Computational Discrete Dislocation Plasticity

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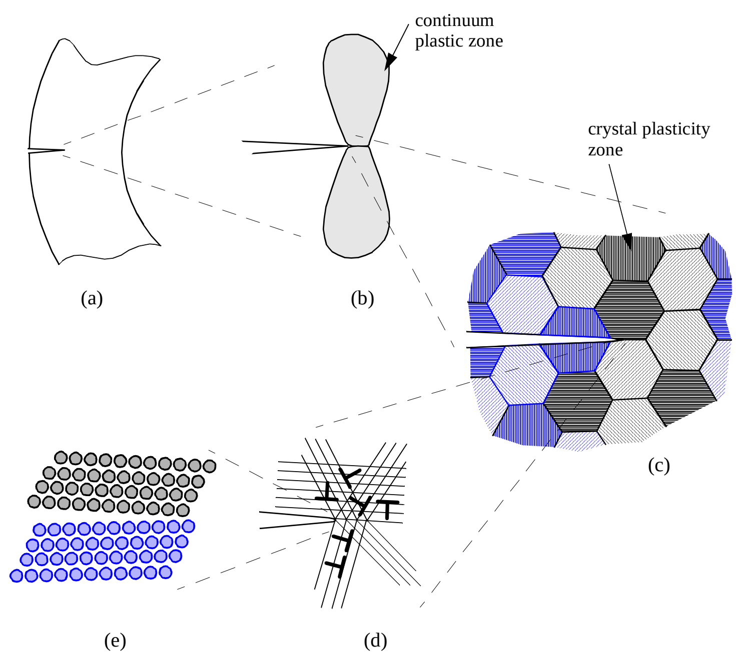
- What is discrete dislocation plasticity?
- What does discrete dislocation plasticity predict?
- What are the implications for phenomenological modeling?
- Whither discrete dislocation plasticity?

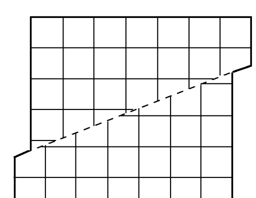
Discrete Dislocation Plasticity

- Continuum description of plastic deformation in crystalline solids where the deformation mechanism is dislocation glide.
- Dislocations are treated as discrete entities and modeled as line singularities in an elastic solid.
  - Elasticity – accurately represents dislocation fields beyond $5b - 8b$ from the core.
- Description between atomistics and a size-independent continuum.



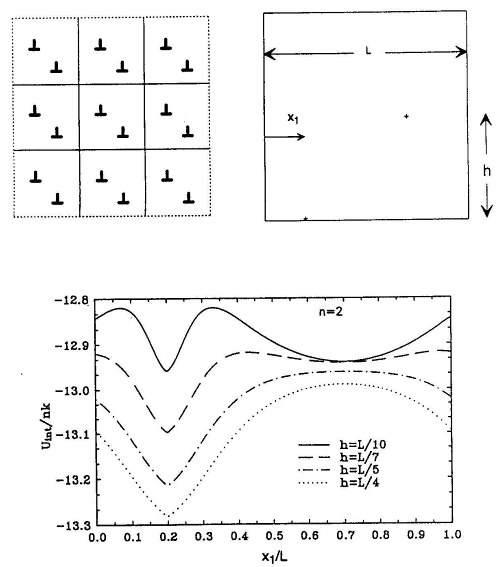
Discrete Dislocation Plasticity

- A material length scale is introduced – the Burgers vector magnitude b – other material length scales may dominate that scale with b. (size matters)
- The dislocation stress field is long range – $\sigma_{ij} \propto f_{ij}/r$. (organized dislocation structures can evolve)
- Plastic deformation arises from the nucleation and glide of dislocations. (dissipation and hysteresis)
- The total displacement field is not a continuous single valued function – $\oint_\Gamma u_{i,j} dx_j \neq 0$. (highly localized deformations; new free surface)

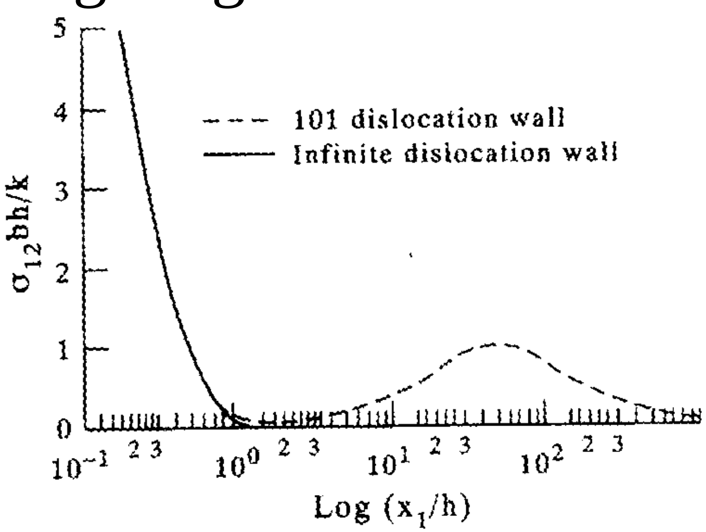


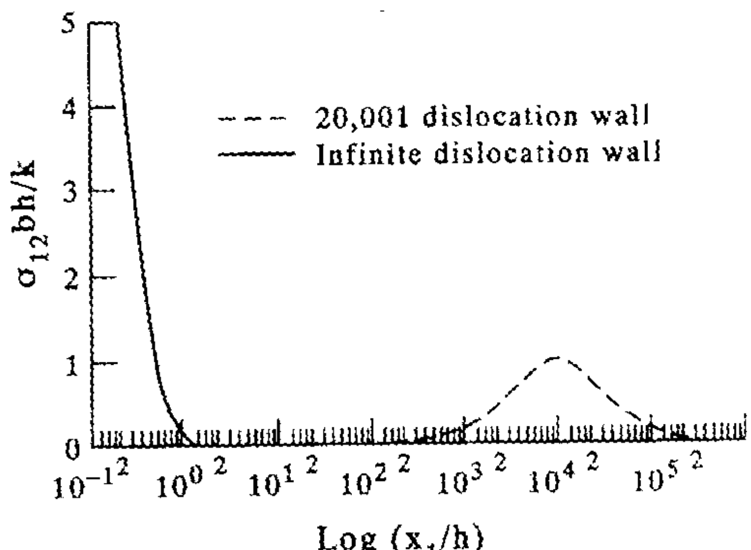
Equilibrium Dislocation Structures

- Non-uniqueness.



- Long range stresses.





Lubarda *et al.*, *Acta Mat.*, 41, 625, 1993.

Discrete Dislocation Plasticity

1. Unit process modeling – the interaction between dislocations and specific microstructural features; for example dislocation-precipitate interactions.
2. Macroscopic constitutive modeling – the stress-strain response of a representative volume element.
3. Formulate and solve general boundary value problems where plastic flow is represented by the collective motion relatively large numbers of discrete dislocations.
   - Plastic flow phenomena on a size scale of $\approx 0.1\ \mu$m to $\approx 100\ \mu$m.
   - Critical deformation and fracture processes take place at this scale.
   - The stress-strain response and the evolution of the dislocation structure are coupled and sensitive to the boundary value problem specification.

Mechanics Framework

- Strain-displacement (small deformations):

$$\epsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

- Momentum balance (quasi-static):

$$\frac{\partial \sigma_{ij}}{\partial x_j} = 0 \qquad \sigma_{ij} = \sigma_{ji}$$

- Constitutive relation (isotropic linear elastic):

$$\sigma_{ij} = \frac{E}{1+\nu}\left(\epsilon_{ij} + \frac{\nu}{1-2\nu}\epsilon_{kk}\delta_{ij}\right)$$

Mechanics Framework

- Long range interactions between dislocation come directly from elasticity theory.
- Constitutive rules are needed *at least* for dislocation glide, annihilation and nucleation.
  - To a certain extent, what constitutive rules are needed depends on the level of modeling, e.g. 2D vs. 3D, and on the resolution – dislocation-dislocation interactions can be well-represented by elasticity theory with near atomic resolution.

