Continuum Models of Dislocation Dynamics and Dislocation Structures

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Gordon Research Conference on Physical Metallurgy
The Holderness School, Plymouth, NH
July 27, 2004
Outline

• The case for multiscale simulation
• The case for multiscale modeling
• The lengthscale hierarchy of polycrystalline metals
• The quasicontinuum method
• Phase-field dislocation dynamics
• Subgrid models of martensite
• Subgrid models of dislocation structures
Machining – Experimental Validation

Chip Morphology Validation
(Courtesy of Third Wave Systems Inc)

(Courtesy of IWH, Switzerland) FE simulation

(Marusich and Ortiz, IJNME ’95)
Machining – Experimental Validation

(Courtesy of Third Wave Systems Inc)

Cutting Force Validation

- General trends predicted, but discrepancies remain!

Residual Stress Validation
Validation and Verification

- Fidelity of simulation codes is critically limited by uncertainties in engineering (empirical) material models

- Main sources of error and uncertainty
  - Discretization errors (spatial + temporal)
  - Uncertainties in data:
    - Material properties
    - Model geometry
    - Loading and boundary conditions...
  - Empiricism of constitutive models

- Need to reduce uncertainty in engineering constitutive models for codes to be predictive!
Limitations of empirical models

- Conventional engineering plasticity models fail to predict earing in deep drawing.
- Prediction of earing requires consideration of polycrystalline structure, texture development.

Deep-drawn cup

Grain structure of polycrystalline W
(Courtesy of Clyde Briant)
Limitations of empirical models

- Conventional plasticity models fail to predict scaling, size effects.

Hall-Petch scaling

\[ \tau \sim \frac{1}{\sqrt{d}} \]

Lamellar structure in shocked Ta
(MA Meyers et al. ’95)

Dislocation pile-up at Ti grain boundary
(I. Robertson)

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The case for multiscale computing

- Empirical models fail because they do not properly account for microstructure
- The empirical approach does not provide a systematic means of eliminating uncertainty from material models
- Instead, concurrent multiscale computing:
  - *Model physics at first-principles level, fine lengthscales*
  - *Compute on multiple lengthscales simultaneously*
  - *Fully resolve the fine scales*
- Bypasses the need to model at coarse lengthscales
Metal plasticity - Multiscale modeling

Lattice defects, EoS

Dislocation dynamics

Subgrain structures

Polycrystals

Engineering calculations

Time

ns, µs, ms

Length

nm, µm, mm
Multiscale computing - Feasibility

ASCI computing systems roadmap

- Computing power is growing rapidly, but...
Multiscale computing – Feasibility

• Computing power is growing rapidly, but $10^9 << 10^{23}$

Ta quadrupole (T. Arias ’00)

FCC ductile fracture (Courtesy F.F. Abraham) (F.F. Abraham ’03)

Au nanoindentation (Knap and Ortiz ’03)
Multiscale computing – Feasibility

Polycrystalline W (Courtesy of C. Briant)

Grain-boundary sliding model
Single-crystal plasticity model

(A.M. Cuitiño and R. Radovitzky ´02)
Multiscale computing – Feasibility

Cold-rolled @ 42% polycrystalline Ta

Experimental cold-rolled texture

(A.M. Cuitiño and R. Radovitzky ´03)

Pole figure
Multiscale computing – Feasibility

DNS of polycrystals: Convergence

Coarse mesh
192 elmts/grain

Intermediate mesh
1536 elmts/grain

Fine mesh
12288 el/grain

(A.M. Cuitiño and R. Radovitzky '03)

- Numerical convergence extremely slow!

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Multiscale computing - Feasibility

- ~ $10^9$ elements at our disposal ($10^6$ elements/processor x 1000 processors)
- ~ 1000 elements/coordinate direction
- ~ 20 elements/grain/direction (8000 elements/grain)
- ~ 50 grains/direction (125K grains)
- ~ 2.5 mm specimen for 50 $\mu$m grains
- Not enough for complex engineering simulations!
- Subgrain scales still unresolved, need modeling!
Metal plasticity - Multiscale modeling

- Lattice defects, EoS
- Dislocation dynamics
- Subgrain structures
- Length and time scales

Engineering calculations
Accessible to direct numerical simulation

Polycrystals
Accessible to first-principles calculations

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The case for multiscale modeling

• It is not possible to fully resolve material and deformation microstructures in complex engineering applications directly by brute force.

