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Predicting fatigue crack initiation in metals using dislocation dynamics simulations

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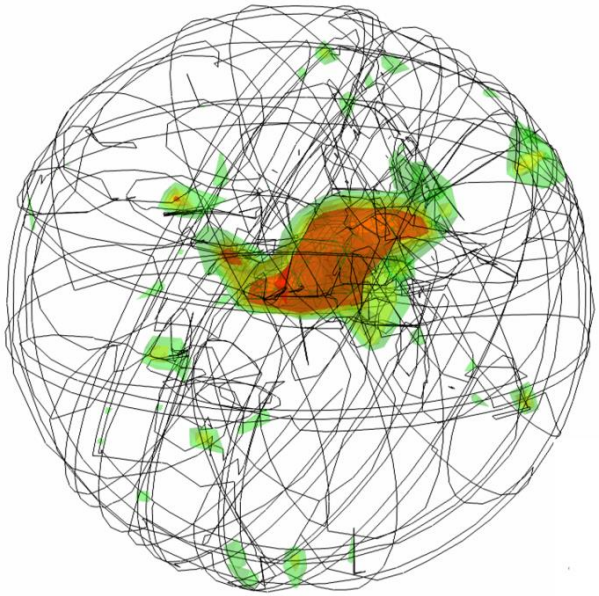
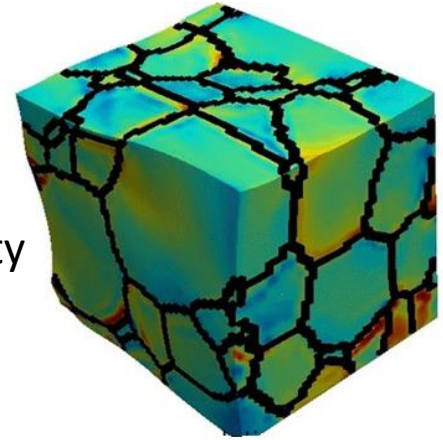
International Workshop on the Environmental Damage in Structural Materials Under Static Load/Cyclic Loads at Ambient Temperatures
May 31, 2016

Agenda

1. Problem statement
2. Energy based theories
3. 3D Cyclic Dislocation dynamics
4. Energy in dislocation networks
5. Multi-scaling: Efficiency factor and crystal plasticity



3D cyclic dislocation dynamics



Crystal plasticity

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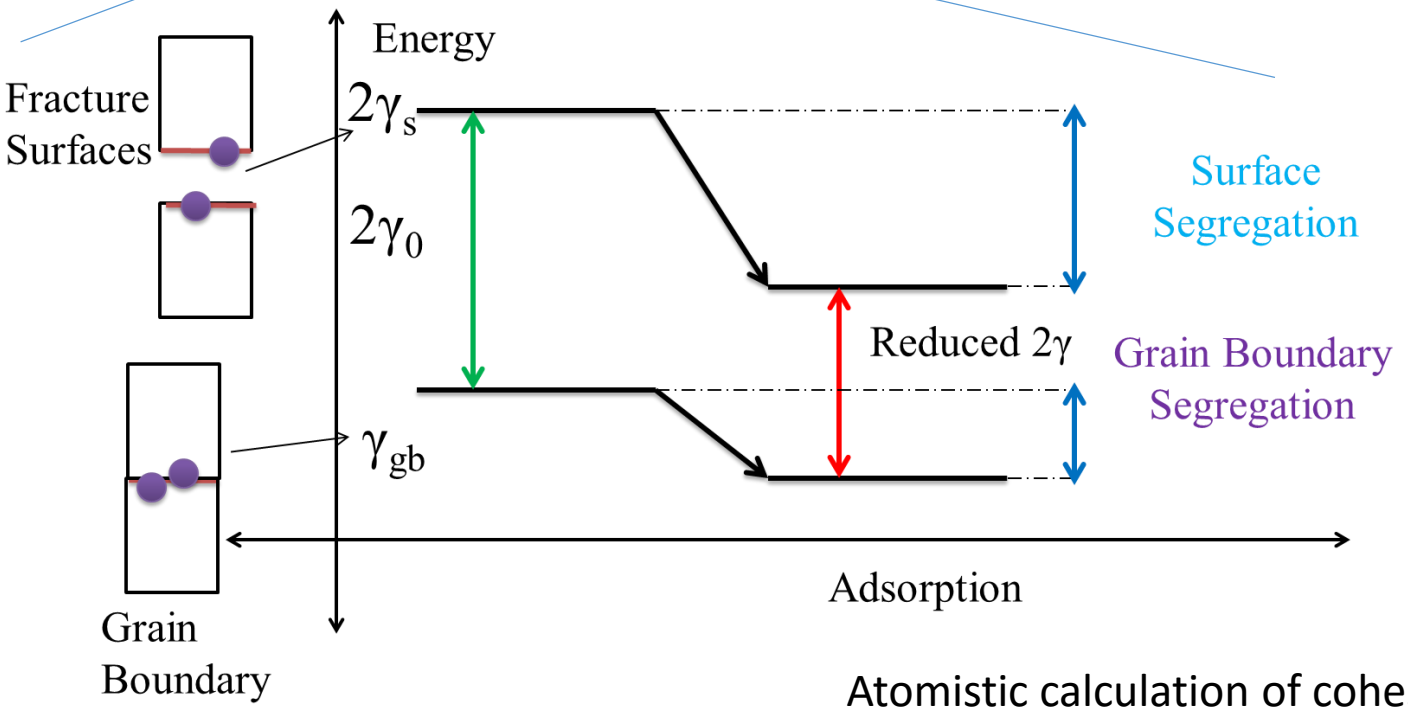
Energy model of fracture

$$G = 2\gamma - E_{el} + \gamma_p$$

Energy model of fracture

Chemistry

$$G = 2\gamma - E_{el} + \gamma_p$$



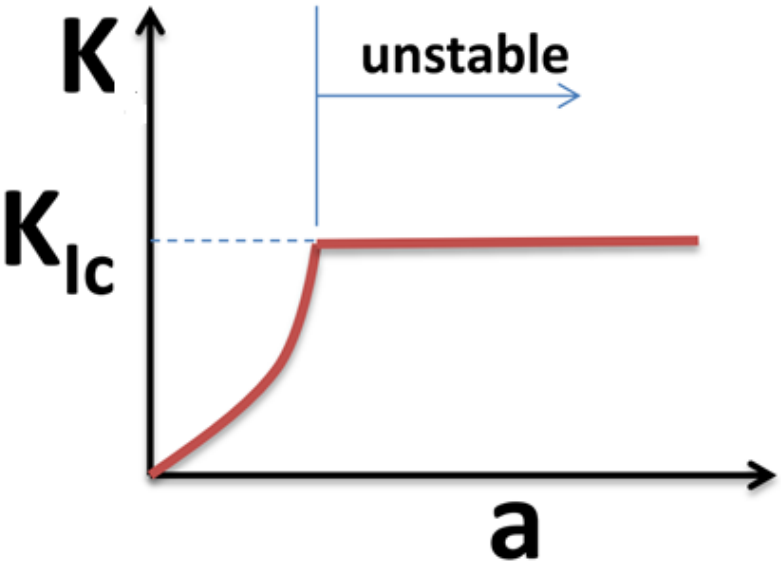
Atomistic calculation of cohesive energy

Energy model of fracture

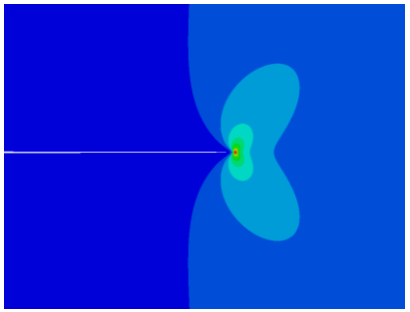
Mechanics

$$G = 2\gamma - E_{el} + \gamma_p$$

Elastic energy release rate (LEFM)



$$E_{el} = (1 - \nu)\frac{K^2}{2\mu}$$



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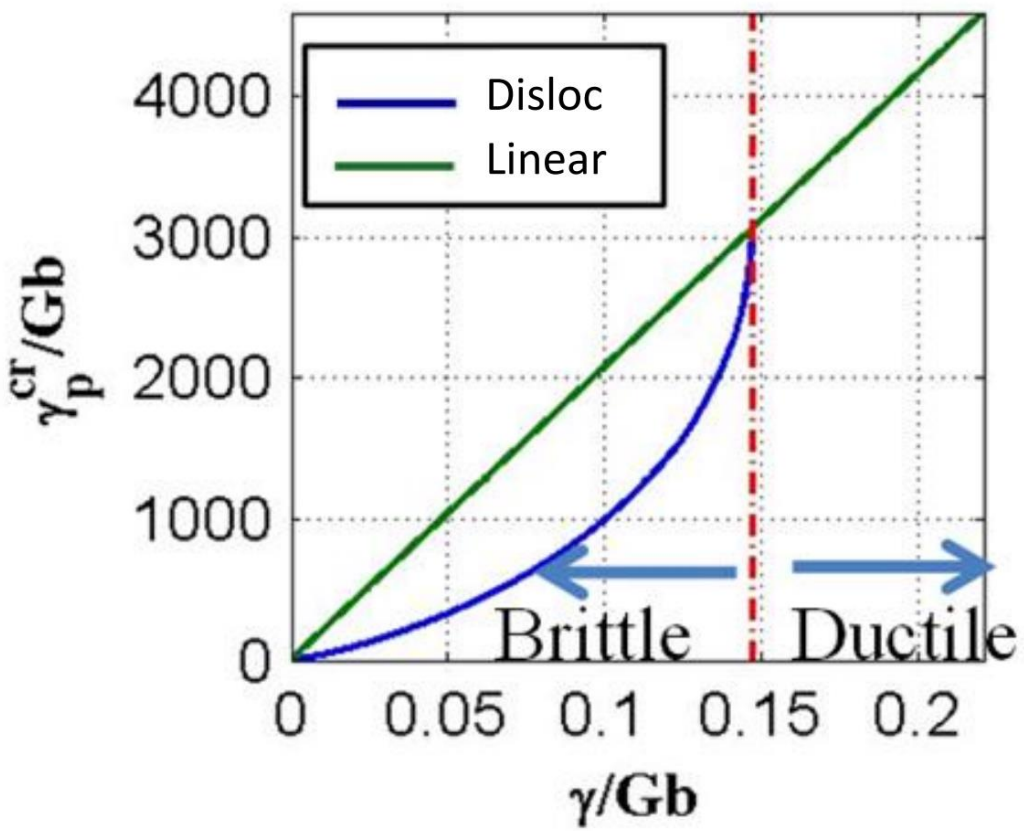
Energy model of fracture

$$G = 2\gamma - E_{el} + \gamma_p$$

- There is no "first principles" model to predict γ_p (yet)
- γ_p = stored energy (eg. Dislocation structure) + heat energy
- Most of the energy is heat (>95%).