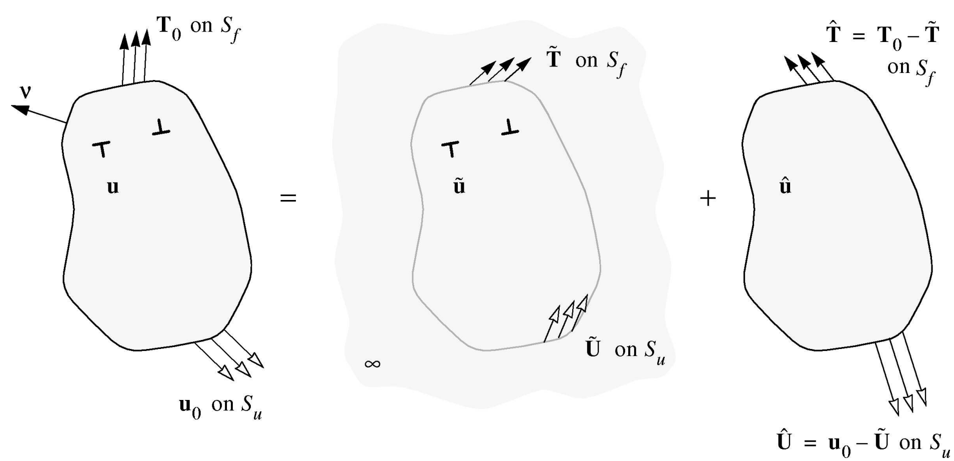
Boundary Value Problems

$$u_i = \tilde{u}_i + \hat{u}_i\,, \quad \epsilon_{ij} = \tilde{\epsilon}_{ij} + \hat{\epsilon}_{ij}\,, \quad \sigma_{ij} = \tilde{\sigma}_{ij} + \hat{\sigma}_{ij}.$$

- ($\tilde{\ }$) fields – sum of the explicitly known singular equilibrium fields of the individual dislocations, e.g. $\tilde{\sigma}_{ij} = \sum_k \sigma_{ij}^{(k)}$.
- ($\hat{\ }$) fields – image fields that correct for the boundary conditions and are non-singular.

$$\hat{\sigma}_{ij,j} = 0 \qquad \hat{\sigma}_{ij} n_j = T_i^0 - \tilde{T}_i \text{ on } S_f \qquad \hat{u}_i = u_i^0 - \tilde{u}_i \text{ on } S_u$$

$$\int_V \hat{\sigma}_{ij} \delta \hat{u}_{i,j} dV = \int_{S_T} (T_i^0 - \tilde{T}_i) \delta \hat{u}_i dS$$



Boundary Value Problems

Specify:

- Elastic constants; slip systems; dislocation constitutive parameters; dislocation sources and obstacles.
- Use the balance laws and boundary conditions to determine the evolution of the dislocation structure and the mechanical response.

The stress-strain response and the evolution of the dislocation structure are strongly coupled and are outcomes of the boundary value problem solution.

- Appropriate specification of boundary conditions is extremely important.
- The slip is embodied in the explicitly known $(\tilde{\ })$ fields – the numerics do not have to attempt to resolve slip.

Computational Procedure

1. At time t the state of the body is known including $\sigma_{ij}(x_k, t)$ and the positions of all dislocations.
2. An increment of loading is prescribed.
3. The state of the body at $t + dt$ needs to be determined.
   - Calculate the dislocation interaction force.
     - Multi-body interaction calculation.
   - Calculate the change in dislocation structure caused by dislocation nucleation, dislocation annihilation, etc.
     - Evaluation of constitutive rules.
   - Calculate the image fields for the updated dislocation arrangement, i.e. the $(\hat{\ })$ fields.
     - Finite element calculation.

Dislocation Constitutive Rules – 2D

- Glide component of the Peach-Koehler force.

$$f^{(k)} = \mathbf{n}^{(k)} \cdot \left[\hat{\boldsymbol{\sigma}} + \sum_{j \neq k} \boldsymbol{\sigma}^{(j)} \right] \cdot \mathbf{b}^{(k)}$$

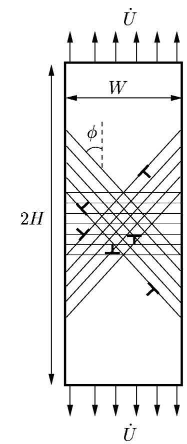
- Dislocation nucleation (Frank-Read sources) – nucleation occurs when $f^{(k)}$ at a source reaches $b\tau_{\rm nuc}$ during $t_{\rm nuc}$.
- Dislocation motion – $v^{(k)} = f^{(k)}/B$ or

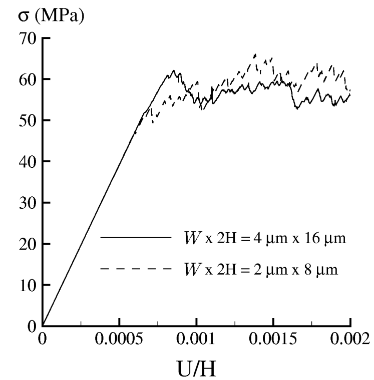
$$v^{(I)} = \begin{cases} \left(f^{(I)} - b\tau_{\rm f}\,\mathrm{sign}(f^{(I)})\right)/B & \text{if } |f^{(I)}| > b\tau_{\rm f}; \\ 0 & \text{otherwise} \end{cases}$$

- Dislocation annihilation – annihilation distance $L_{\rm e}$.
- Obstacles – pin dislocations and release them once $f^{(k)}$ attains $b\tau_{\rm obs}$.

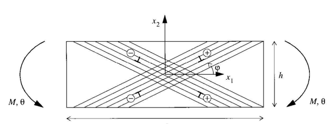
GNDs and Size Effects

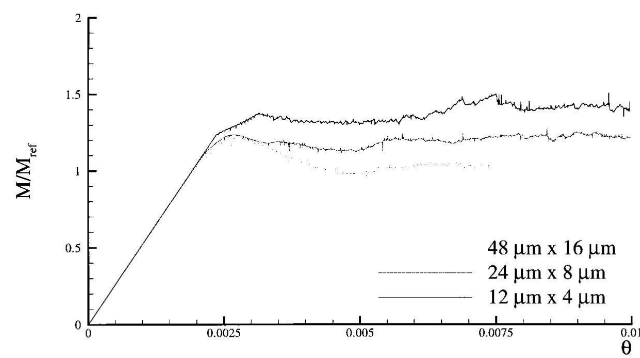
- Tension.





- Bending.

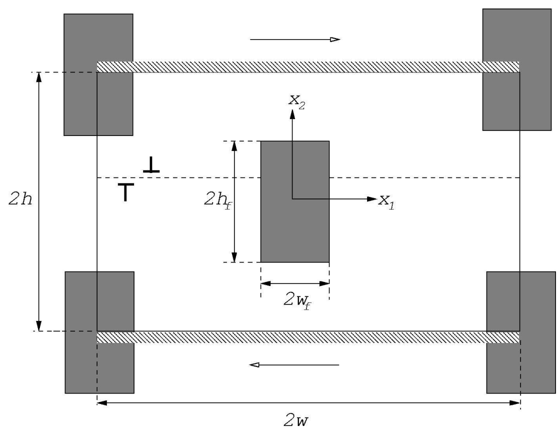


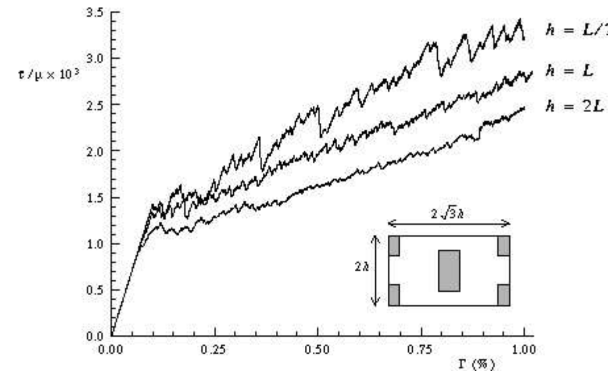


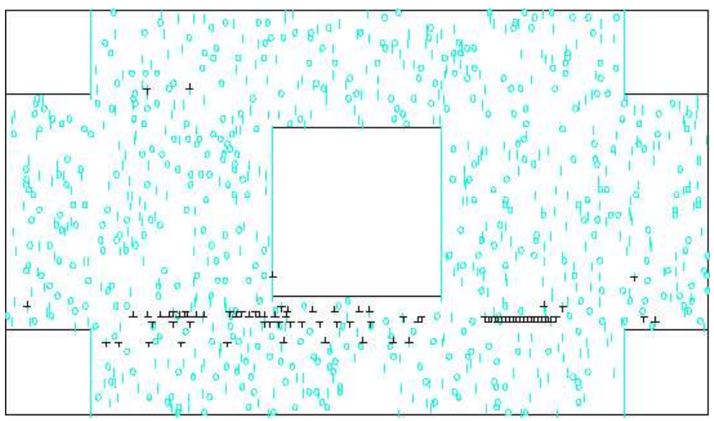
The stress-strain response and the evolution of the dislocation structure are outcomes of the boundary value problem solution.

Cleveringa *et al.*, *Int. J. Plast.*, 15, 837, 1999.

