A Combined Discrete-dislocation/Scale-dependent Crystal Plasticity Analysis of Deformation and Fracture in Nanomaterials

Presented by:

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Objective

Compare the results of analyses in which two material models, that take different approaches to model plasticity, are used to simulate deformation and fracture in single crystal solids of the mesoscale size range (fraction of micrometer to approximately 100μm) where the geometric length scale is of the same order as relevant material length scales.

Overview of Presentation

I. Brief Description of Models

✍ Discrete Dislocation Model
(Van der Giessen, Needleman 1995)

✍ Crystal Plasticity Model

II. Results and Comparison

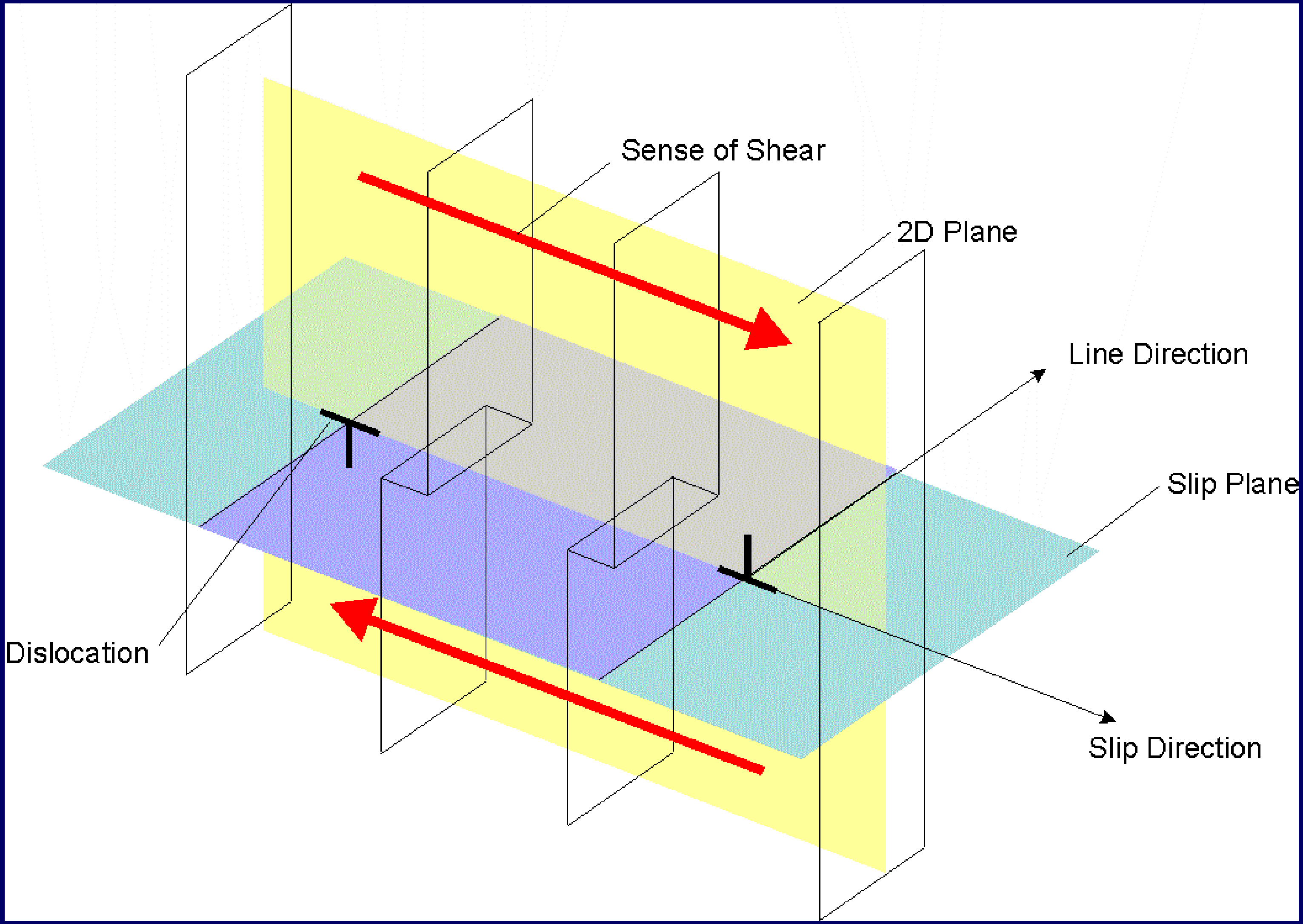
✍ Micro-beam Bending

✍ Mode I Crack

III. Conclusions

Lattice Slippage (Dislocation Loop 2D)

Principle cause of plastic deformation in crystalline solids is lattice sliding, or the expansion of dislocation loops



Discrete Dislocation Model

(Van der Giessen and Needleman, 1994)

Incorporates effects of movement, generation/annihilation, and interaction of dislocations into materials' plastic stress-strain responses

Simplifications

- ✍ 2D plane strain
- ✍ Dislocations ~ discrete, infinitely long, straight-line defects residing in a linear-elastic solid, and of the edge type
- ✍ Evolution of dislocation structure
  - *long range interactions* between dislocations and stress field
  - *short range interactions* (nucleation, annihilation)

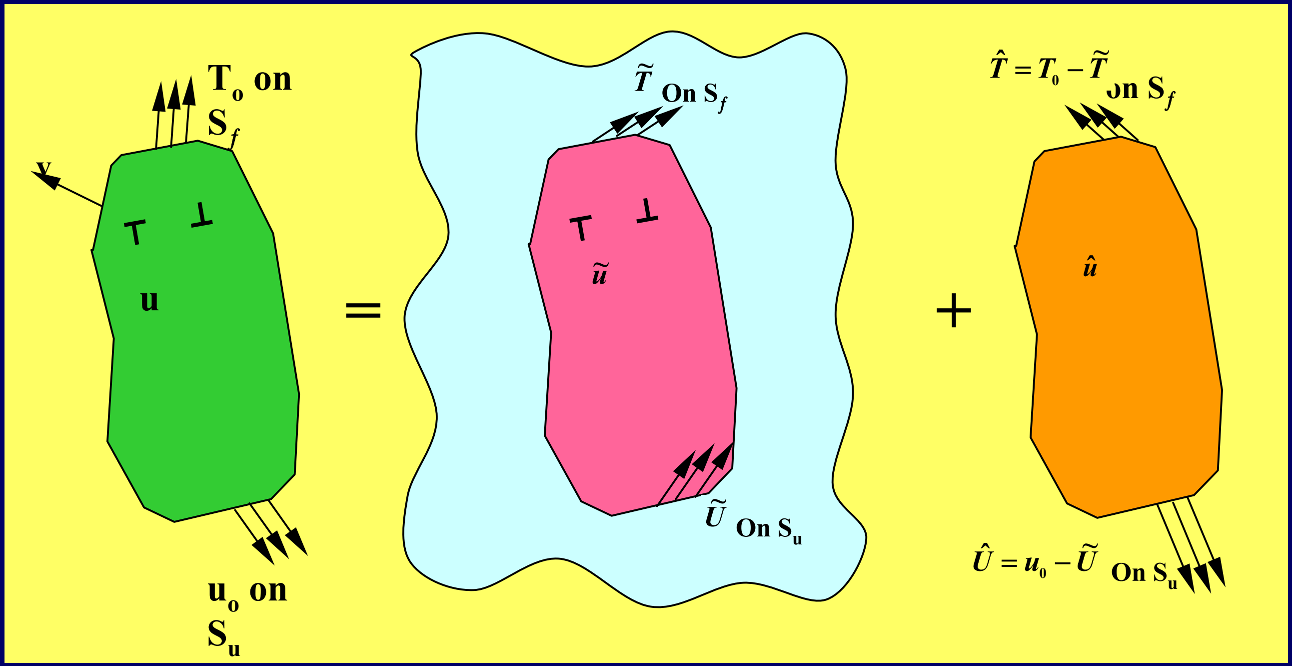
Discrete Dislocation Formulation

Evolution of deformation state and dislocation structure

1. Dislocation configuration known, body in equilibrium with applied tractions and displacements
2. For an increment in loading, boundary value problem solved to determine equilibrium stress fields
3. Long and short range interactions considered to determine new dislocation structure

Discrete Dislocation Formulation
(Decomposition of B.V.P.)