Energy model of fracture

$$G = 2\gamma - E_{el} + \gamma_p$$



Plastic work can be estimated from experiments (2γ: DFT, E_{el}: Experiments, G=0 at fracture), can be plotted in terms of γ (see my poster)

Incremental Energy Model

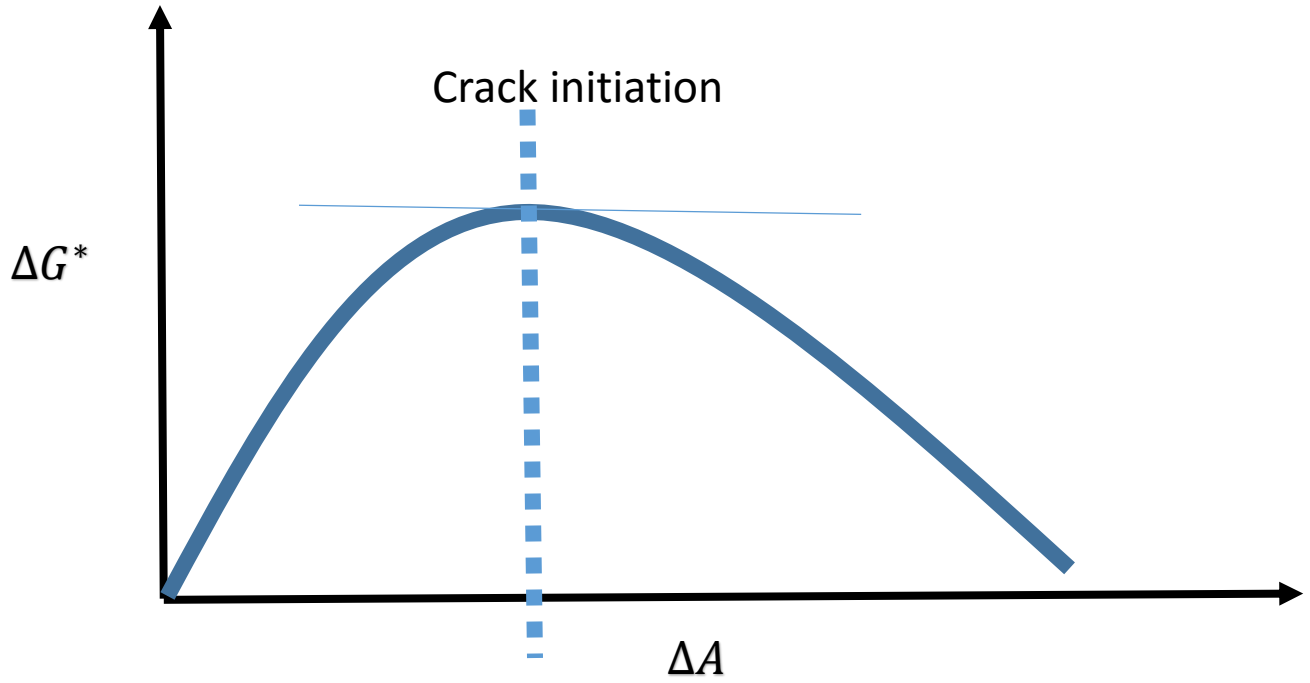
$$\Delta G^* = 2\gamma\Delta A - E_{el}^{\Delta A} - E_{stored} + \delta_{diss}$$

- Perform energy balance at the moment the crack forms
- Thermal dissipation neglected at that instant.
- The surface energy is balanced by the release of elastic energy and the removal of stored dislocations.
- Approach brings in crack size ΔA: not so popular!
- Terms are about the same order of magnitude

Mura and Nakasone, *A Theory of Fatigue Crack Initiation in Solids*, J. Appl. Mech., 57 (1990)

Incremental Energy Model

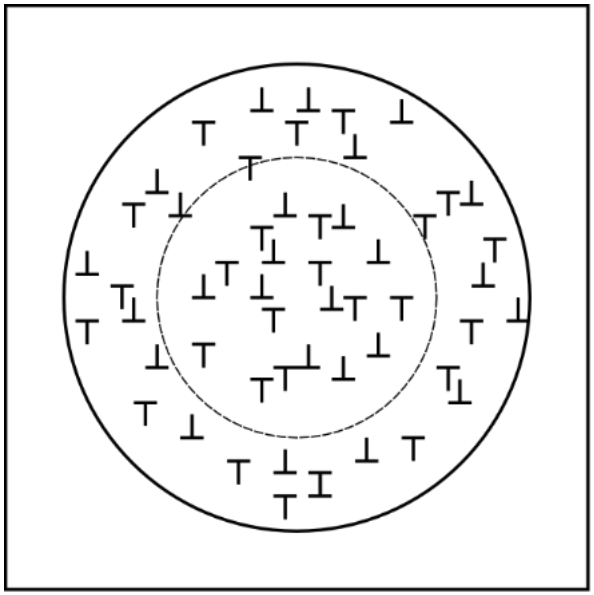
$$\Delta G^* = 2\gamma\Delta A - E_{el}^{\Delta A} - E_{stored} + \delta_{diss}$$

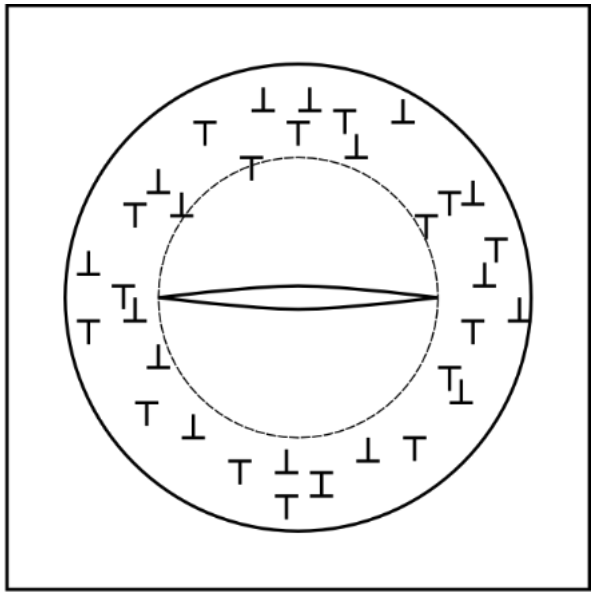


Mura and Nakasone, *A Theory of Fatigue Crack Initiation in Solids*, J. Appl. Mech., 57 (1990)

Increment in crack size

ΔA (crack area) is total length of dislocations times the Burger's vector

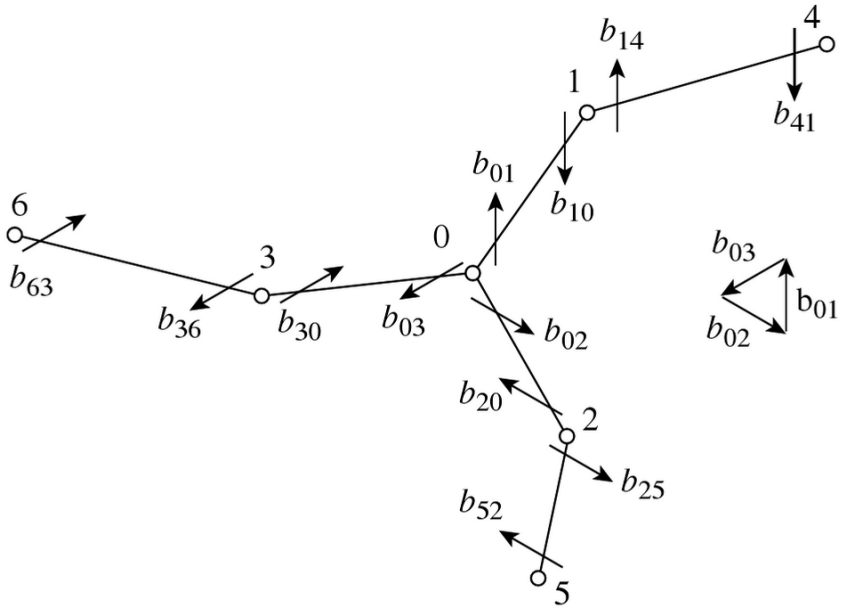




Dislocation dynamics can predict stored energy AND crack size.
Avoids difficulties associated with modeling thermal effects.

Dislocation Dynamics – General

- Only model the dislocation line – no atoms
- Discretize the dislocations into line segments, evolve using Peach-Kohler force
- Advantages:
  - DD: micrometers and microseconds vs Atomistic models: nanometers, nanoseconds
  - Can model at grain level, with slip reactions vs homogenized forms in crystal plasticity
- Disadvantages:
  - O(N^2)-Problem → high strain values (>1%) difficult to obtain
  - Topology of dislocations changes, causing continuous remeshing
  - Computationally expensive



[1] Bulatov, Vasily, Cai, *Computer Simulations of Dislocations*

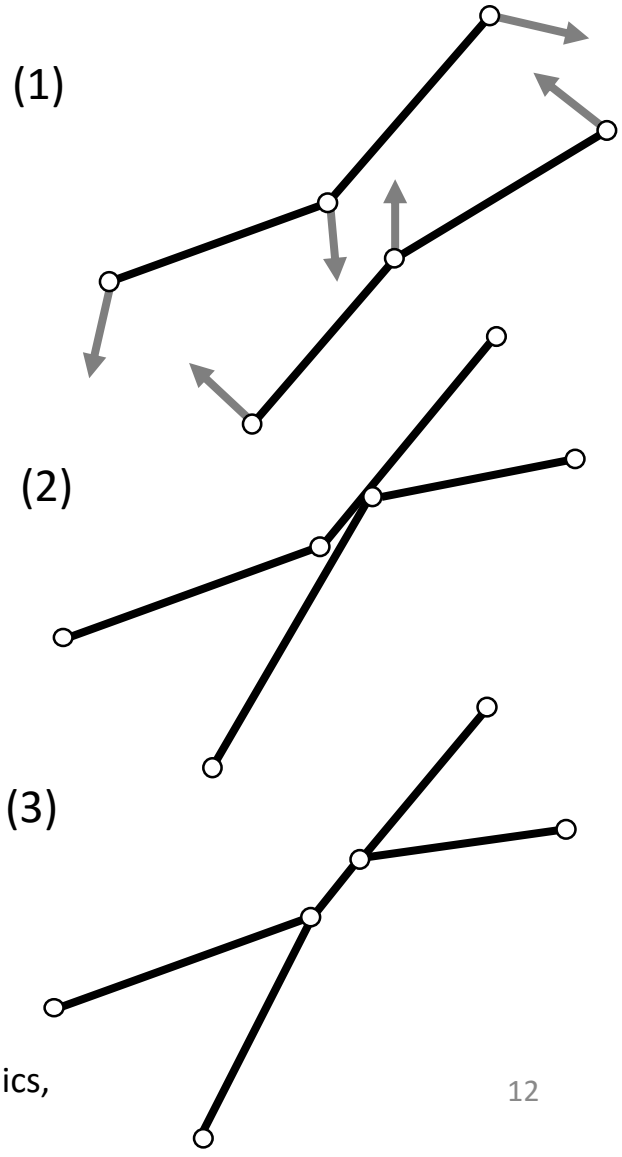
Dislocation Dynamics

- Steps for a DD calculation:
  1. Calculate the force on each node
  2. Move the dislocations according to a mobility function
  3. Apply topological changes: Split, Merge, Remesh
- Nodal force: elastic force + core-energy contribution

$$\mathbf{f}_i = -\frac{\partial E_{\text{tot}}(\{\mathbf{r}_i, \mathbf{b}_{ij}\})}{\partial \mathbf{r}_i}$$

$$E_{\text{tot}}(C) = E_{\text{el}}(C, r_c) + E_{\text{core}}(C, r_c)$$

- Elastic force is due to long range effects that can be captured from continuum mechanics
- Core energy due to local effects of highly distorted atoms close to dislocation, where continuum mechanics cannot be used



[1] Arsenlis et al., Enabling strain hardening simulations with dislocation dynamics, Modelling Simul. Mater. Sci. Eng., 15 (2007) 553-595

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Dislocation Dynamics

- Mobility function: velocity as function of force

$$\mathbf{v}_i = \mathbf{M}(\{\mathbf{f}_j\})$$

- Would lead to curved dislocation segments → invert, implicitly define velocity
- This represents motion in over damped regime

$$\mathbf{f}^{\text{drag}}(\mathbf{x}) = -\mathcal{B}(\boldsymbol{\xi}(\mathbf{x})) \cdot \mathbf{v}(\mathbf{x})$$

