Simulation of Ductile Yield and Plastic Deformation: Size/Rate/Temperature Effects

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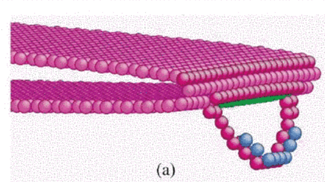
Questions about dislocation nucleation at a crack tip:

Should we expect Arrhenius behavior?
Is there only one relevant energy barrier?
How does the activation energy depend on stress intensity factor?

T. Zhu, J. Li, S. Yip, PRL 2004

Calculated activation energy for half-loop nucleation in Cu at one value of the applied load

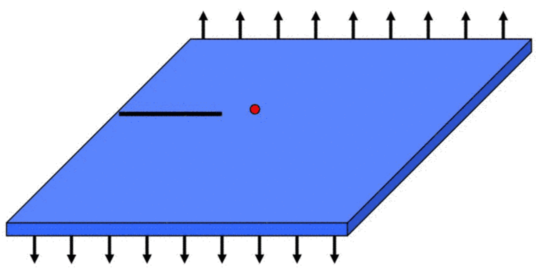


Our approach:

Simulate repeated emission events at different values of T, load
Determine activation energy from an Arrhenius plot
Includes effects of both nucleation and mobility

Strategy: simulate in 2-d, then compare with analytical solution

Consider problem in two dimensions...



Crack in a finite thin strip
Loaded in mode III
Screw dislocations nucleate
as points at crack tip

Apply subcritical load
$\rightarrow$ at T=0, no nucleation
$\rightarrow$ at T>0, thermal activation

Dislocations nucleate at crack tip, annihilate on opposite free surface

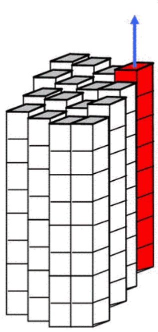
Idealized molecular dynamics:

- antiplane displacements only- 2-d strain field z(x,y)

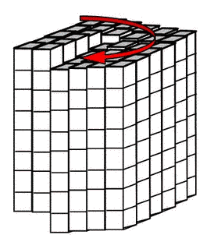
- idealized simple potential between columns

$$H = \sum_{<i,j>} -K_{ij} \cos\left(\frac{z_i - z_j}{a}\right) + \frac{1}{2} m \sum_i \left(\frac{dz_i}{dt}\right)^2$$

Potential Kinetic



2-d strain field



Screw dislocation

System can only contain straight screw dislocations;
no loops or half-loops

Screw dislocation nucleates as straight line

Idealized molecular dynamics:

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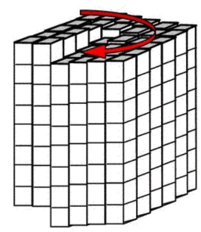


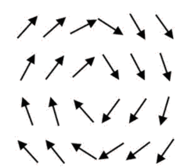
Screw dislocation

This is just the XY "rotor" model

$$H = \sum_{<i,j>} -K_{ij} \cos(\theta_i - \theta_j) + \frac{1}{2} I \sum_i \left(\frac{d\theta}{dt}\right)^2$$

Column height z_i maps to XY spin orientation θ_i

Screw dislocation maps to a vortex



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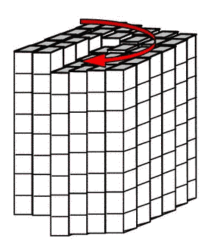

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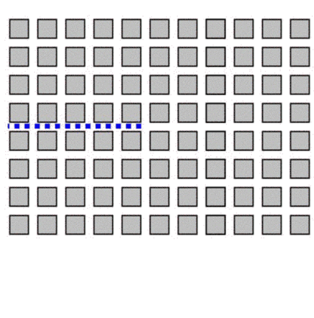
$$H = \sum_{<i,j>} -K_{ij} \cos(\theta_i - \theta_j) + \frac{1}{2} I \sum_i \left(\frac{d\theta}{dt}\right)^2$$

Top view



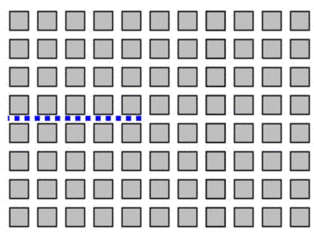
Introduce a crack by setting the interaction K_{ij} =0 on broken bonds

…no elastic interaction between columns on opposite sides of crack

- Derive eqn. of motion from Hamiltonian
- Load forces applied at edges of cell
- Apply thermostat on edges of cell
- Other bonds cannot break

→ Crack can only emit pure screw dislocations
→ Crack cannot extend
→ Pure, ideal ductile response