- ~ Infinite linear elastic medium with *n* dislocations
- ^ Modified boundary condition form of original problem w/o dislocations



$$u = \tilde{u} + \hat{u}, \quad \varepsilon = \tilde{\varepsilon} + \hat{\varepsilon}, \quad \sigma = \tilde{\sigma} + \hat{\sigma}\,; \text{ in V}$$

Discrete Dislocation Formulation
(Long Range Dislocation Interactions)

Long range interactions among dislocations and between dislocations and applied stress field

- ✍ Dislocation glide allowed on well-defined slip planes (drag controlled motion)

$$v^i = f^i / B$$

$$f^i = n^i \cdot \left(\hat{\sigma} + \sum_{j \neq i} \tilde{\sigma}^j \right) \cdot b^i \quad \text{(Peach-Koehler force)}$$

Discrete Dislocation Formulation
(Short Range Dislocation Interactions)

Short range interactions between dislocations

Nucleation (Frank-Read type point sources)

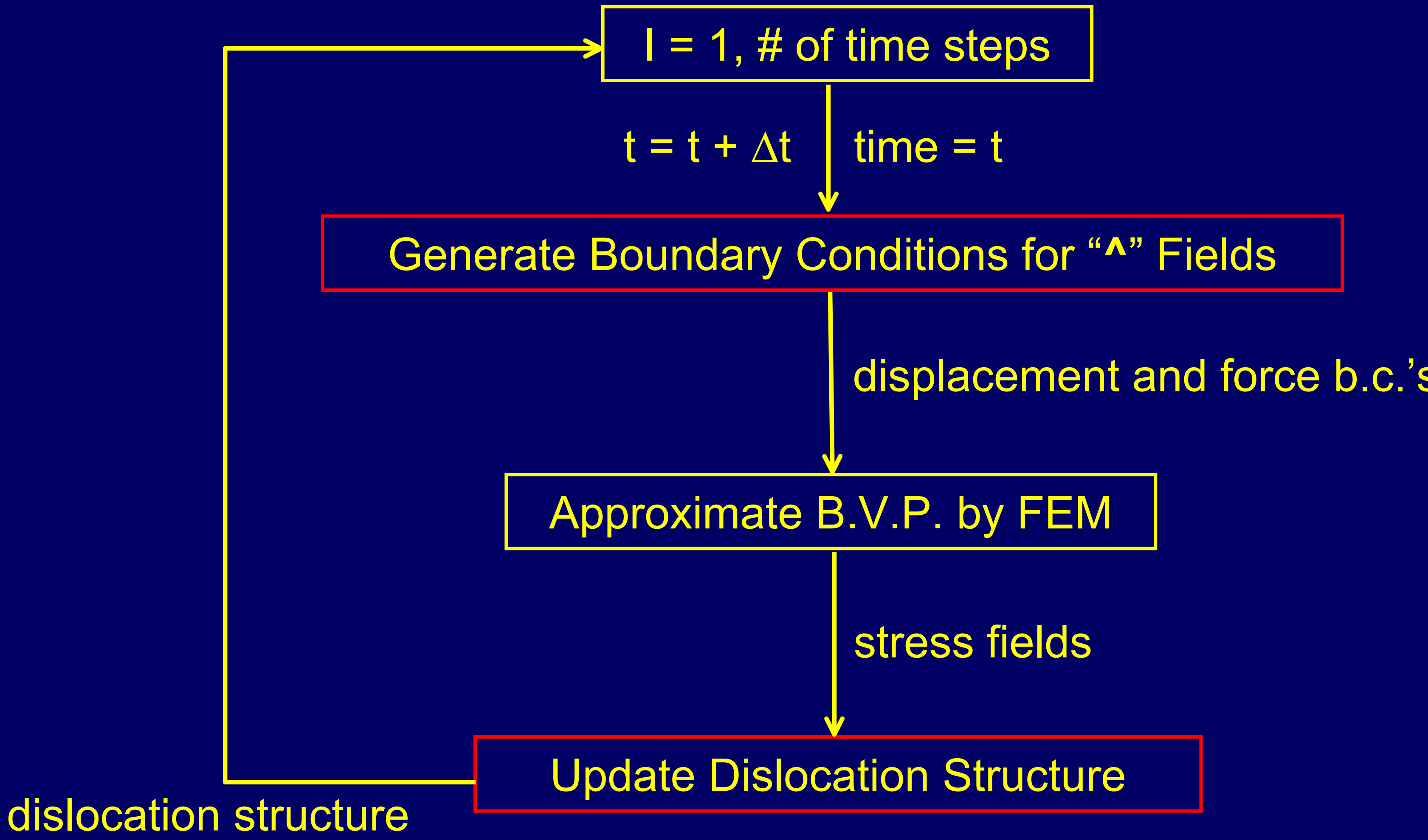
- if Peach-Koehler force exceeds critical value $\tau_{nuc} b$, *a* dislocation dipole is formed at distance

$$L_{nuc} = \frac{E}{4\pi\left(1-\nu^{2}\right)}\frac{b}{\tau_{nuc}}$$

Annihilation

- two dislocations of opposite Burgers vector on the same plane annihilate when within critical distance

Implementation
(Euler Forward Time Integration)



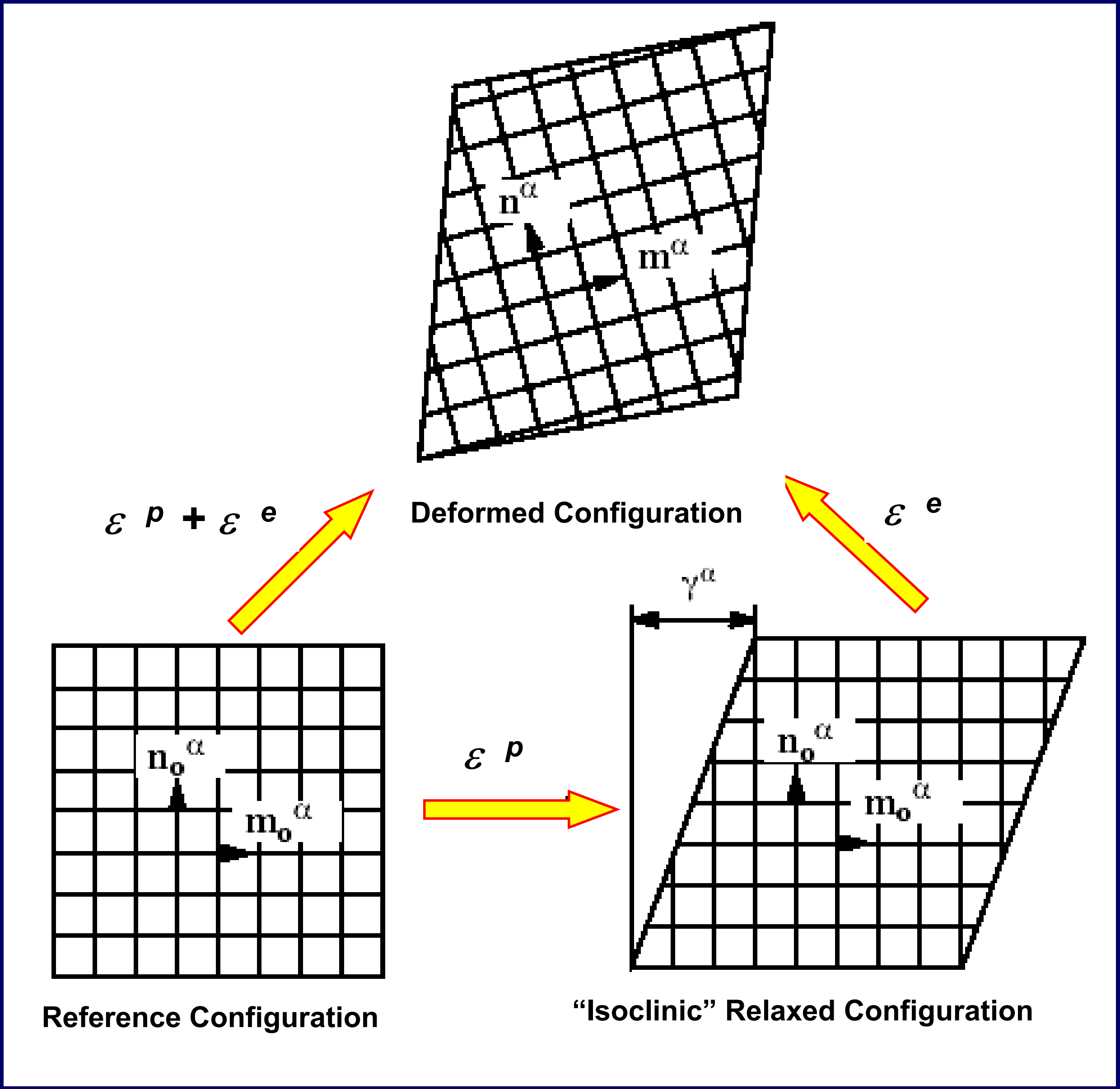
Crystal Plasticity Model

Plastic deformation (slip) occurs only on particular material dependent planes

Deformation decomposition for single crystal

- ✍ Elastic distortion of the lattice (stretching of atomic bonds)
- ✍ Sliding on slip planes which leaves the lattice undisturbed (atomic plane slippage)