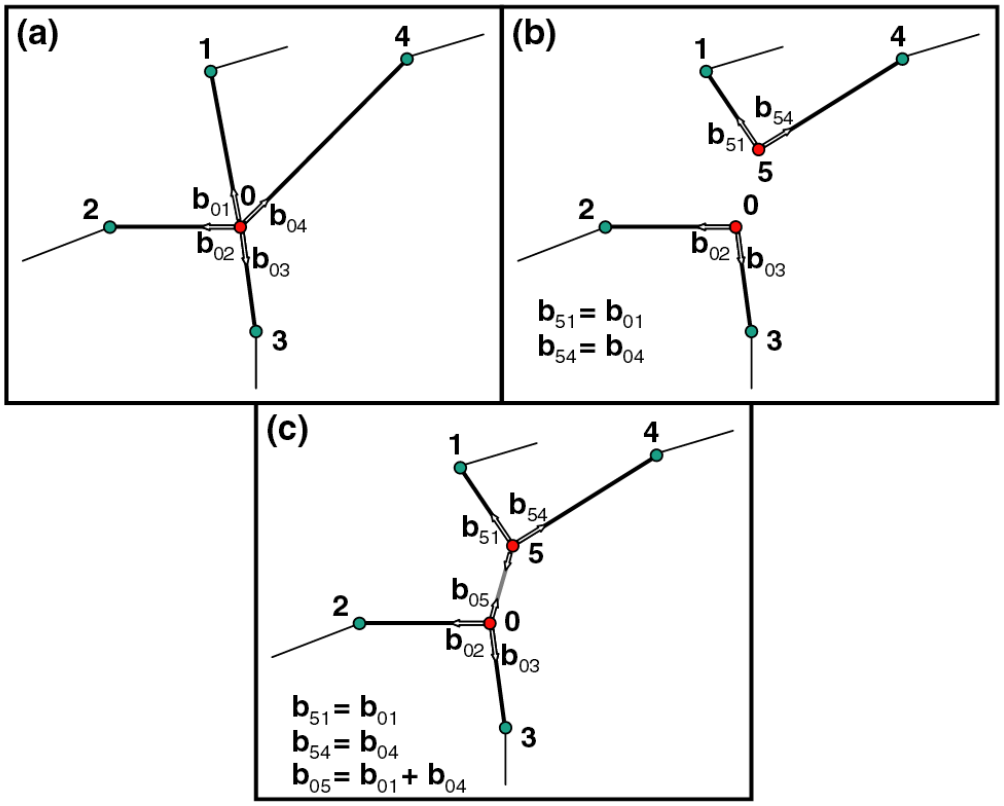
- The mobility functions are the material model of DD code (prefer certain glide planes over others …)
- With forces and velocities defined, calculate the next time step: $\boldsymbol{X}_i^{t+\Delta t} = \boldsymbol{X}_i^t + \boldsymbol{V}_i^t \, \Delta t$ (explicit)

$$\boldsymbol{X}_i^{t+\Delta t}(n+1) = \boldsymbol{X}_i^t + \frac{1}{2}(\boldsymbol{V}_i^{t+\Delta t}(n) + \boldsymbol{V}_i^t)\Delta t$$

(implicit, iterative)

Topological changes

- When dislocations collide/ annihilate/ change size need to change discretization
- Core reactions need to be derived from DFT/ MD
- Only two operations defined in ParaDiS: *split node* and *merge node*



Example - split node:

(a) Initial network

(b) Remove connections of node 0 to 1 and 4 and connect to new node 5

(c) Connect 0 to 5 and conserve Burgers vector

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New additions to DD code

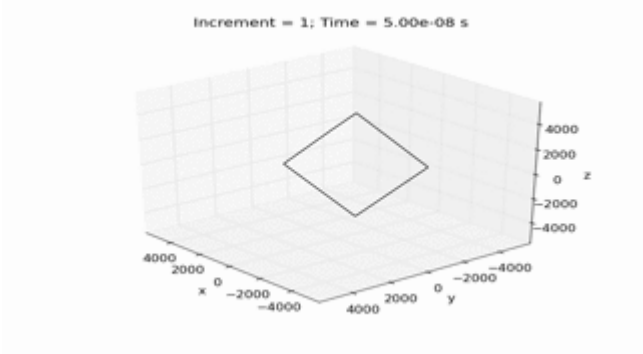
- Energy calculations for every mechanism
  - damping, annihilation, core, interactions, self energy
    - External and internal work
  - Test energy conservation for different loading cases
  - Enable cyclic stress driven loading
- Grain boundary mechanism – pile-ups
- Quasi-Newton implicit solver

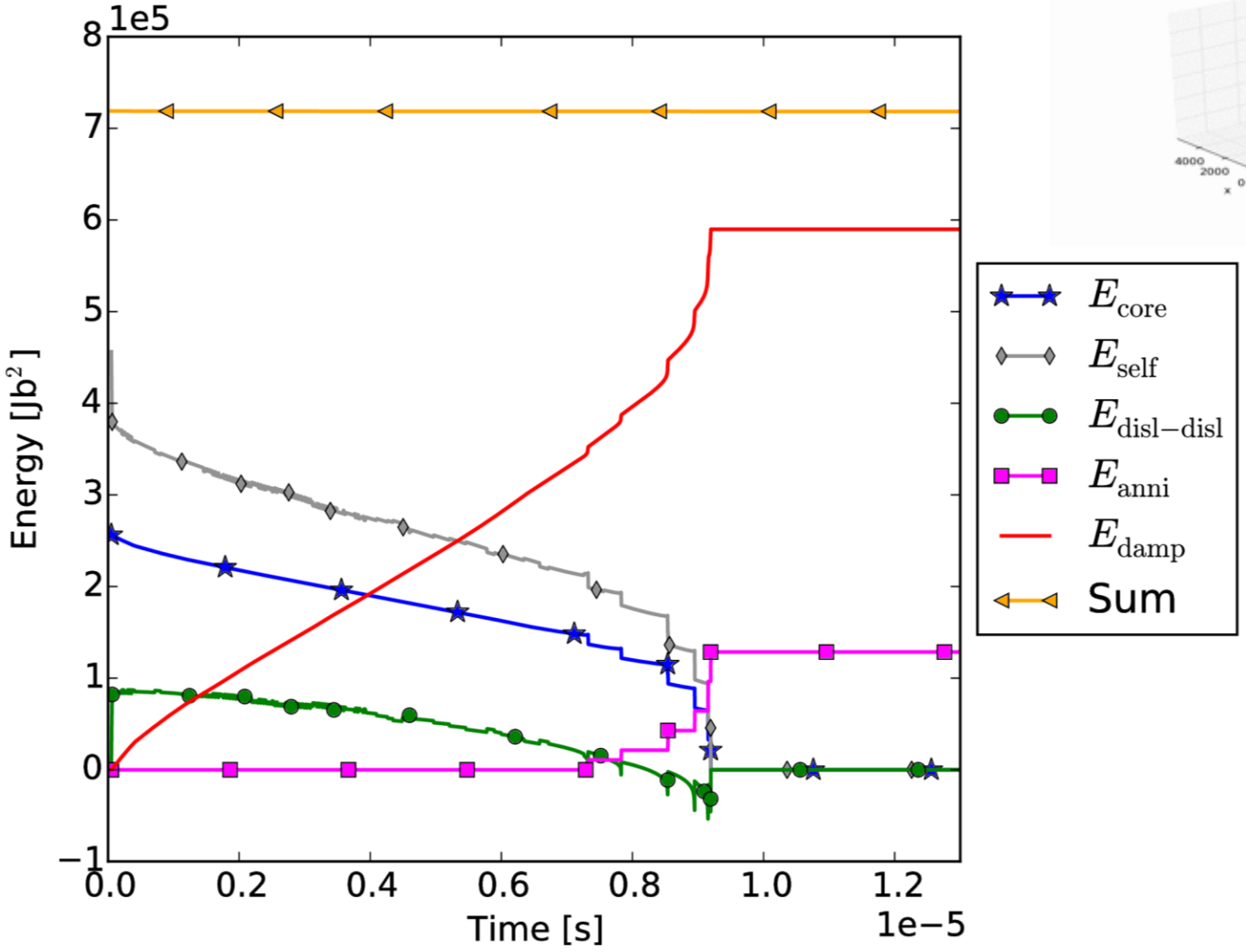
Energy contributions in DD simulations

- Annihilation energy – Energy associated with topological operations, that are not accompanied by movement
- Damping of moving dislocations $E_{\text{damp}} = \int_0^t \sum_{\text{nodes}} \boldsymbol{F}_i \circ \boldsymbol{v}_i \mathrm{d}t$
- Internal elastic energy $E_{\text{el,int}} = \frac{\sigma_{\text{ext}}^2}{E} V/2$
- External Work $W_{\text{ext}} = \int_V \int_0^{\varepsilon} \sigma_{\text{ext}} \mathrm{d}\bar{\varepsilon} \mathrm{d}V = \int_V \int_0^t \sigma_{\text{ext}} \dot{\varepsilon} \mathrm{d}t \mathrm{d}V$
- Core energy
- Energy of elastic dislocation field (self and interaction) see Cai et al. (2006)

