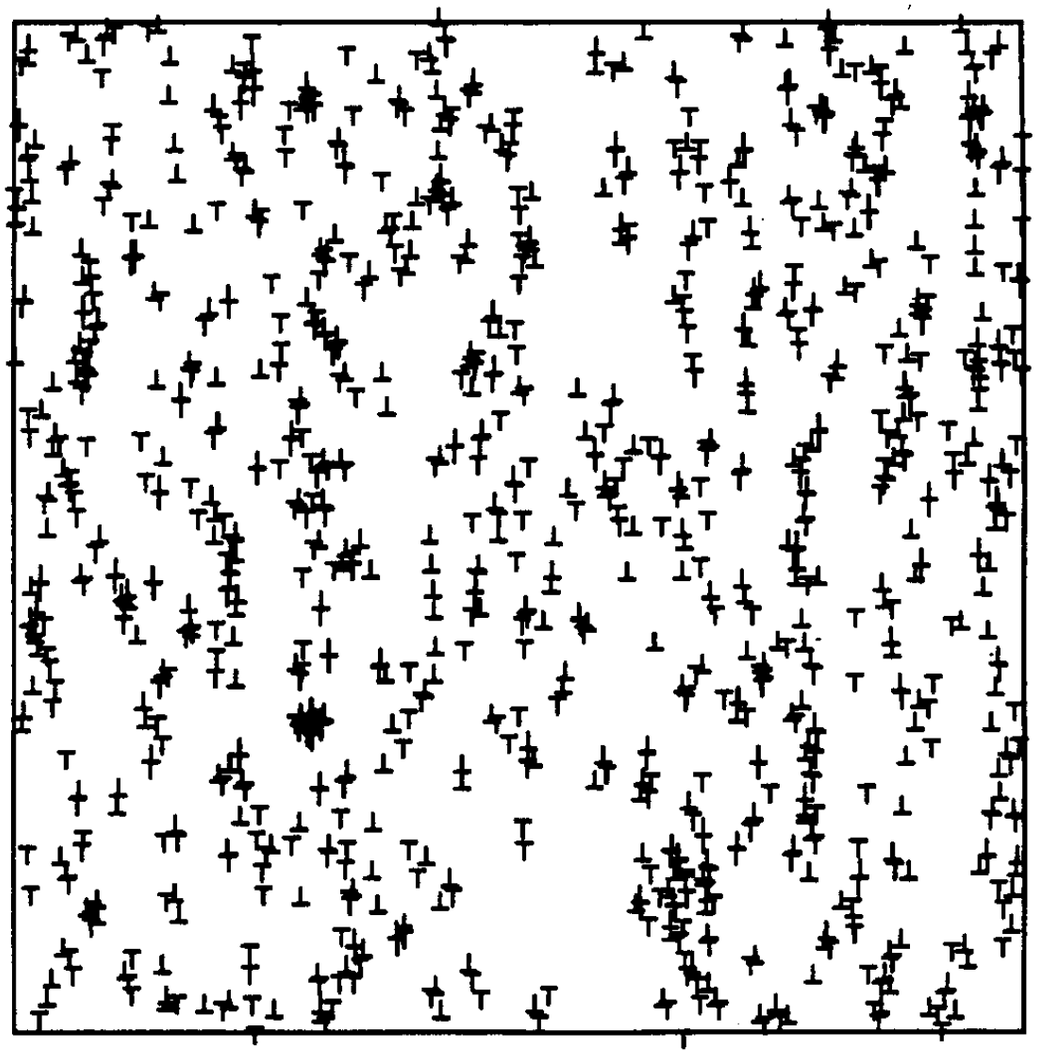
Not quite converged (τ=0)

At converged solution:
straight lines alternating
+ and - dislocations with
spacing 1/2 the cutoff
distance

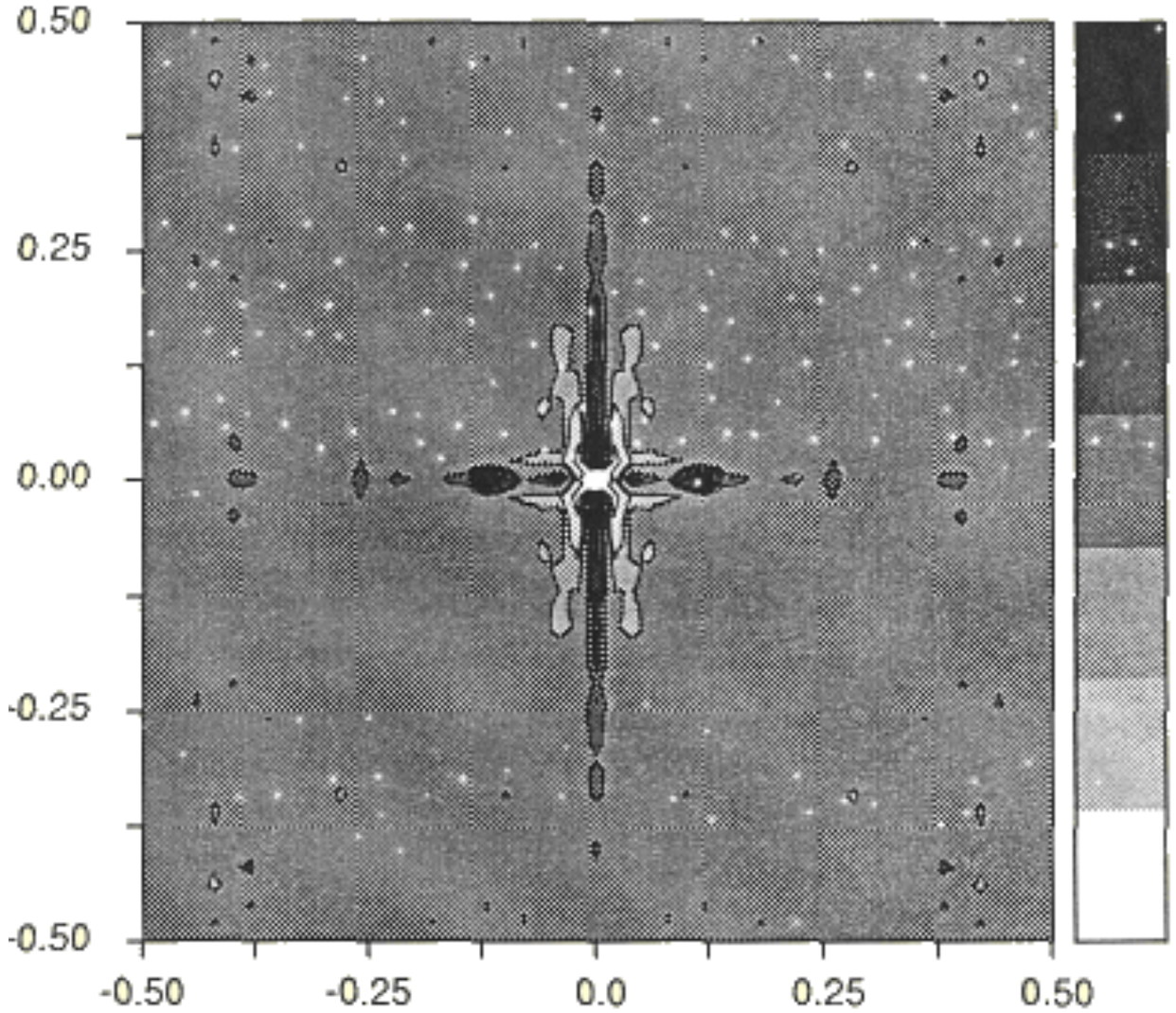


“Dislocation distributions in two dimensions,” A. N. Gulluoglu, D. J. Srolovitz, R. LeSar, P. S. Lomdahl, Scripta Metallurgica 23, 1347-1352 (1989).

Results: all interactions to infinity



sign-weighted pair correlation function



shows importance of knowing how to carry out the simulation!

"Dislocation distributions in two dimensions," A. N. Gulluoglu, D. J. Srolovitz, R. LeSar, P. S. Lomdahl, Scripta Metallurgica 23, 1347-1352 (1989).

Your assignment ...

We will email you a zipped folder called LeSarDD.zip.

In this folder is a file (DislocationDynamics.pdf) that contains a description of how to implement (in MATLAB) the 2D modeling I just described.

DislocationDynamics.pdf also contains some exercises to consider.

There is also a folder called code that contains 2 other folders. The one called DD2D contains MATLAB code for this problem.

2D models show interesting behavior, but ...

- many interesting simulations have been done with these 2D (2.5 D) models

- Alan Needleman and Erik van der Giessen in particular have done very nice work, including coupling to continuum models

- However, dislocation plasticity is 3D

- Michael Zaiser (Erlangen) once describe these 2D simulations as “cubist” representations of plasticity

La Femme Au Miroir
Fernand Leger, 1920

discrete dislocation simulations in 3D

- include dislocations moving along all active slip planes to examine evolution and response

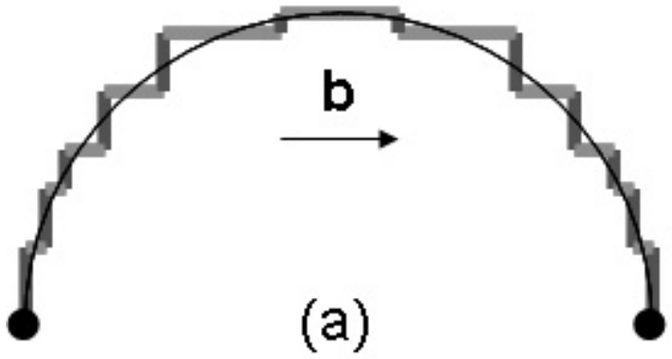
- pioneering simulations by Kubin (early 90s). Many groups doing lovely work: Kubin and "offspring" (Devincre, Madec, Fivel, ...), Bulatov, Cai, Weygand, Gumbsch, Schwarz, Ghoniem, Wang, El-Awady, Zhou, ...

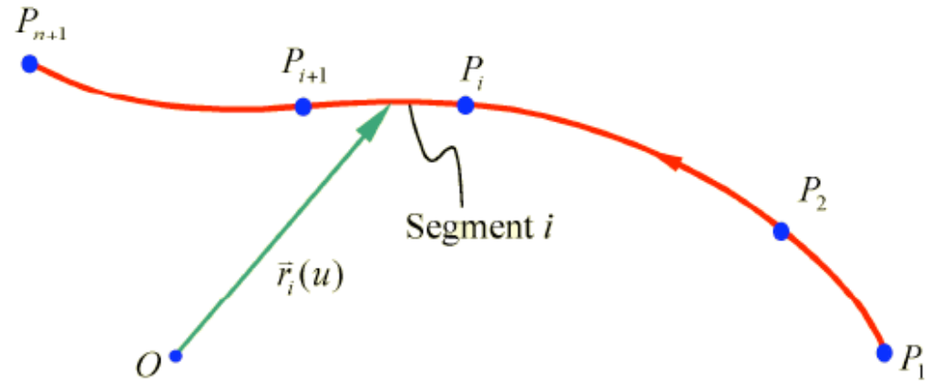
- such simulations require (a partial list):
  1. representation of dislocations in space
  2. description of interactions (forces)
  3. boundary conditions
  4. description of dynamics
  5. approximations, models, etc.

Step 1: approaches to representing dislocations

methodologies fall into two classes

- discrete linear segments
  - pure edge/pure screw (Kubin and company)
  - mixed edge and screw (ParaDis, PARANOID)



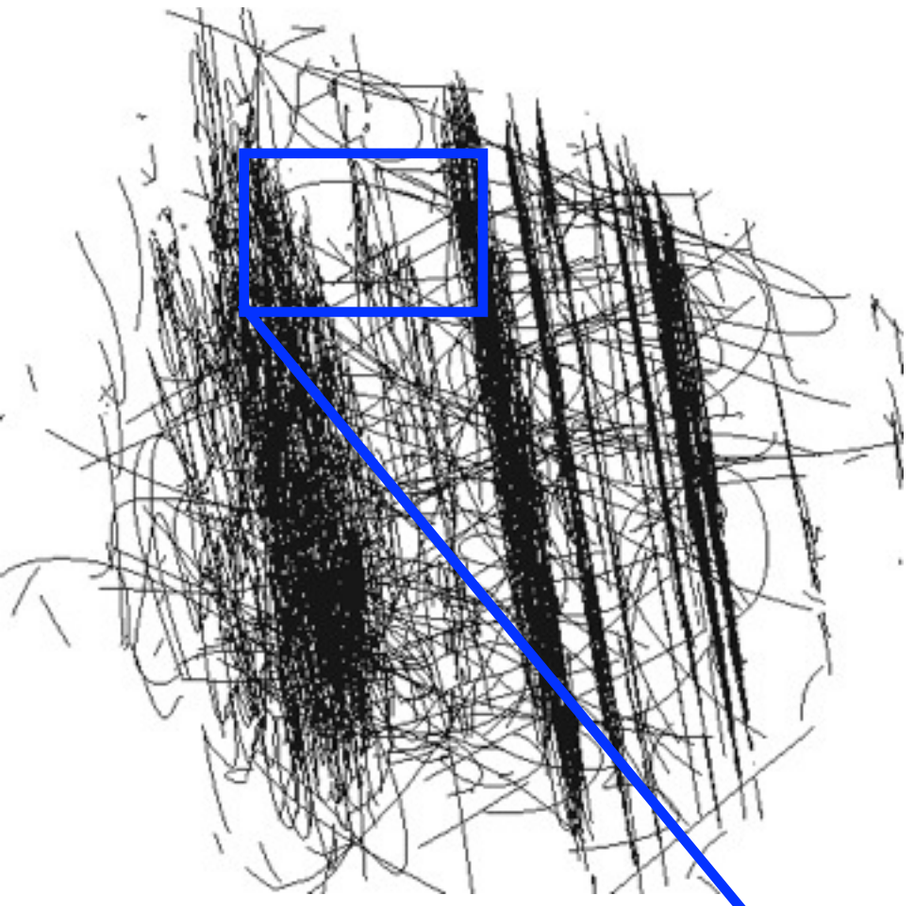


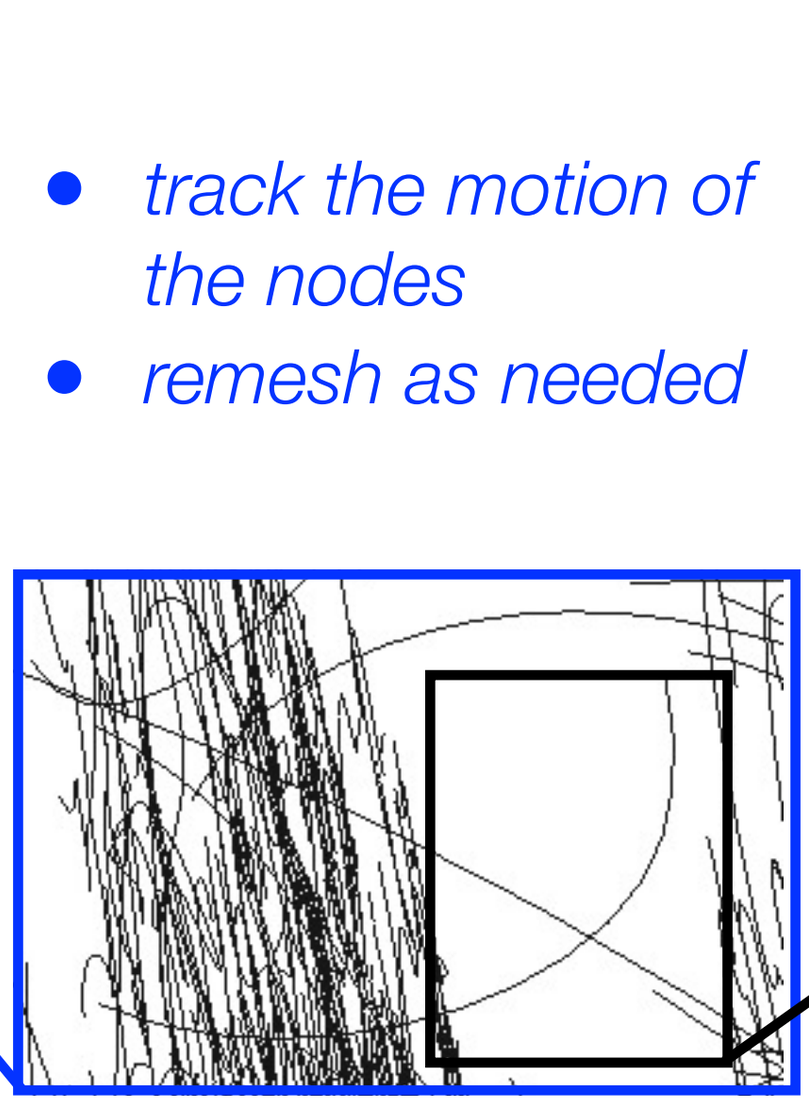
- curvilinear dislocations
  - parametric dislocations of Ghoniem
  - nodal points plus interpolation
  - numerical integration along curves

Ghoniem, Tong, and Sun, Phys. Rev. B 61, 913 (2000);
Wang, Ghoniem, Swaminarayan, and LeSar, J. Comp. Phys. 219, 608 (2006)

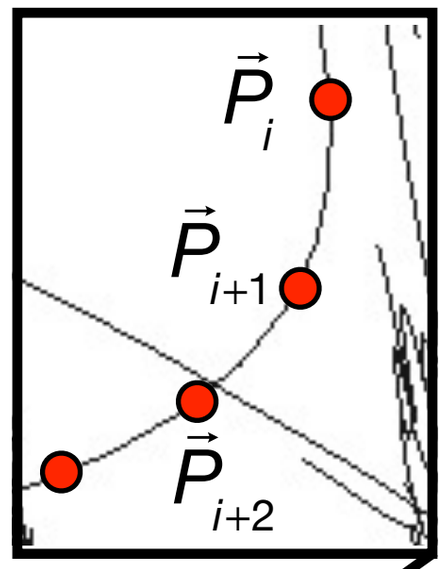
Step 1: parametric dislocations

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





- *track the motion of the nodes*
- *remesh as needed*

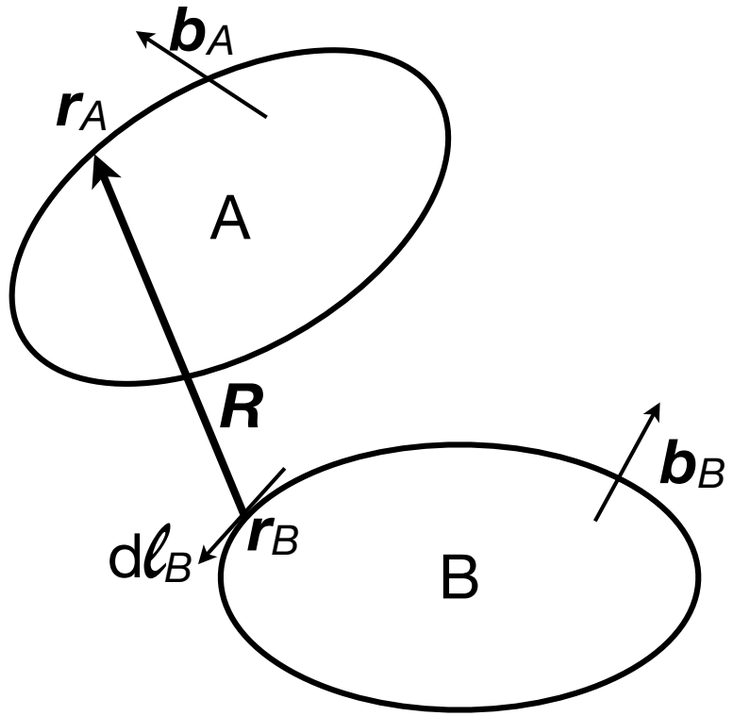


Ghoniem, Tong, and Sun, Phys. Rev. B 61, 913 (2000);
Wang, Ghoniem, Swaminarayan, and LeSar, J. Comp. Phys. 219, 608 (2006)