Deformation Decomposition



Crystal Plasticity Formulation

Decomposition of total strain rate into elastic distortion and sliding on slip system α

$$\dot{\varepsilon} = \dot{\varepsilon}^e + \dot{\varepsilon}^p$$

where,

$$\dot{\varepsilon}^e = C^{-1}[\dot{\sigma}], \quad \dot{\varepsilon}^p = \sum_{\alpha} \dot{\gamma}^{\alpha} P^{\alpha}$$

and,

$$P^{\alpha} = \frac{1}{2}\left[m^{\alpha} \otimes n^{\alpha} + n^{\alpha} \otimes m^{\alpha}\right]$$

Crystal Plasticity Formulation

Rate form of constitutive law

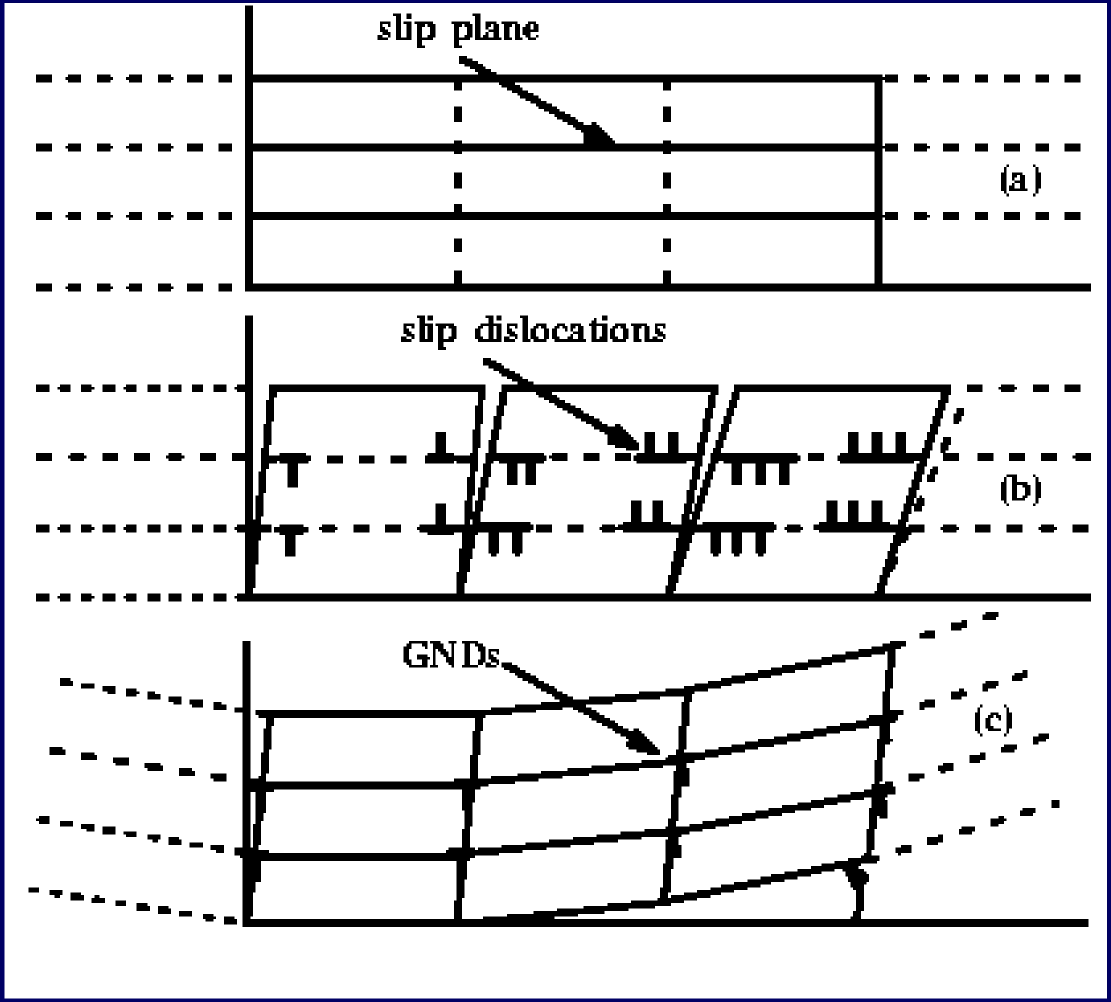
$$\dot{\sigma} = C\left[\dot{\varepsilon} - \sum_{\alpha} \dot{\gamma}^{\alpha} P^{\alpha}\right]$$

Viscoplastic material, rate of shear strain and shear stress related through power law relation

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0 \left[\frac{\tau^{\alpha}}{s^{\alpha}}\right]^{1/m} sign(\tau^{\alpha})$$

$$\dot{s}^{\alpha} = f\left(\gamma^{\beta}, \dot{\gamma}^{\beta}\right)$$

Nonlocal Crystal Plasticity (GNDs)



Original Continuum

Gradient in plastic shear

GNDs required to maintain continuity

Incorporation of Nonlocal effects into Crystal Plasticity Model

Revised form of slip resistance evolution equation

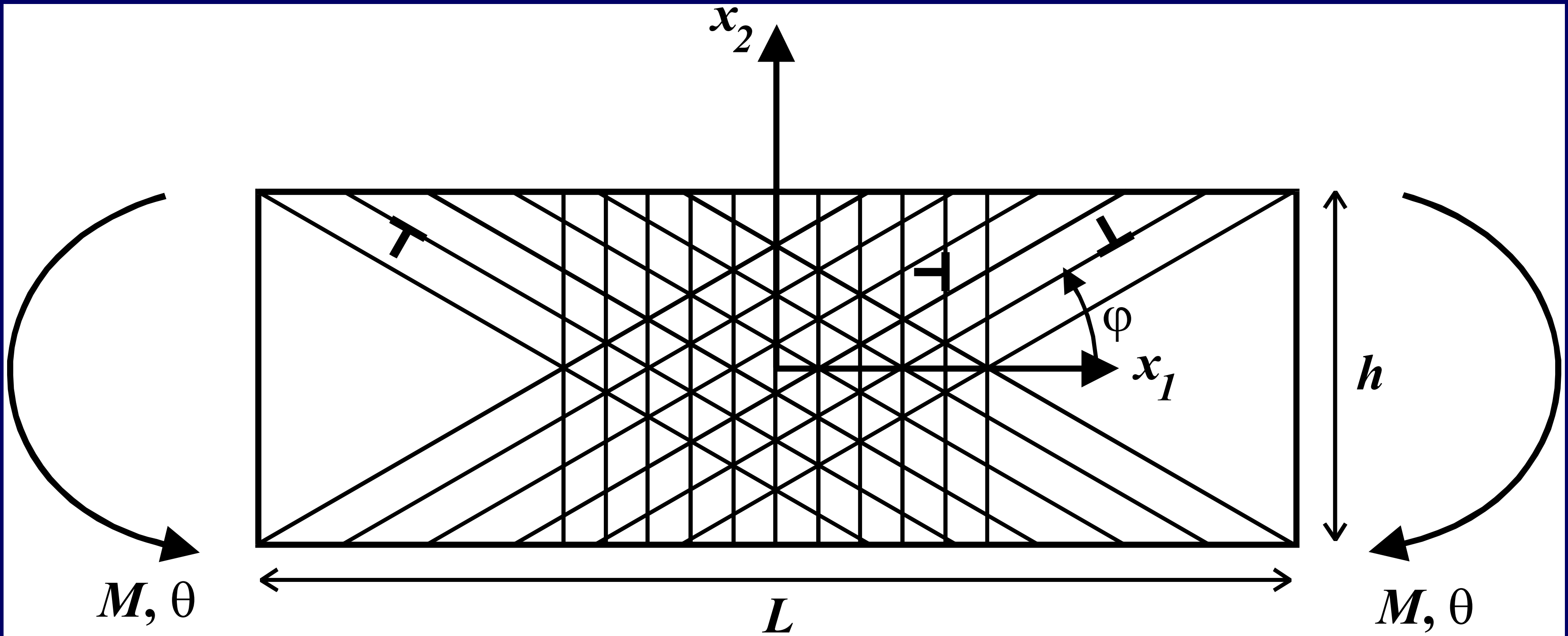
$$\dot{s}^{\alpha} = f\left(\gamma^{\beta}, \dot{\gamma}^{\beta}, \nabla\dot{\gamma}^{\beta}\right)$$

Implementation in ABAQUS/Standard
(User Material (UMAT) Subroutine)

Increment description (starting time = 0)