Top view



Introduce a crack by setting the interaction $K_{ij}=0$ on broken bonds

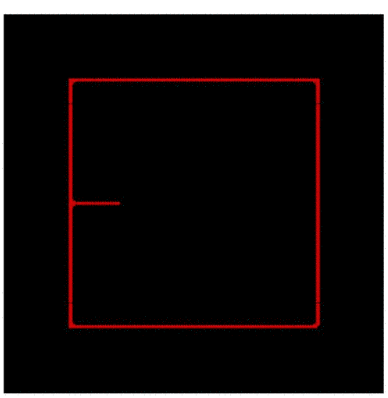
…no elastic interaction between columns on opposite sides of crack

100 x 100, crack length =20

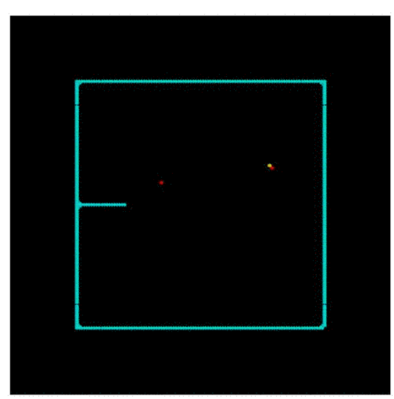
Low temperature

Defects nucleate one at a time at the crack tip

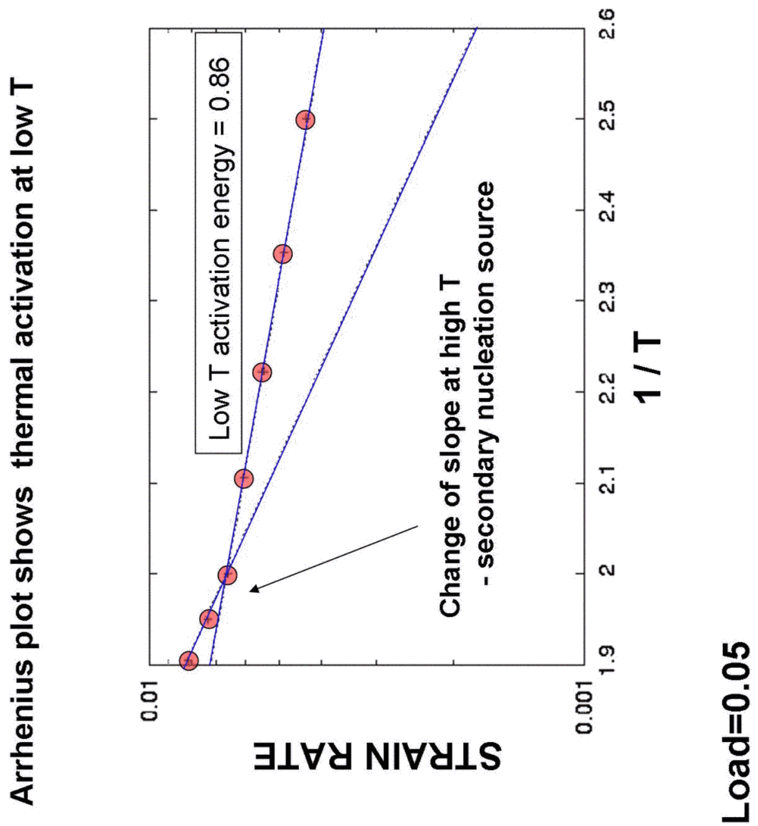
High temperature
(Note: $T_{KT}=0.895$)
Nucleation rate limited by mobility
Occasional nucleation at wall