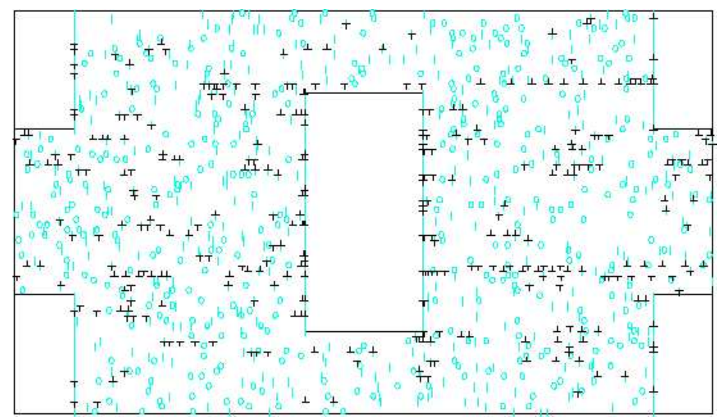
GNDs and Size Effects







material (i)

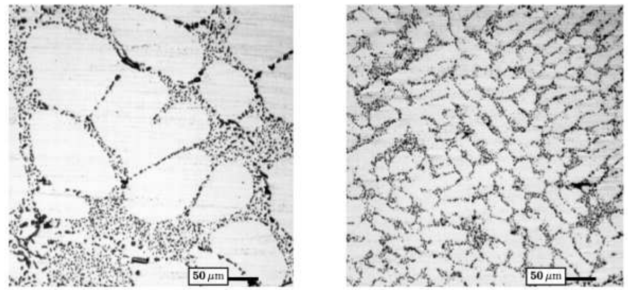


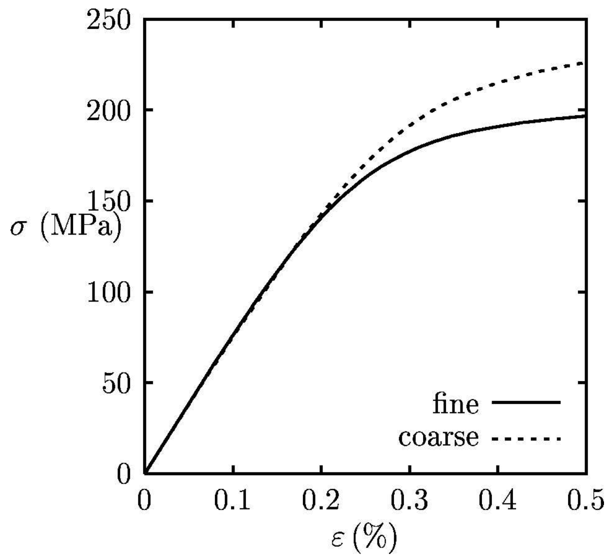
material (iii)

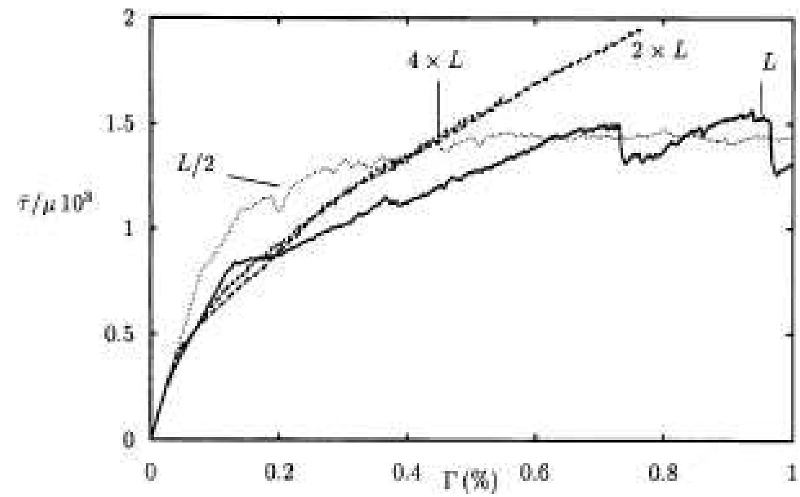
GNDs lead to increased hardening and size dependence.

Cleveringa *et al.*, Acta Mat., 45, 3163, 1997; J. de Phys. IV, 8 P4, 83, 1998.

Smaller can be Softer



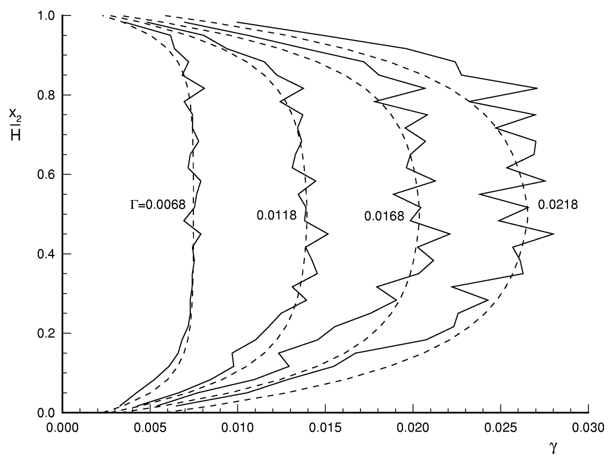


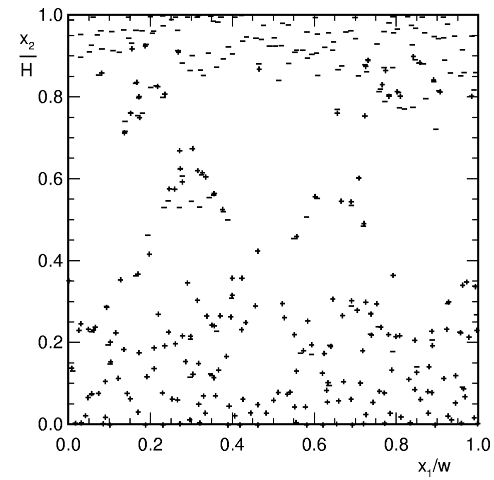


For cast A356 Al alloys, smaller is softer experimentally and in the discrete dislocation calculations.

Benzerga et al., Acta. Mat., 49, 3071, 2001.

Boundary Layers and Material Properties



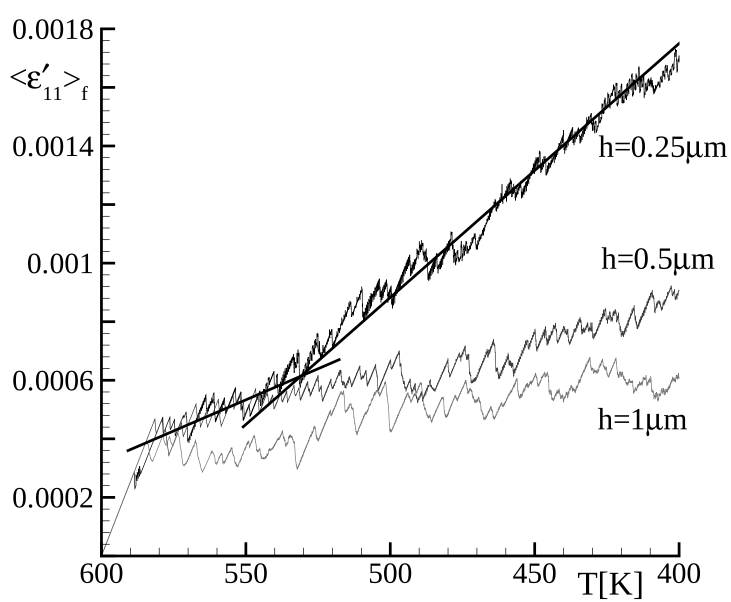


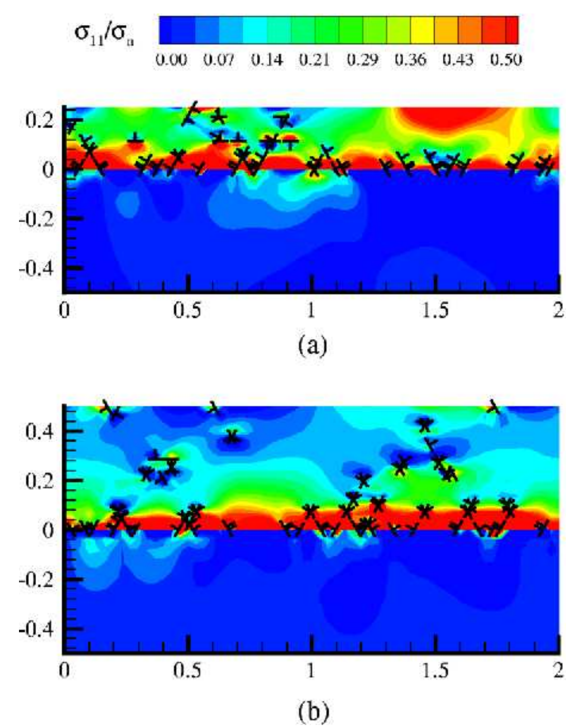
- A strain gradient arises as a consequence of the constraint of the interfaces on dislocation motion.
- A boundary layer does not develop with a sufficiently large τ_f.
- Do materials with high values of τ_f exhibit size effects due to GNDs but not due to boundary layers?
  - If so, what are the implications for phenomenological models?