1. Subroutine first returns elastic estimate of material Jacobian $\partial\Delta\sigma / \partial\Delta\varepsilon$ for a perturbation about time = 0
2. Strain increment guesses passed to subroutine by ABAQUS
3. Slip resistance s^{α} guessed
4. Stress σ (t+Δt) determined by nonlinear equation solver
5. New s^{α} computed
6. Repeat from 4 until convergence of s^{α}
7. Material Jacobian and stress σ (t+Δt) passed to ABAQUS
8. Check if equilibrium satisfied, if not, repeat from 2

Beam Bending
(B.V.P. and Slip Plane Orientation)



$\varphi = \pm\, 30°, 90°$

Initial Conditions (Beam Bending)

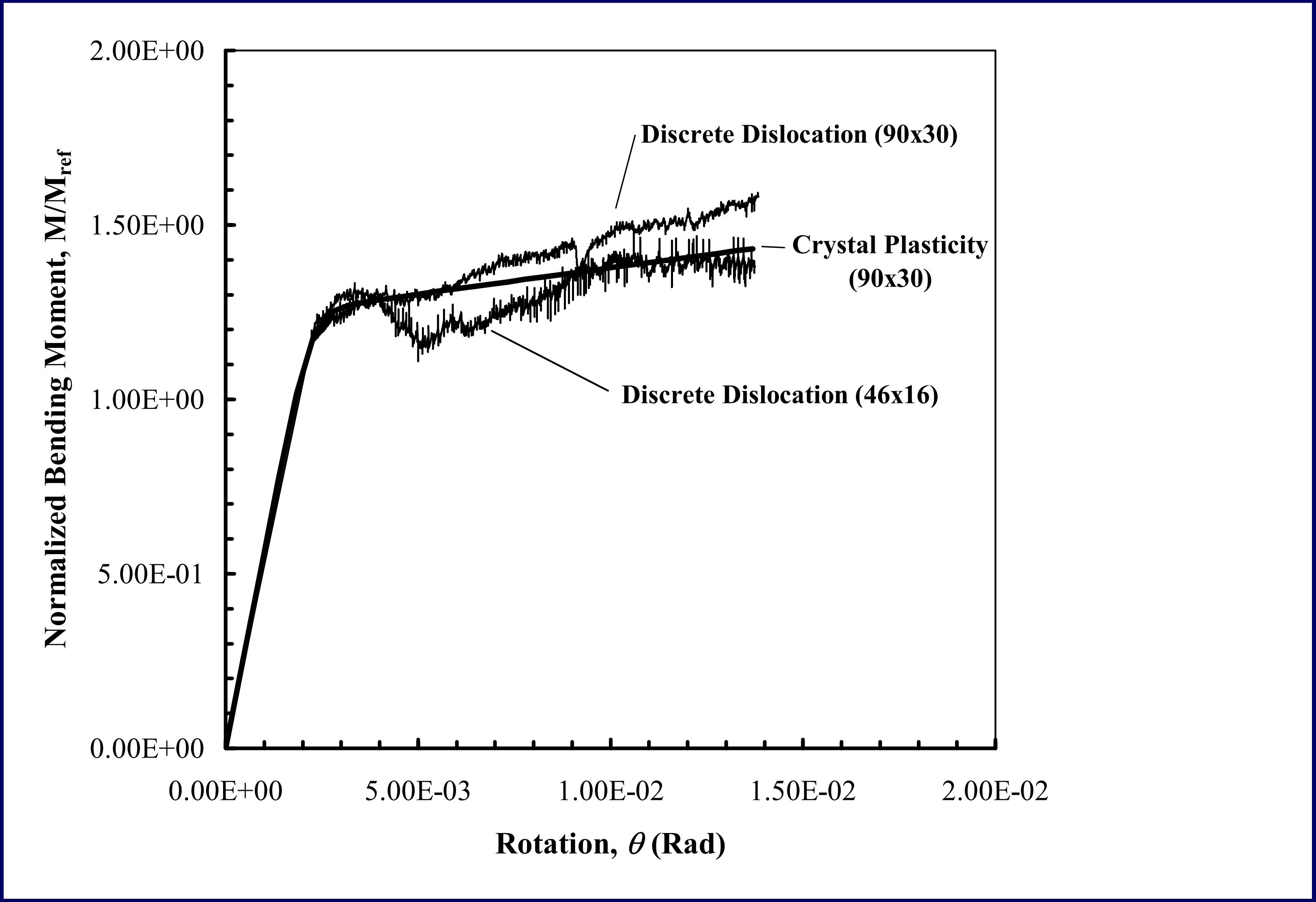
Discrete Dislocation Plasticity Analysis

- *Source distribution* (random spatial distribution, Gaussian source strength distribution)
- Initially, dislocation free crystal

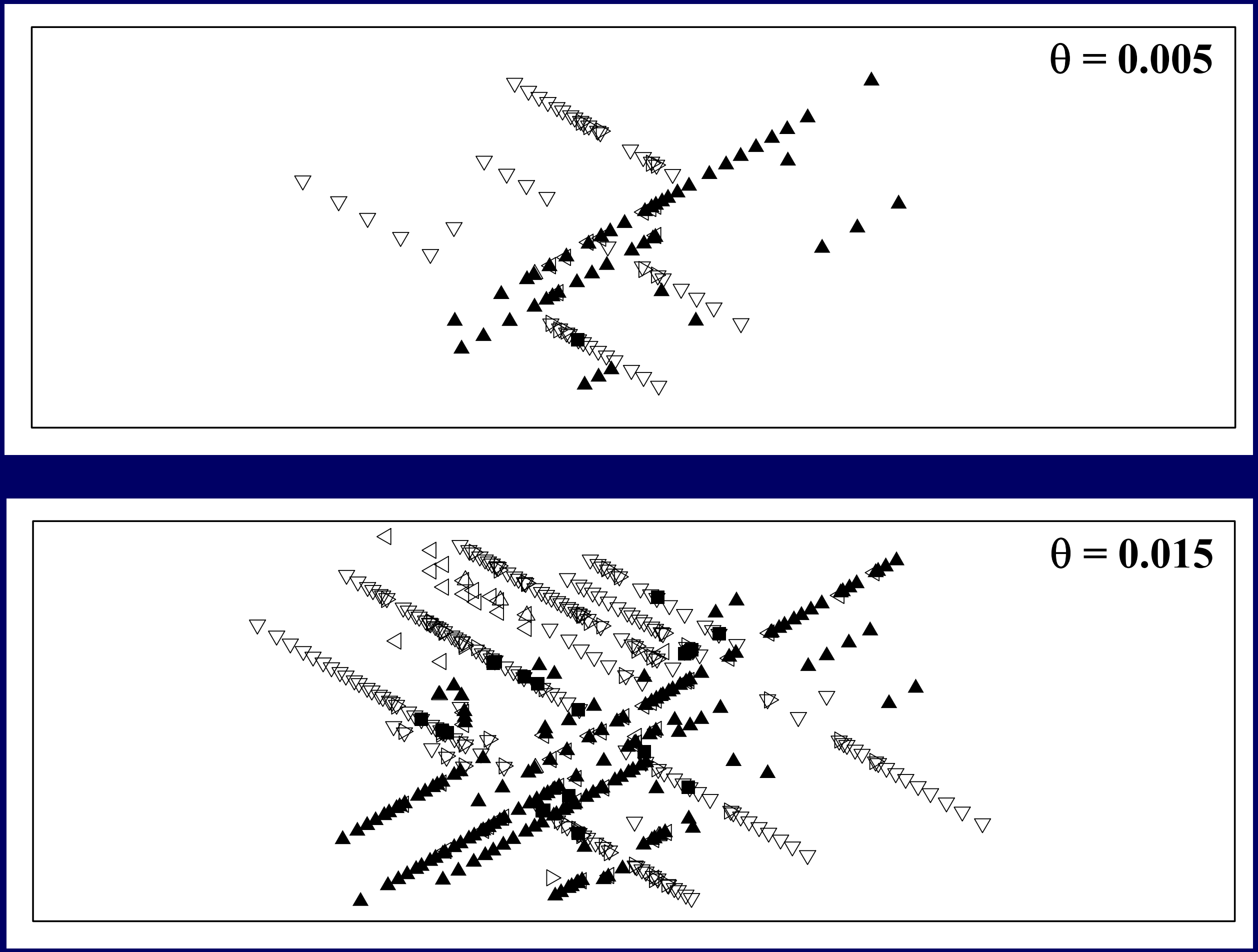
Crystal Plasticity Analysis

- Distribution of initial slip resistance consistent with source strength distribution of discrete dislocation analysis