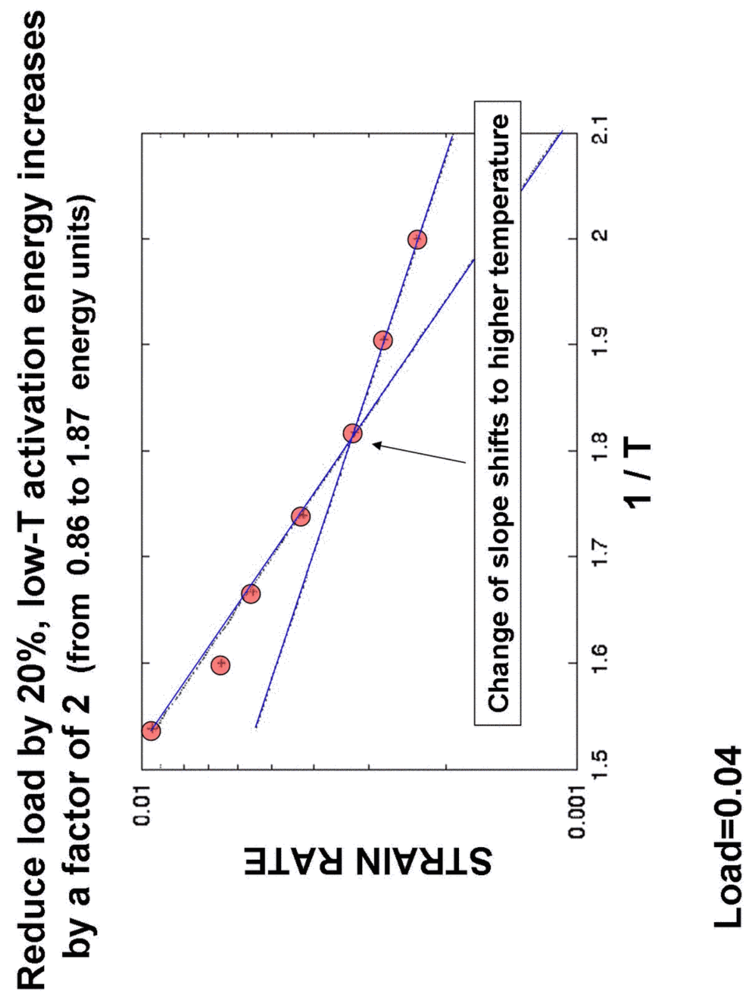


T = 0.35



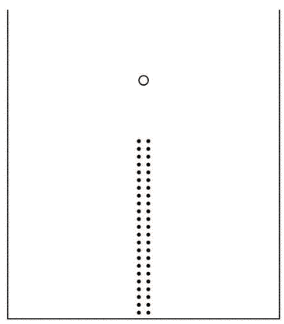
T = 0.5


Arrhenius plot shows thermal activation at low T
Low T activation energy = 0.86
Change of slope at high T
- secondary nucleation source
STRAIN RATE
0.01
0.001
1.9
2
2.1
2.2
2.3
2.4
2.5
2.6
1 / T
Load=0.05


Reduce load by 20%, low-T activation energy increases
by a factor of 2 (from 0.86 to 1.87 energy units)
Change of slope shifts to higher temperature
STRAIN RATE
0.01
0.001
1.5
1.6
1.7
1.8
1.9
2
2.1
1 / T
Load=0.04

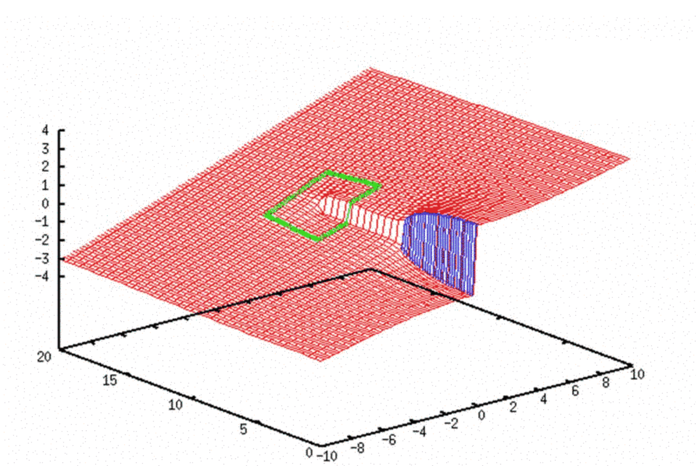
2-d analytical calculation: dislocation escape from crack tip

Need to know the effective potential experienced by a screw dislocation near a crack tip at Temperature=0, under shear load



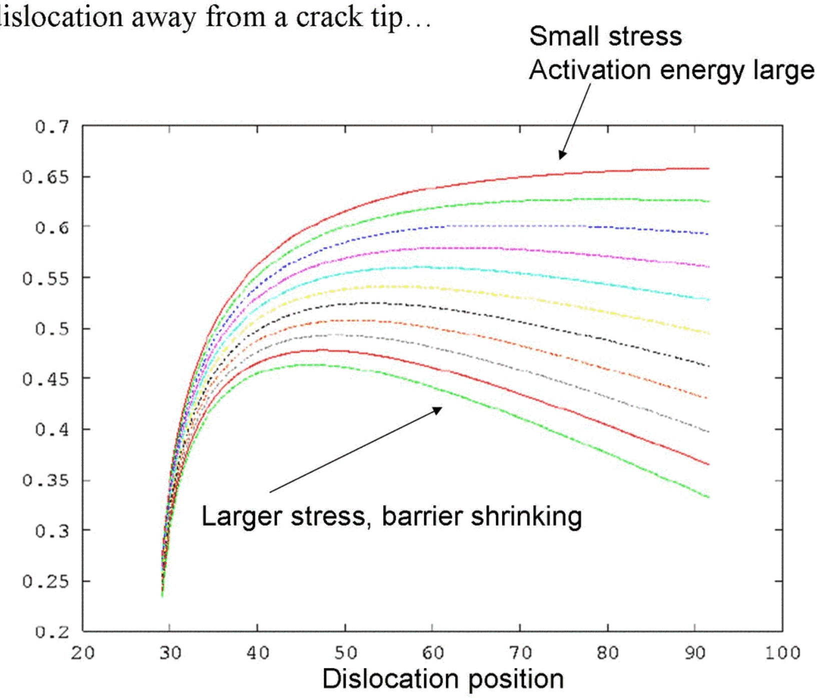
Solve via conformal mapping

Work by Sergio Picozzi



Analytical solution for screw dislocation near a crack tip in a strip with a sharp crack—from conformal mapping calculation