Step 2: stresses and forces

$$\vec{F} = \left(\vec{b}\cdot\sigma\right)\times\hat{\xi}$$

force on dislocation calculated from stress: Peach-Koehler Force



stress comes from many sources

$$\sigma^{(a)} = \sigma_{ext} + \sigma_{defect} + \sigma_{self} + \sum_{b\neq a}\sigma^{(ab)}$$

stress from an individual dislocation

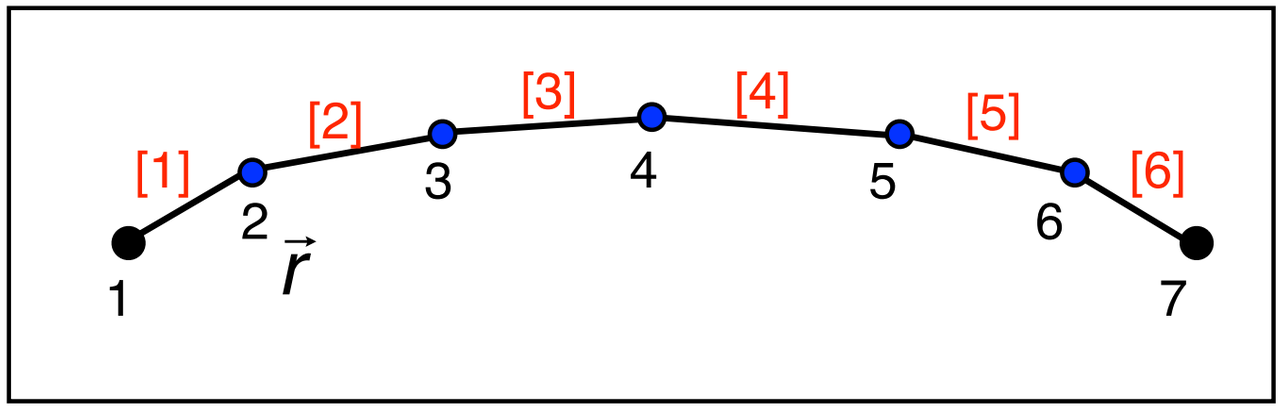
$$\sigma_{ij} = \frac{\mu b_n}{8\pi}\oint\left[R_{,mpp}\left(\varepsilon_{jmn}d\ell_i + \varepsilon_{imn}d\ell_j\right) + \frac{2}{1-\upsilon}\varepsilon_{kmn}\left(R_{,ijm} - \delta_{ij}R_{,ppm}\right)d\ell_k\right]$$

$$R_{,ijk} = \frac{\partial^3 R}{\partial x_i\,\partial x_j\,\partial x_k} \sim \frac{1}{R^2}$$

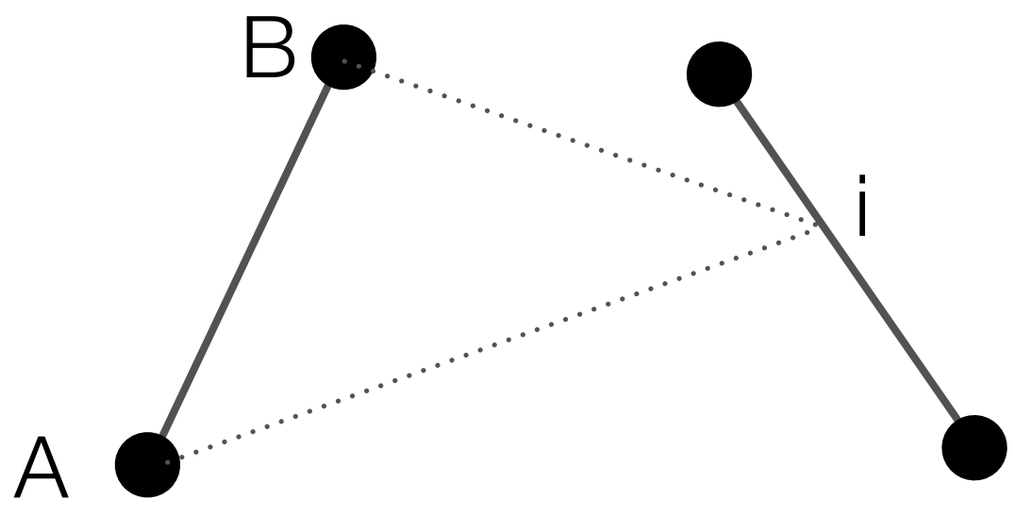
evaluated numerically: $\oint f(r)\,d\ell \rightarrow \sum_{\alpha=1}^{N_{segment}}\sum_{q=1}^{N_{\text{int}}} w_q f(r_{\alpha q})$

basic method: Wang, Ghoniem, Swaminarayan, and LeSar, J. Comp. Phys. 219, 608 (2006)

Step 2: stresses and forces



if use discrete linear segments



stress at point i from a segment from A to B is an analytic expression made up of more tensors

from stress can find the force.

below we will discuss how to calculate stress on nodes from stress on segments

see Hirth and Lothe, *Theory of Dislocations*
Devincre, Solid State Comm 93, 875 (1995)

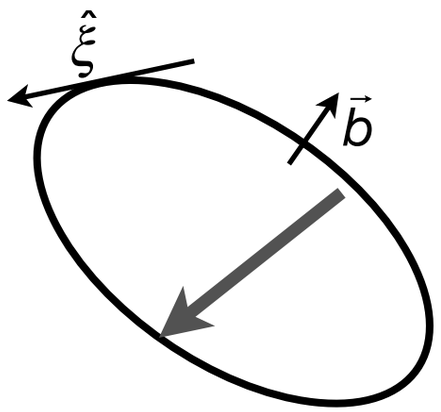
Step 2: self stresses

Two terms:

- core energy increases with length of dislocation so it **opposes dislocation growth**:

$$\frac{E_{core}}{L} = T = \alpha \mu b^2$$

- interaction of one part of a dislocation with itself



Step 4: equations of motion and dynamics

- full equation of motion (required at least at large $\dot{\varepsilon}$):

$$m\vec{a} = \vec{F} - \gamma\vec{v}$$

- over-damped limit (ignore inertial effects): $\vec{v} = \vec{F} / \gamma$
- for force velocity: determine forces on the nodes and solve the equations of motion

$$\vec{r}(t+\delta t) = \vec{r}(t) + \vec{v}(t)\delta t$$

- time step limited by largest force

Note: as we shall discuss below, the forces and velocities of the nodes requires some attention.

"Dislocation motion in high-strain-rate deformation," Wang, Beyerlein, and LeSar, Phil. Mag. 87, 2263 (2007).

Step 5: some approximations

dislocation reactions

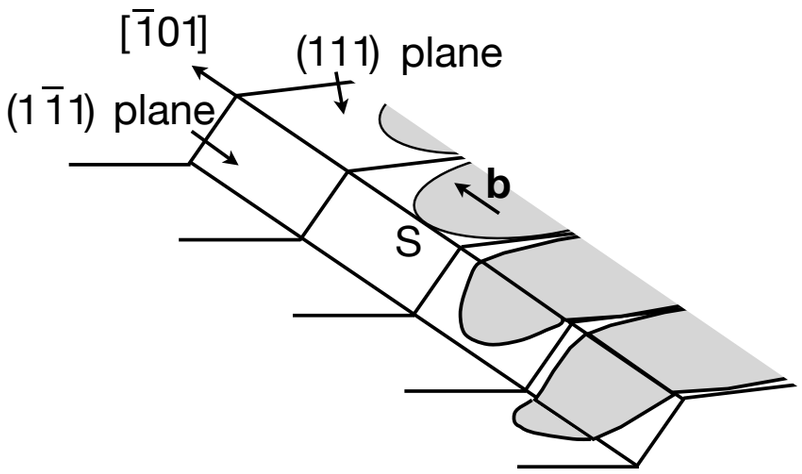
- treated with models
- ignore partials (more on this below)

coupling of dislocation motion to geometry

- we ignore the effects of lattice rotations caused by the dislocations
- many issues with boundary conditions, with the modeling of bulk plasticity being much more challenging than modeling of small-scale plasticity

Step 5: models

cross slip:



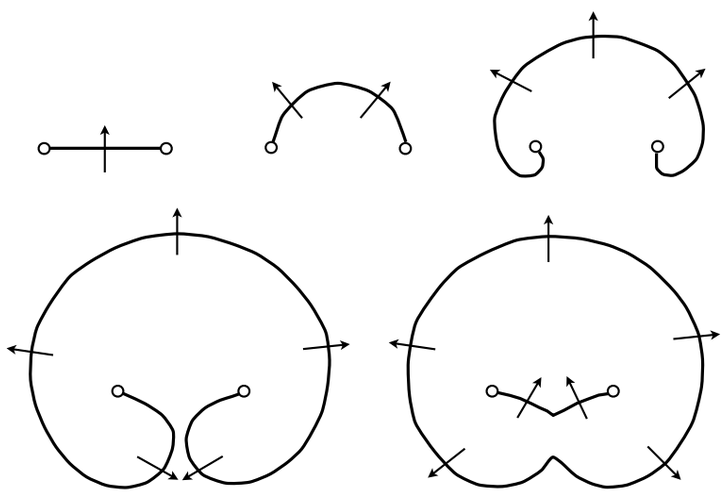
A Monte Carlo method is used to determine whether cross-slip is activated.

$$P = \frac{L}{L_o}\frac{\delta t}{\delta t_o} e^{\left[-\frac{V}{k_B T}\left(\tau_o - \tau_{CS}\right)\right]} \qquad for\ \tau_{CS} < \tau_o$$

$$P = 1 \qquad for\ \tau_{CS} > \tau_o$$

Kubin LP et al., Scripta Mater. (1992)

Frank-Read sources, annihilation, and junction forming



annihilation

junction

what else should we include:

e.g., climb, ...?

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Summary of the approximations

- all atomistic-based processes described with models
- most codes ignore partial dislocations
- most materials are anisotropic not isotropic
- we ignore the effects of lattice rotations caused by the dislocations (except as a post-process)
- boundary conditions are a challenge, with the modeling of bulk plasticity being more challenging than modeling of small-scale plasticity
- we typically approximate long-range interactions
- ...

steps in a simulation

- choose initial conditions and stress
  - place dislocations randomly on possible slip planes
- calculate total stresses on each node by integrating over all dislocations and find forces
- calculate if cross slip occurs
- solve equations of motion (nodes move)
- check for junctions, annihilations, etc.
- repeat

from movement of dislocations, calculate plastic strain

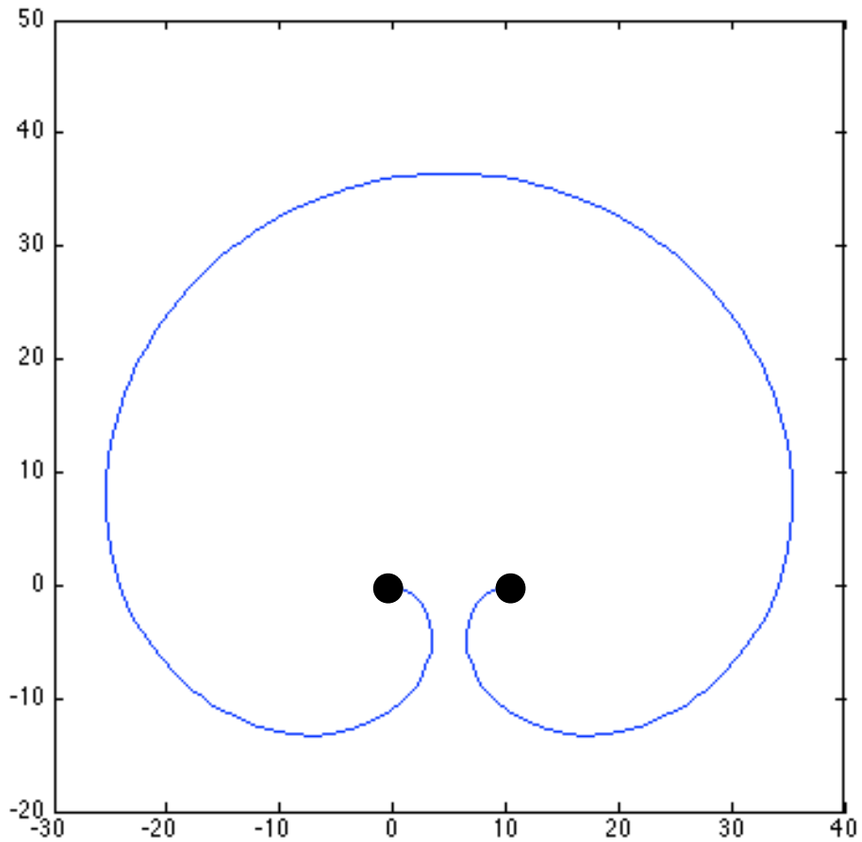
analyze dislocation structures, densities, etc.

An example:
a simple Frank-Read Source

example: a line-tension based Frank-Read source

DislocationDynamics.pdf also contains an explanation of this model. A folder called DDFR in the folder “code” contains MATLAB code this model.

The goal is to simulate:



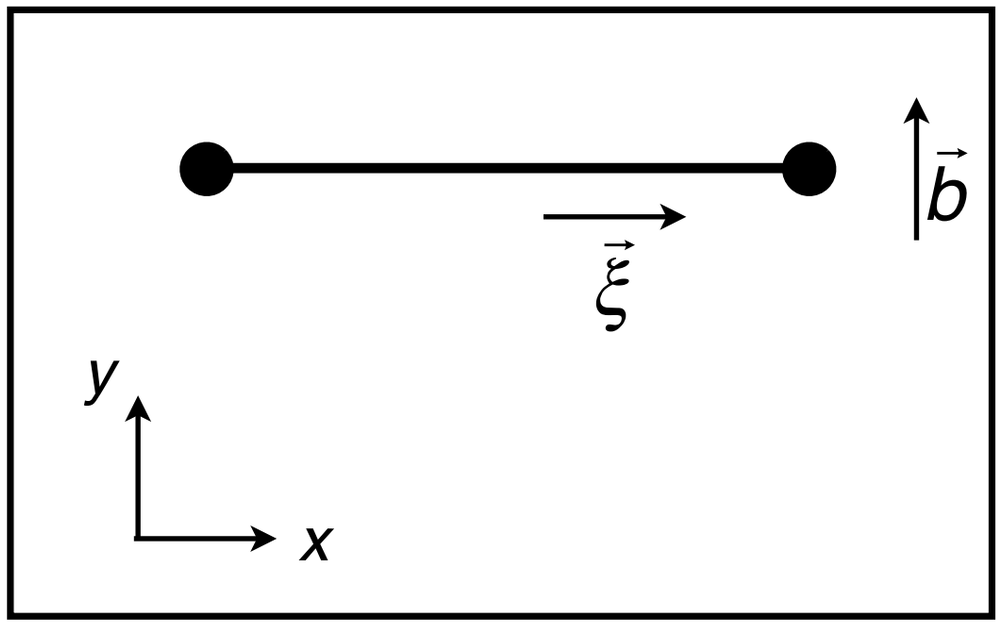
Nota bene: for a more complete discussion, see

Computer Simulations of Dislocations, V. V. Bulatov and W. Cai, (Oxford University Press, New York, 2006

and for more complete MATLAB codes, see

http://micro.stanford.edu/~caiwei/Forum/2005-12-05-DDLab/

the model



We start with a dislocation pinned at both ends.

This segment has

$\vec{b} = b(0,1,0)$ and $\hat{\xi} = (1,0,0)$

and is thus what kind of dislocation?

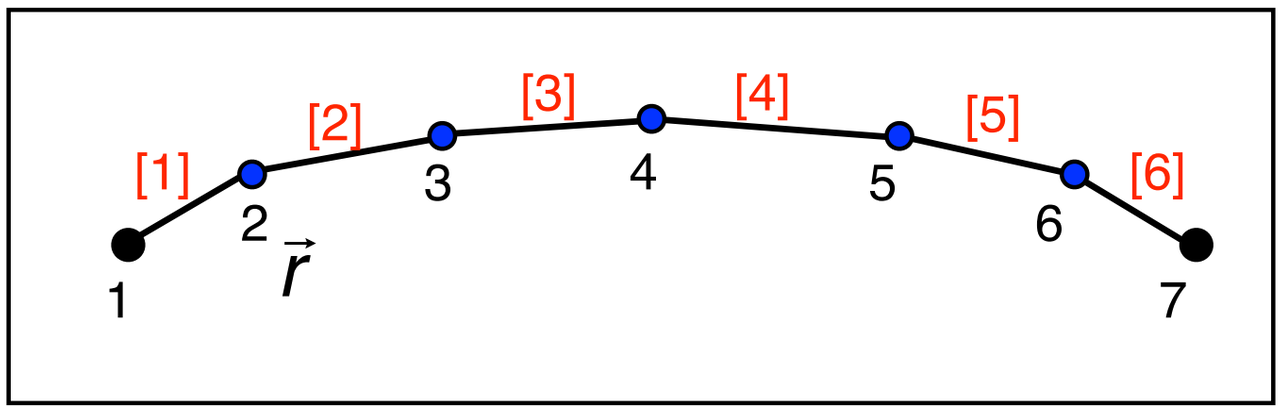
The glide plane is in the *xy* plane. The forces in the glide plane are:

$$\frac{\vec{F}}{L} = \left(\vec{b} \cdot \boldsymbol{\sigma}\right) \times \hat{\xi}$$

$$\frac{\vec{F}}{L} = b\sigma_{yz}\left(-\xi_y, \xi_x\right) = b\,\tau\left(-\xi_y, \xi_x\right)$$

representation of the dislocation and nodal forces

Add nodes to dislocation and connect with straight segments.