Shu et al., J. Mech. Phys Solids, 49, 1361, 2001.

Boundary Layers and Source Limited Plasticity

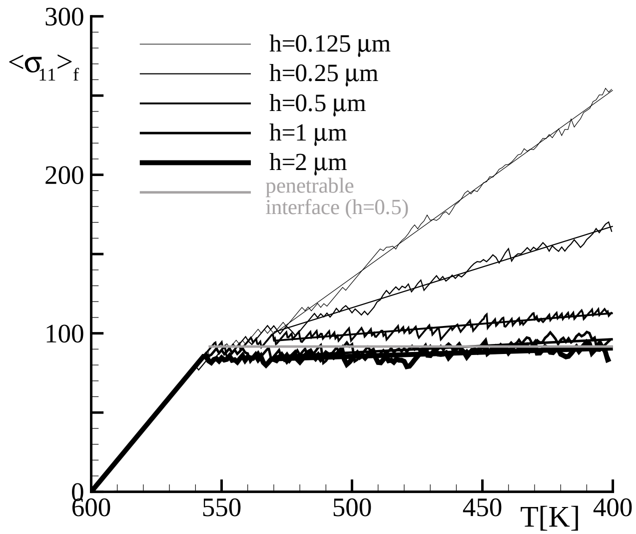
- Cooling from a stress-free state.
- There is a rather abrupt change in the hardening rate for thinner films due to the back stress generated by the boundary layer dislocations.

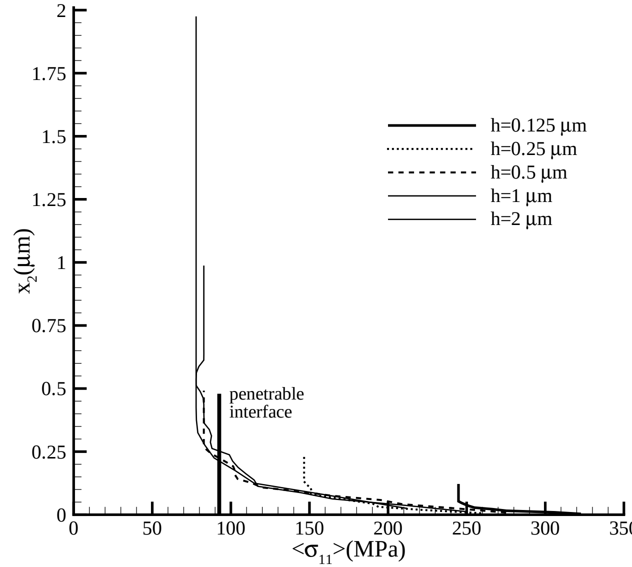




Nicola et al., J. Appl. Phys., 93, 5920, 2003.

Boundary Layers and Source Limited Plasticity





- For a sufficiently thick film, there is a film thickness independent boundary layer and

$$\sigma = \sigma_b \frac{1-h_l}{h} + \sigma_l \frac{h_l}{h} \qquad \sigma = \sigma_b + (\sigma_l - \sigma_b) h_l h^{-1}$$

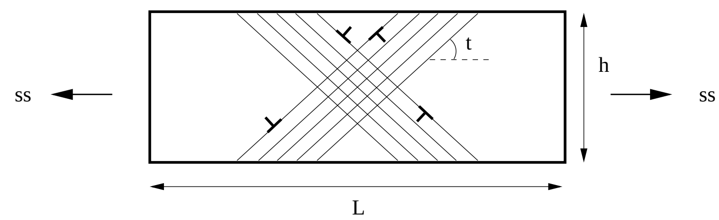
- For a sufficiently thin film, nucleation is inhibited throughout the film, the size effect becomes more pronounced and the scaling changes.

Nicola et al., submitted, 2004.

Size Effects

- Geometrically necessary dislocations arising from imposed strain gradients.
  - Modeled by a wide variety of nonlocal plasticity theories.
- Boundary layers that arise where an overall homogeneous response is possible.
  - Requires a nonlocal plasticity theory with higher order boundary conditions.
- Microstructures where smaller is softer.
- Source limited plasticity.
  - Can these be modeled by nonlocal plasticity theory?
- What are appropriate length scales and scalings for the various origins of size effects? Do these evolve? How?

Sensitivity to Perturbations



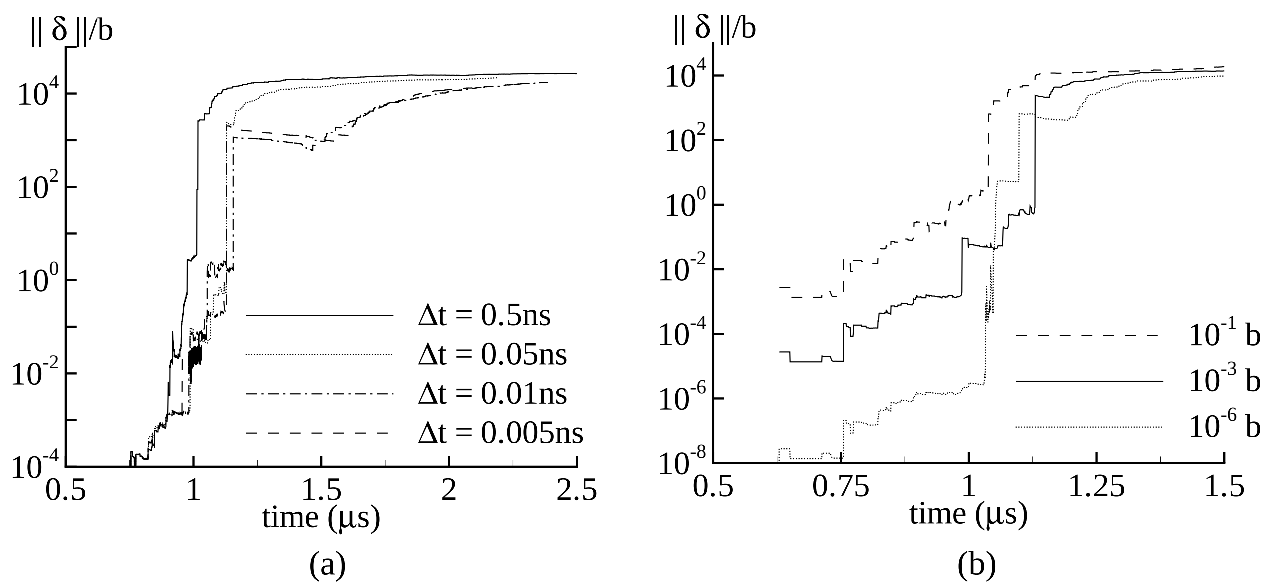
- Plane strain tension with positions of nucleation sites or dislocation positions perturbed.
- No overall instability.
- The system is termed chaotic if small perturbations in the initial configuration are amplified exponentially with time.

Deshpande et al., Scripta Mat., 45, 1047, 2001.

Sensitivity to Perturbations

- Dislocation dynamics can exhibit extreme sensitivity to small perturbations – chaotic in this sense.
- Two cases; dislocations (or sources) at x_0 and $x_0 + \delta_o$ at t_0.

$$\|\delta(t)\| = \frac{1}{N}\sum_{I=1}^{N}\sqrt{(x_p^{(I)}(t) - x_u^{(I)}(t))^2 + (y_p^{(I)}(t) - y_u^{(I)}(t))^2}$$



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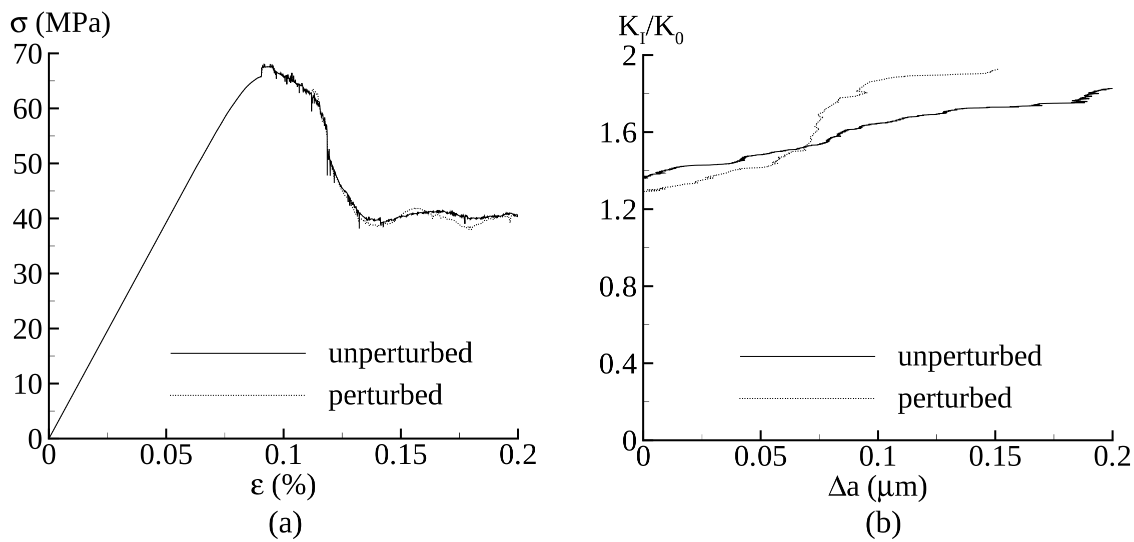


Stress-strain   Fracture

Deshpande et al., Scripta Mat., 45, 1047, 2001

Sensitivity to Perturbations

- Which behaviors are sensitive to tiny variations in initial conditions and which are not?
- What are the relative roles of statistical and geometrically necessary dislocations?
- Are there inherent limits to the controllability of dislocation based phenomena?