Pulling a dislocation away from a crack tip…

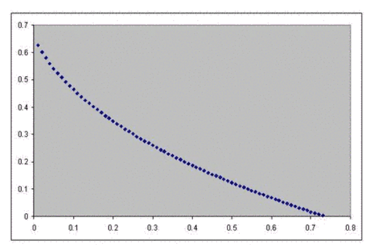


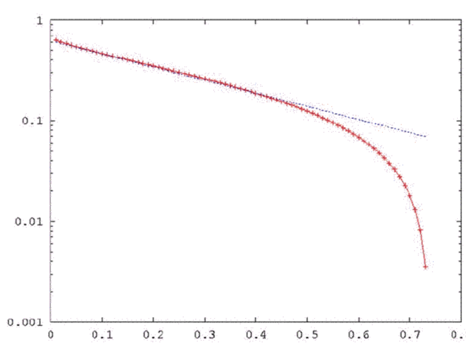
For large enough stress, barrier vanishes entirely.

Result from analytic calculation:

Barrier drops exponentially with load

-- activation volume not well defined
-- stress at crack tip also not well defined!





Energy barrier $\sim e^{-\alpha \cdot load}$

What we learned:

-2-d dislocation nucleation rate at a crack tip shows Arrhenius behavior; slope changes when secondary source activated

- Activation energy highly sensitive to applied stress intensity factor
  … increased by factor of 2 when load reduced by 20%

- Concept of activation volume not well defined
  (Not big surprise; stress at crack tip not well defined either)

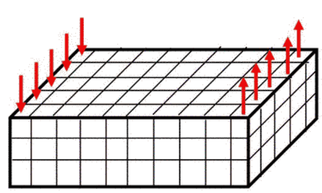
- Analytical calculation suggests that energy barrier drops exponentially with applied load

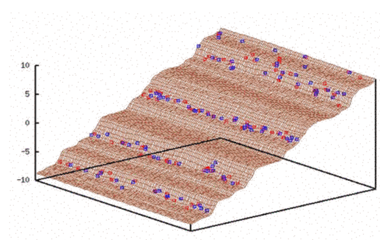
Still to figure out:

Does this tell us anything new about nucleation in 3-d???

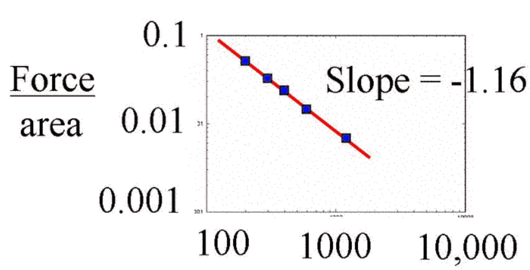
Good model for nucleating vortices from a notch in a superconducting thin film?

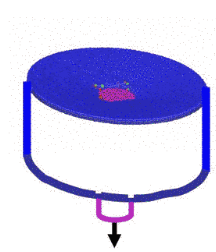
Other fun things to do with this idealized model….





Formation of shear bands

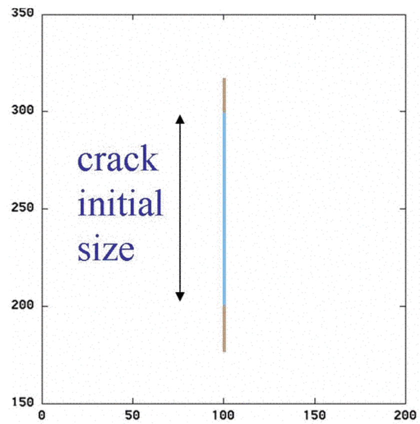




Size effects in plastic flow

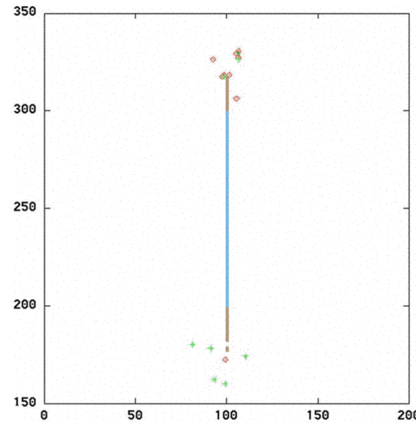
If add bond-breaking rules, apply constant strain rate, see brittle-ductile transition– “toy model”