Force on segment *i* is constant along the segment:

$$\vec{F}_i^s = b\,\tau\left(-\xi_y, \xi_x\right)\ell_i$$

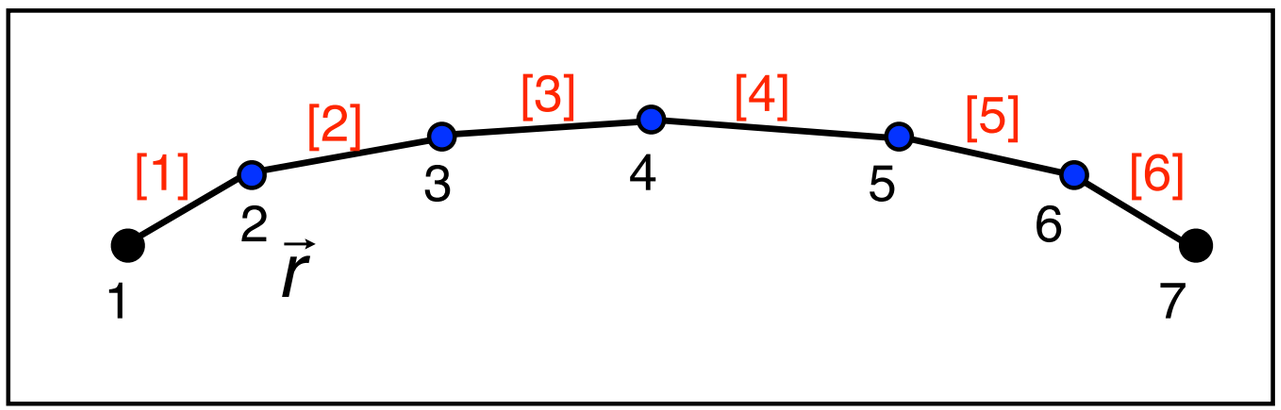
Force on node *i*:

- weighted average of force on segments
- for constant force on segments $\vec{F}_i = \left(\vec{F}_i^s + \vec{F}_{i+1}^s\right)/2$

Line tension force on *i*: $\vec{F}_i^\ell = E_\ell\left(-\hat{\xi}_{i-1} + \hat{\xi}_i\right)$

- E_ℓ is the line energy

velocity



velocity of a node is dependent on velocity of the segment

- each point on the segment has a different force, and thus different velocity (v = M F)
- as Bulatov and Cai describe, the velocity is a weighted average
- they give an approximate expression, which we use

$$\vec{v}_i^{\,n} \approx \frac{\vec{F}_i^{\,n}}{B\left(\ell_{i-1} + \ell_i\right)/2}$$

use Euler equation (or something better) for EOM

limitations of model code

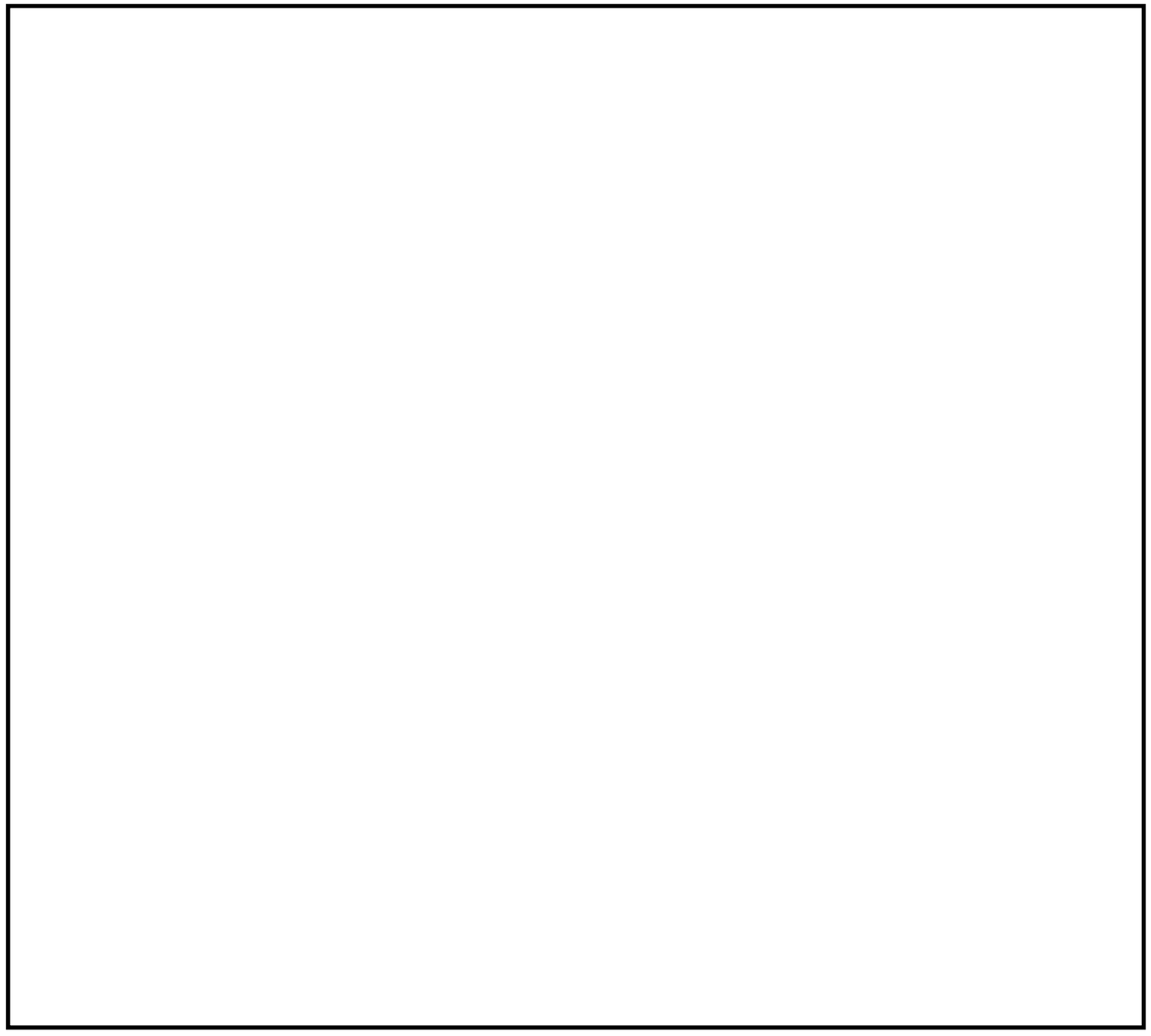
- no interactions between segments
- no annihilation
- ...

However, it will show you how the basic method works.

And you can make movies.

a better calculation of an FR source

operation of a source in a thin film



Applications

1. Some successes: small-scale plasticity

dislocation dynamics simulations have proven very successful for small-scale systems

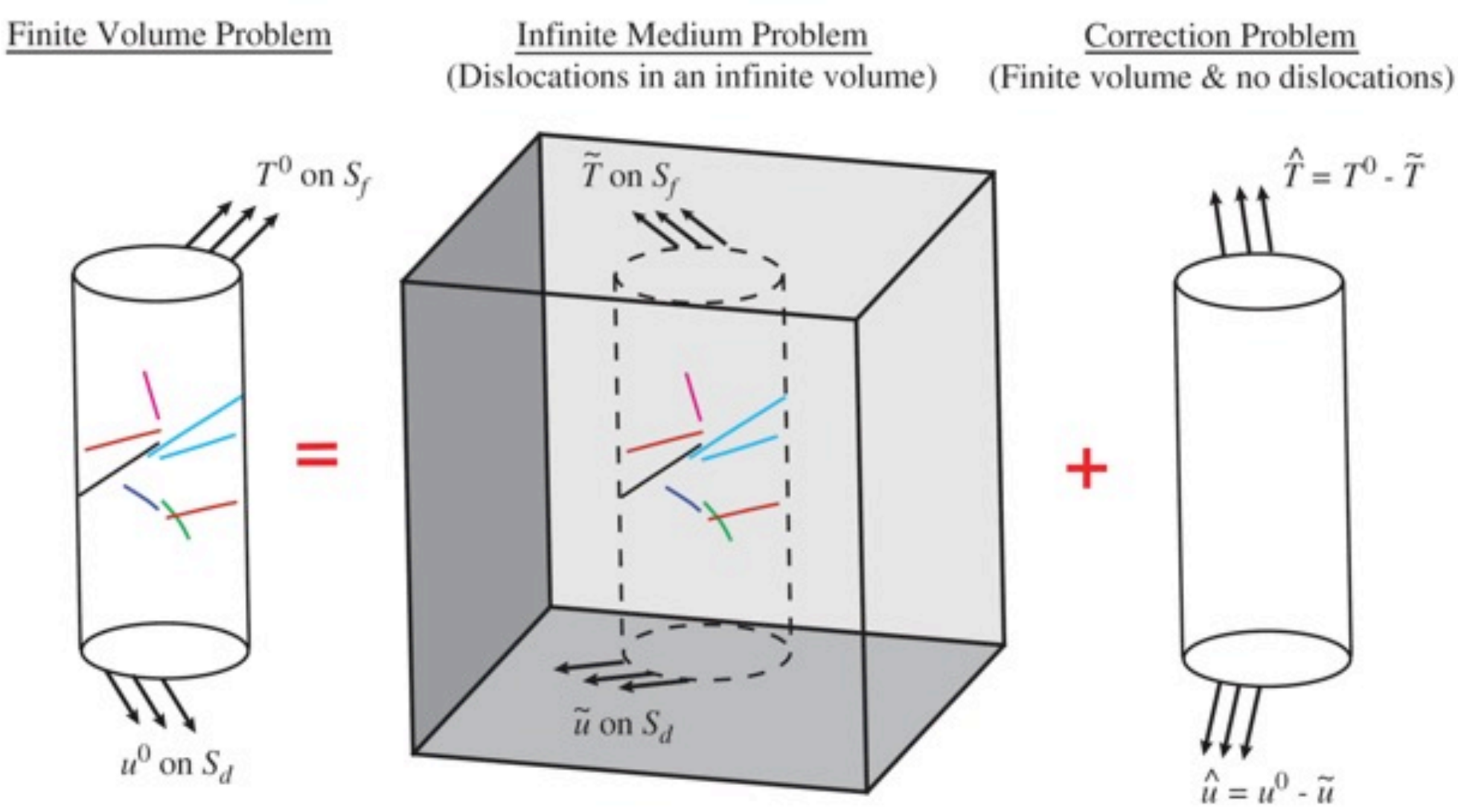
4 examples showing how changes in interfaces change plasticity:

- *small scales with free surfaces (micropillars)*[1,2]
- small scales with coated surfaces (micropillars)[3]
- *polycrystalline thin films with free surfaces*[4]
- polycrystalline thin films with coated surfaces[5]

[1] *Zhou, Biner and LeSar, Acta Mater. 58, 1565 (2010).*
[2] *Zhou, Beyerlein and LeSar, Acta Mater. 59, 7673 (2011).*
[3] *Zhou, Biner and LeSar, Scripta Mater. 63, 1096 (2010).*
[4] *Zhou and LeSar, Int. J. Plasticity 30-31, 185 (2012).*
[5] *Zhou and LeSar, Comput. Mater. Sci. 54, 350 (2012).*

small scale plasticity is the perfect problem for DDD - small numbers of dislocations and straightforward boundary conditions

free surfaces: boundary element method



Total displacement and stress fields:

$$u_{ij} = \tilde{u}_{ij} + \hat{u}_{ij} \qquad \sigma_{ij} = \tilde{\sigma}_{ij} + \hat{\sigma}_{ij}$$

$\hat{u}_{ij}$ and $\hat{\sigma}_{ij}$ are the image fields that enforce the boundary conditions.

$\tilde{u}_{ij}$ and $\tilde{\sigma}_{ij}$ are the displacement and stress fields in an infinite medium from all dislocations.

El-Awady, Biner, and Ghoniem (2008)

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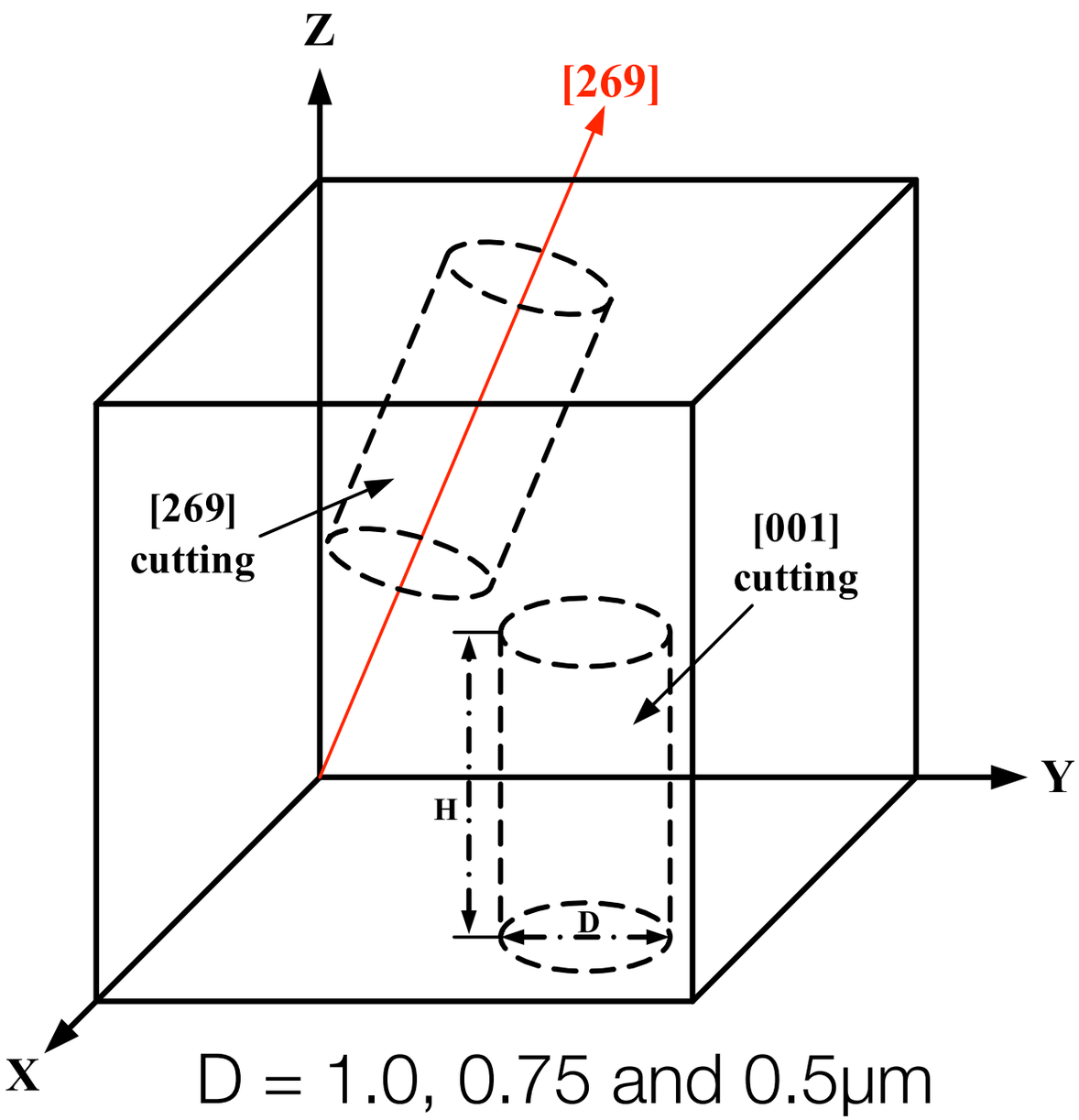
sample preparation (no ions required)



D = 1.0, 0.75 and 0.5μm

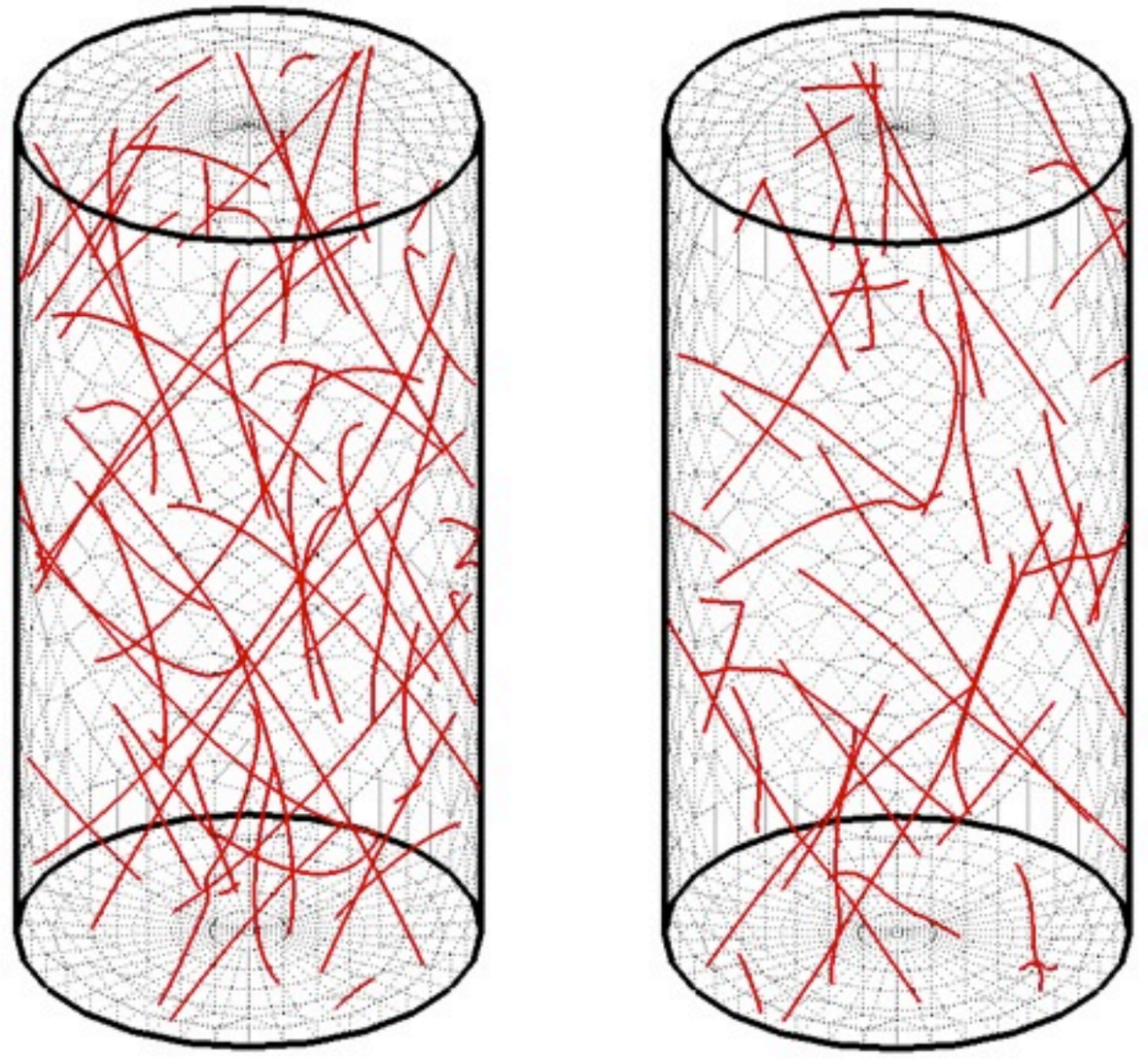
D : H = 1 : 2

Before relaxation

Density = 2.7×10^{13} m^{-2}

After relaxation

Density =1.8×10^{13} m^{-2}



(Dotted lines are BEM meshes)

- initial conditions shown to have large effect of calculated response in small systems: Motz, Weygand, Senger, Gumbsch, Acta Mater 57, 1744 (2009).