- Sum has to be constant

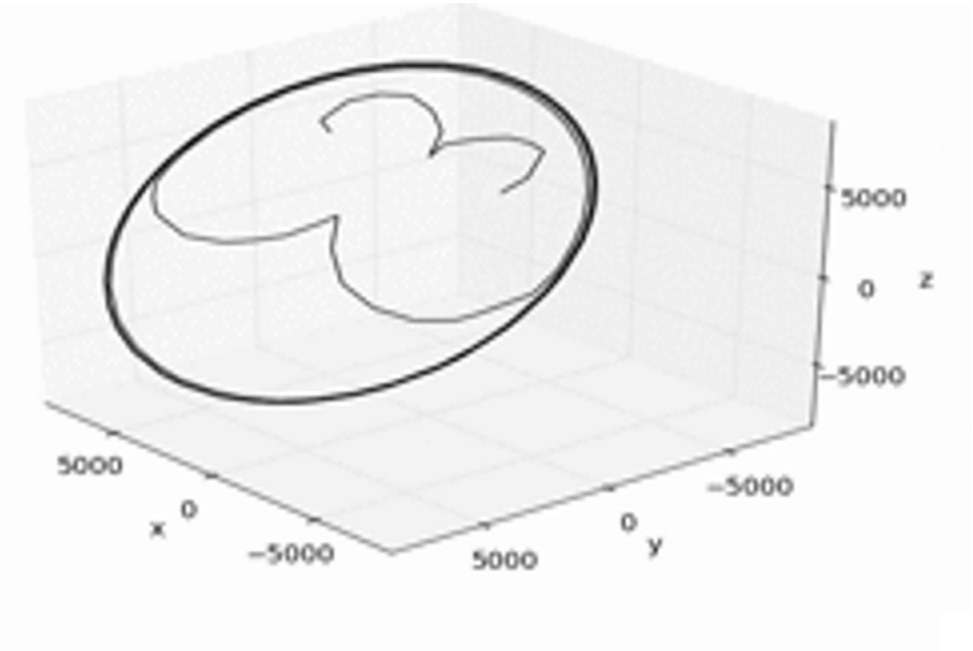
Collapsing loop

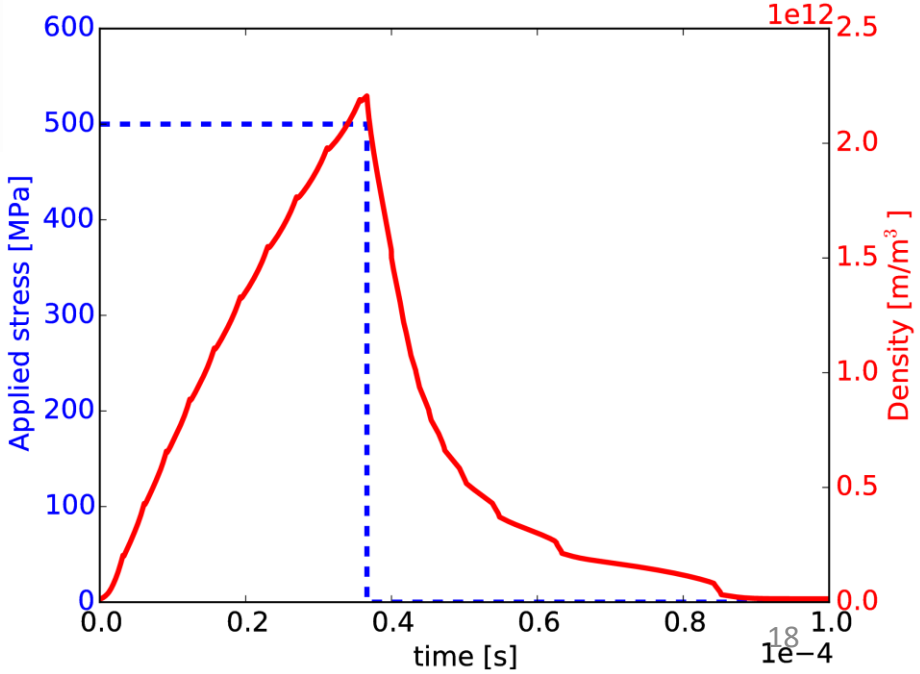




- No external work applied
- All initial elastic energy of the loop went into dissipation (movement of loop) and annihilation (‘dissipation without movement’)
- Sum is constant

Frank-Read Source





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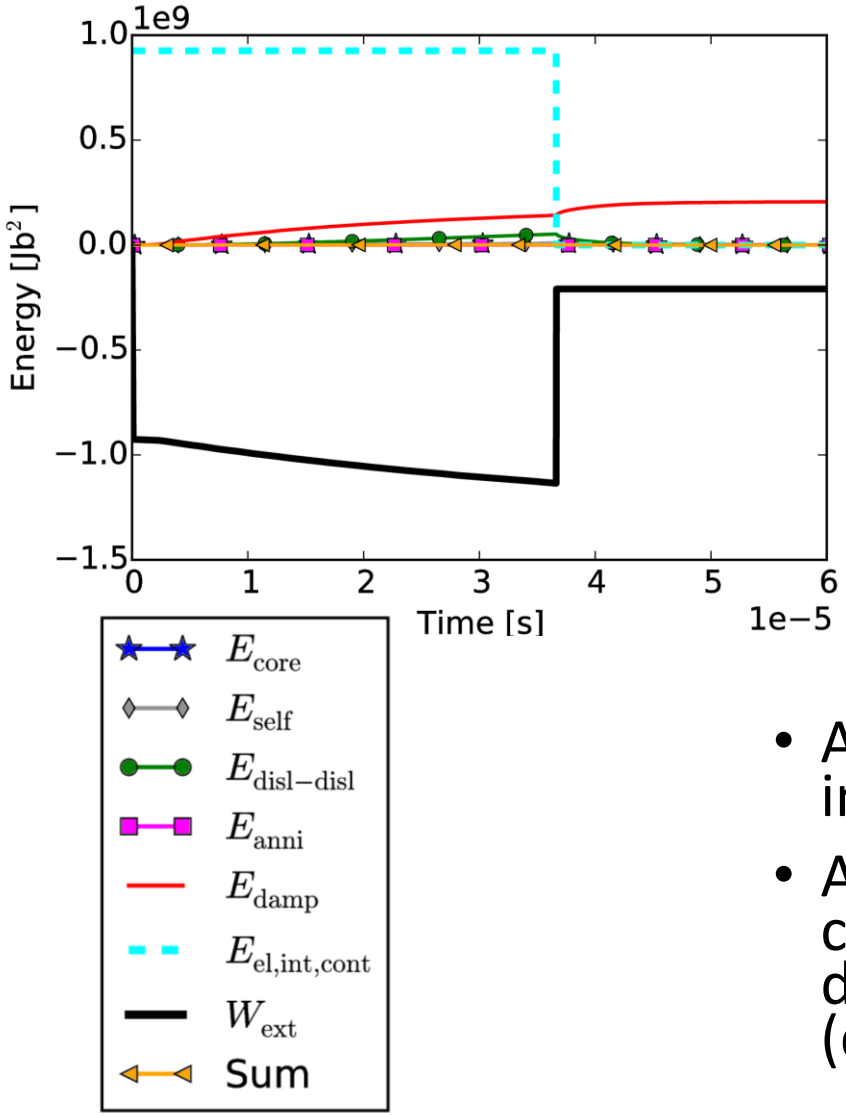
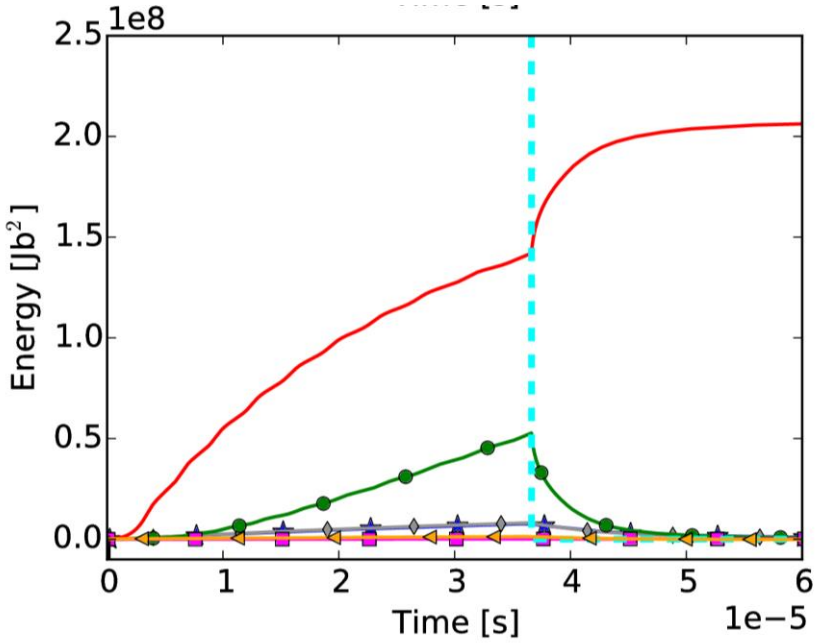
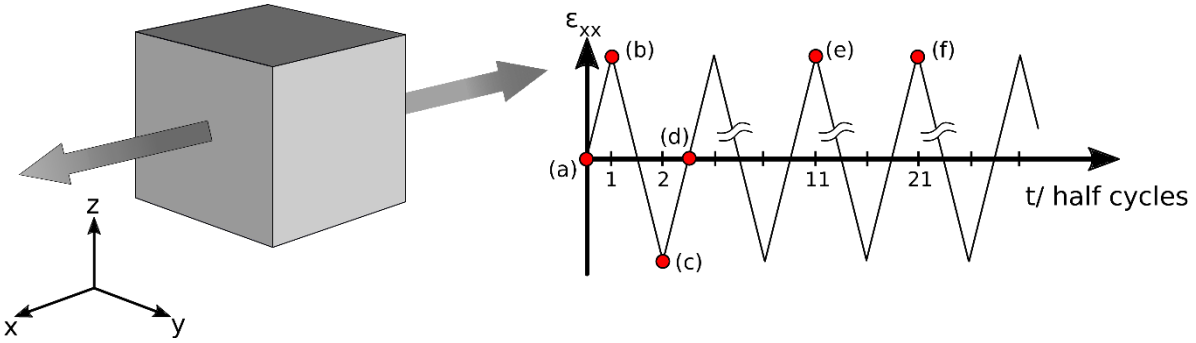


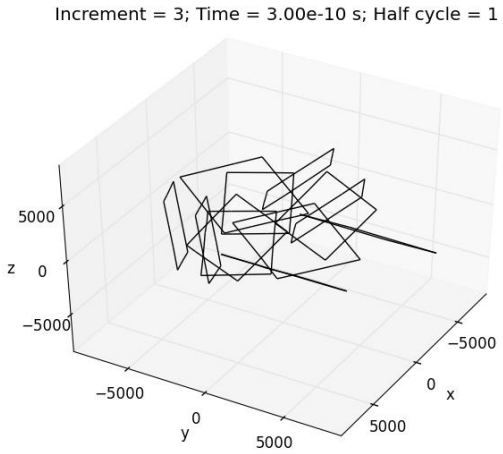


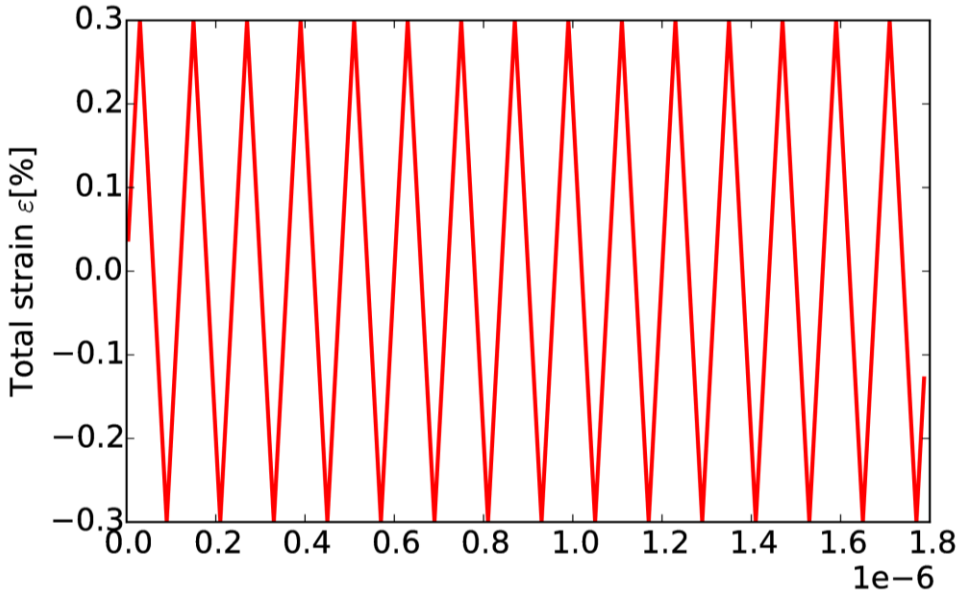
- At beginning elastic energy increases
- After external load removed, load collapses and internal energy of dislocations dissipated to heat (damping)

Cyclic loading

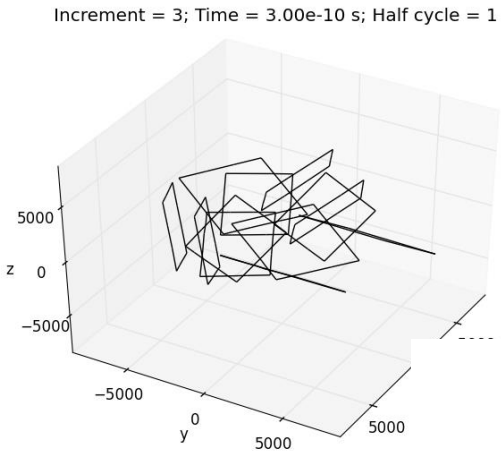
- Largest ever fatigue DD simulation till date – 40 cycles, 6 weeks on 128 CPUs
- French Group Depres, Fivel – 20 cycles
- Density increases with number of cycles