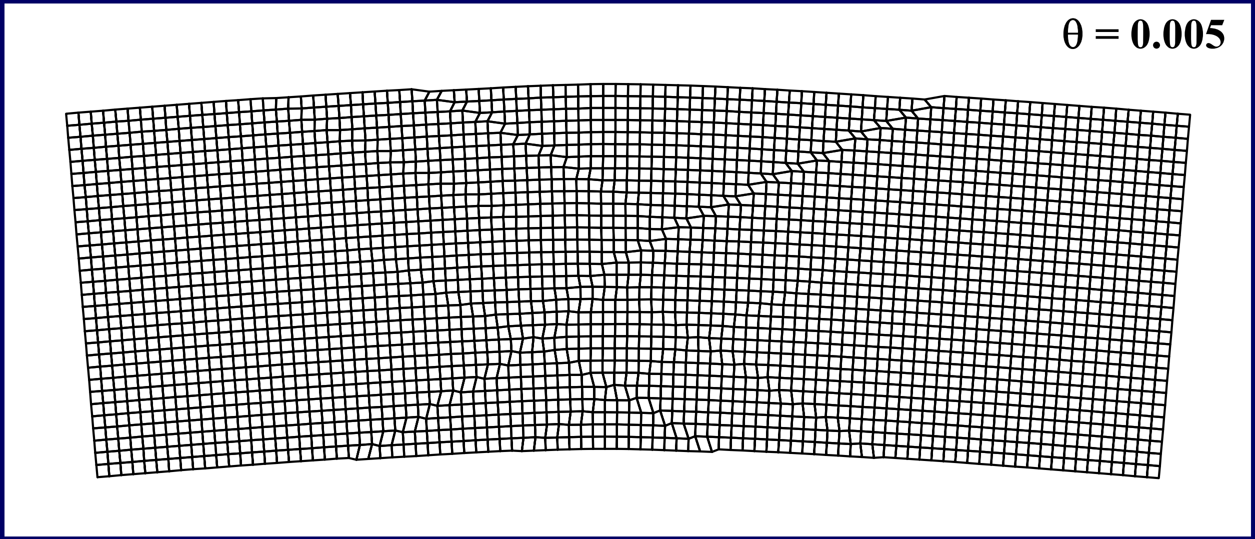
Discrete Dislocation Beam Bending
(Normalized Bending Moment vs. Rotation)

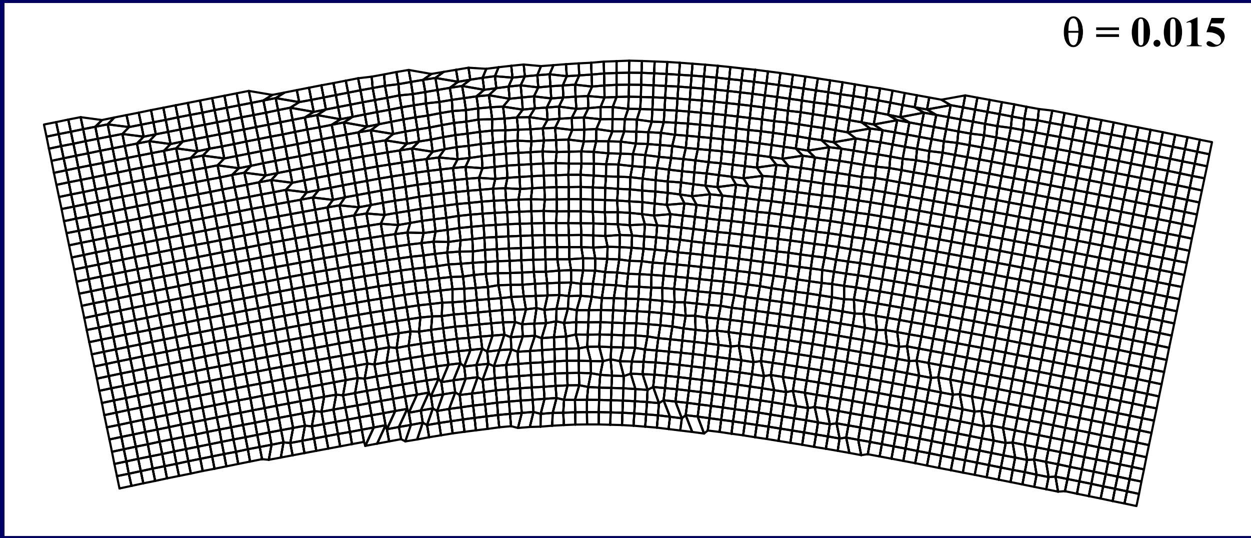


Discrete Dislocation Beam Bending
(Dislocation Configurations)

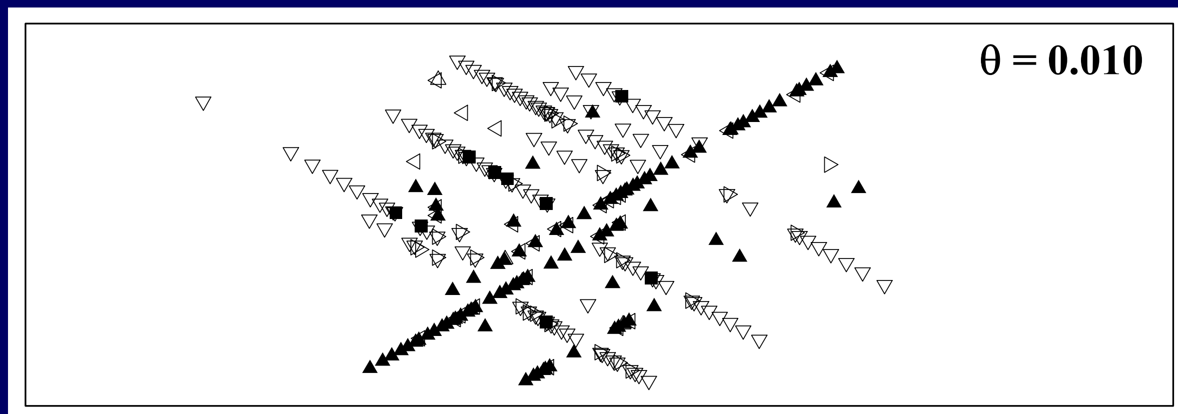


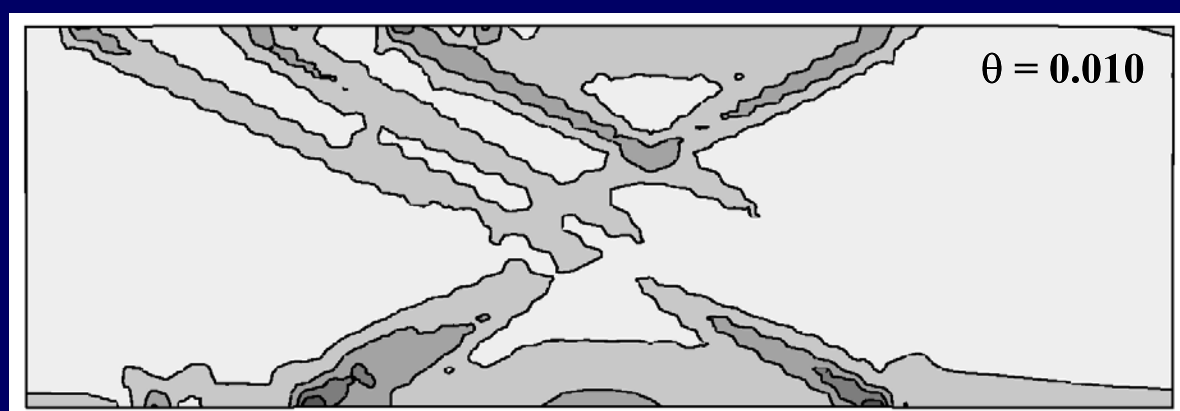
Discrete Dislocation Beam Bending
(Deformed Shapes)