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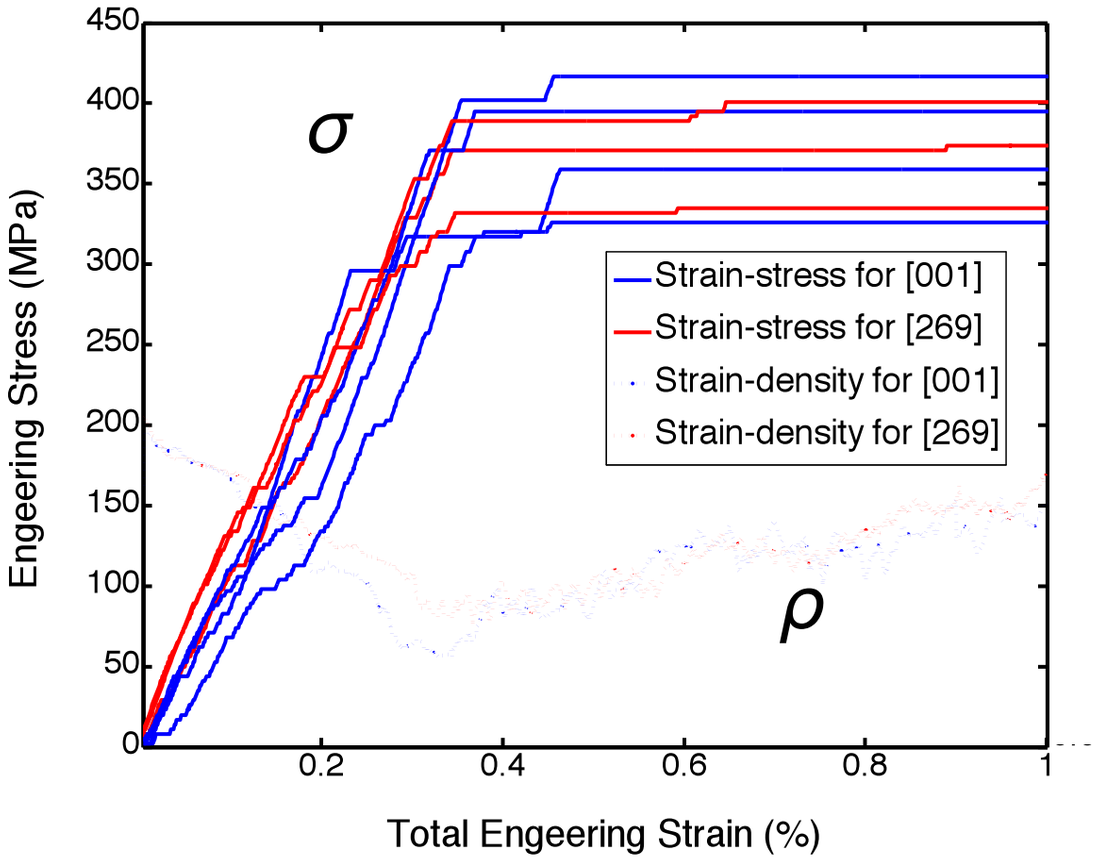
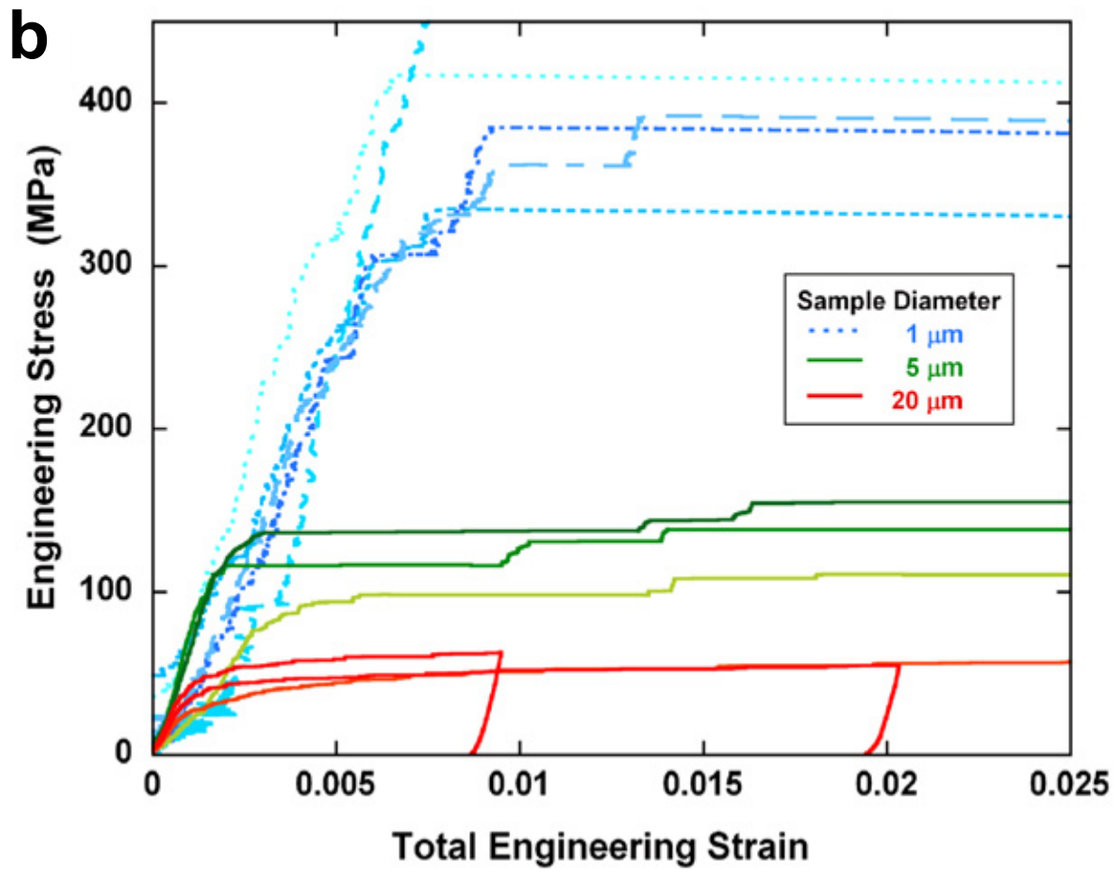
stress-strain behavior of Ni



1 micron samples

calculated

onset of flow:
ε ~ 0.003



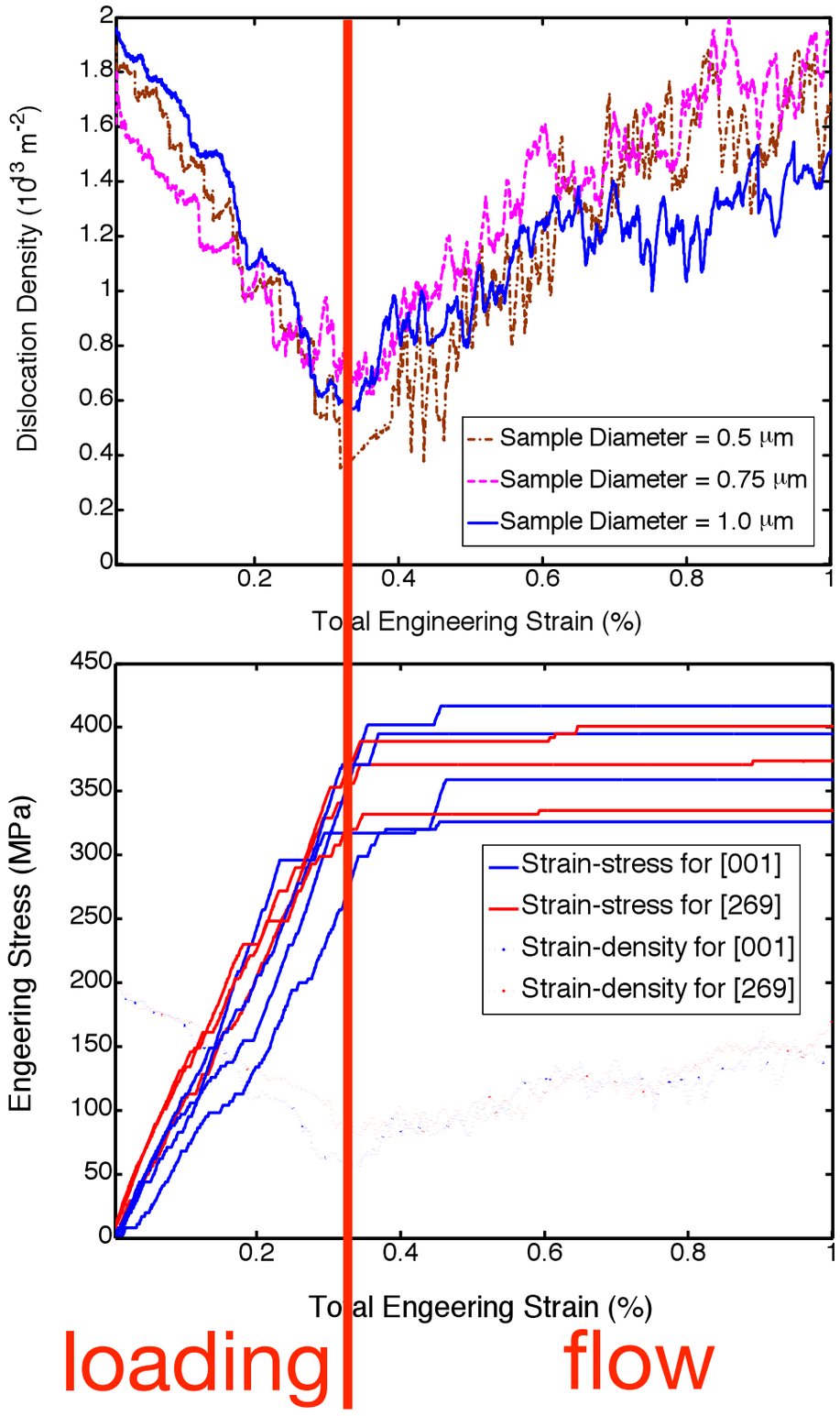
1 micron samples

experimental

onset of flow:
ε ~ 0.008

differences arise from: strain rate, equation of motion, …

loading and flow

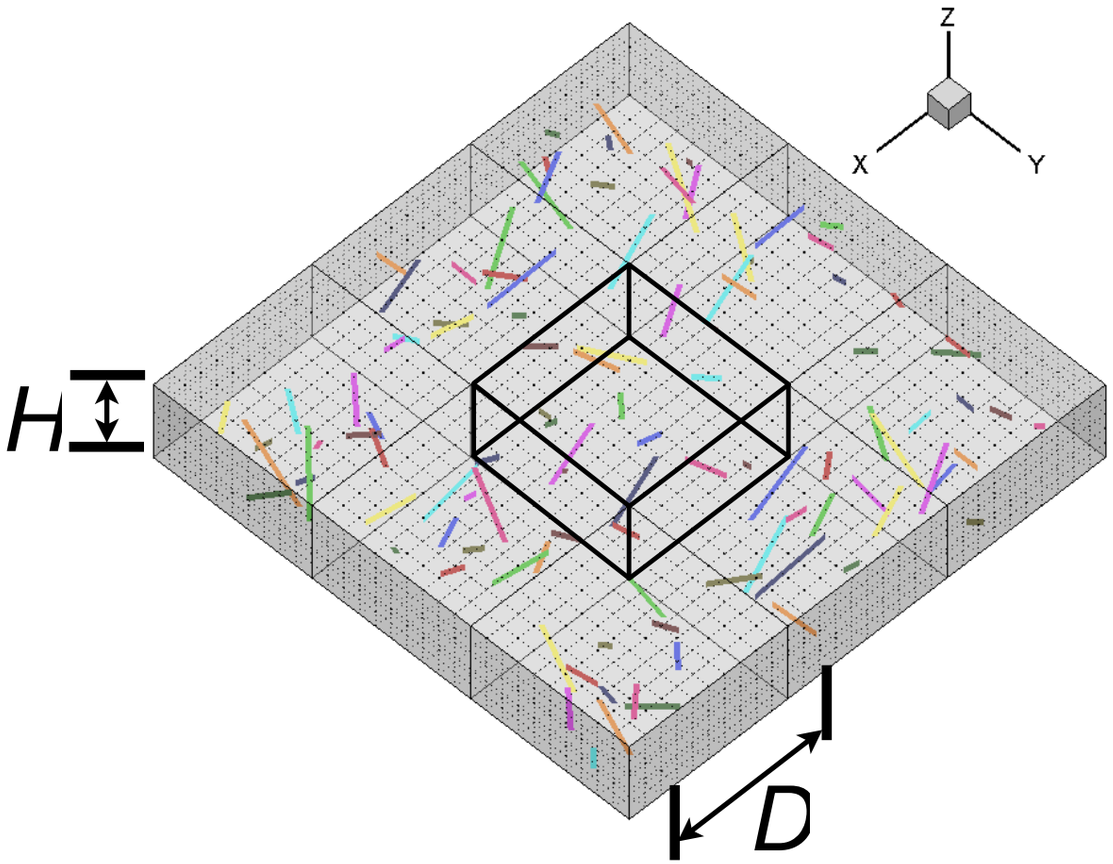


loading regime: intermittent flow, but are they avalanches?

see “Scale free intermittent flow in crystal plasticity,” Dimiduk, Woodward, LeSar, and Uchic, Science 312, 1188 (2006).

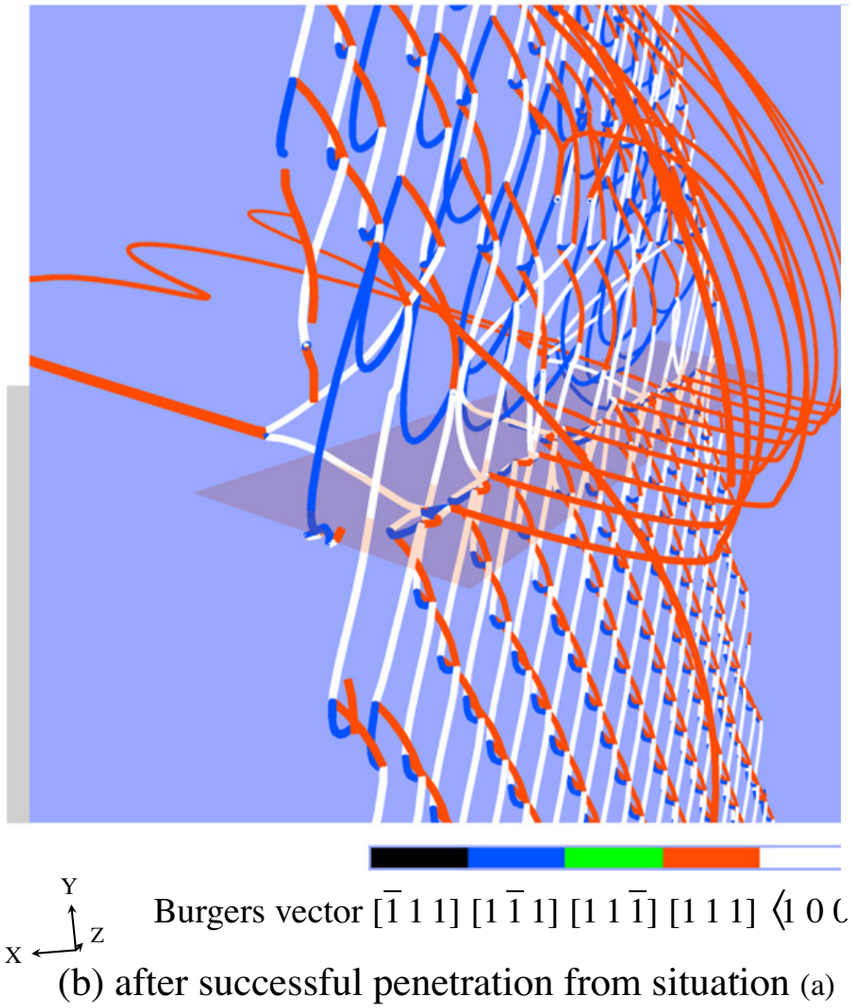
a simple model for a free-standing polycrystalline thin film

simulation cell

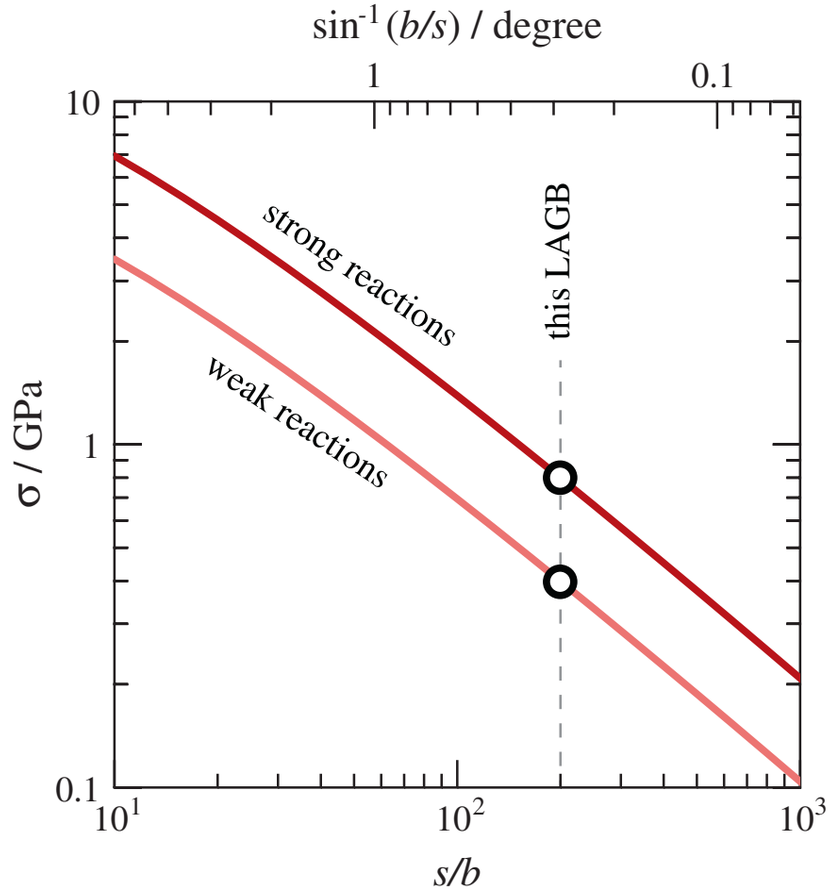


- free surfaces on all sides
- 9 grains, all with same orientation
- tension under constant strain rate
- all stress-strain-density behavior calculated from internal grain only, averaged over 10 realizations

DD model of dislocation-grain boundary interactions



(b) after successful penetration from situation (a)