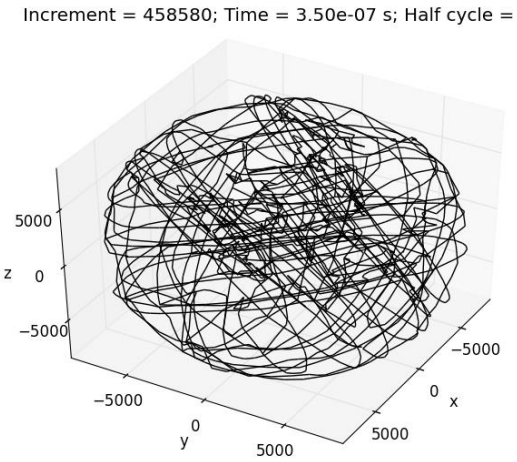


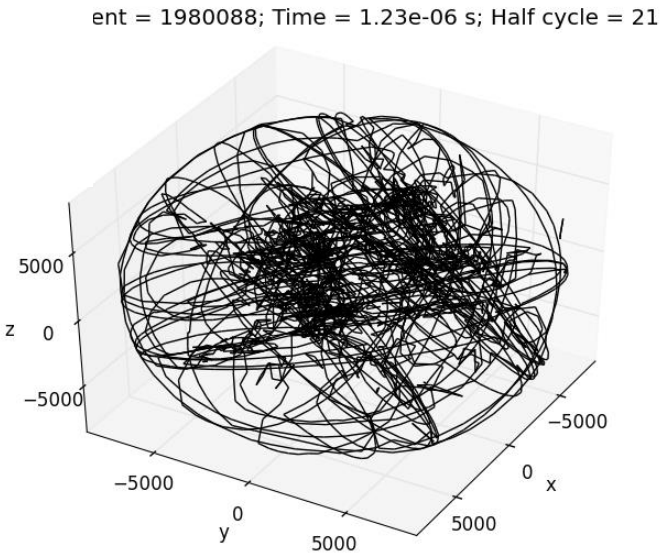


Initial and final state



$$\Delta G^* = 2\gamma\Delta A - E_{el}^{\Delta A} - E_{stored}$$

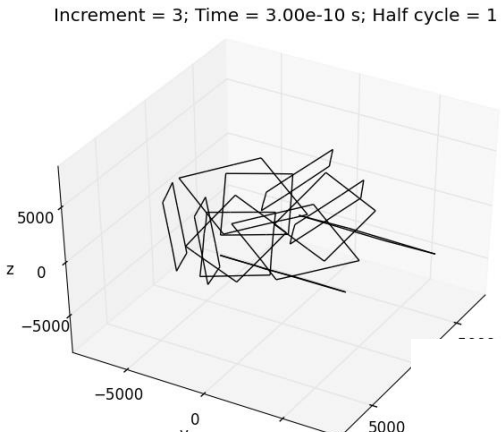




Persistent dislocations over number of cycles

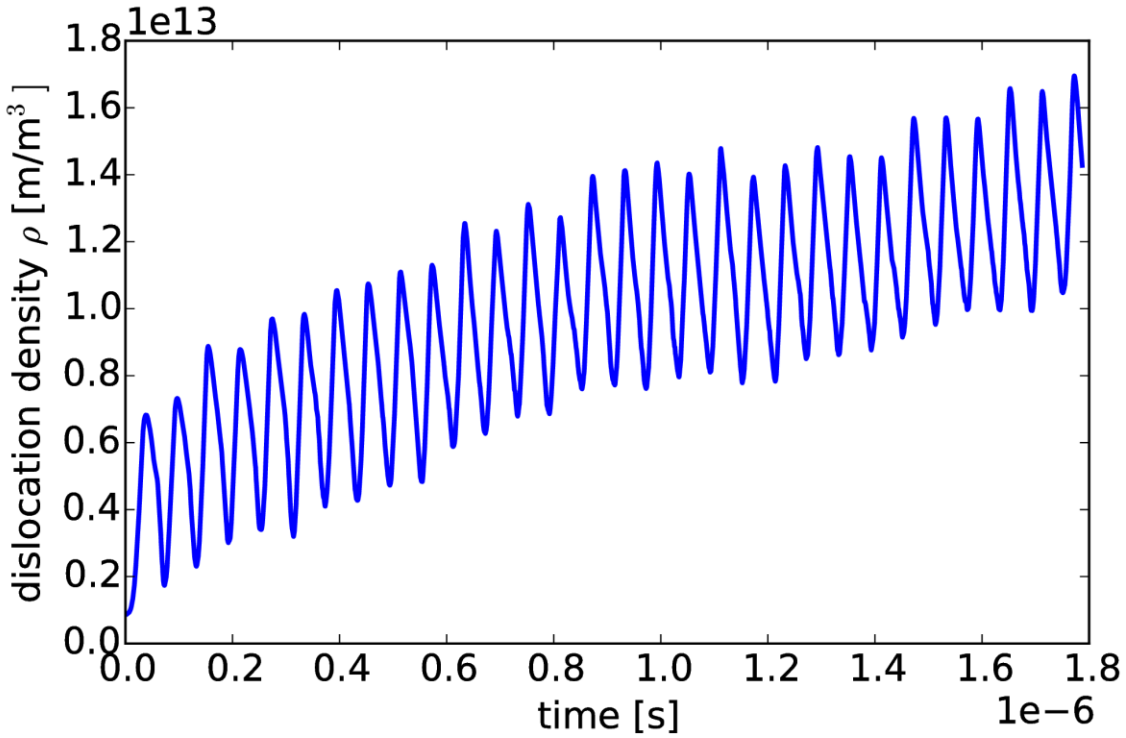
Chemical effects can be added as an osmotic force: (Future work)

Initial and final state

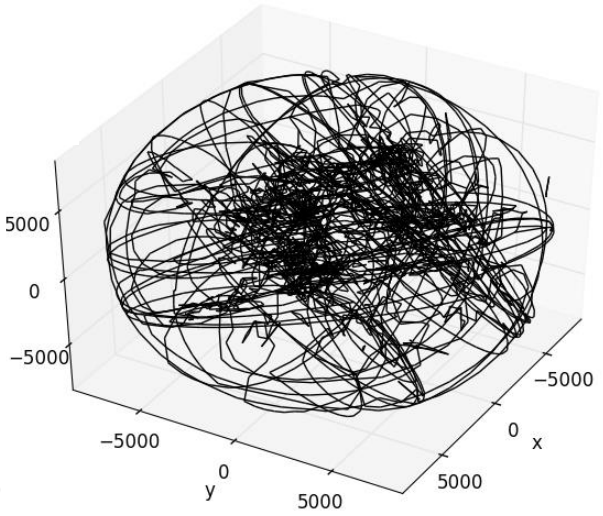


$$\Delta G^* = 2\gamma\Delta A - E_{el}^{\Delta A} - E_{stored}$$

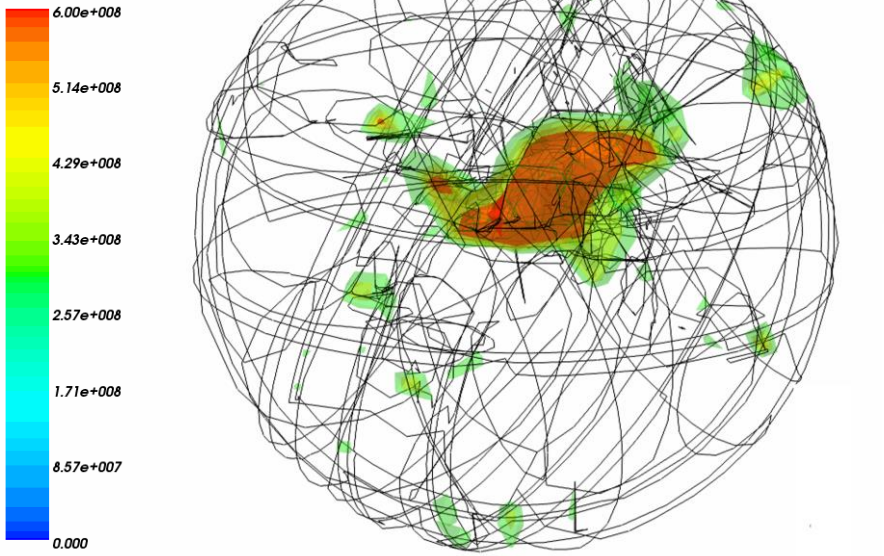
Increment = 458580; Time = 3.50e-07 s; Half cycle = 7