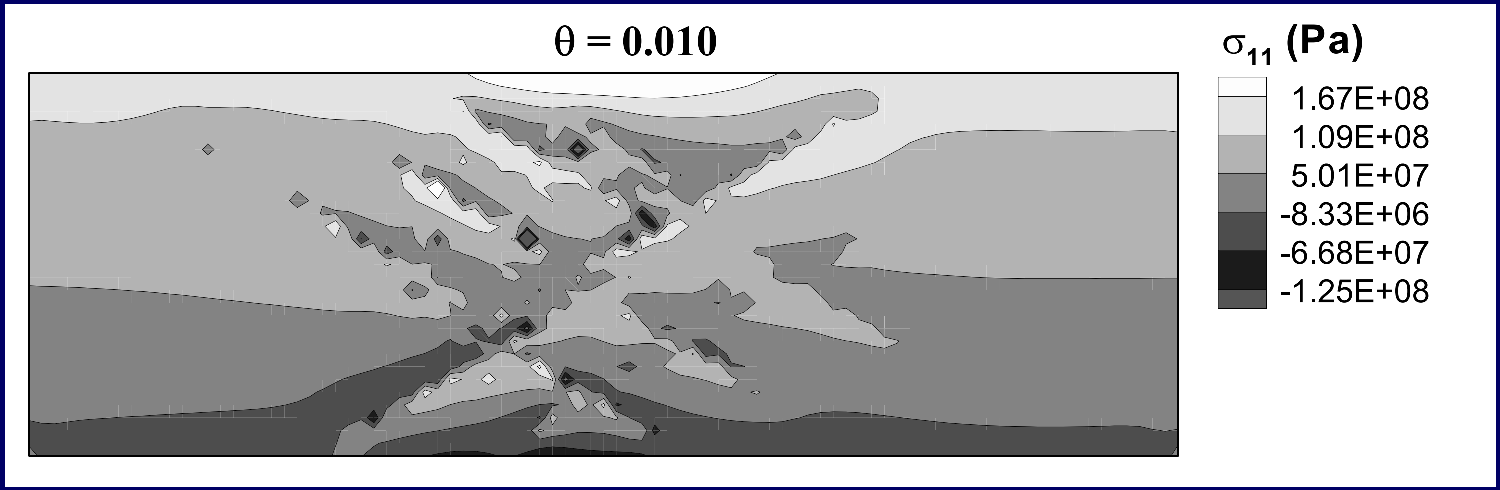


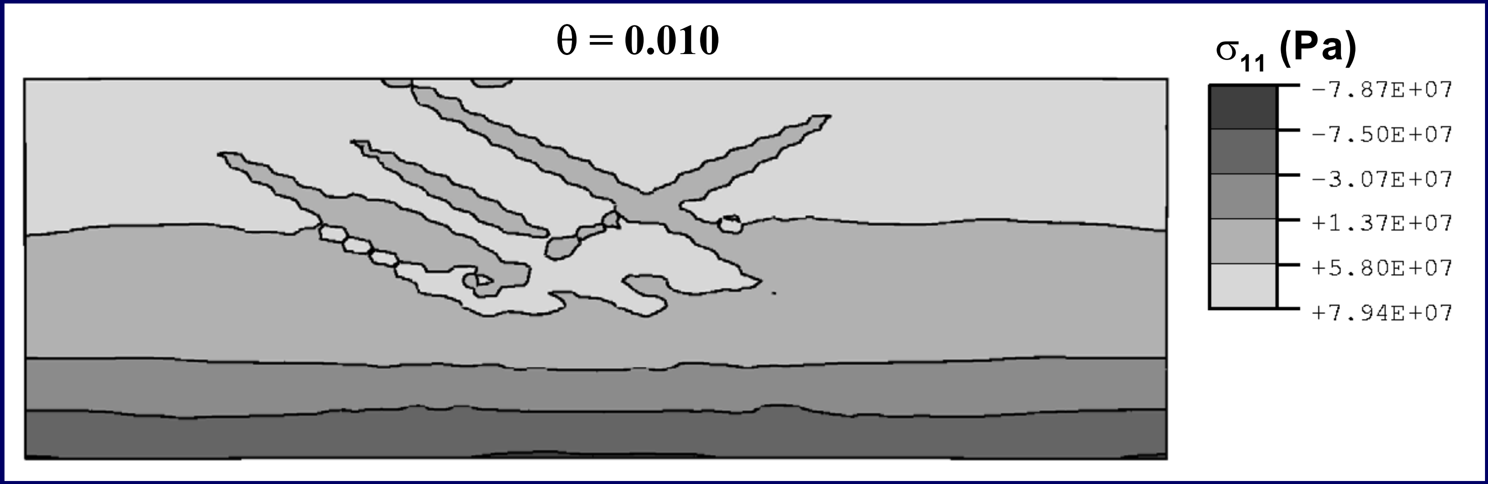
Discrete Dislocation/Crystal Plasticity Comparison (dislocations, plastic strain)





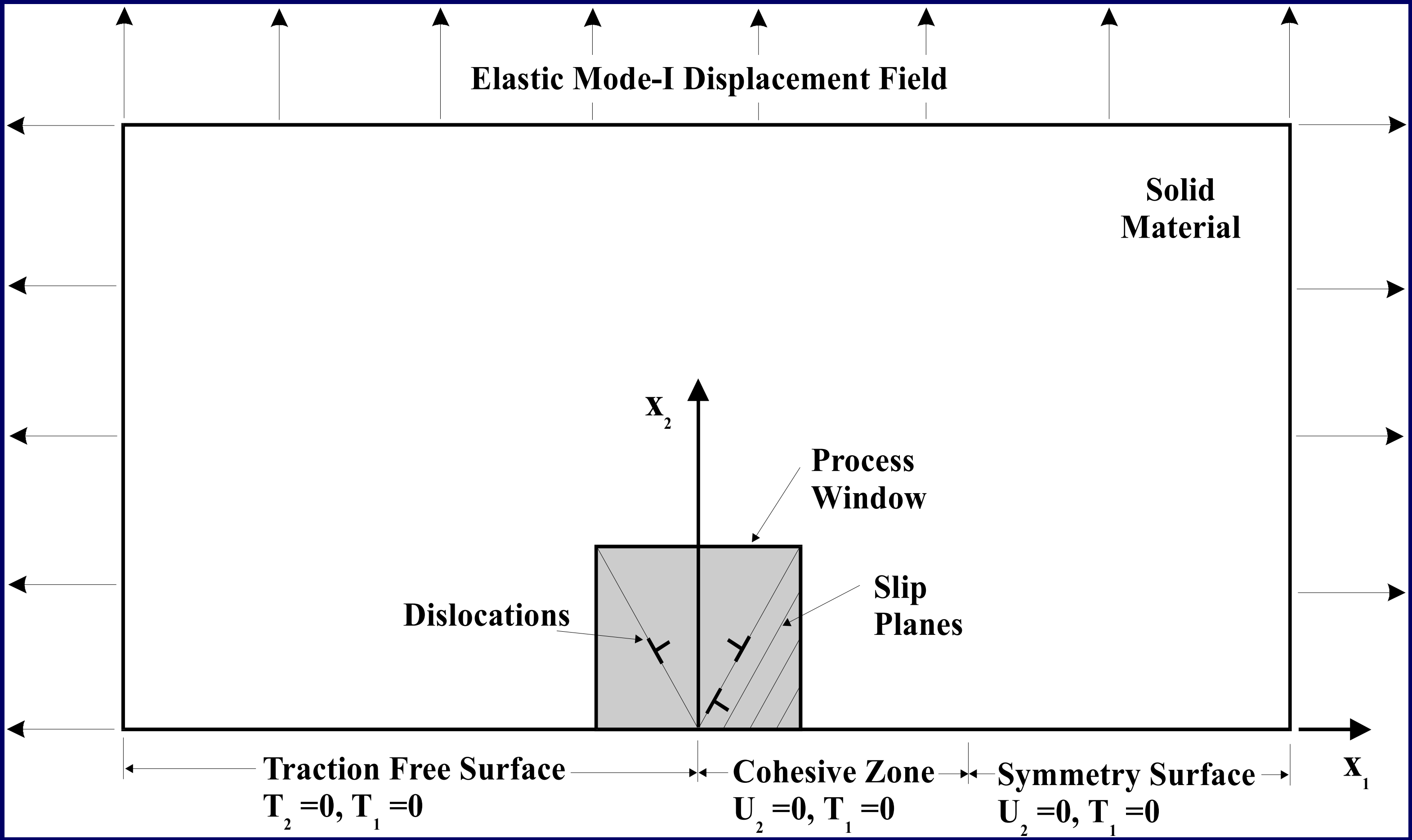
Discrete Dislocation/Crystal Plasticity Comparison (stress)