Statistical Effects

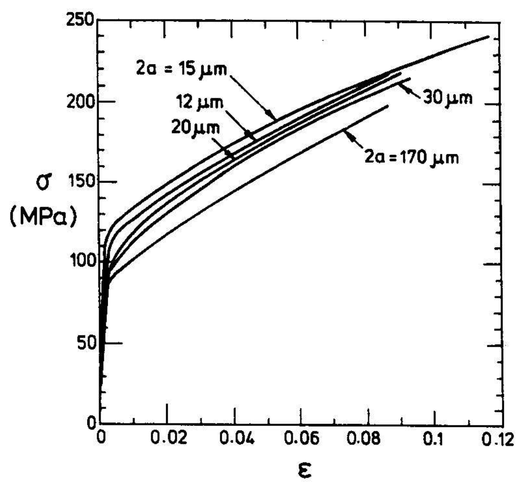
- From the discreteness of dislocation sources (source locations can matter).
  - Continuum plasticity theories, local and gradient, presume that if field variables at a material point satisfy a plastic flow condition that there is a source at that material point to produce the necessary dislocations.
  - At sufficiently small scales, this is not necessarily the case.
- From the chaotic nature of dislocation interactions.

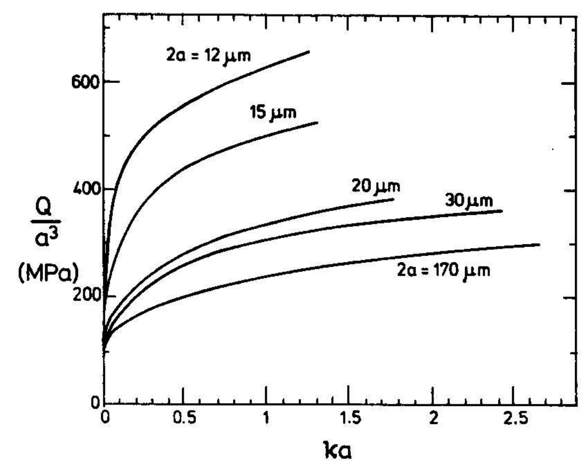
What are the limits to a deterministic description of plastic flow?

When is a single discrete dislocation calculation insufficient and an ensemble of calculations needed?

Size Effects and Fracture

- An observed increase in strength at micron size scales is associated with the dislocation structures induced by plastic deformation gradients (GNDs), e.g. Fleck et al. (1994).



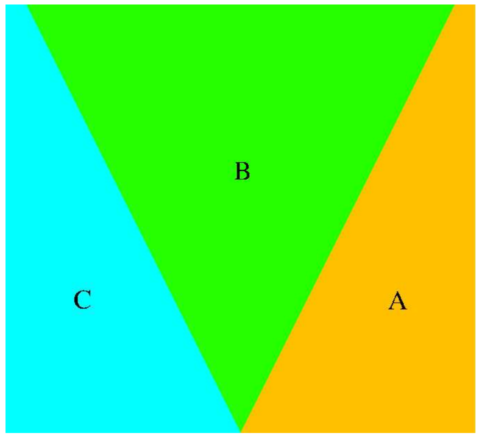


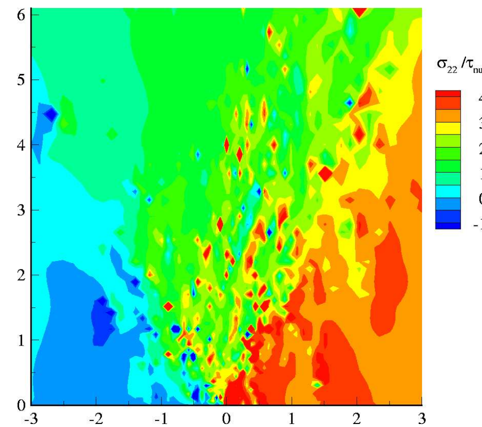
- Crack tip deformation fields give rise to large plastic deformation gradients.

Dislocations play a dual role in fracture: (i) plastic flow caused by their motion increases the resistance to crack growth; (ii) local stress concentrations associated with organized dislocation structures promote crack growth.

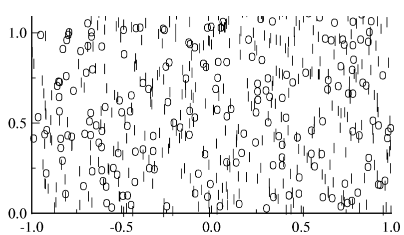
Stationary Crack – Two Slip Systems

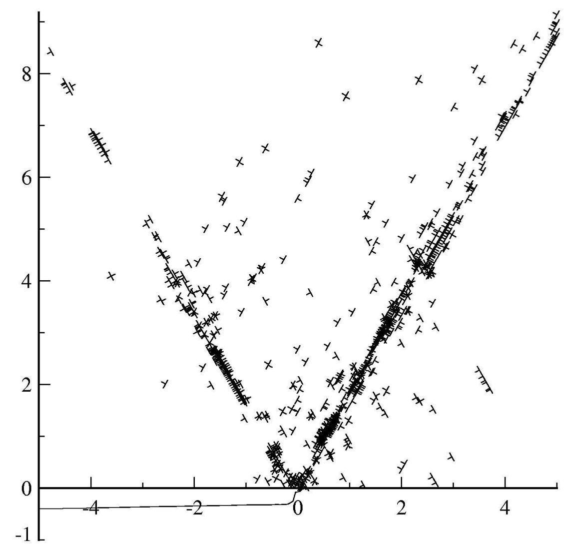
- Classical crystal plasticity – sectors of constant stress, Rice (1987).





- Dislocation structure.





Many internal sources – no special dislocation nucleation from the crack tip.

Crack Growth

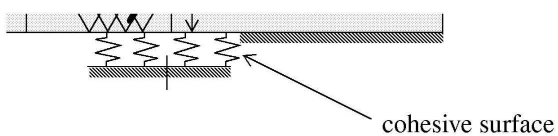
Cohesive surface framework.

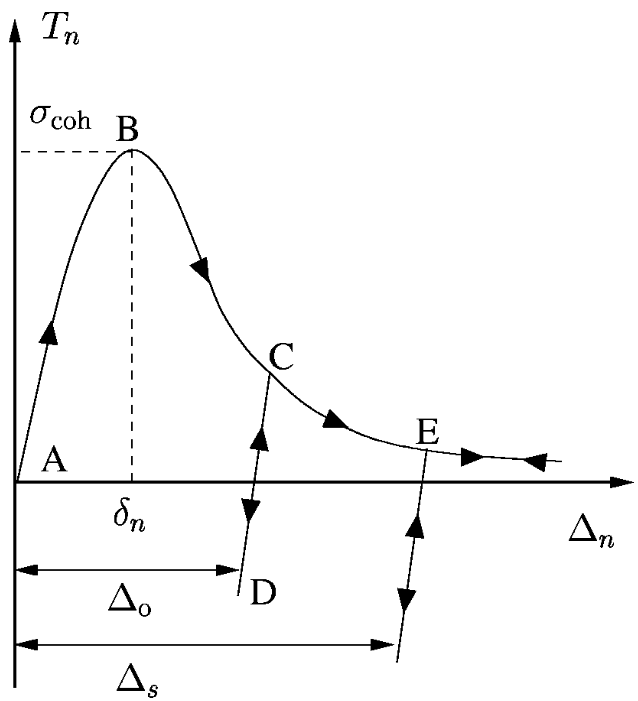
- The location of one or more cohesive surfaces is specified.
- Two constitutive relations – a bulk constitutive relation and a cohesive constitutive relation.
- A characteristic length is introduced.
- No crack tip singularity.