ent = 1980088; Time = 1.23e-06 s; Half cycle = 21

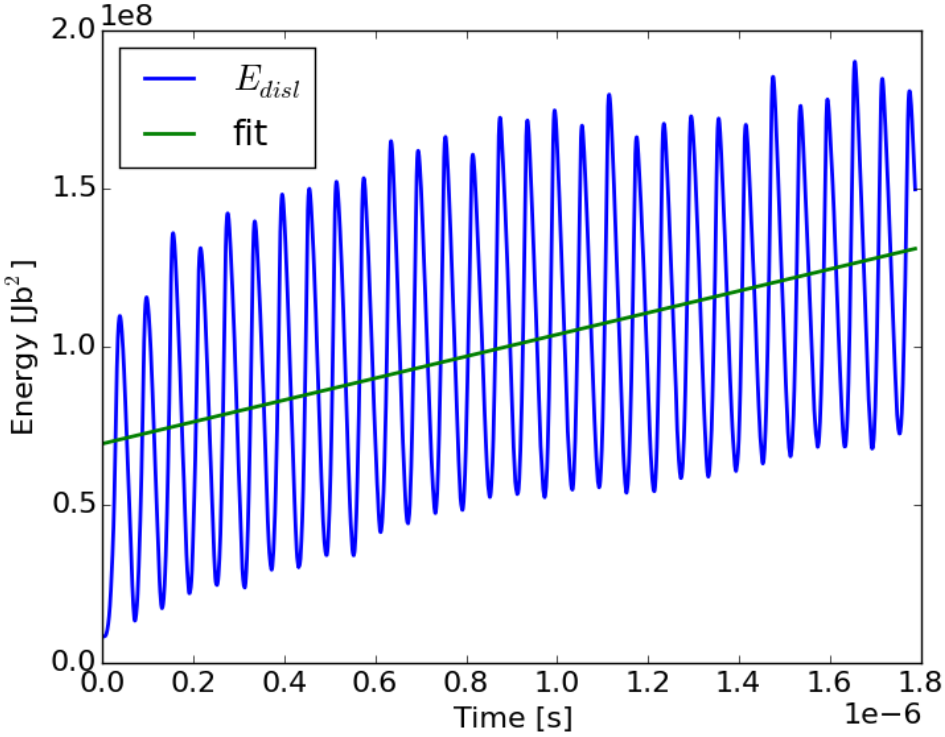


Cyclic loading – Increase in density



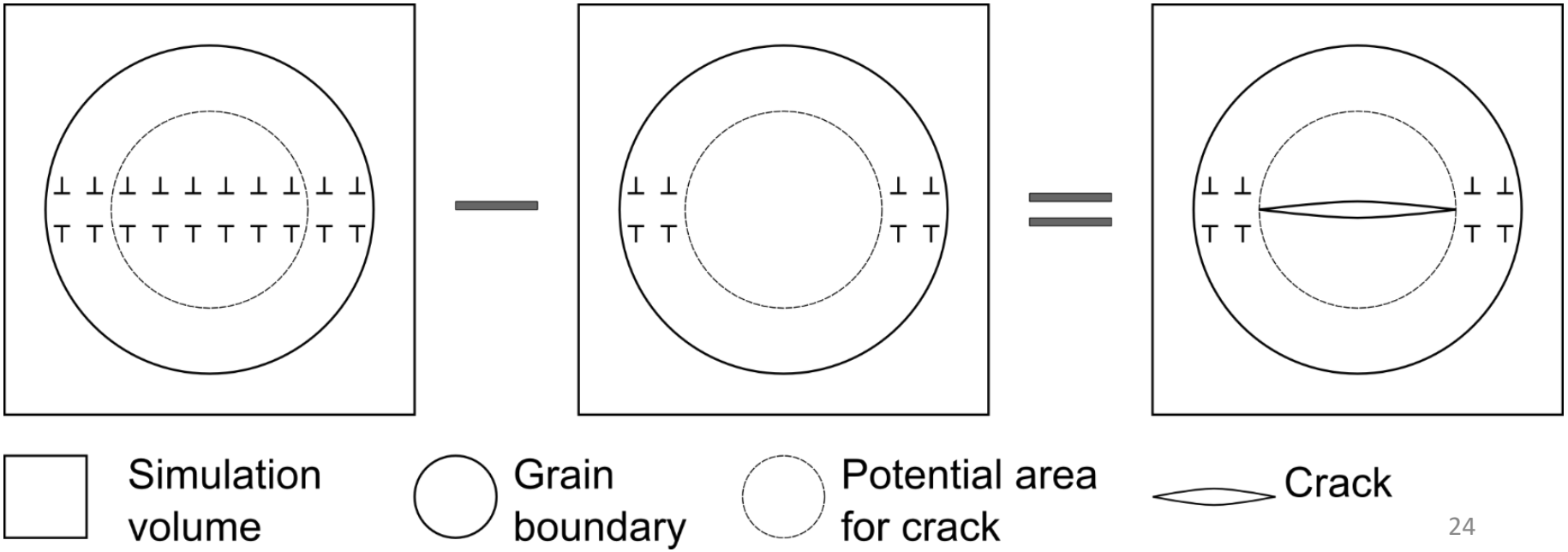
Dislocation density [m/m^3]

After 20 cycles



Partial energies

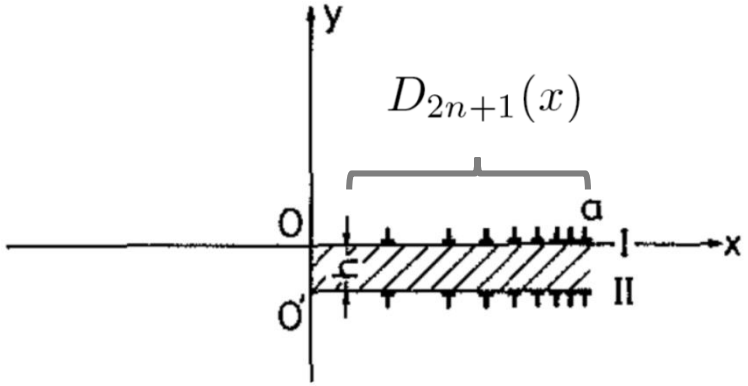
- Some dislocations are very far spaced out, unlikely to form one (contiguous) crack
- Remove only some dislocations in area where dislocation density is highest
- As before: total energy of all dislocations (and possible external elastic field) MINUS energy of remaining dislocations after crack is formed EQUAL to energy of the crack
- IMPORTANT: The dislocations removed should be able to form a surface of the size of the crack



Modelling dislocation density evolution analytically

Mura and Nakasone, *A Theory of Fatigue Crack Initiation in Solids*, J. Appl. Mech., 57 (1990)

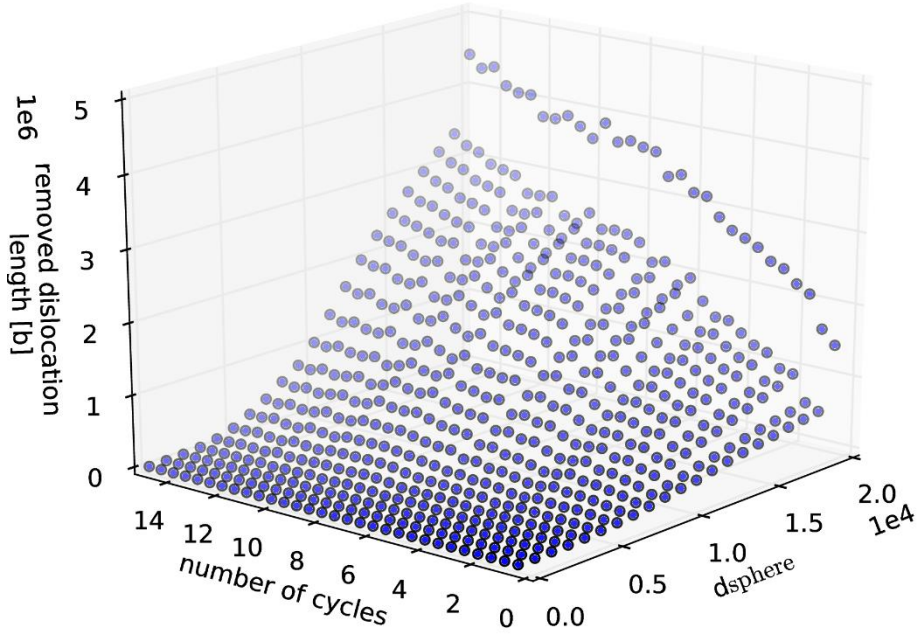
Dislocation accumulation is typically modeled as linear with number of cycles

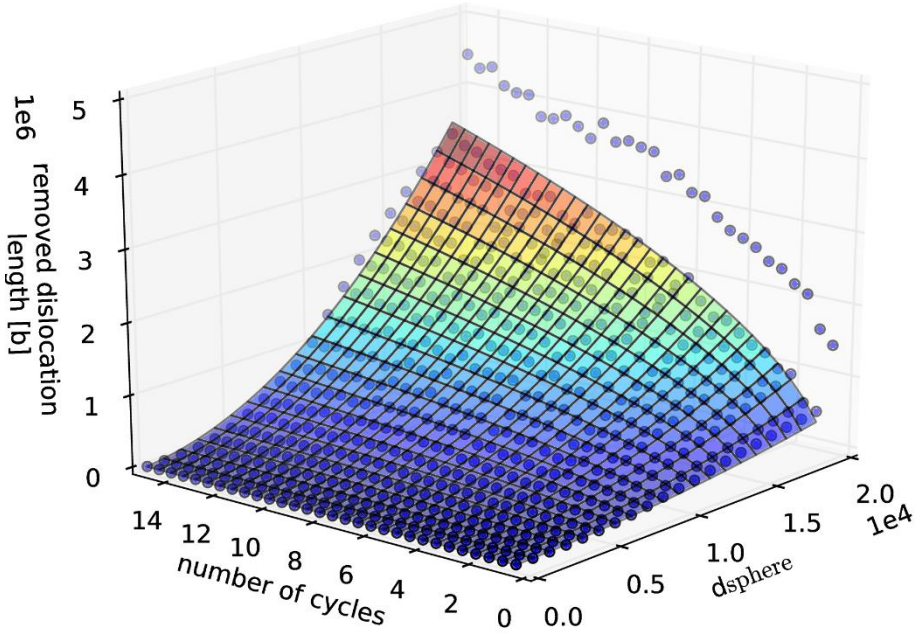


$$D_{2n+1}(x) \approx n\Delta D$$
$$\approx n(\Delta\tau - 2\tau_f)x/[\pi A(\sqrt{a^2 - x^2}]$$

D- dislocation distribution, $D = f(x, n)$
n- number of cycles
$\Delta\tau$- applied cyclic shear stress
τ_f- frictional stress
x- coordinate
A - $\mu b/2\pi(1-\nu)$
a- half length of PSB

Dependence of dislocation length on cycles and volume





- Assume up to quadratic increase in space and square root in w.r.t number of cycles

$$l = \left(C_{l1}d + C_{l2}d^2\right)\left(\sqrt{n} + C_{l3}\right)$$

$C_{\ell 1}, C_{\ell 2}, C_{\ell 3}$ .. some fitting constants

n .. number of cycles

d .. diameter of sphere used to remove the dislocations

Dependence of dislocation length on cycles and volume

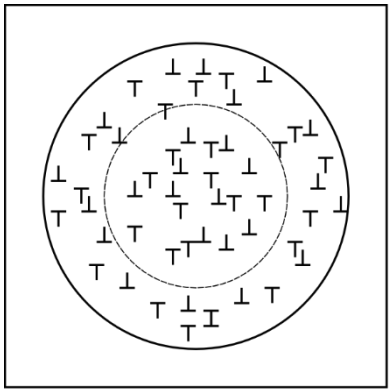
- At any given point in time the dislocation removed in the test volume should form a crack of comparable size:

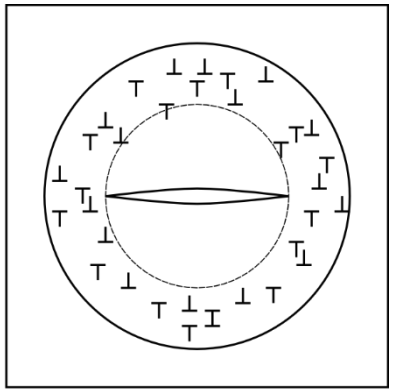
$$bl = \frac{\pi}{4} d^2$$

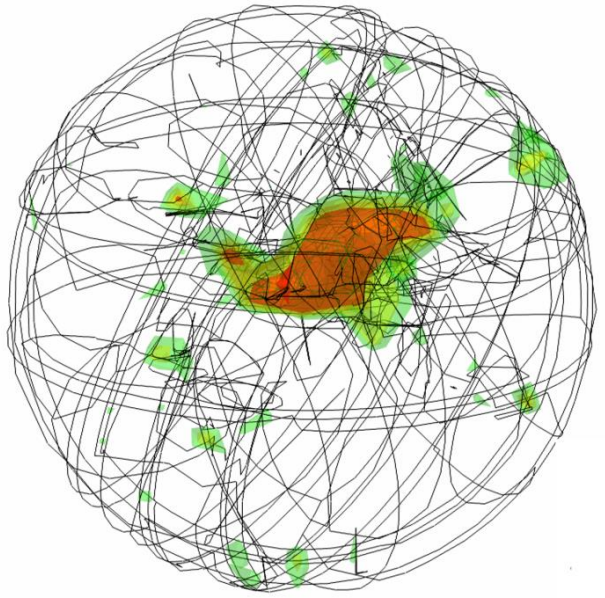
$$l = \left(C_{l1} d + C_{l2} d^2\right)\left(\sqrt{n} + C_{l3}\right)$$

$$d = \frac{C_{l1}\left(\sqrt{n} + C_{l3}\right)}{\pi/(4b) - C_{l2}\left(\sqrt{n} + C_{l3}\right)}$$