Low T, high strain rate



Brittle—just bond breaking

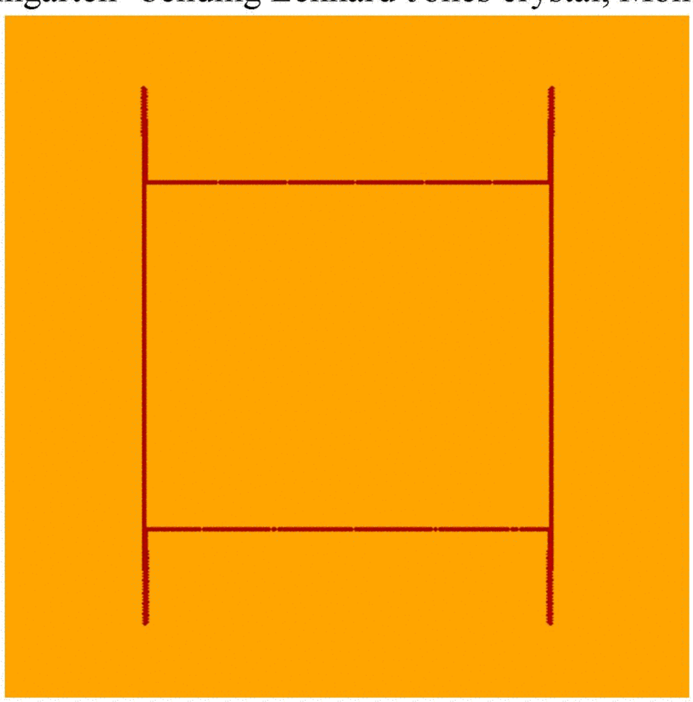
High T, low strain rate

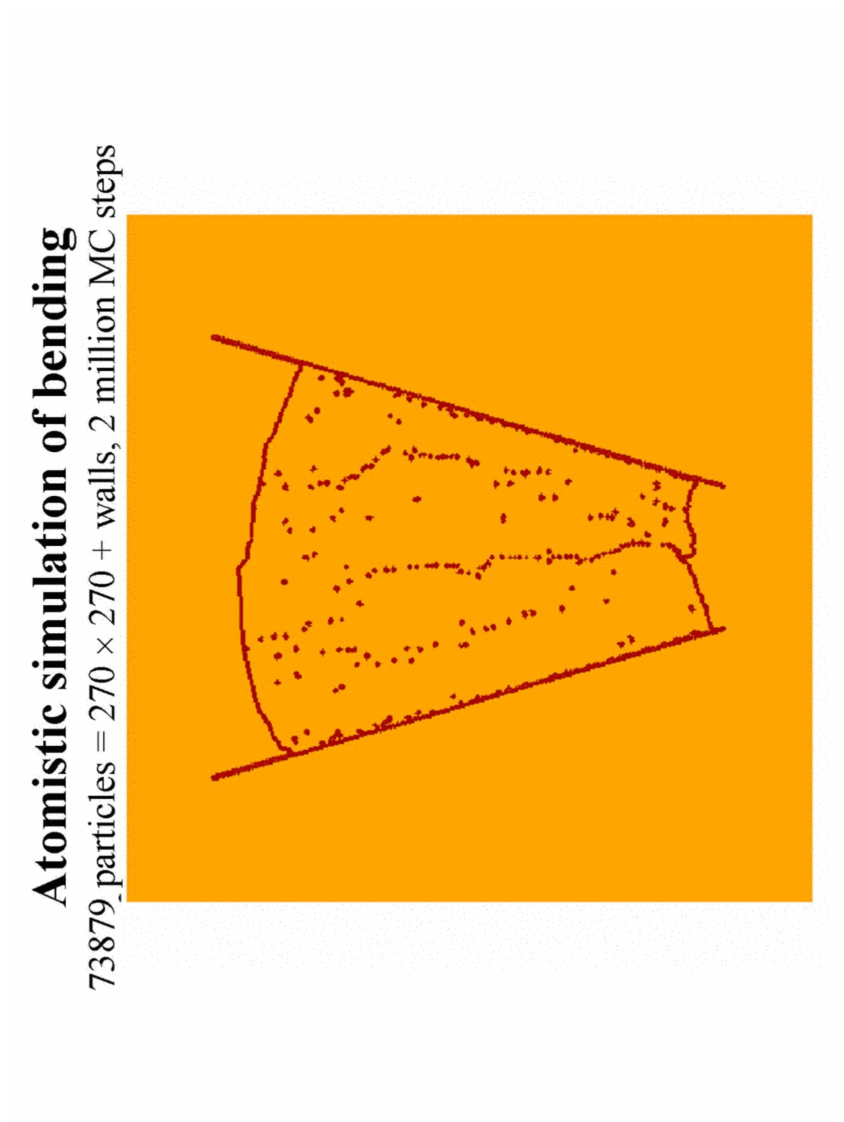


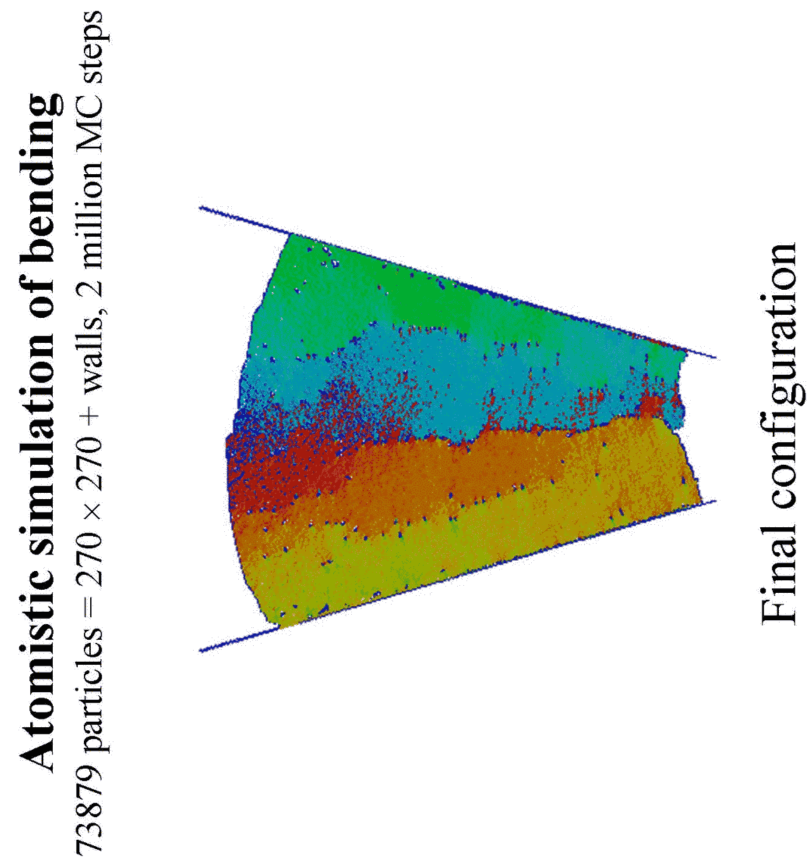
Ductile—crack arrests, emits dislocations; new cracks nucleate ahead of crack tip, coalesce

Dislocation patterning in 2-d

Scott Weingarten--bending Lennard-Jones crystal, Monte Carlo




Atomistic simulation of bending
73879 particles = 270 × 270 + walls, 2 million MC steps

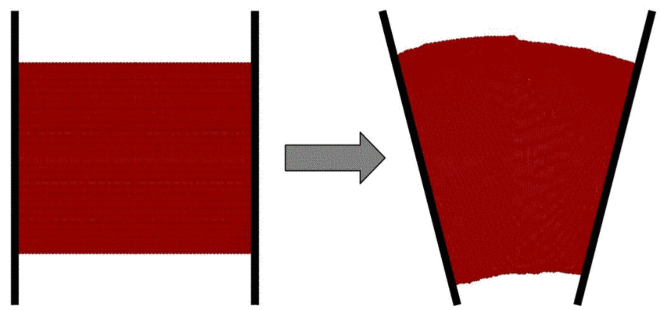

Atomistic simulation of bending
73879 particles = 270 × 270 + walls, 2 million MC steps
Final configuration

Simulation Technique

- 2-D Lennard-Jones single crystal, triangular lattice
- Rigid walls rotate, apply compressive strain
- System evolves via off-lattice Monte Carlo (Metropolis algorithm)
- Effective strain rate depends on MC steps per bend increment

Why Monte Carlo?

- System is always driven toward thermal equilibrium
- No thermal gradients or shockwaves
- No momentum, dislocation motion always overdamped