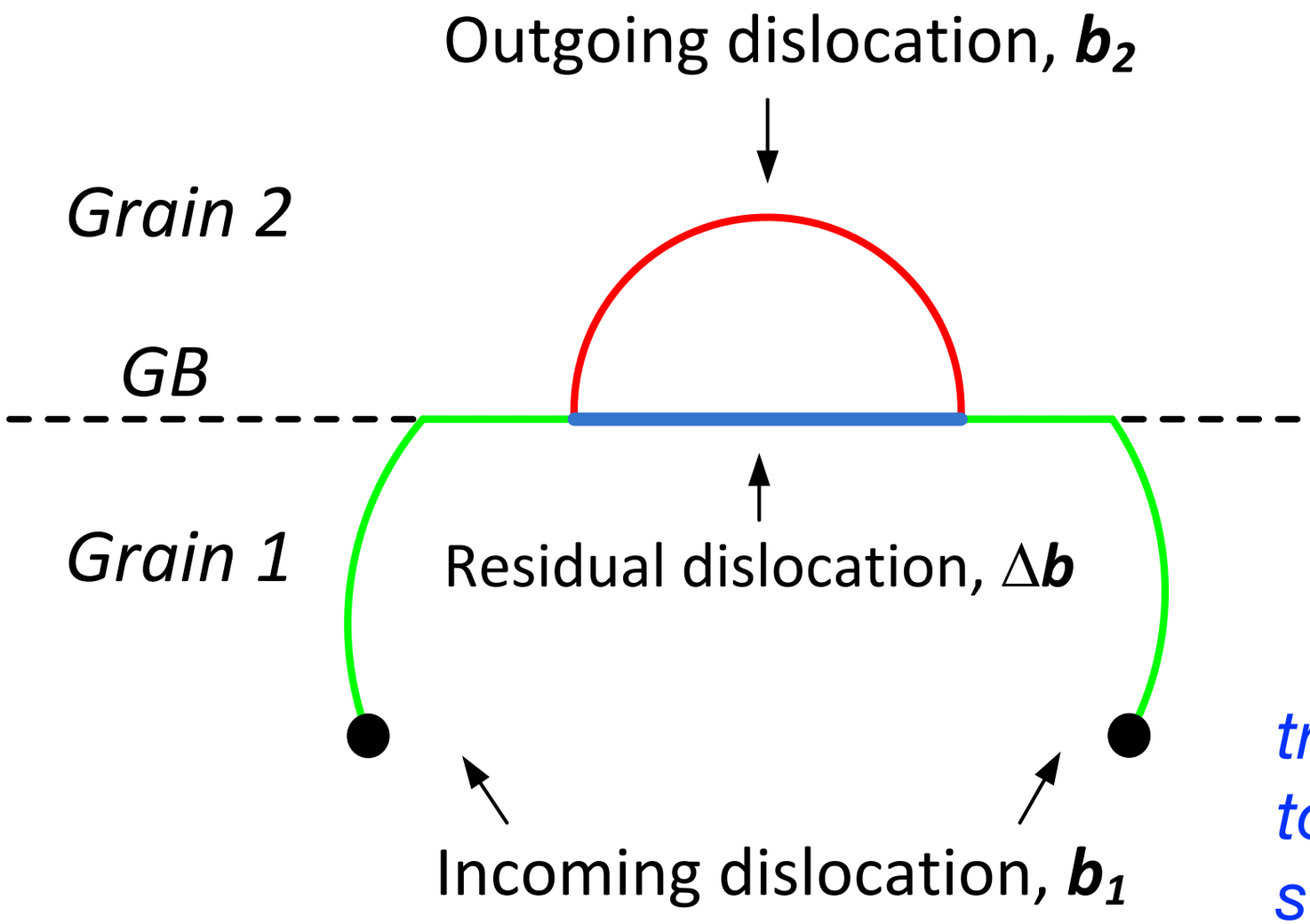
- low angle GB (0.3°) modeled with interpenetrating mesh of dislocations
- modeled transmission of dislocations through the LAGB

- atomistic simulations are also being done, but each orientation and dislocation are different

Simulation of dislocation penetration through a general low-angle grain boundary
B. Liu, P. Eisenlohr, F. Roters, D. Raabe, Acta Mater 60, 5380 (2012)

transmission model at grain boundaries

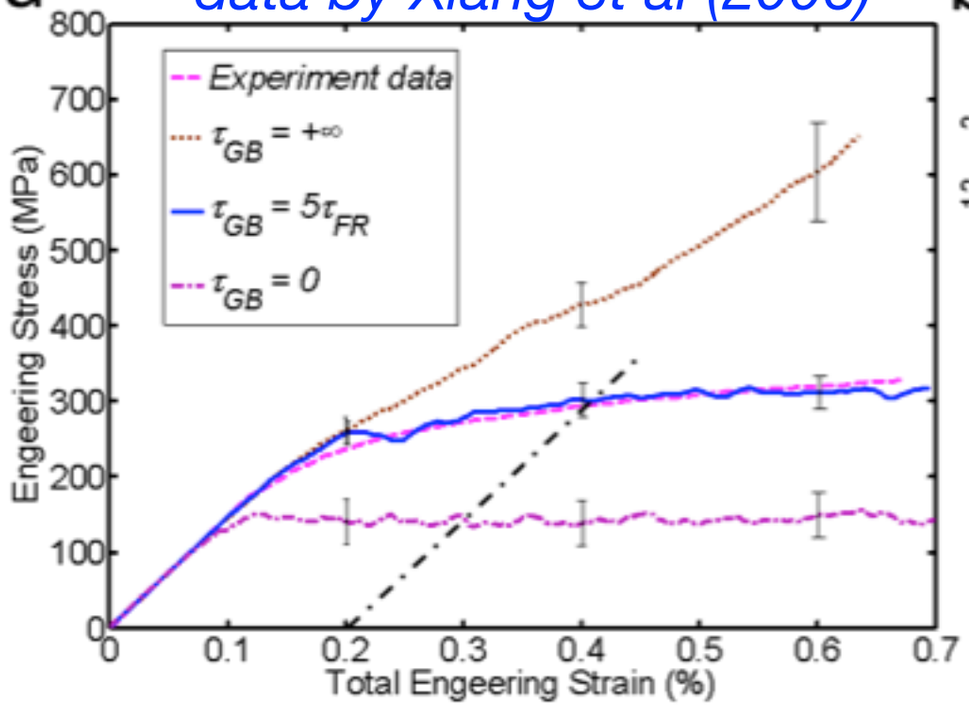
grain boundary/dislocation interactions (de Koning et al. 2002)

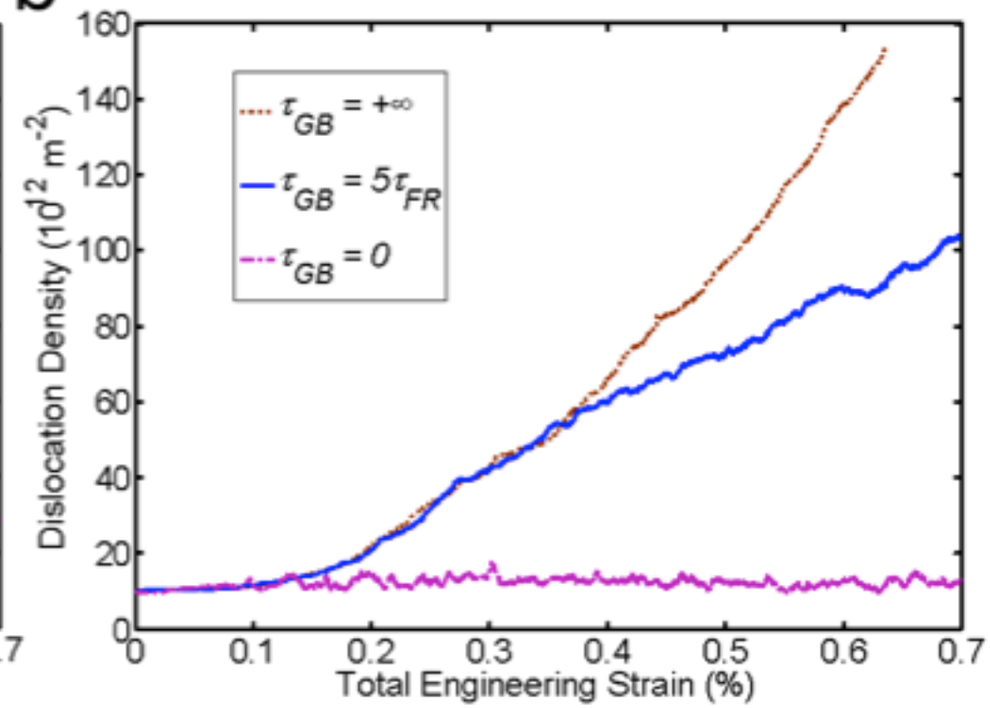


transmission stress adjusted to match experimental stress-strain relation

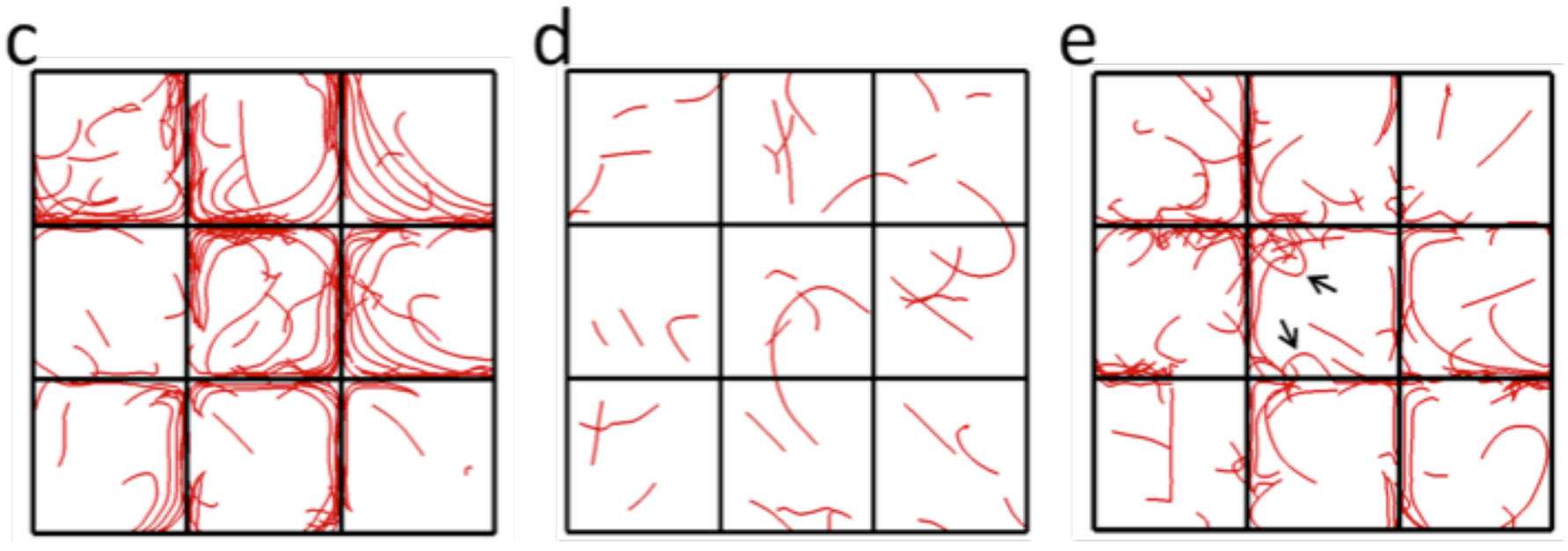
setting transmission stress: τ_{GB}

data by Xiang et al (2006)

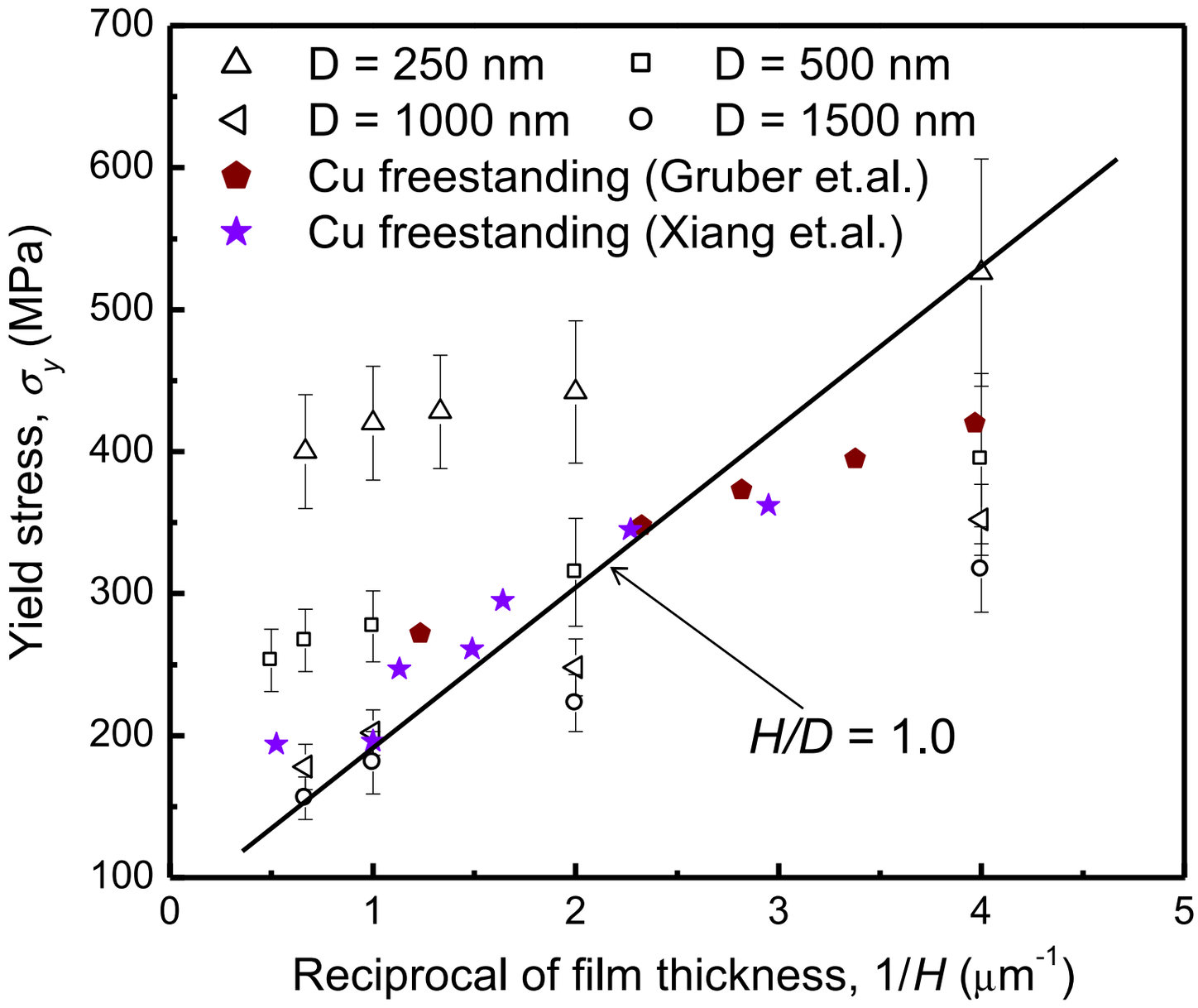




$\tau_{GB} = 5\ \tau_{FR}$



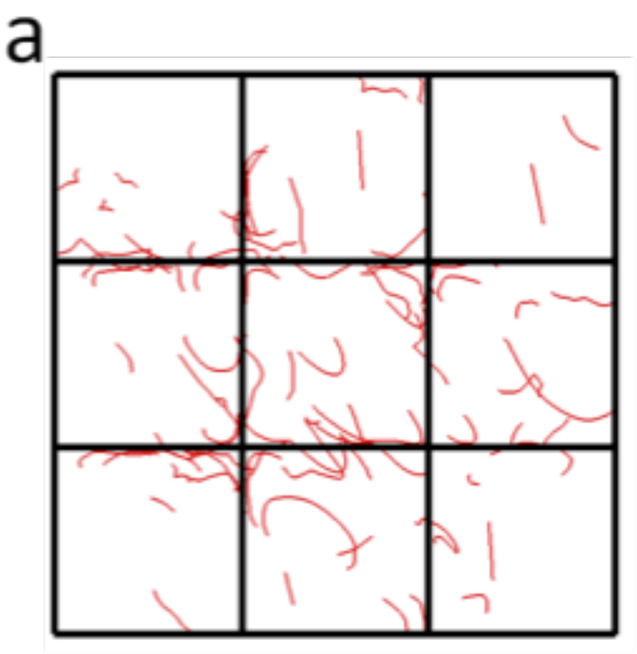
comparison with experiment

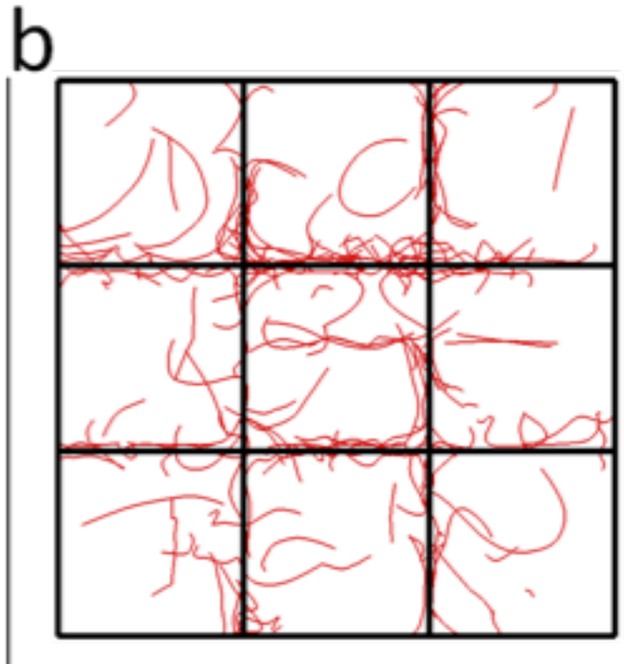


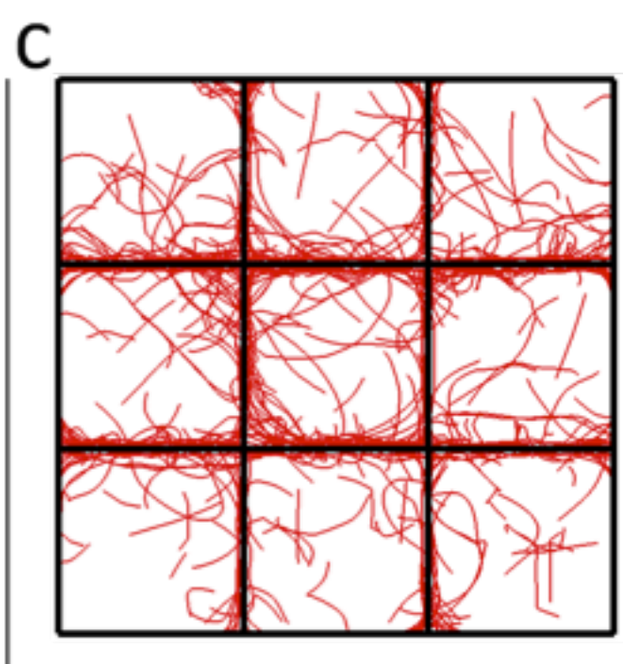
Excellent agreement with experimental stress-strain behavior, but ...

is this a definitive test of the method?