Principle of virtual work:

$$\int_V \sigma_{ij}\delta\epsilon_{ij}dV - \int_{S_{\mathrm{coh}}} T_i\delta\Delta_i dS = \int_{S_{\mathrm{ext}}} T_i\delta u_i dS$$

Cohesive Constitutive Relation

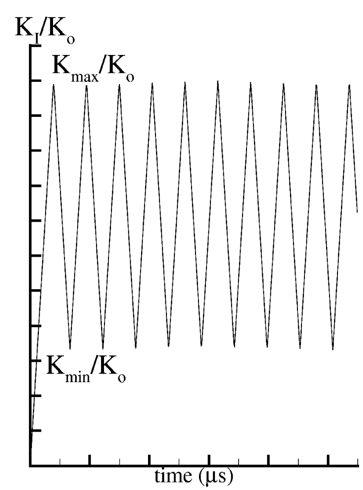




$$K_0 = \sqrt{\frac{E\phi_n}{1-\nu^2}}$$

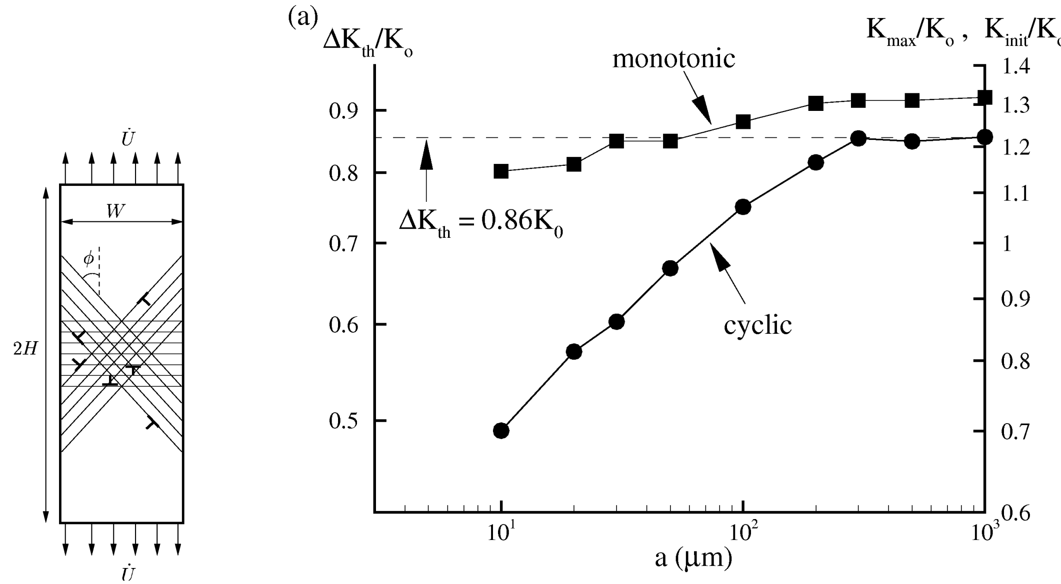
Hysteresis and Fatigue Crack Growth

- Crack growth under cyclic loading that occurs even when the driving force for crack growth is smaller than what is needed for crack growth under monotonic loading conditions.
  - Because of the anti-shielding character of the near tip dislocation structure, decohesion can occur under cyclic loading conditions in circumstances where it is precluded under monotonic loading conditions.
- Hysteresis is necessary for fatigue.



Short Crack Effect

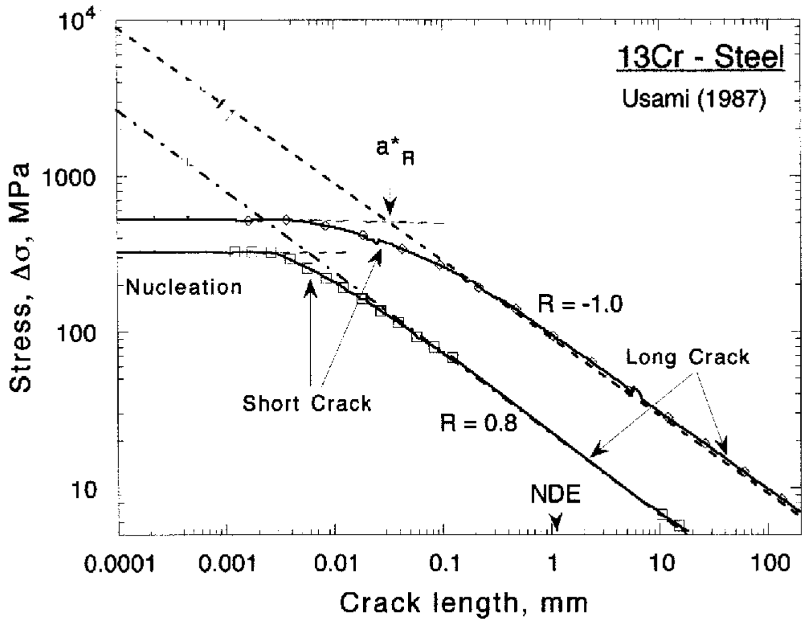
Edge cracked specimen.

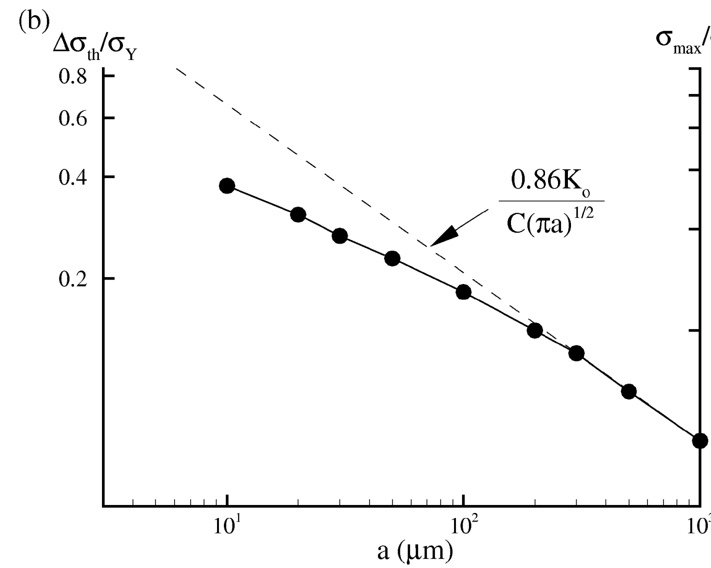


- For $a < 100\mu$m cyclic crack growth occurs with $K_{\max} < K_0 = \sqrt{E\phi_n/(1-\nu^2)}$.
  - K_0 is a measure of the work of separation, ϕ_n, which must be supplied locally for crack growth to occur.
  - $K_{\max} = C\sigma_{\max}\sqrt{\pi a}$ is a measure of the applied stress; due to the anti-shielding nature of the dislocation structure, the "local K" can be greater than $K_{\max}$.

Deshpande et al., Acta Mat., 51, 1, 2003.

The Kitagawa-Takahashi Diagram



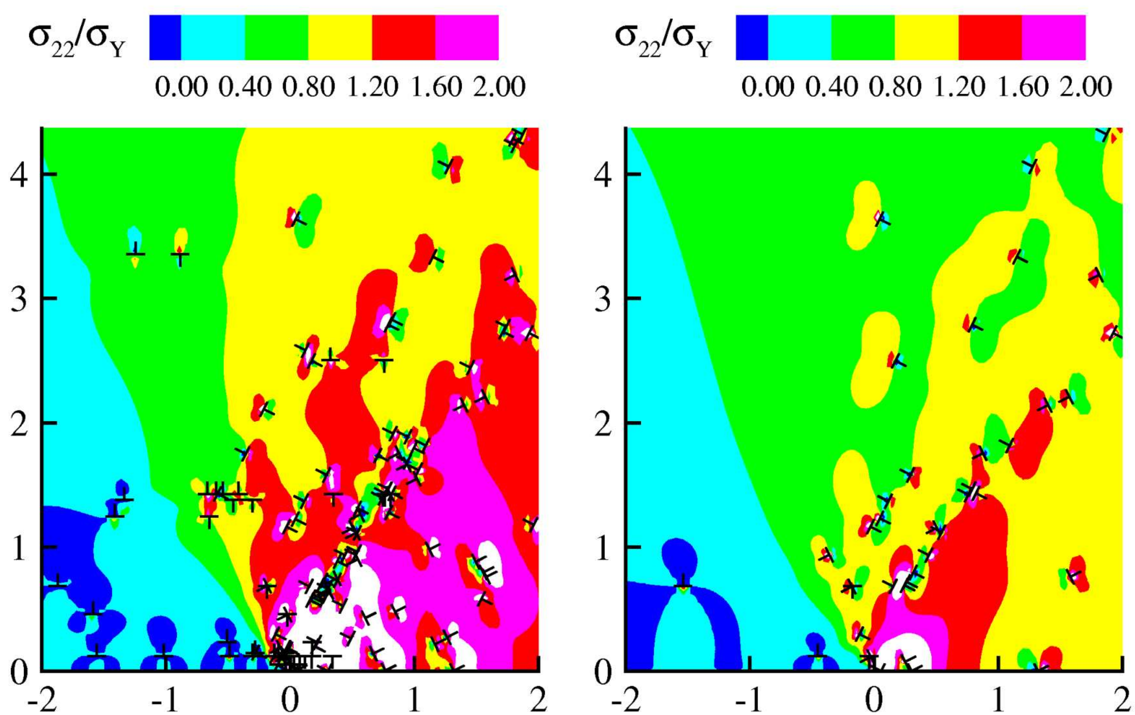


- $\sigma_{\max}/\sigma_{\mathrm{Y}} < 1 \rightarrow K_{\max}/K_0 < 1$ for $a \approx 10\mu$m, where K_0 is the critical stress intensity factor for elastic crack growth.