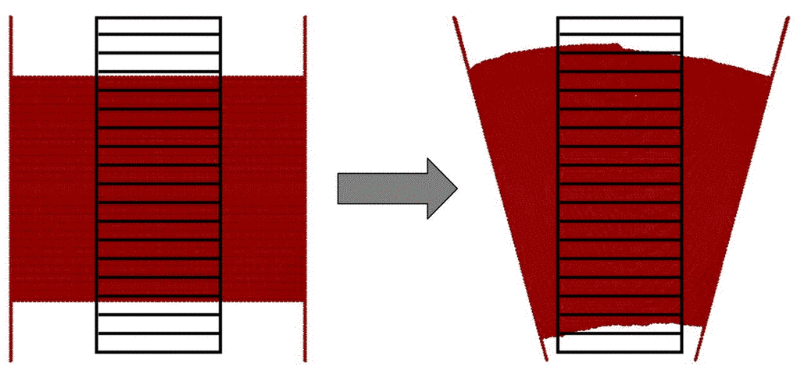


Mechanical Response quantified via calculation of the Bending Moment

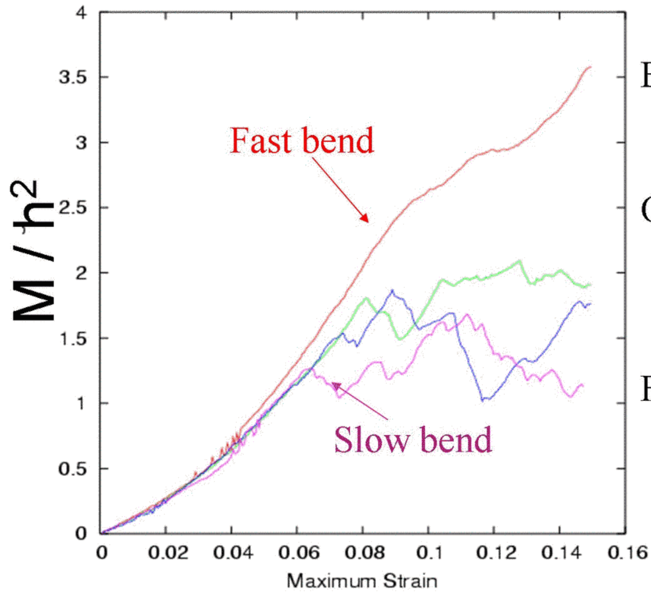
Bending moment: $M = \int \sigma_{xx}(y) y dy$

Stress calculated from interatomic forces in each layer, integrated numerically

Calculated using middle half of crystal, away from contact force:



Mechanical response depends on strain rate



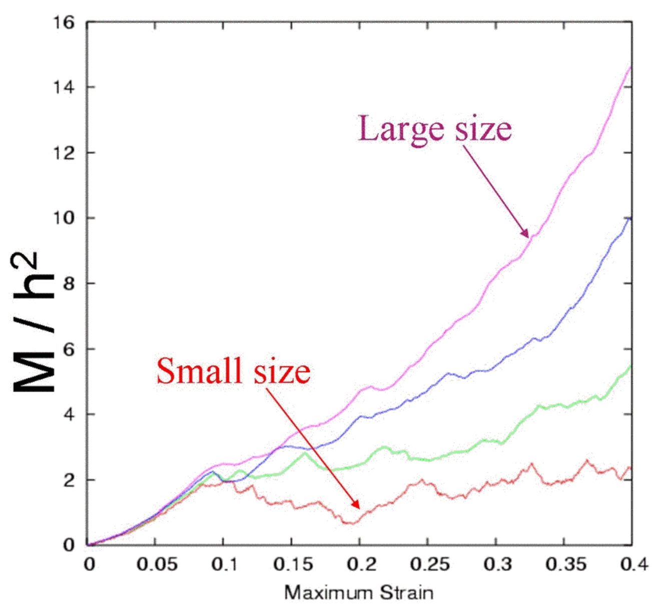
Bending moment vs. maximum strain

One crystal size, 73879 particles (270×270)+walls

Four different strain rates

Simulations approach (but don't reach) quasistatic limit

Size effect at constant strain rate: Inverse Size Effect



Bending moment vs. maximum strain

Four different crystal sizes

Same strain rate (number of MC steps/bend)

Results in an apparent REVERSE size effect: larger → stronger

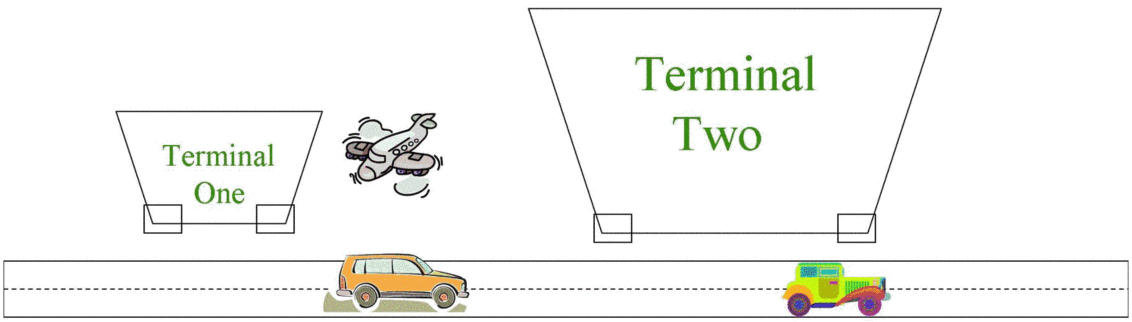
Inverse size effect in single crystal

If scale system size by a factor of 2 with same strain rate,
…should have 4 times as many total dislocations