dislocation structures

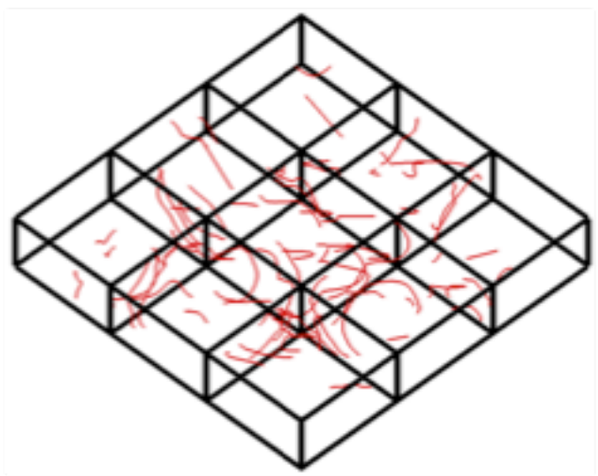




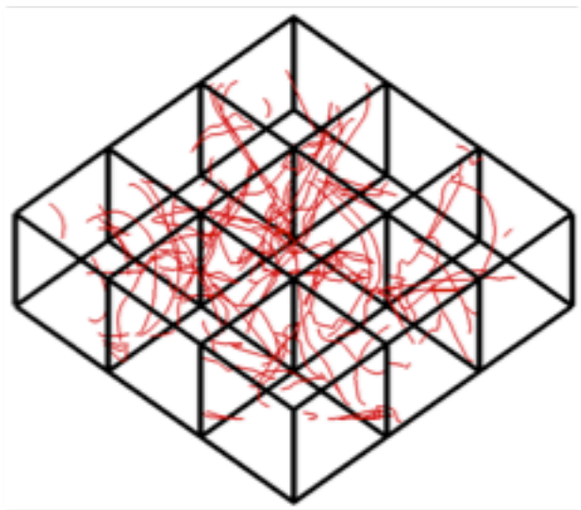


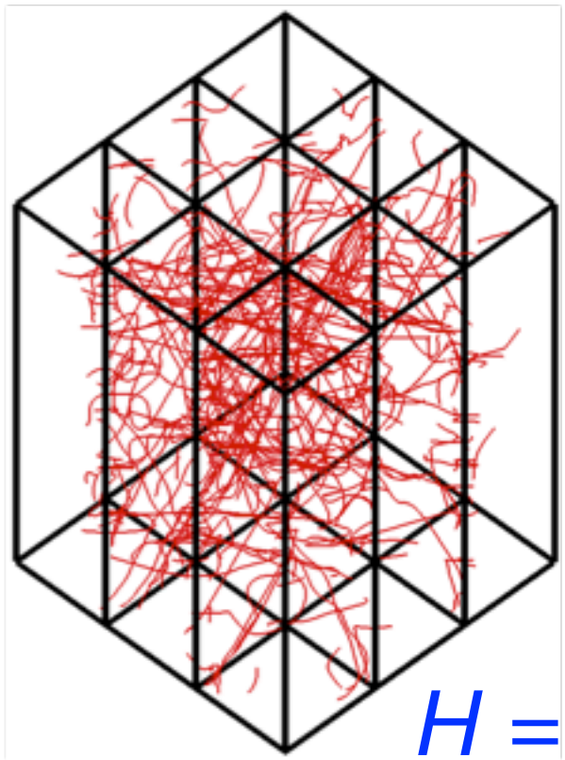
D = 500 nm

H = 250 nm



H = 500 nm



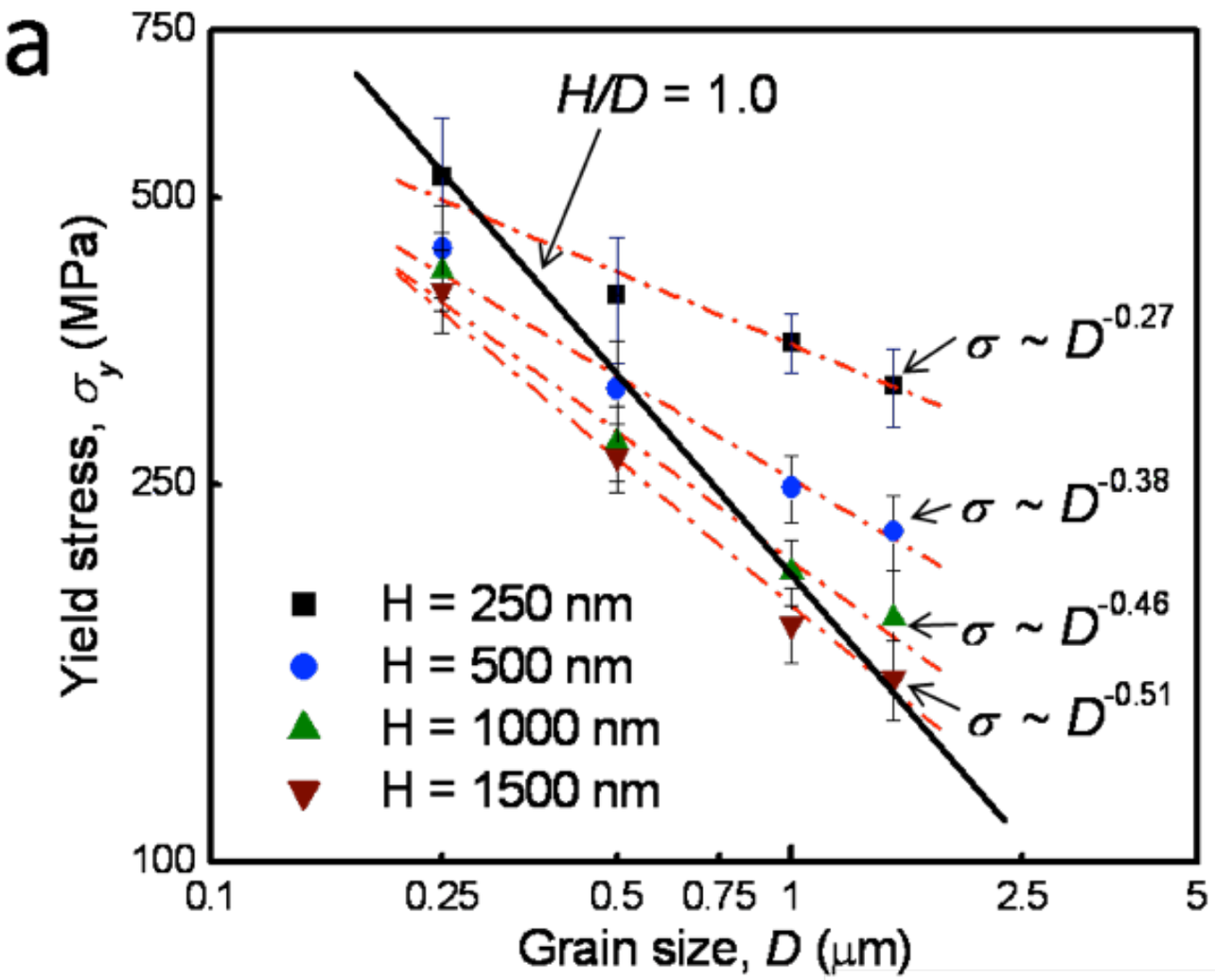


H = 2 µm

dependence on *D* and *H*

- dependence of yield stress on *D* as a function of film thickness

- approaches Hall-Petch relation for thick films (H = 1.5 μm)



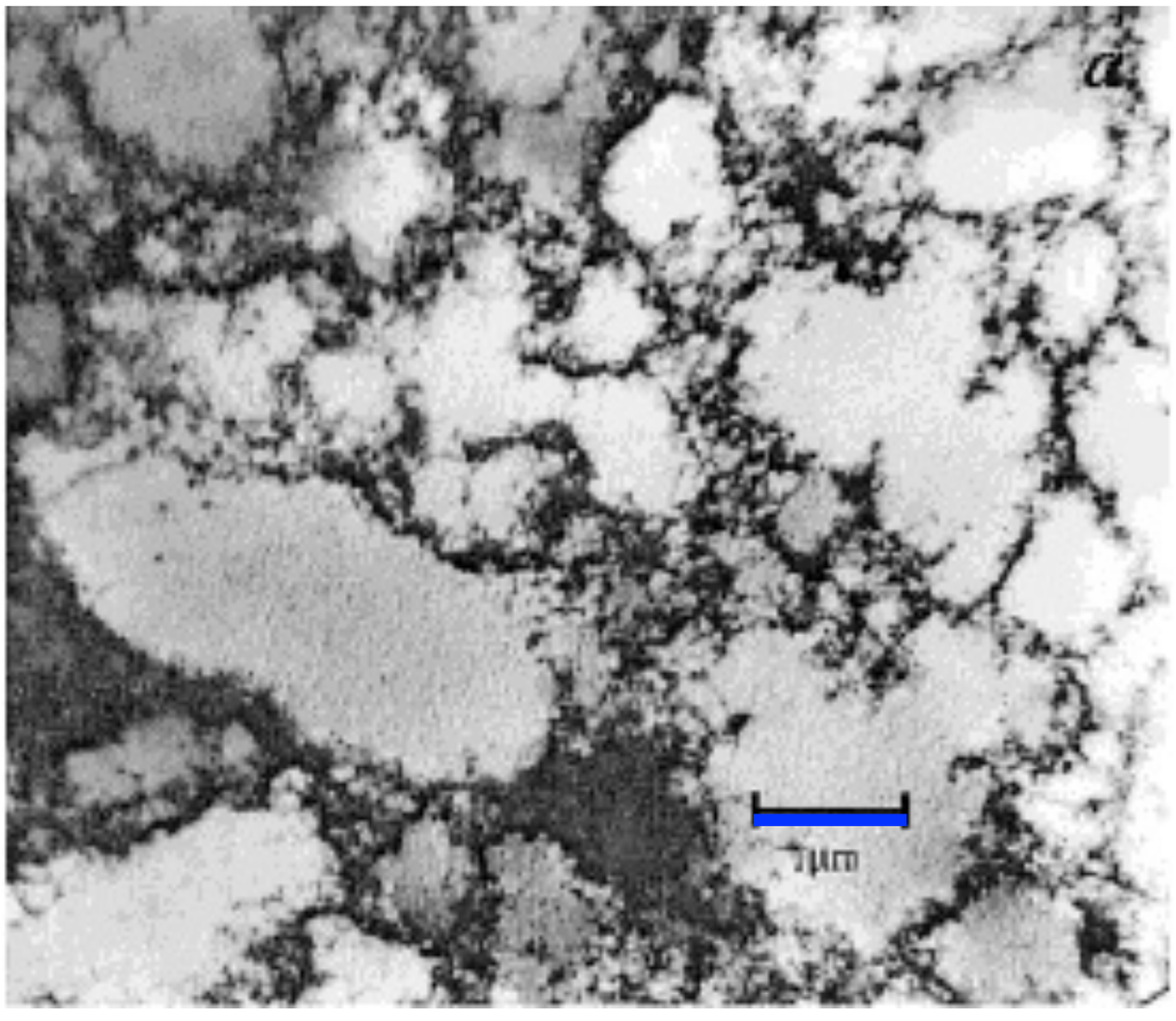
outlook

- for small-scale samples, DD simulations have led the way in developing understanding of the deformation mechanisms
- by controlling physics, we can examine the role of different physical processes (e.g., cross slip)
- limited by the assumptions mentioned earlier
- with better connection to experiments (esp. structure), we should be able to examine the “correctness” of the predictions, which can guide the development of better models

A challenge: bulk plasticity

2. Can we model with DD the development of dislocation substructures?

Single crystal Cu in single slip: Stage III



1 μm

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

we will use as an example a study of high strain rate response done in collaboration with Los Alamos

computational challenges

the dislocation density increases with stress $\rho^{1/2} \propto \tau$

- calculations slow with increasing stress, with the computational time per time step increasing as

$$n_{node} \propto L \propto \rho \propto \tau^2 \qquad t_{comp} \propto n_{node}^2 \propto \tau^4$$

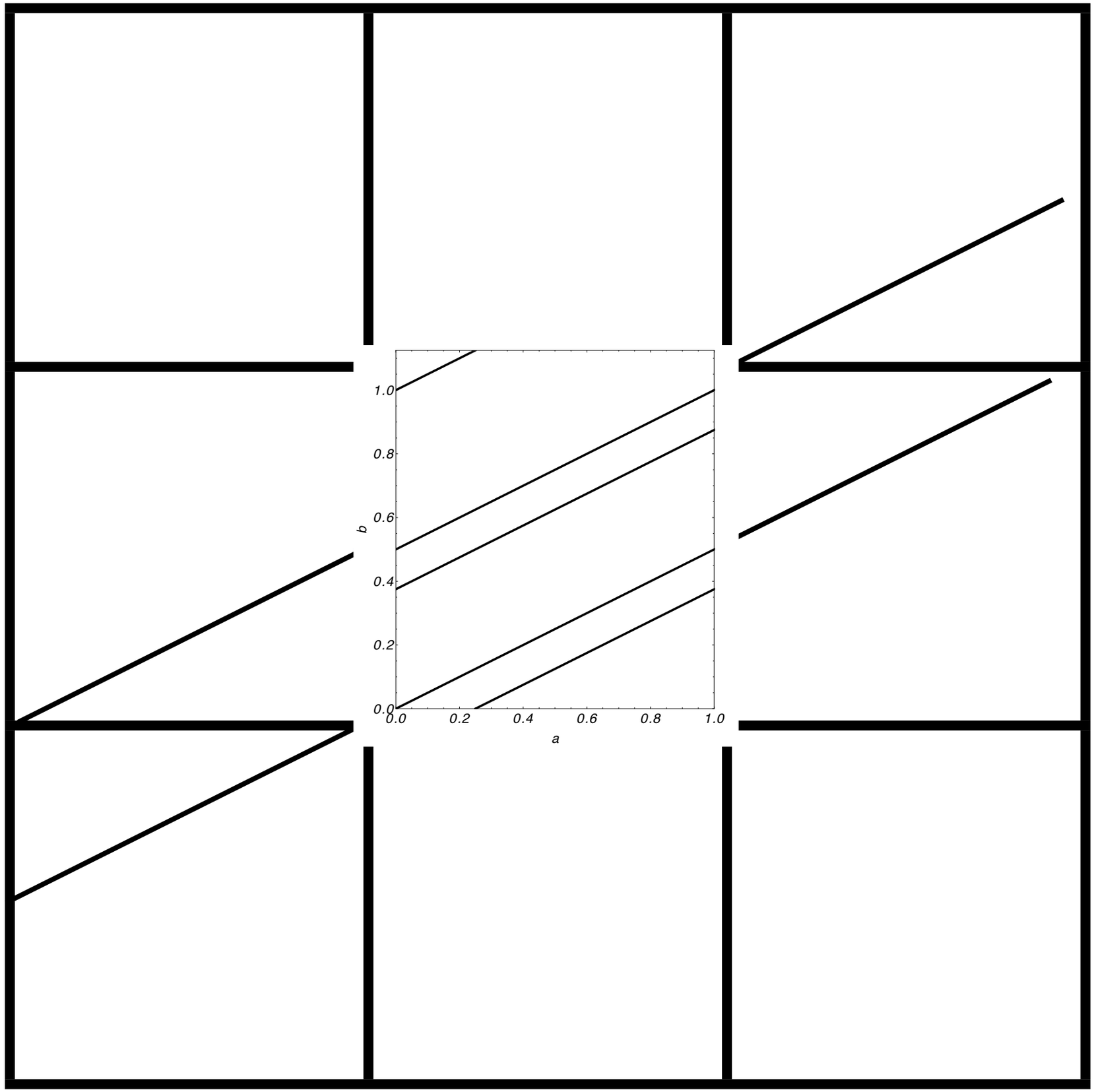
time steps decrease with increasing dislocation density

- typically use dynamic time stepping because of very large dislocation interaction stresses (based on a maximum distance a dislocation can move)
- time steps are small (can be as small as 10^{-10} sec)
- as density increases, have more pileups and larger stresses and thus smaller time steps: $\delta t \sim 1/\tau$

boundary conditions

- must have transport of dislocations into and out of the simulation cell
- periodic boundary conditions can be a problem.
  - Madec, Devincre and Kubin, “On the use of periodic boundary conditions in dislocation dynamics simulations”, Solid Mechanics and Its Applications **115**, 35-44 (2004)
- can avoid many of these issues with large cells (slow calculations), but still have long-ranged interactions
- may be best to use large cylinders whose properties seem to be bulk-like

periodic boundary conditions

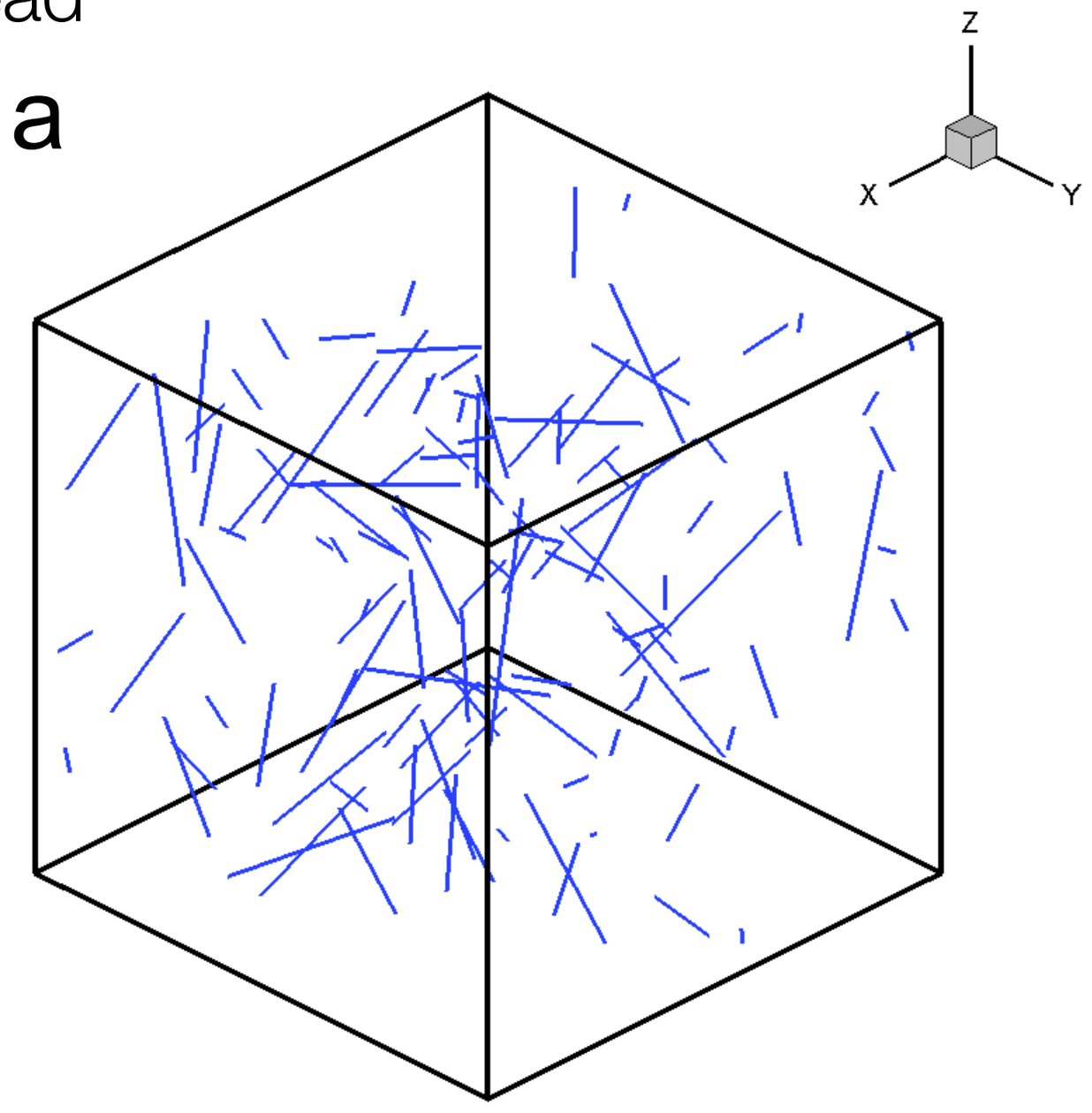


a typical initial structure

assume an initial set of Frank-Read sources randomly placed on available slip systems

under stress, they bow out and interact with other dislocations

as the length of dislocations increases, so does the complexity of the microstructure