$$\frac{K_{\max}}{K_0} \approx \left(\frac{\sigma_{\max}}{\sigma_{\mathrm{Y}}}\right) \frac{\sqrt{a/\delta_n}}{\sqrt{E\sigma_{\mathrm{coh}}/\sigma_{\mathrm{Y}}^2}} \approx \left(\frac{\sigma_{\max}}{\sigma_{\mathrm{Y}}}\right) \frac{\sqrt{a/\delta_n}}{E/\sigma_Y} \approx \left(\frac{\sigma_{\max}}{\sigma_{\mathrm{Y}}}\right)$$

Short Crack Effect

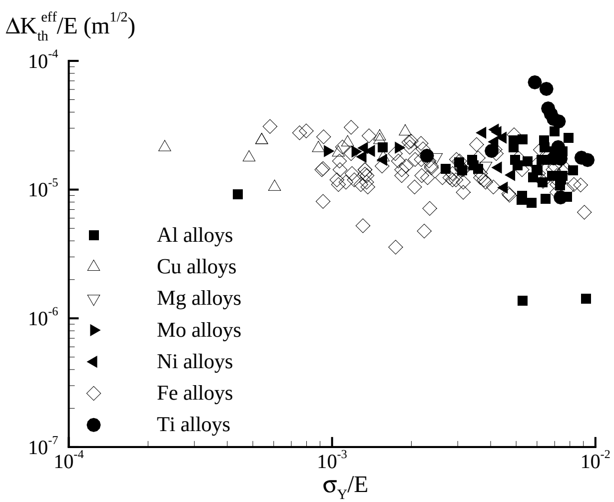
- For crack sizes of $\approx 5\mu$m and smaller, the high stress region near the crack tip is not large enough to nucleate and move many dislocations at $\sigma_{\max} < \sigma_Y$. Since fatigue requires irreversibility, fatigue crack growth is precluded.

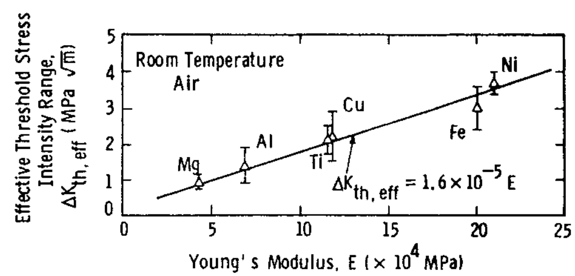


(a) (b)

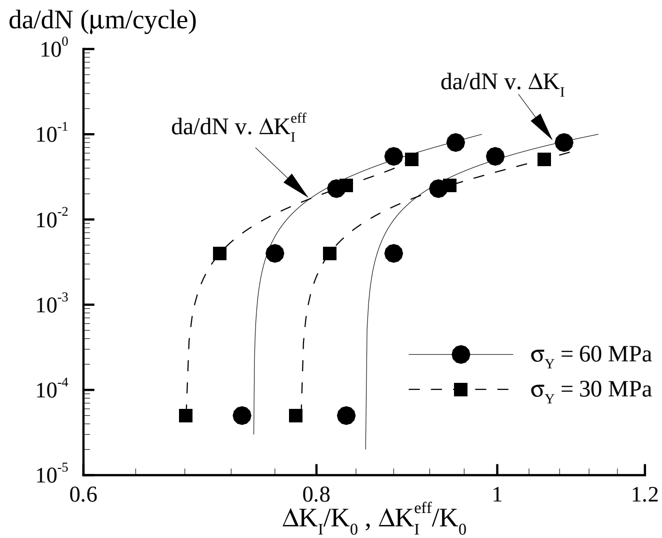
Scaling with Material Properties

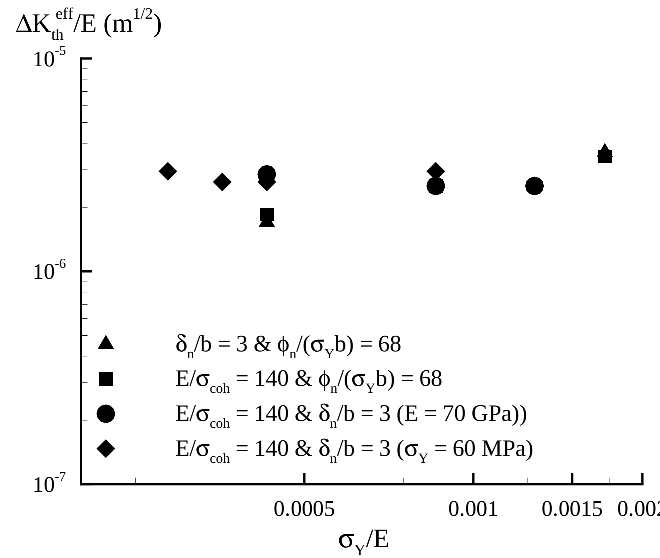
- The fatigue threshold is relatively independent of the material's yield strength, Kang *et al*. (1992).
- Scaling with Young's modulus is seen, Liaw *et al*. (1983).
- da/dN is not sensitive to $\sigma_{\rm Y}$ in the lower Paris law regime.





Scaling with Material Properties





- $\Delta K_{\rm th}^{\rm eff} \propto K_0 = \sqrt{\frac{E\phi_n}{1-\nu^2}}$ $(\phi_n = e\sigma_{\rm coh}\delta_n)$ with some deviation occurring for very low $\sigma_{\rm Y}$.
  - Vary material – $\sigma_{\rm coh} \propto E \rightarrow \Delta K_{\rm th}^{\rm eff} \propto E\sqrt{\delta_n}$.
  - Fix material, vary ϕ_n – $\Delta K_{\rm th}^{\rm eff} \propto \sqrt{\phi_n}$.

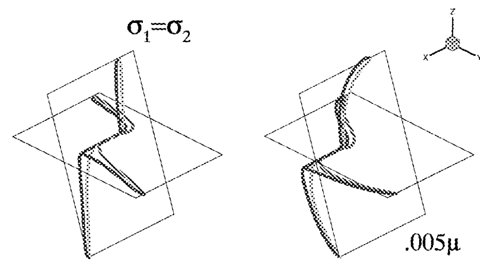
Deshpande et al., Acta Mat., 51, 4637, 2003.

Fracture and Fatigue

- The local stress concentrations associated with organized dislocation structures play a key role.
  - Current nonlocal plasticity theories can, at least in principle, account for the associated stress increase.
- In discrete dislocation plasticity, hysteresis is a natural outcome of the solution of boundary value problems under cyclic loading and is key for fatigue.
  - Current nonlocal plasticity predictions for hysteresis?
  - Current nonlocal plasticity predictions for scaling with material parameters?
- Source limitation effects can come into play.
  - Not modeled by current nonlocal plasticity theories.
- Dislocation nucleation from the crack tip.
- Finite geometry changes – crack tip blunting.

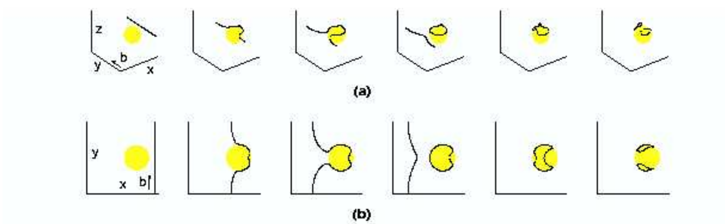
3D Discrete Dislocation Plasticity

- Representation of 3D dislocation fields in anisotropic solids.
  - Nodal methods



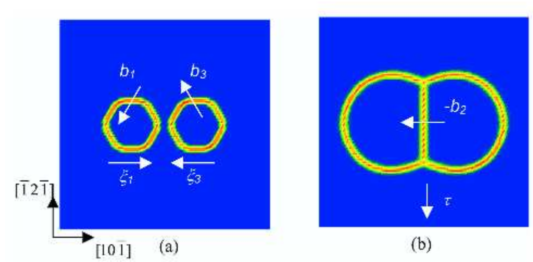
Shenoy et al., Phys. Rev. Lett., 84, 1491, 2000.