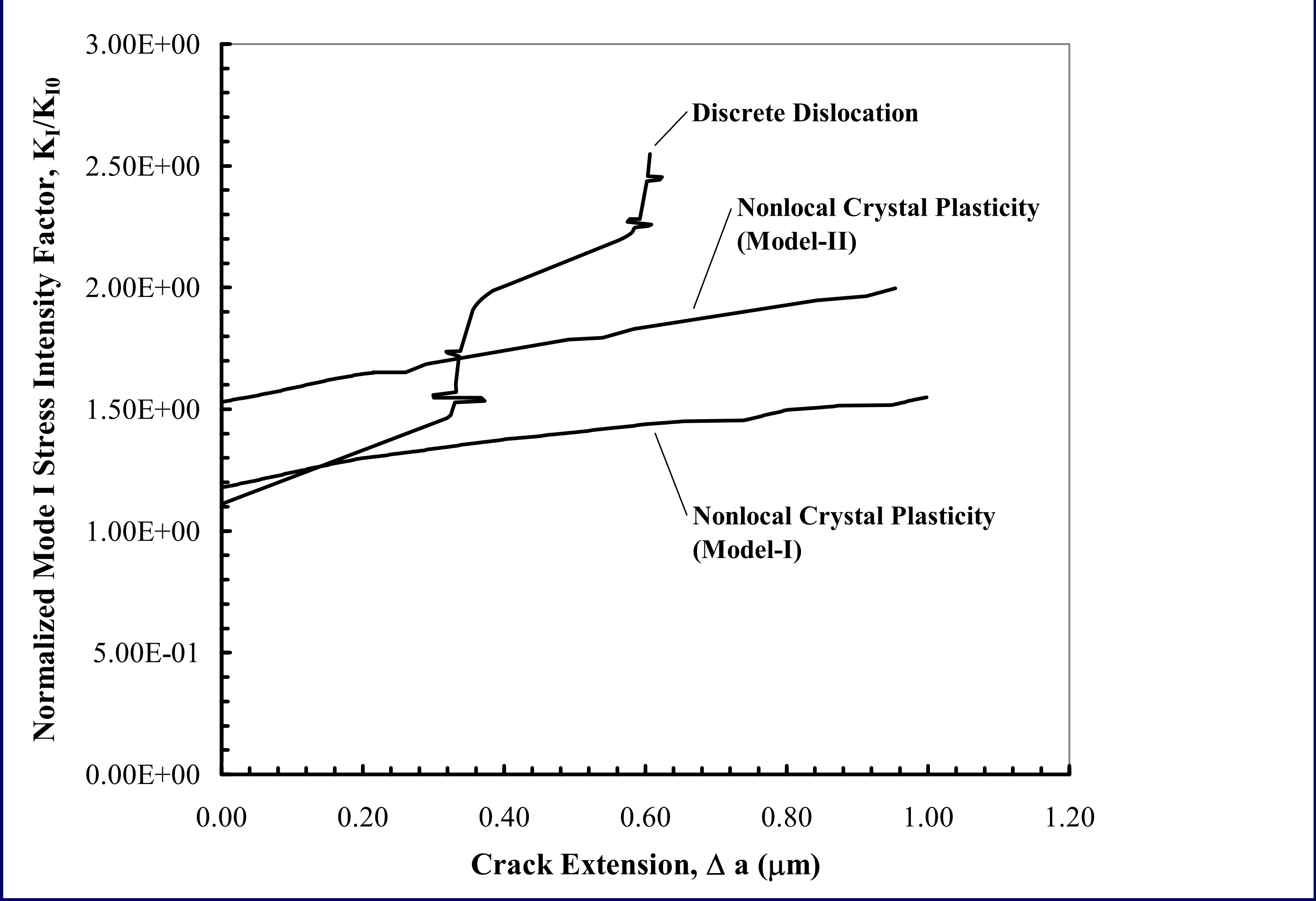
Discrete Dislocation Mode I Crack

(B.V.P. and Slip Plane Orientation)

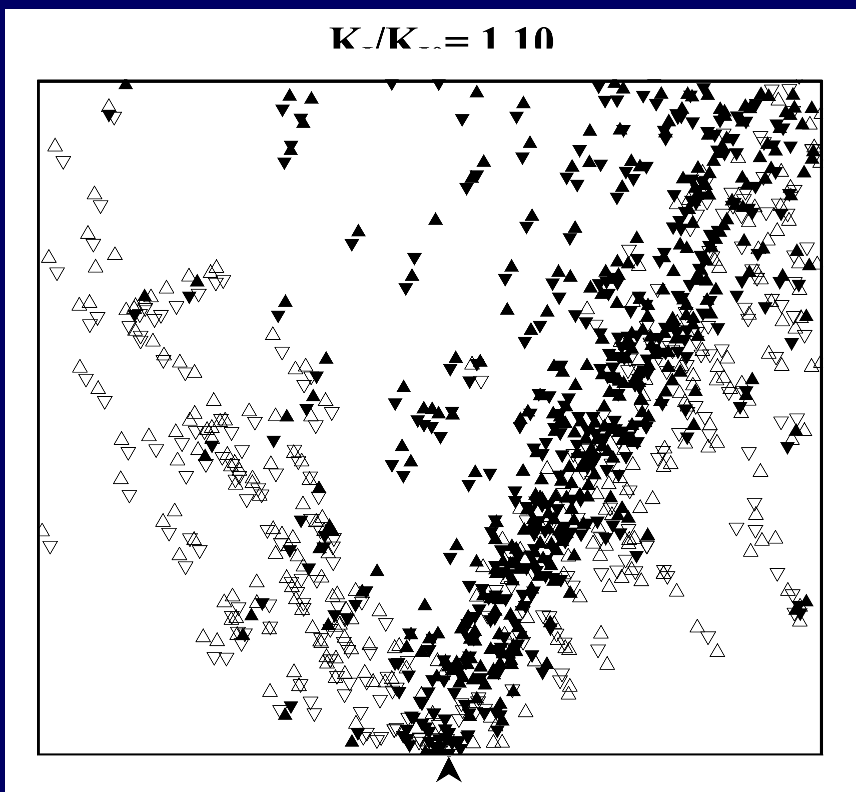


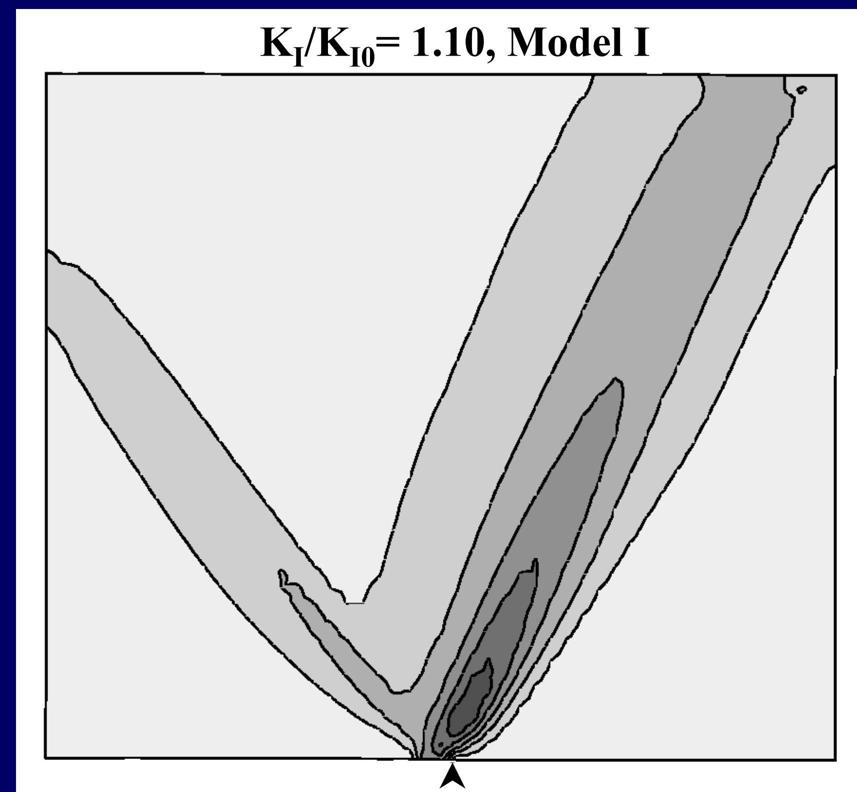
$\varphi = \pm 60°$

Discrete Dislocation Mode I Crack
(K_I/K_0 vs. Crack Length)



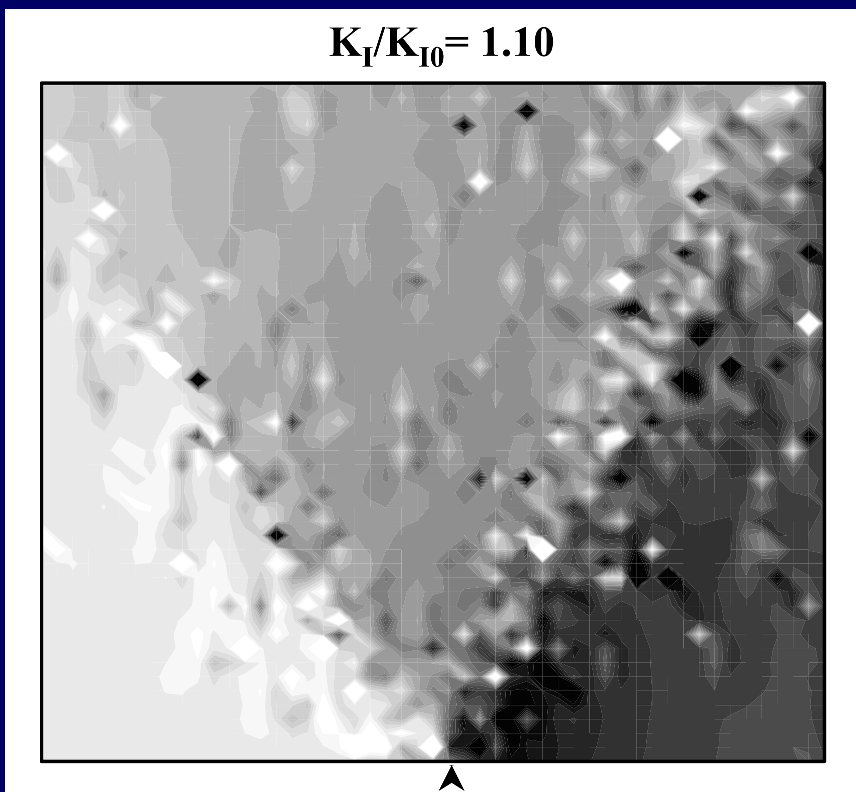
Discrete Dislocation/Crystal Plasticity Comparison (dislocations, plastic strain)