5 μm cube

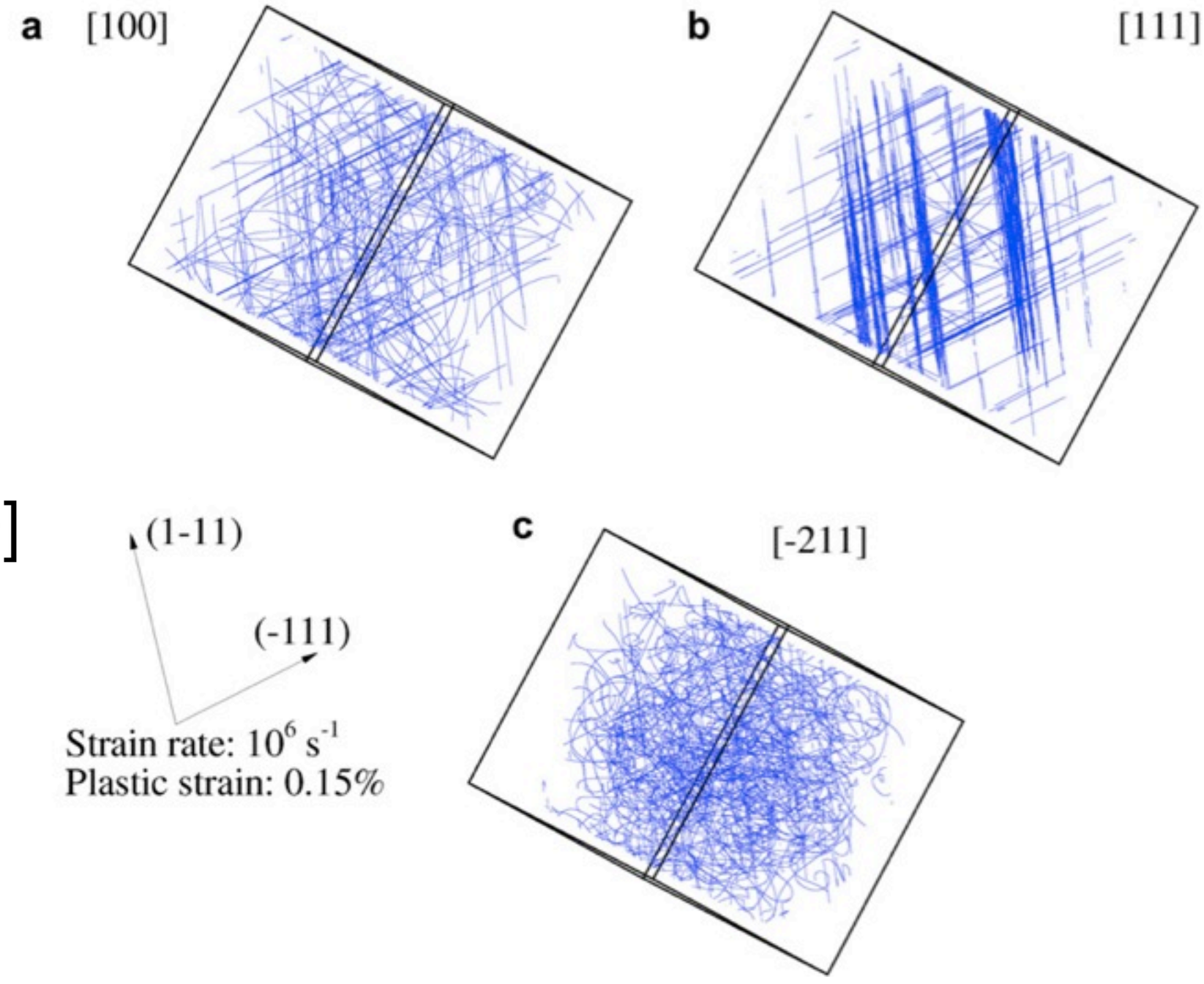
studies at high strain rate on Cu single crystals

effects of loading on dislocation microstructures and deformation

Schmid factors:

$[111] < [\bar{2}11] < [100]$

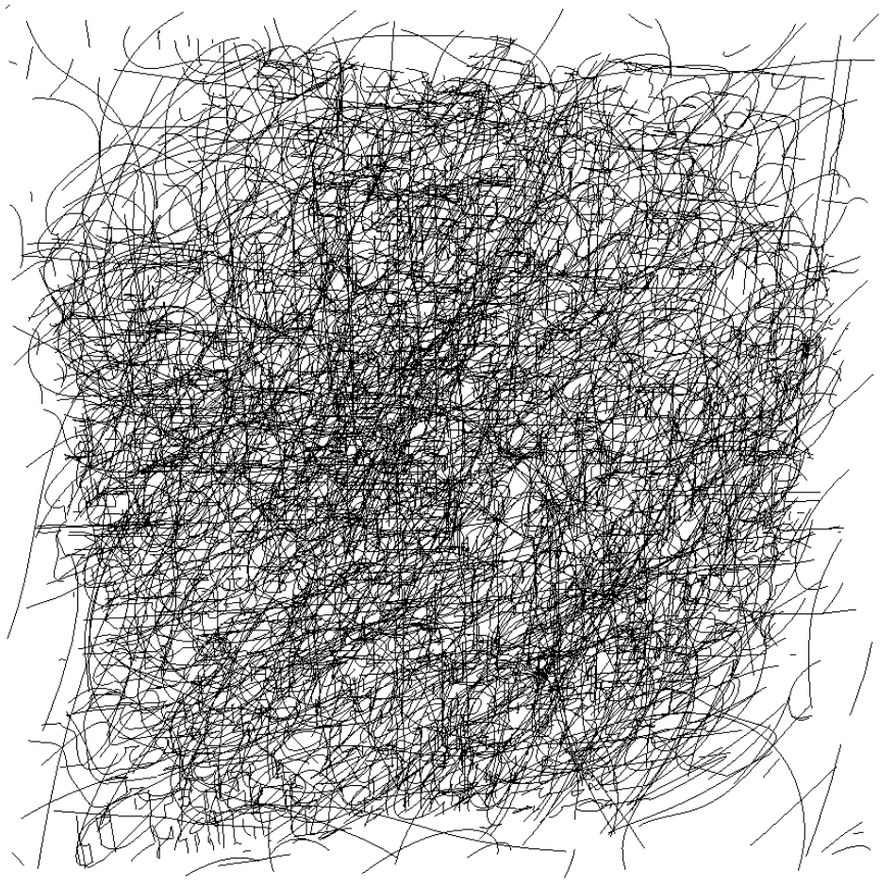
interest in high rates: e.g., impact damage



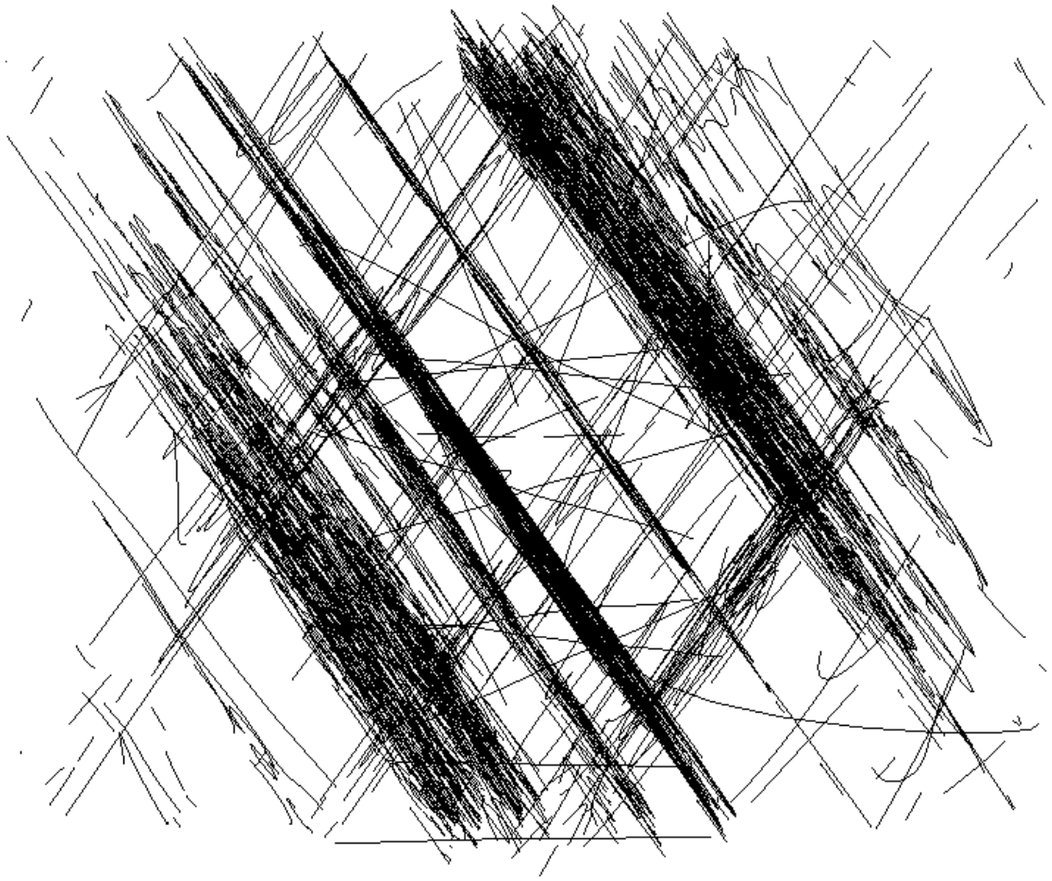
5 μm cubes

"Plastic anisotropy in fcc single crystals in high rate deformation," Wang, Beyerlein, and LeSar, IJP 25, 26-48 (2009)

slip bands in [111] loading



viewed along [100]



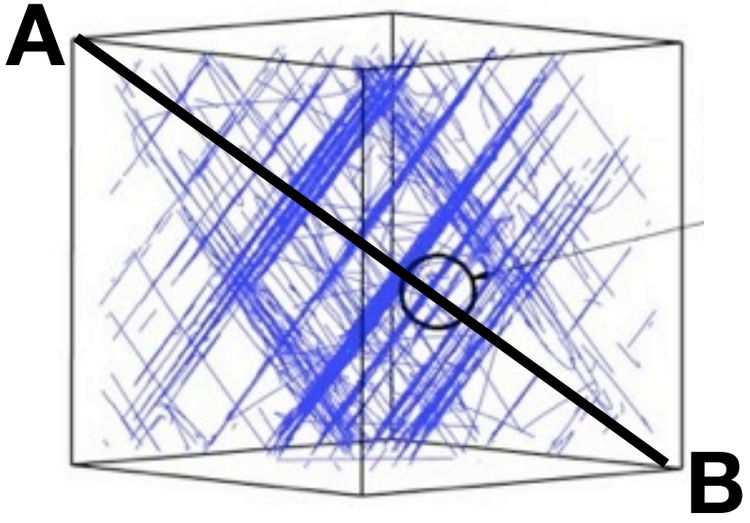
viewed along [110]

5 μm cube

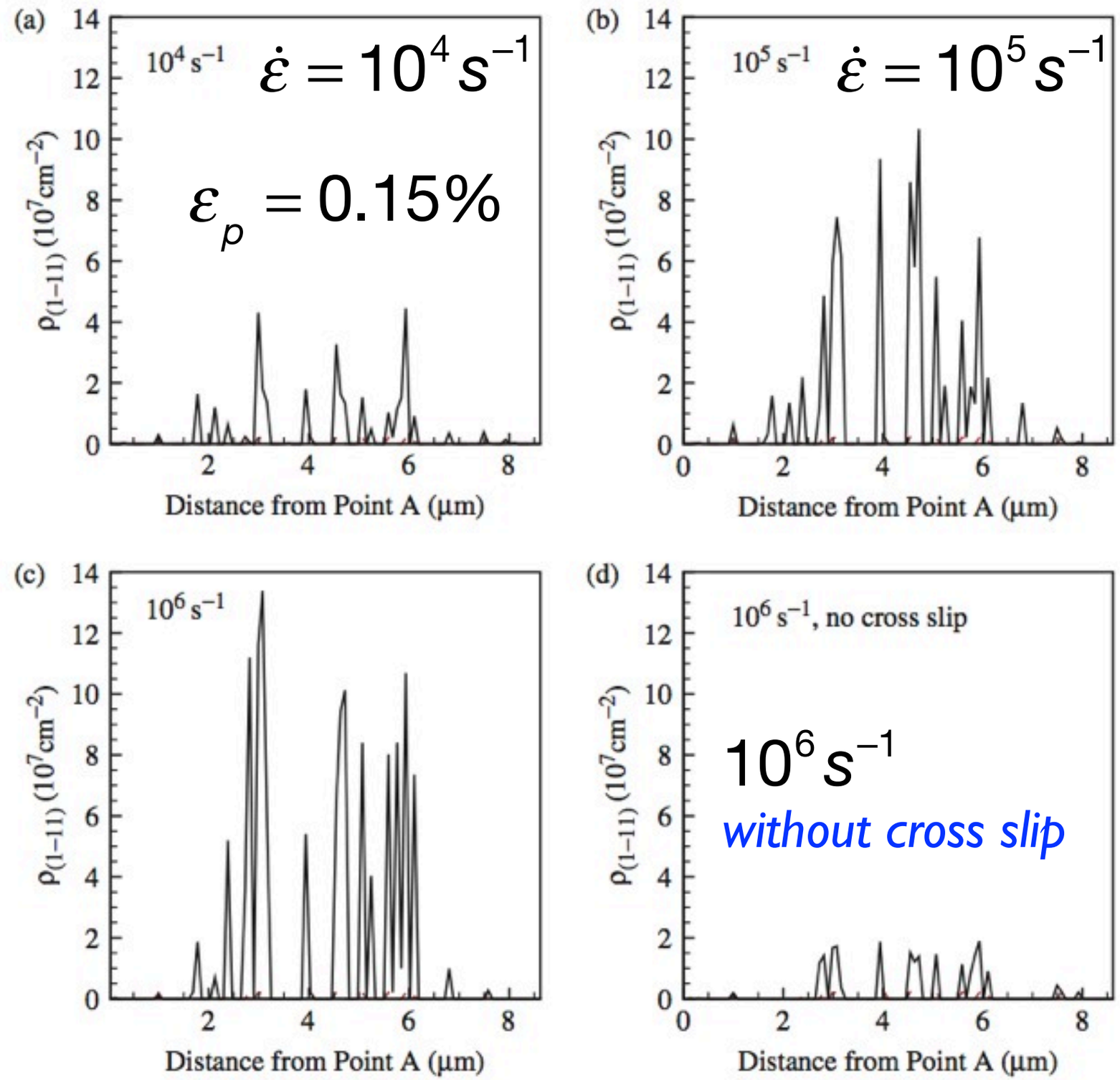
Is this an artifact of the boundary conditions?

"Plastic anisotropy in fcc single crystals in high rate deformation,"
Wang, Beyerlein, and LeSar, IJP 25, 26-48 (2009)

dislocation density on $\left[1\bar{1}1\right]$ slip planes

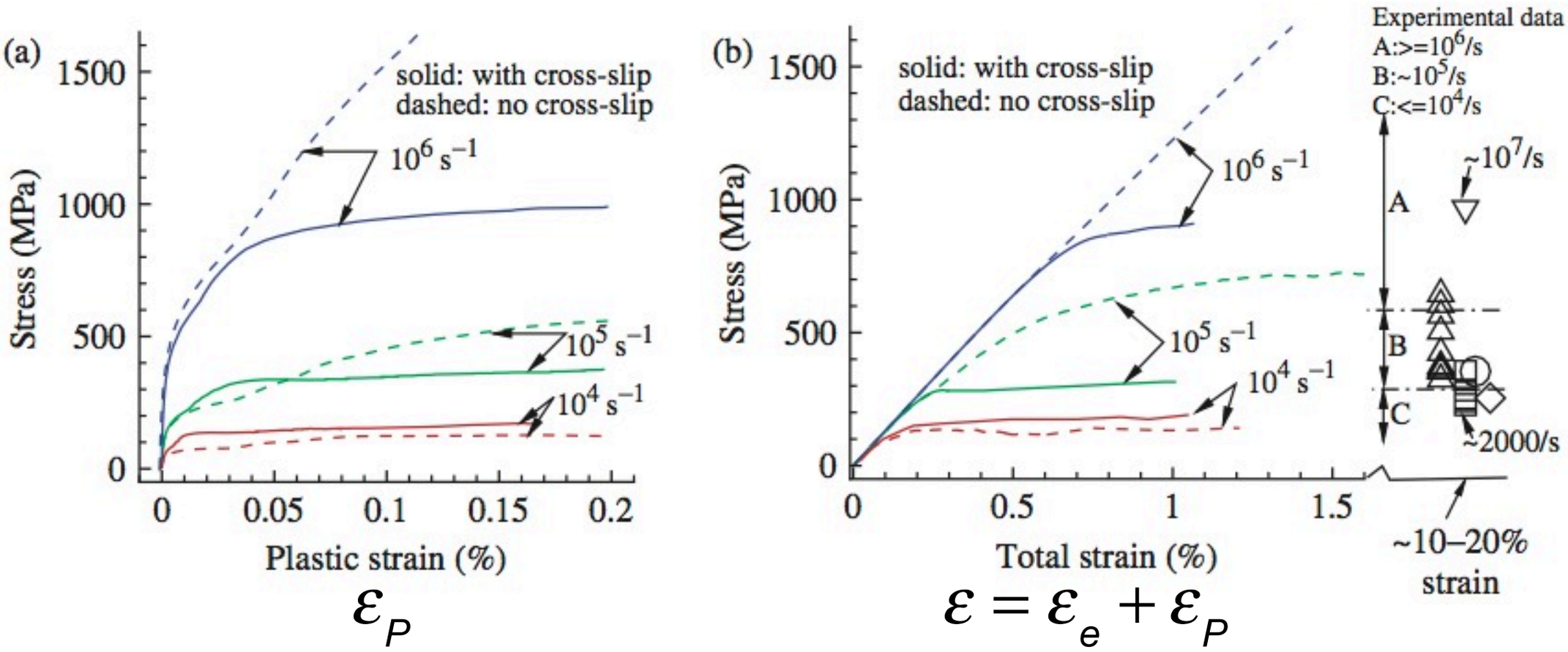


- slip bands are approximately 0.2 μm wide
- band spacing varies between 0.1-1 μm
- spacing between fine bands within bands is 0.01 μm



81

hardening



- high-rate behavior differs from that at low rates, which is controlled by obstacles and thermal activation
- *essentially all dislocations are glissile*
- slip bands act as “deformation highways”: processes in slip-band formation are the dominant deformation mechanisms

  What is the effect of the boundary conditions?