Currently dislocations in sphere are removed







Doing the numbers

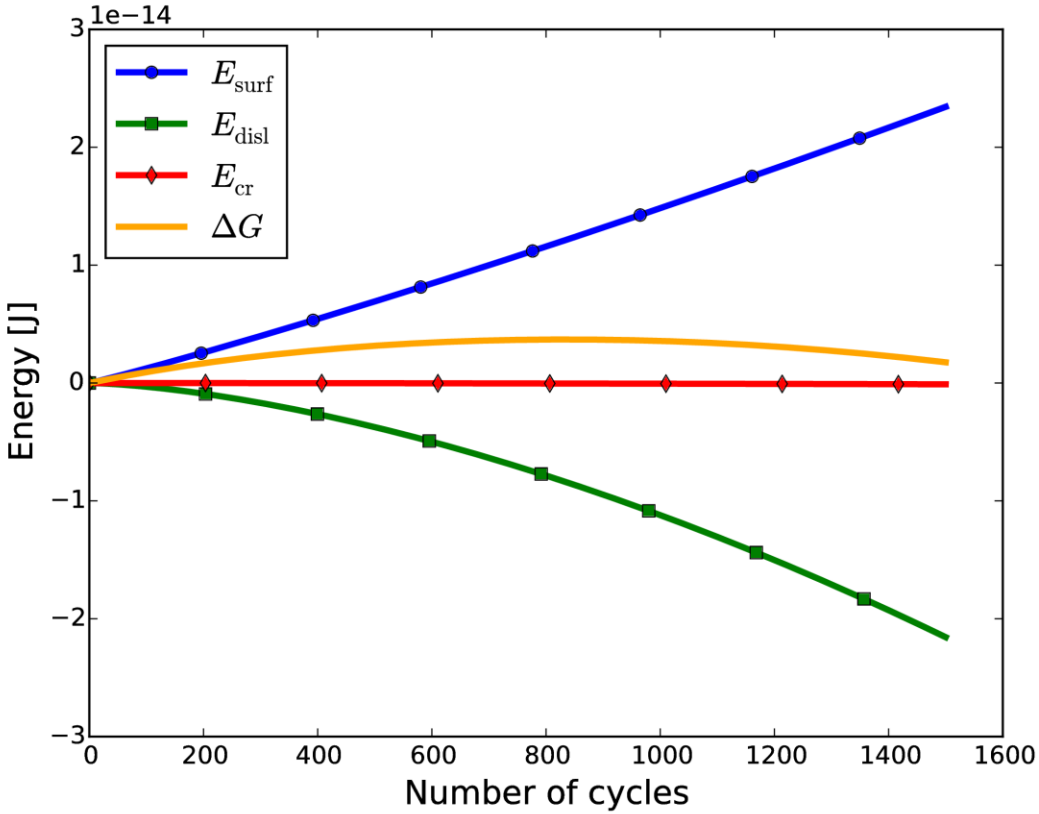
$$\Delta G = E_{\text{surf}} - E_{\text{disl}} - E_{\text{cont}}$$

$$d = \frac{C_{l1}\left(\sqrt{n}+C_{l3}\right)}{\pi/(4b)-C_{l2}\left(\sqrt{n}+C_{l3}\right)}$$

$$E_{\text{surf}} = 2\gamma\frac{\pi}{4}d^2$$

$$E_{\text{disl}} = C_{d1}d^2\left(n^{0.5}+C_{d2}\right)$$

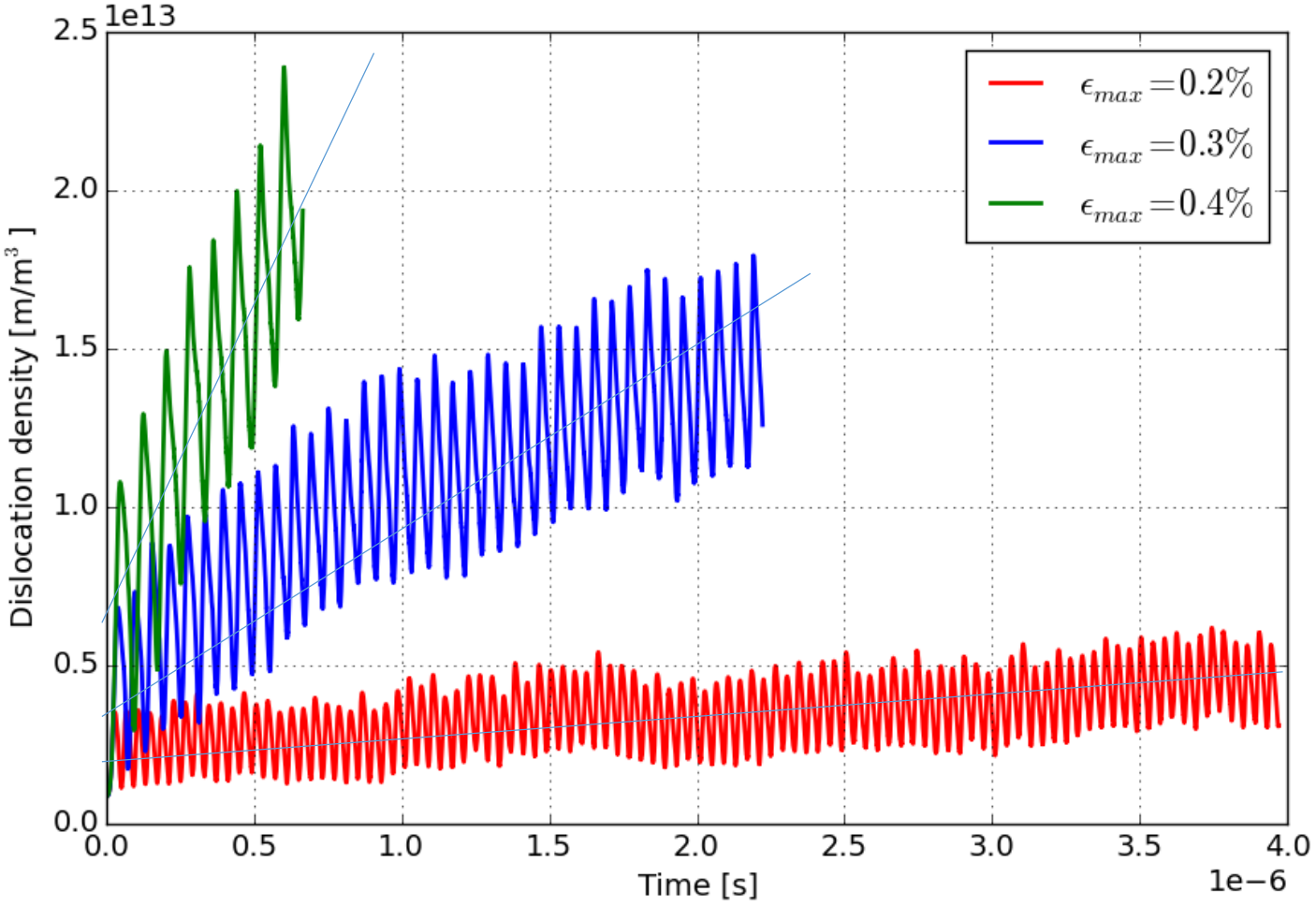
$$E_{\text{cont}} = \frac{8(1-\nu^2)}{3E}\sigma^2 d^3$$



Incubation crack we found is 150 nm

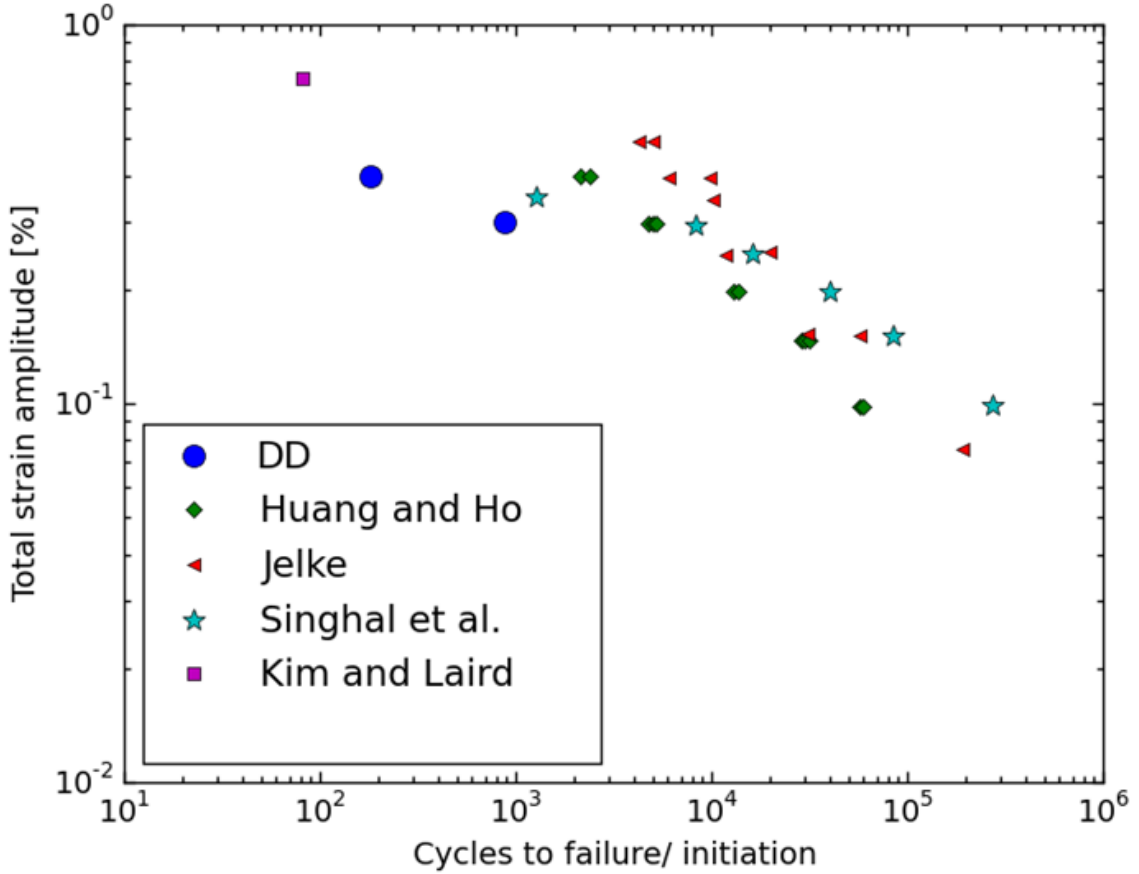
Varying maximum strain

- As expected: higher maximum load leads to increase in dislocation density
- Incubation crack sizes and critical cycles will be different
- Could be linear with respect to cycles – Mura.