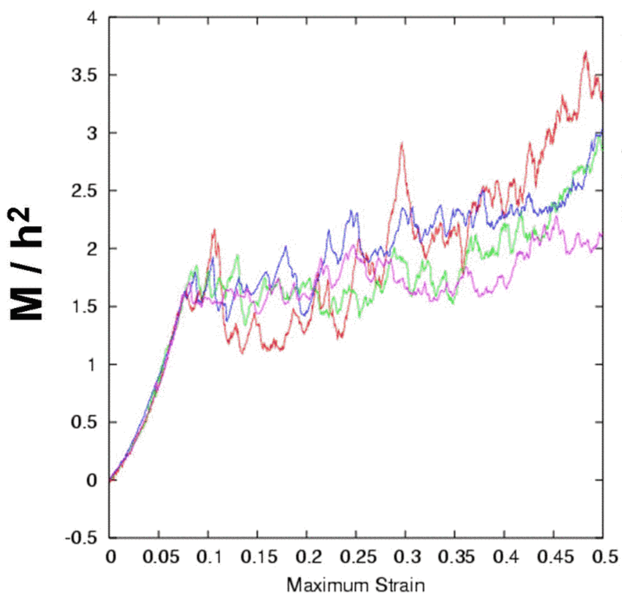
Dislocation nucleation rate at corners can't rise by a factor of 4

Larger system has too few dislocations → stress rises
→ higher bending moment

Inverse size effect due to dislocation "starvation"



Size effect disappears when steps/bend scaled with area: increase atoms by 4, increase cpu time by 16



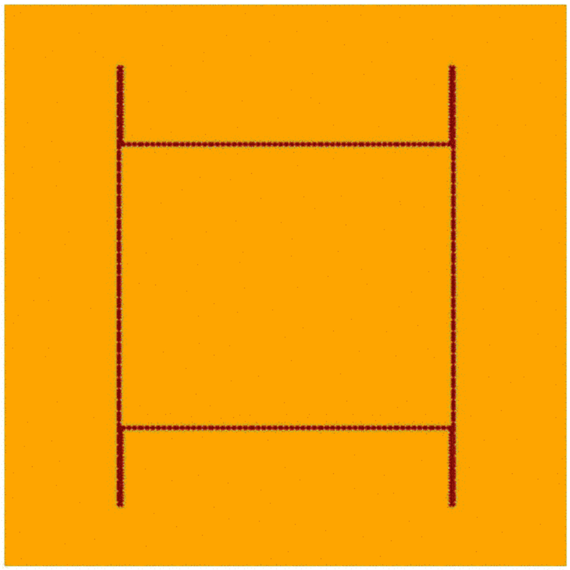
Bending moment vs. maximum strain

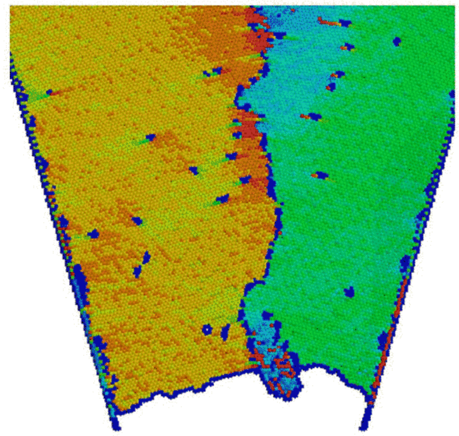
Number of MC steps/bend scaled to area:

Particles	Steps/Bend
90 × 90	25
180 × 180	100
270 × 270	225
360 × 360	400

No Size Effect!!!

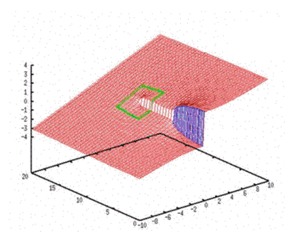
Grain ejection… hillock formation?



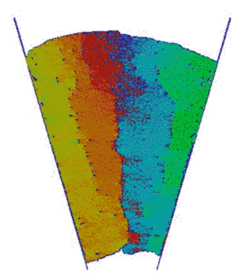


Mechanics of materials in 2-d

Even without entanglement and other 3-d effects, we get…

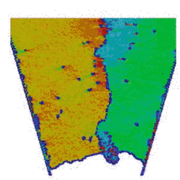


- Thermal activation at a crack tip
  - Arrhenius behavior
  - Change of slope with activation of secondary source
  - Analysis--Activation energy drops exponentially with load



- Dislocation patterning
  - shortage of sources → reverse size effect
    - size effect goes away when strain rate scaled

- Grain boundary instability
  - hillock formation/grain ejection



Question for future work…

Is coalescence of dislocations into grain boundaries a phase transition?