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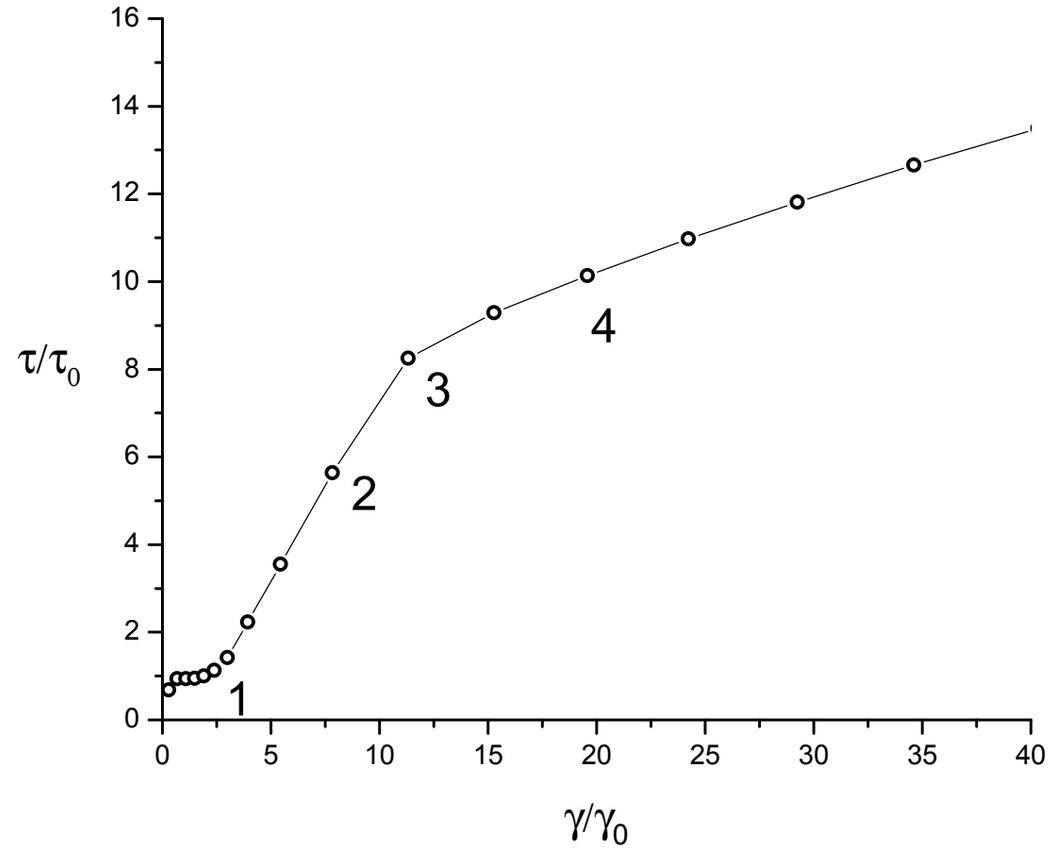
3. stage II hardening by DD simulations

Kubin et al. used DD to examine the hardening rate based on calculating the mean free path of the dislocations along various slip planes (replacing dependence on experiment in Kocks model), assuming uniform densities per slip system.

Application to various metals at room temperature:

- they obtain qualitative, but not quantitative agreement with experiment.
- in many ways a 2D model (mean free path on different slip systems)



Kubin, Devincre, and Hoc, Intl. J. Mater. Res. (2009).
Devincre, Hoc, Kubin, Science 320, 1745 (2008)

Model not essentially different from the 2D phase-field modeling of Koslowski et al., PRL 93, 265503 (2004)

stage II: their conclusions

1. they have not solved stage II, though they made progress

2. they believe that it is possible

3. they cannot predict the transition between stages

“There is presently no generally accepted theory explaining how and why organized dislocation microstructures emerge during plastic flow.” Kubin, Devincre, and Hoc, Intl. J. Mater. Res. (2009).

IV. some more examples

- **strain hardening**: e.g., Kubin and coworkers mapped out aspects of Stage II strain hardening in *fcc* crystals, Devincre, Hoc, and Kubin, Science **320**, 1745 (2008); Kubin, Devincre, and Thierry, Intern. J. Mater. Res. **100**, 1411 (2009).

- **fatigue**: Fivel and coworkers applied 3D dislocation simulations to the early stages of fatigue, with applications to fatigue in: steel [Déprés, Robertson, and Fivel, Phil. Mag. **84**, 2257 (2004); *ibid.* **86**, 79 (2006)], *fcc* materials [Déprés, Fivel, and Tabourot, Scripta Mater. **58**, 1086 (2008)], and precipitation hardened materials [Shin, Robertson, and Fivel, Phil. Mag. **87**, 3657 (2007)]

- **silicon**: see work from K. W. Schwarz, for example, with PARANOID code

- Others of note: Weygand/Gumbsch/... : many calculations, including small-scale plasticity

Outlook and needs

Summary of some of the approximations

- all atomistic-based processes described with models
- most codes ignore partial dislocations
- interactions are long-ranged
- most materials are anisotropic not isotropic
- we ignore the effects of lattice rotations caused by the dislocations (except as a post-process)
- boundary conditions are a challenge, with the modeling of bulk plasticity being much more challenging than modeling of small-scale plasticity
- ...
- *we need more sensitive tests to tell us what is and is not important. Structures matter so microscopy is key.*

Outlook for calculating bulk mechanical properties

- Simulations are limited by: size, boundary conditions, and all the approximations mentioned above.
- Limited success for DD in modeling dislocation substructure development.
- Thus, prediction of hardening has not been possible.
- “The present dislocation-based models for strain hardening still have difficulties integrating elementary dislocation properties into a continuum description of bulk crystals or polycrystals. As a consequence, current approaches cannot avoid making use of extensive parameter fitting.” - Devincre, Hoc, Kubin, Science 2008.

Needs

- Better connection to experiment: "The feedback loop between theory, simulation and experiment for plasticity and property modeling," T. M. Pollock and R. LeSar, Current Opinion in Solid State and Material Sciences 17, 10-18 (2013).
- As noted above, we need to link to experimentally measured dislocation substructures
- We will do this in collaboration with Marc DeGraef, using methods he discussed Monday
- With better connection to experiments (esp. structure), we should be able to examine the "correctness" of the predictions, which can guide the development of better models.

(S)TEM Defect Simulations

Darwin-Howie-Whelan equations:

$$\frac{\mathrm{d}S_{\mathbf{g}}(z)}{\mathrm{d}z} = 2\pi \mathrm{i} s_{\mathbf{g}} S_{\mathbf{g}}(z) + \mathrm{i}\pi \sum_{\mathbf{g}'}{}' \frac{e^{-\mathrm{i}\alpha_{\mathbf{g}-\mathbf{g}'}(\mathbf{r})}}{q_{\mathbf{g}-\mathbf{g}'}} S_{\mathbf{g}'}(z)$$

Displacement field

$$\frac{1}{q_{\mathbf{g}}} \equiv \frac{1}{\xi_{\mathbf{g}}} + \mathrm{i}\frac{e^{\mathrm{i}(\theta'_{\mathbf{g}}-\theta_{\mathbf{g}})}}{\xi'_{\mathbf{g}}} \qquad \alpha_{\mathbf{g}}(\mathbf{r}) \equiv 2\pi \mathbf{g} \cdot \sum_{i=1}^{N_d} \mathbf{R}_i(\mathbf{r}) = 2\pi \mathbf{g} \cdot \mathbf{R}_t(\mathbf{r})$$

Extinction distance — Absorption length

Reformulate as a matrix problem:

Scattering matrix

$$\frac{\mathrm{d}\mathbf{S}(z)}{\mathrm{d}z} = \mathrm{i}\mathcal{A}(\mathbf{r})\mathbf{S}(z) \longrightarrow \mathbf{S}(\epsilon) = e^{\mathrm{i}\mathcal{A}\epsilon}\mathbf{S}(0) = \mathcal{S}(\epsilon)\mathbf{S}(0)$$

Propagation = scattering matrix product

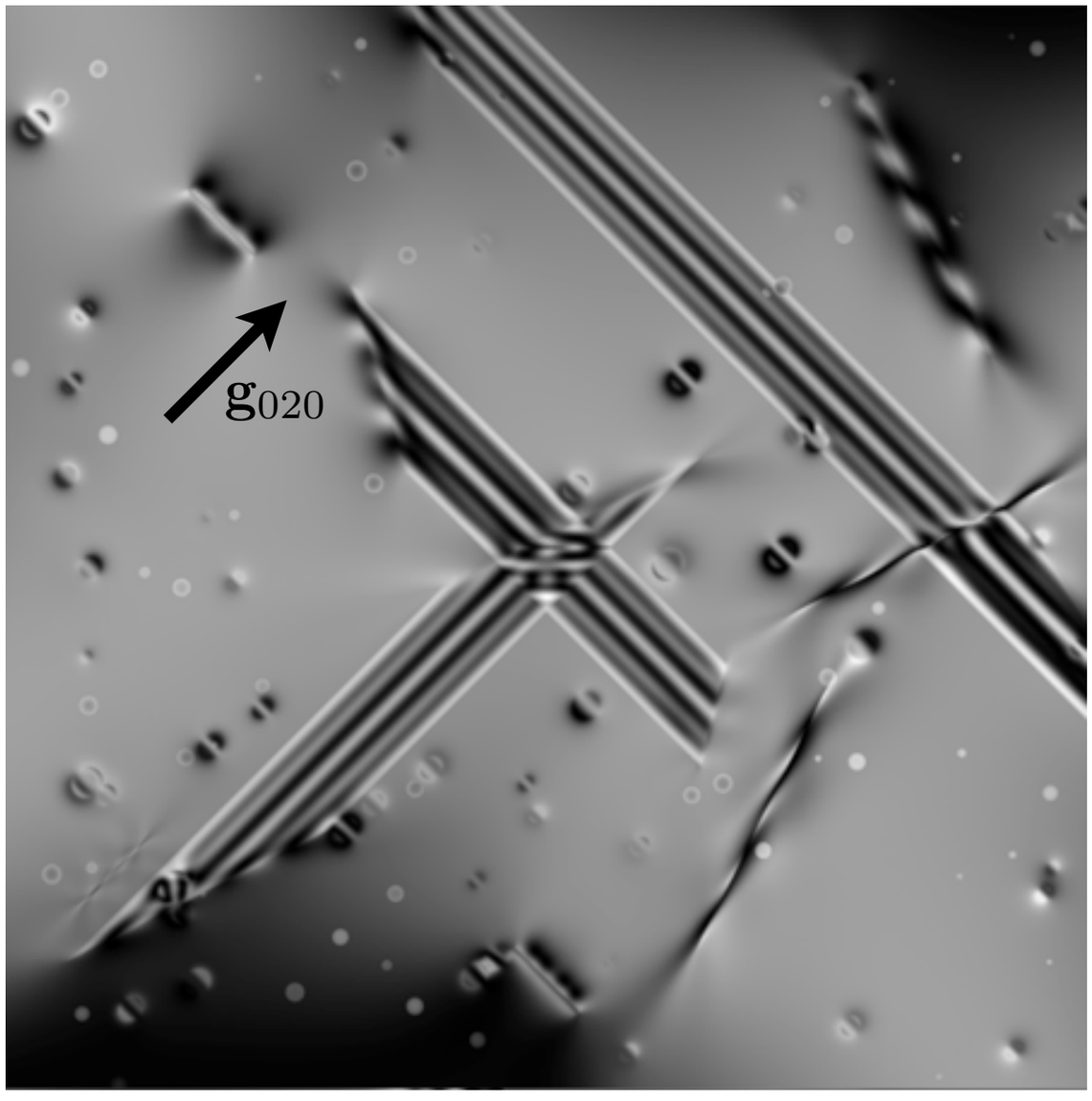
From: Marc De Graef

$$\mathbf{S}(z) = \mathcal{S}(z_m)\mathcal{S}(z_{m-1})\cdots\mathcal{S}(z_2)\mathcal{S}(z_1)\mathbf{S}(0)$$

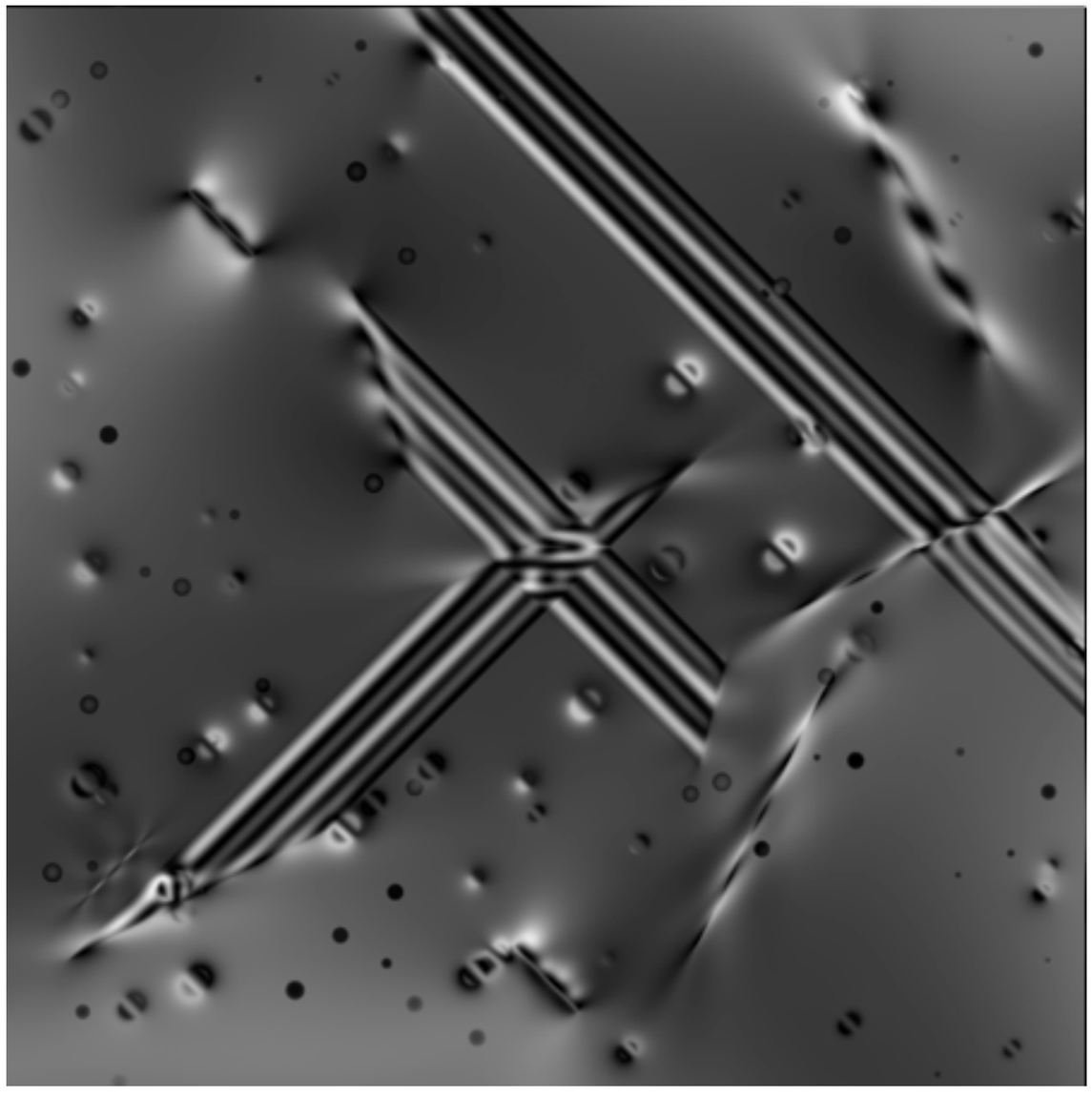
Example
parallel illumination

From:
Marc De Graef

fcc-Al, 200 keV
100 nm foil, "slightly bent"
6 perfect dislocations, 3 stacking faults
50 spherical voids, 50 spherical inclusions
(020) systematic row, 9 beams



bright field



dark field

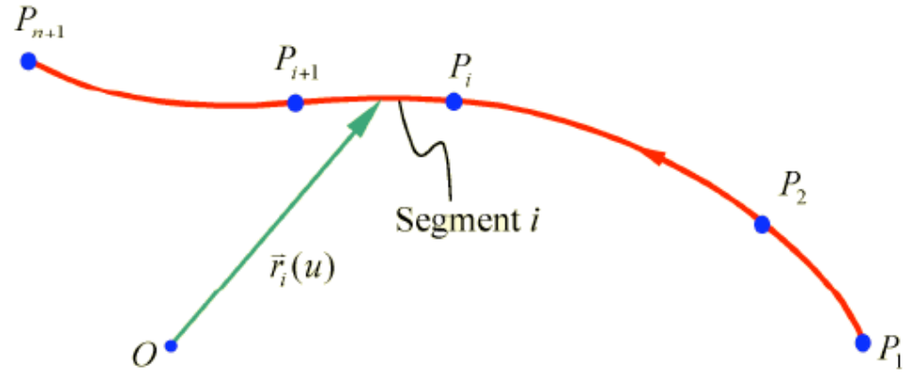
Calculated (S)TEM results

- calculation of the displacements

$$u_i\left(\vec{R}\right) = -\frac{b_i\Omega}{4\pi} + \frac{1}{8\pi}\oint\left[\varepsilon_{ikl}b_l R_{,pp} + \frac{1}{(1-\nu)}\varepsilon_{kmn}b_n R_{,mi}\right]d\ell'_k$$

$$R_{,ij} = \frac{\partial^2 R}{\partial X_i \partial X_j}$$

$$\oint f(r)d\ell \rightarrow \sum_{\alpha=1}^{N_{segment}}\sum_{q=1}^{N_{int}} w_q f(r_{\alpha q})$$



- Complication: Ω is discontinuous in dislocation plane.
- From displacements, we will calculate the expected STEM signal, enabling us to better compare with data.

acknowledgements

who did the work:

- Caizhi Zhou, MUST
- Zhiqiang Wang, U. North Texas
- Irene Beyerlein, Los Alamos
- Sriram Swaminarayan, Los Alamos
- Marisol Koslowski, Purdue University

collaborators:

- Nasr Ghoniem, UCLA
- Dennis Dimiduk and coworkers, Air Force Research Laboratory

Questions?