• Instead, multiscale modeling:
  – Identify relevant structures and mechanisms at all lengthscales.
  – Bridge lengthscales by:
    • Building models of effective behavior (coarse graining).
    • Computing material parameters from first principles (parameter passing).

• Approaches?
Multiscale modeling - Approaches
Multiscale modeling - Approaches

- Lattice defects, EoS
- Dislocation dynamics
- Subgrain structures
- Polycrystals
- Engineering calculations
- Quasi-continuum

Time scale: ns, µs, ms
Length scale: nm, µm, mm

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Quasicontinuum - Reduction

Quasicontinuum – Cluster sums

Merging of clusters near atomistic limit
Quasicontinuum - Adaptivity

- \( E(K) \equiv \text{Lagrangian strain in simplex } K \)
- Refinement criterion: Bisect \( K \) if \( |E(K)| \geq TOL \frac{b}{h(K)} \)

Longest-edge bisection of tetrahedron (1,4,a,b) along longest edge (a,b) and of ring of tetrahedra incident on (a,b)
QC - Nanoindentation of [001] Au

- Nanoindentation of [001] Au, 2x2x1 micrometers
- Spherical indenter, R=7 and 70 nm
- Johnson EAM potential
- Total number of atoms \( \sim 0.25 \times 10^{12} \)
- Initial number of nodes \( \sim 10,000 \)
- Final number of nodes \( \sim 100,000 \)

Detail of initial computational mesh

(Knap and Ortiz, *PRL* 90 2002-226102)
QC - Nanoindentation of [001] Au

7 nm indenter, depth = 0.92 nm
QC - Nanoindentation of [001] Au

7 nm indenter, depth = 0.92 nm
QC - Nanoindentation of [001] Au

70 nm indenter, depth = 0.75 nm
QC - Nanoindentation of [001] Au

70 nm indenter, depth = 0.75 nm
QC - Nanovoid cavitation in Al

- 72x72x72 cell sample
- Initial radius $R=2a$
- Total number of atoms $\sim 16 \times 10^6$
- Initial number of nodes $\sim 34,000$

Close-up of internal void

(Marian, Knap and Ortiz ’04)
QC - Nanovoid cavitation in Al

Initial elastic regime, following the interatomic potential's shape

1st yield point

Hardening regime: dislocation locking

2nd yield point: possible material failure (under investigation)

\( p \) (GPa)

\( \varepsilon_v \) (%)

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Dislocation structures, first yield point
QC - Nanovoid cavitation in Al

Dislocation structures, hardening stage

Dislocation types:

A - Conventional
\( \frac{1}{2}\langle 110\rangle \{111\} \)

B - Anomalous
\( \frac{1}{2}\langle 110\rangle \{001\} \)
QC - Nanovoid cavitation in Al

Dislocation structures, second yield point

Unconfined plastic flow carried by conventional $\frac{1}{2}\langle 110 \rangle \{ 111 \}$ dislocations
Quasicontinuum

- The Quasicontinuum method is an example of a multiscale method based on:
  - Kinematic constraints (coarse-graining)
  - Clusters (sampling)
  - Adaptivity (spatially adapted resolution)
- The Quasicontinuum method is an example of a concurrent multiscale computing: it resolves continuum and atomistic lengthscales concurrently during same calculation
- Challenges:
  - Dynamics (internal reflections)
  - Finite temperature (heat conduction)
  - Transition to dislocation dynamics
Multiscale modeling - Approaches

- Lattice defects, EoS
- Dislocation dynamics
- Subgrain structures
- Length
- Time

- Polycrystals
- Engineering calculations
- Phase-field DD

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Phase-field dislocation dynamics

- Irreversible accommodation of shear deformation by crystallographic slip
- Volterra dislocation: $[u] = b$, on slip area
Phase-field dislocation dynamics