  - Level set methods.



Xiang et al., Acta Mat., 52, 1745, 2004.

  - Phase-field methods.



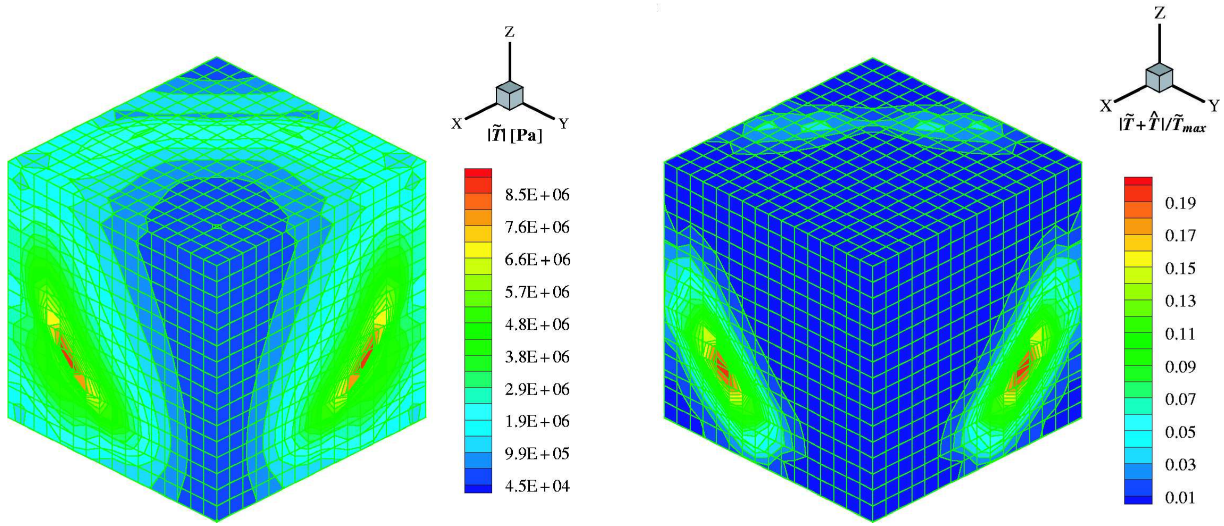
Shen et al., Acta Mat., 51, 2595, 2003.

3D Discrete Dislocation Plasticity

- Efficient and accurate 3D multi-body interaction computations.
  - Multipole methods.

    Lesar, Rickman, Phys. Rev. B, 65, 144110, 2002

- Accurate image force calculations particularly when a dislocation intersects a free surface.



Weygand et al., Model. Simul. Mat. Sci. Eng., 10, 437, 2002.

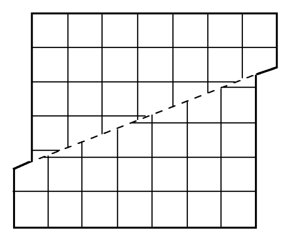
How much can be learned from incorporating 3D physics into a 2D computational framework?

Modeling Needs

- Finite deformations.
- Dislocation nucleation.
- Interaction of dislocations with grain boundaries and interfaces.
- Multi-scale connections.
- Direct incorporation of temperature dependence.
- Multi-physics and multi-mechanism modeling.

Finite Deformations

- Lattice rotations can play a dominant role in the deformation response of crystalline solids.
- Geometry changes significantly affect response in a wide variety of contexts; crack tip blunting; asperity flattening and/or shearing; surface roughening.
- Due to slip new free surface can be created.



- The displacement field is not a continuous single valued function. $\oint_\Gamma u_{i,j} dx_j \neq 0$.

Is it appropriate to insist on compatibility of the *total* displacement field in a nonlocal plasticity theory?

Finite Deformations

- There is strong coupling between finite deformation effects and the discrete dislocation dynamics.
  - Dislocations can change slip planes due to slip on intersecting systems.
  - The slip plane orientation varies due to nonuniform lattice rotations.
  - Nonuniform lattice rotations and elastic anisotropy imply position dependent elastic moduli L_{ijkl} and a polarization stress term enters the boundary value problem for the $(\hat{\ })$ fields.

Deshpande et al., J.Mech. Phys. Solids, 51, 2057, 2003.

Finite Deformations

- A numerical method that allows for the creation of new free surface due to slip.
- A numerical method that allows for resolving the effects of surface steps.

Such methods are under development.

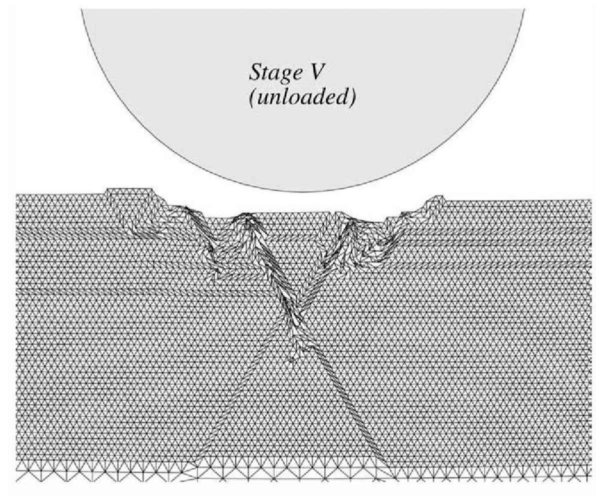
- The creation of new free surface and surface steps is important for coupled mechanical-chemical phenomena.

Dislocation Nucleation

1. Dislocation multiplication by Frank-Read sources is a propagation rather than a nucleation phenomenon.
2. Mesoscale models for dislocation nucleation need to be developed.
   - Dislocation nucleation from crack tips.
   - Dislocation nucleation from surface steps.
   - Grain boundaries and interfaces as sources and sinks for dislocations.

Multi-Scale Modeling

- Direct connections to atomistic and continuum plasticity descriptions are being developed.
  - Defect passing is key.



Miller et al., Acta Mat., 52, 271, 2004.

- Obtaining such solutions is extremely computationally intensive.

Connections

The lower the level of modeling, the greater the computational demands.

- Direct coupling atomistics to discrete dislocation plasticity to continuum plasticity.
- Information passing.
  - From experiment.
  - From lower level modeling.
    - Unit process modeling (atomistics or high resolution discrete dislocation) to discrete dislocation plasticity – nucleation criteria, dislocation motion rules, dislocation interaction rules.
  - To more phenomenological theories.

Connections

- What sort of phenomenological mesoscale plasticity theory is appropriate? When?
  - Statistical theories. Zaiser et al., Phys. Rev. B, 64, 224102, 2001.
  - Field theories. Gurtin, J. Mech. Phys. Solids, 50, 5, 2002.
  - How can direct connections to discrete dislocation plasticity be made?

    Yefimov et al., J. Mech. Phys. Solids, 52, 279, 2004.

    Bittencourt et al., J. Mech. Phys. Solids, 51, 281, 2003.
  - What are the implications of lack of compatibility at the discrete dislocation scale of the total displacement field?

    Deseri, Owen, J. Elast., 70, 197, 2003.
  - Can appropriate boundary conditions for phenomenological mesoscale plasticity theories be determined from discrete dislocation analyses?
  - How useful are isotropic theories of crystalline solids at the mesoscale?

Predictions

- What is needed to obtain quantitatively accurate discrete dislocation plasticity predictions?
- What is worth predicting quantitatively? It should be easier, faster, cheaper to do the predictiction than to do the experiment.
- When are trends and dependence on parameters good enough?

Concluding Remarks

- Features that are key for critical deformation and fracture processes in crystalline solids emerge naturally from discrete dislocation plasticity:
  - Size effects due to gradients either imposed or arising from self-organized dislocation structures.
  - Source limitation effects.
  - Hysteresis leading to fatigue.
- Discrete dislocation plasticity has provided insight into mesoscale deformation and failure processes and even in its current state has the potential to continue to do so.

Concluding Remarks

- Discrete dislocation plasticity provides a conduit for relating atomistic scale information to macro/micro scale behavior.
- Discrete dislocation plasticity can:
  - Provide a framework for assessing the performance and reliability of micro/nano-scale devices and components.
  - Provide a framework for the design of material systems.
  - Provide a quantitative understanding of key fracture and fatigue phenomena.
  - Provide a means of exploring the limits of deterministic predictability of plastic flow and fracture processes and (possibly) the basis for a statistical characterization.
  - Provide a testbed for the development of nonlocal continuum plasticity theories.
- But...

- Significant advances in modeling and in computational methodology are needed before the full potential of discrete dislocation plasticity can be realized.
- Inelastic deformation is often the consequence of more than dislocation glide; models for coupling with other processes (e.g. chemical, diffusional) and other deformation mechanisms (e.g. twinning, phase changes, grain boundary deformation modes) are needed.