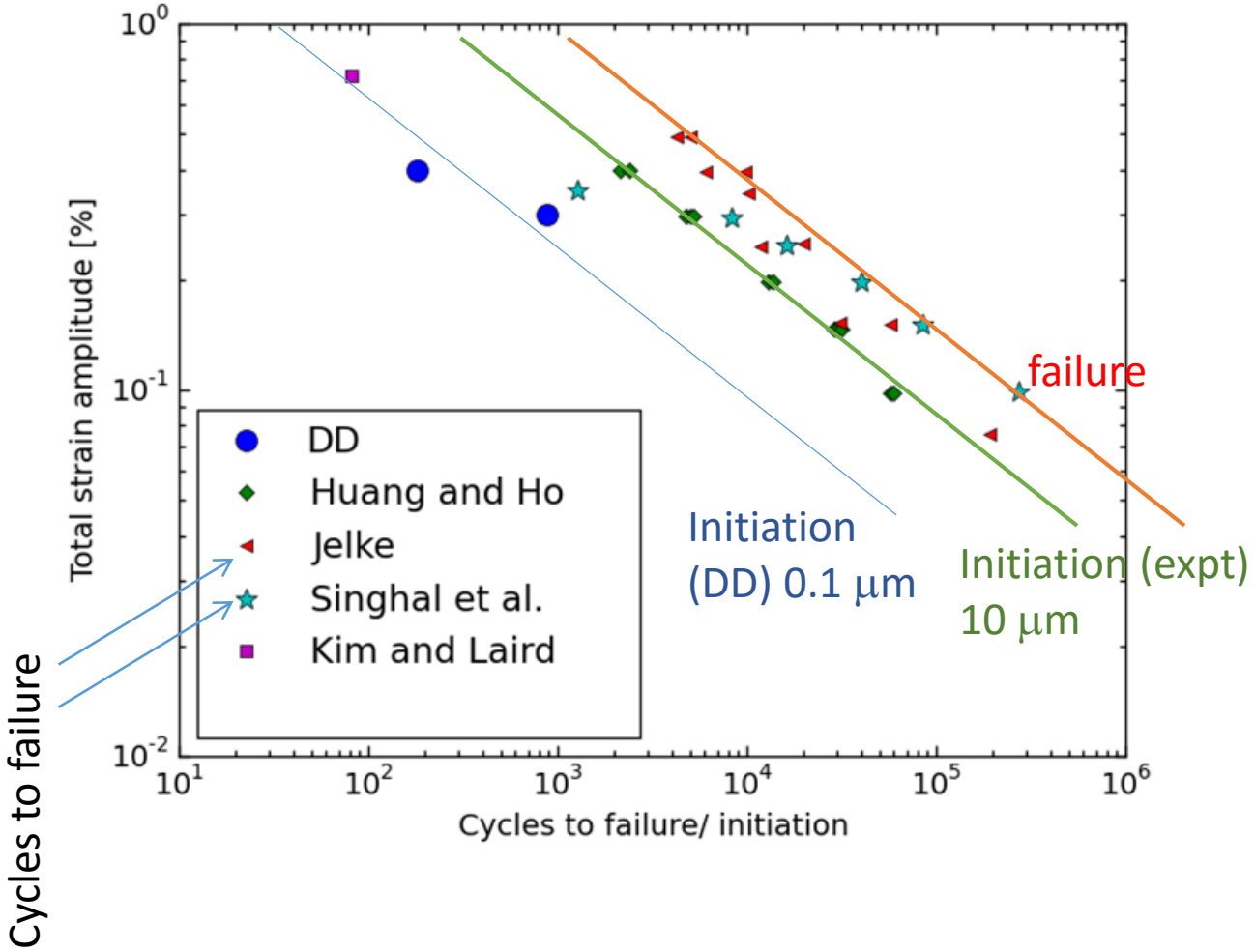
Comparison to experiments

- At higher strain levels: DD conservative
- Experimental: detectable initiation & full failure
- DD results are for initiation



Comparison to experiments

- At higher strain levels: DD conservative
- Experimental: detectable initiation & full failure
- Numerical: initiation



Multiscale crystal plasticity

- Crystal plasticity can be used to compute (total) plastic work
- The total work can be scaled by an efficiency factor to compute the stored energy
- The efficiency factor is obtained from dislocation dynamics

Plastic work in virtual crack

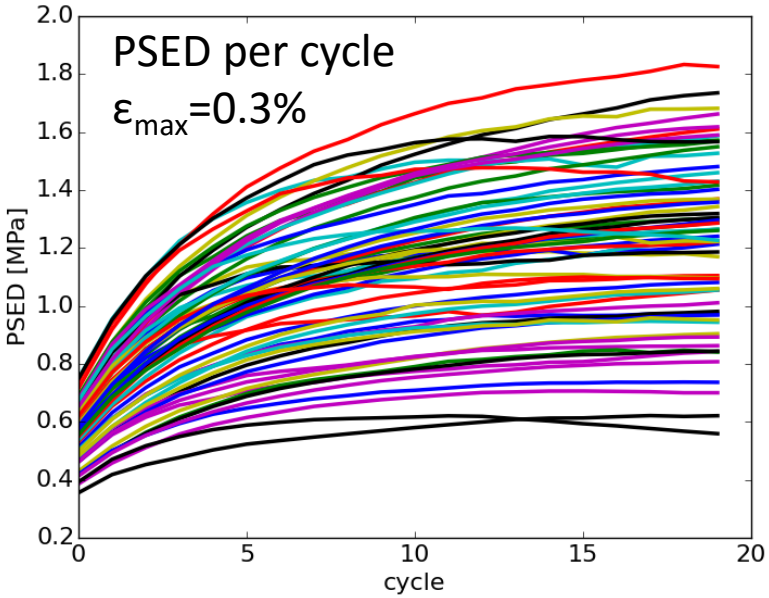
$$\text{Stored energy} = f t_m \int_0^t \sum_\alpha \tau^\alpha \dot{\gamma}^\alpha \mathrm{d}t = \frac{f^* \varpi}{2}$$

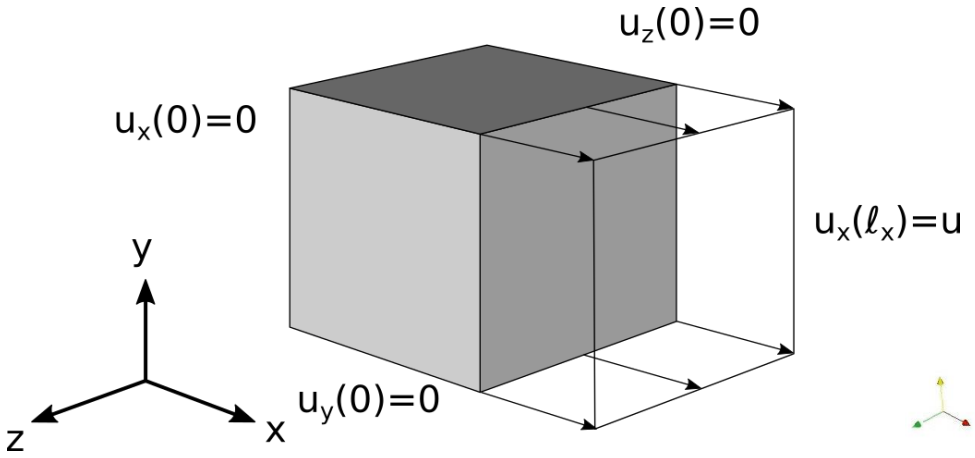
A- Area of crack
f - Efficiency factor
ϖ- Plastic strain energy density
N - Cycles to failure
$\Delta\gamma^\alpha$- Plastic strain increment in system α
τ^α—Resolved shear stress in system α
t^m- Thichness of PSB

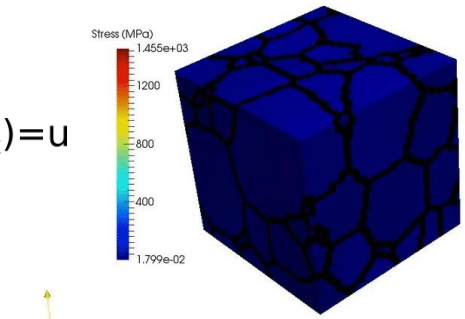
(Li, Shen & Proust, 2015
Fine & Bhat, 2007, Naderi et al (TDA) 2016)

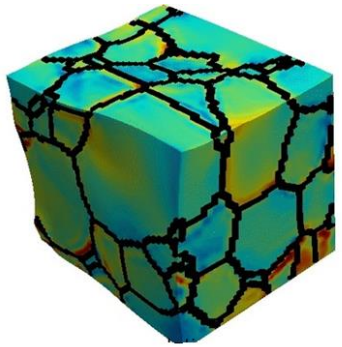
CPFE simulations

- Rate independent CPFE formulation for copper
- Random FCC orientation
- Cyclic loading for 20 cycles
- Plastic Stored Energy Density (J/m^3) for various grains are plotted

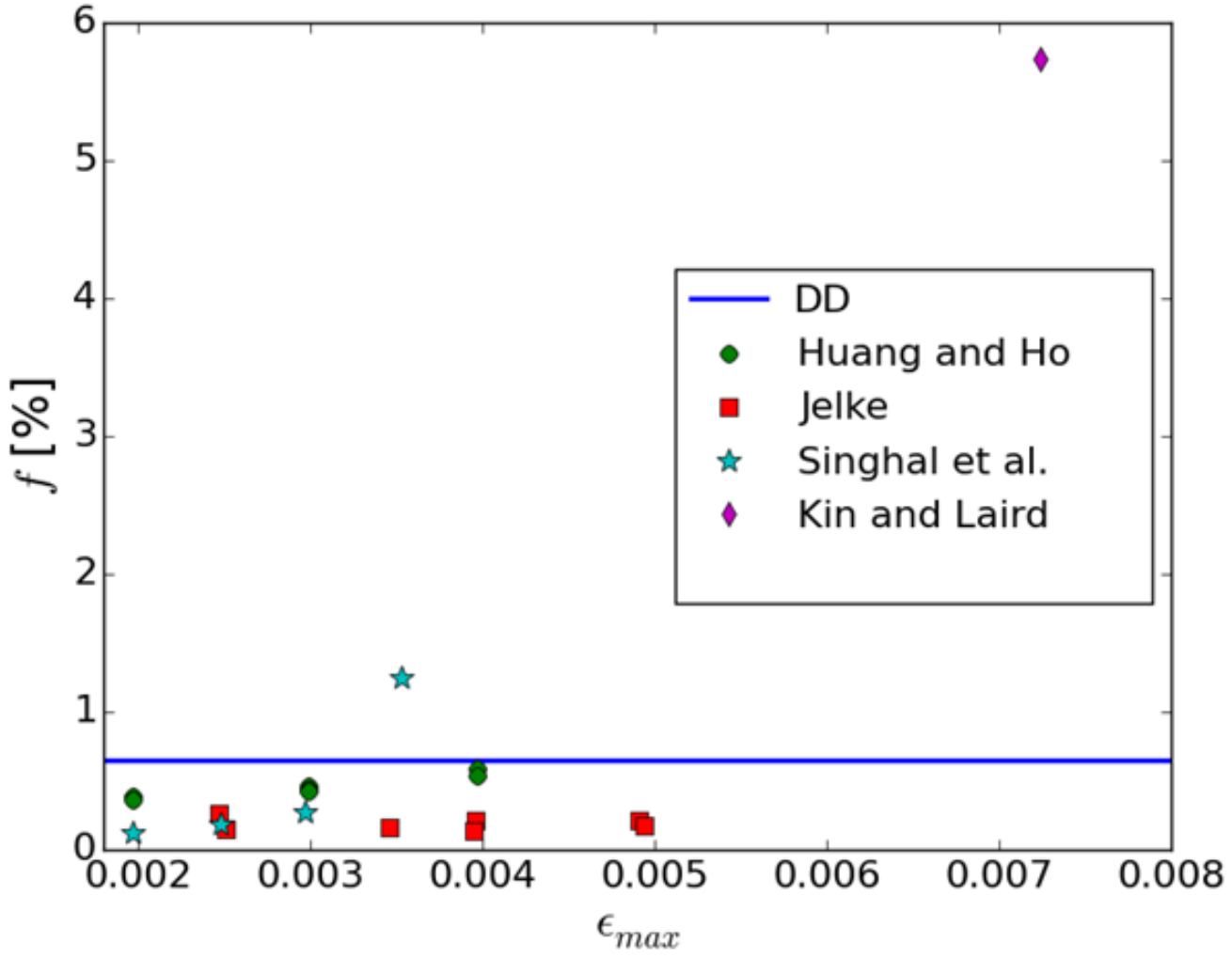








Efficiency factor comparison between DD and CPFE + experiments



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Conclusion

- Performed the largest cyclic dislocation dynamics simulation till date. Accurately computed energy in stored dislocations.
- Showed an incremental energy approach for using DD results
  - Hypothetical crack is inserted and incremental energy balance is calculated
  - Energy stored in dislocation network drives crack
  - Has to balance surface energy change and reduction in continuum energy due to crack
- Showed how to calculate efficiency factor from DD for use in continuum or crystal plasticity calculations
- Future work: Addition of crack tip stress fields. Addition of precipitate structure, addition of chemical effects (solute, environment)

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Thank you for your attention!

Questions?