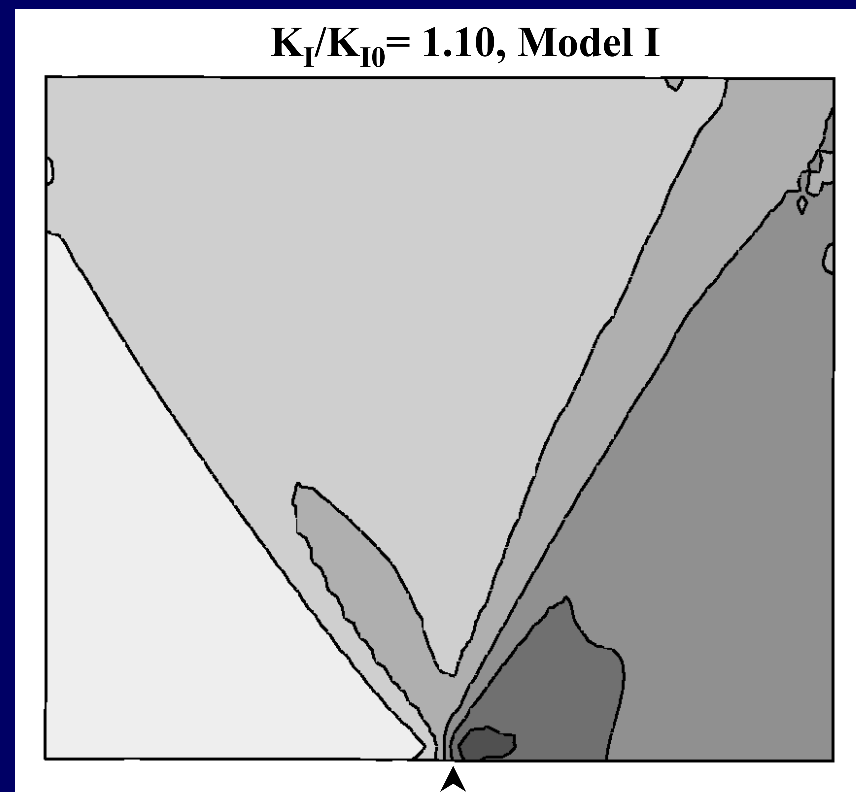




crack initiation

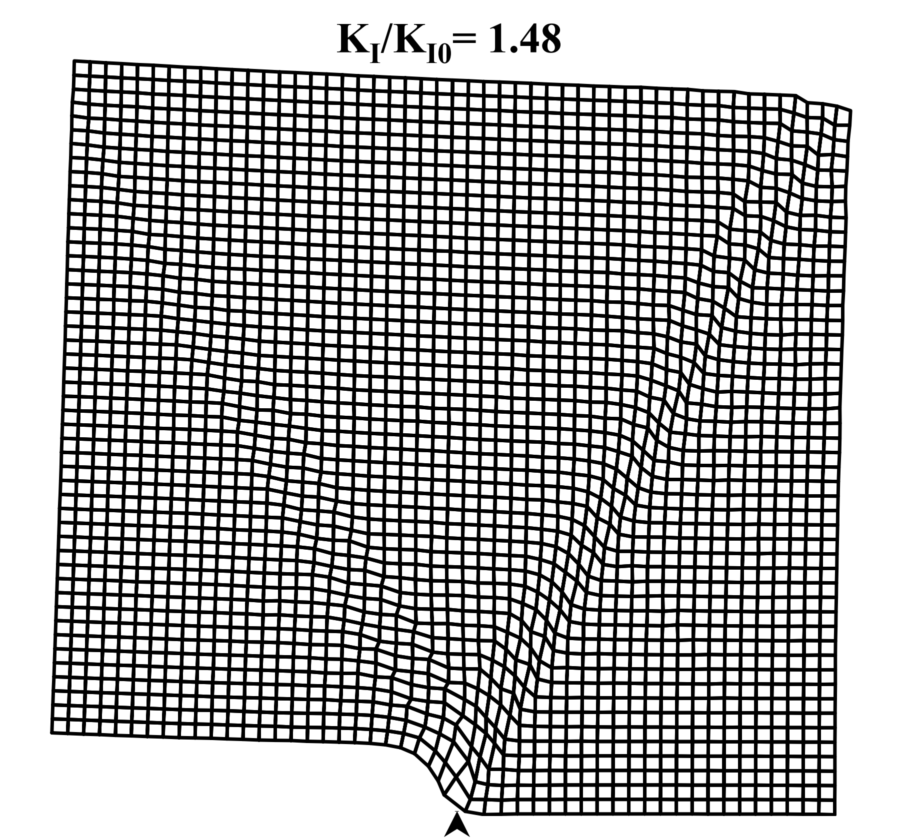
Discrete Dislocation/Crystal Plasticity Comparison (stress)

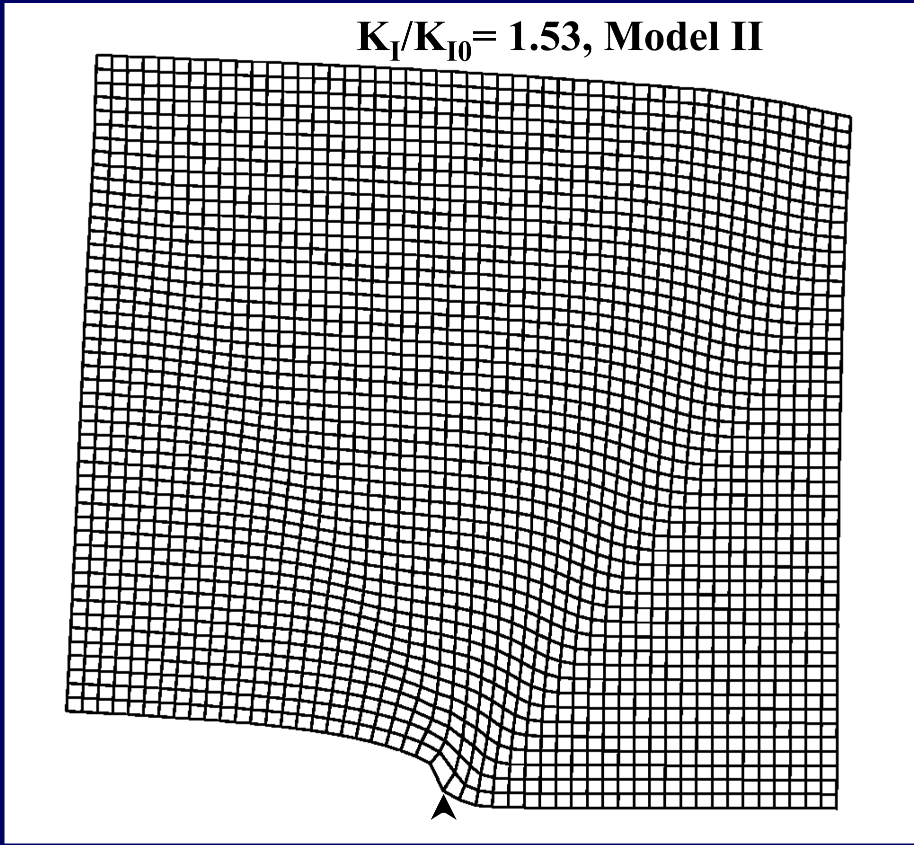




crack initiation

Discrete Dislocation/Crystal Plasticity Comparison (deformation)





Conclusions

- ✍ Micro-beam bending and mode I crack problems in the presence of crystallographic slip were analyzed in a consistent manner using both discrete dislocation and crystal plasticity models.

- ✍ Comparison of the results of the micro-beam bending analyses indicates a similarity in the global responses (bending moment vs. rotation) and some similarities in the plastic deformation patterning, but differences in the amount of deformation band formation and maximum axial stress.

- ✍ Comparison of the results of the mode I crack analyses indicates an inability to simulate the global response (applied loading vs. crack extension) but qualitative and quantitative similarities exist in the deformation and stress fields and the crack profiles.