- Interaction with short-range obstacles:
  - Impenetrable obstacles (pinning)
  - Obstacles of finite strength (dissipative interaction)

(Humphreys and Hirsch '70)
Phase-field dislocation dynamics

(Koslowski, Cuitiño and Ortiz, JMPS ’02)

- Assumption: The energy is of the form

\[ E(u) = \frac{1}{2} \int c_{ijkl} u_{i,j} u_{k,l} \, dx + \int \phi(\|u\|) \, dS \]

- Elastic energy
- Peierls energy

- Piecewise-quadratic Peierls potential:

\[ \phi(\zeta) \]
Phase-field dislocation dynamics

- Problem: Minimize energy $E(u)$ subject to:
  - Interaction with obstacles (pinning or dissipative)
  - Applied shear stress
Phase-field dislocation dynamics

- Phase field $\xi(x)$: Counts (signed) crossings of dislocations over $x \equiv$ Peierls energy well, or phase
- Pinning case can be solved analytically.
- Penetrable obstacle case can be reduced to determining value of phase field on obstacles.
Phase-field dislocation dynamics

Stress-strain curve

Dislocation density

(Movie)
Phase-field dislocation dynamics

Fractal dimension

\[ D \]

\[ \tau_{\text{ext}} \] [MPa]

Cu: Hahner et al., PRL 81, 2470 (1998)

Stage I: \( D \sim 1.9 \)

Avalanches

Miguel (2001)

Simulation

\[ N(A) \]

\[ A[100b^2] \]

\( \tau_E = 1.8 \pm 0.1 \)

Koslowski, Le Sar and Thompson ’04

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Phase-field dislocation dynamics

- Dislocation dynamics approaches rely on *analytical solutions* of linear elasticity to reduce the *dimensionality* of the problem from 3 (crystal) to 1 (dislocation lines): semi-inverse approach.
- Phase-field dislocation dynamics with pairwise Peierls potential reduces dimensionality further, from 3 (crystal) to 0 (point obstacles).
- Challenges:
  - Large three-dimensional ensembles
  - Atomistic dislocation cores
  - Dislocation reactions, junctions
Multiscale modeling - Approaches

- Lattice defects, EoS
- Dislocation dynamics
- Subgrain structures
- Polycrystals
- Engineering calculations
- Lamination

Time scales:
- nm
- µm
- ms
- µs
- ns

Length scales:
- nm
- µm
- mm

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Twinning - Microstructures

(Cu-Al-Ni, C. Chu and R. D. James)
Crystal plasticity - Microstructures

Dipolar dislocation walls

Labyrinth structure in fatigued copper single crystal (Jin and Winter ´84)

Nested bands in copper single crystal fatigued to saturation (Ramussen and Pedersen ´80)

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Crystal plasticity - Microstructures

- Lamellar structures are universally found on the micron scale in highly-deformed crystals
- These microstructures are responsible for the soft behavior of crystals and for size effects

Lamellar dislocation structure in 90% cold-rolled Ta (Hughes and Hansen ‘97)
Lamellar structure in shocked Ta (Meyers et al ‘95)
Microstructures – Sequential lamination
Nematic elastomers - Lamination

\[ W(F, n) = A \text{tr}(FF^T) - B \|F^T n\|^2 \]

(Courtesy of de Simone and Dolzmann)

Central region of sample at moderate stretch
(Courtesy of Kunder and Finkelmann)

Blandon et al. ´93
De Simone and Dolzmann ´00
De Simone and Dolzmann ´02
Commonly observed solid/solid transitions in Fe:

- $\alpha$(bcc) $\rightarrow$ $\varepsilon$(hcp) at $p = 13$ GPa, coexisting phases $p < 20$ GPa (Bundy, 1964)
- $\varepsilon$(hcp) $\rightarrow$ $\alpha$(bcc) at $p \sim 16$ GPa, coexisting phases $p > 5$ GPa
Phase transitions in Fe – Effect of shear

Initial model with 7 total variants (1 bcc/6 hcp)
Phase transitions in Fe – Effect of shear

\[ F = \begin{pmatrix} 1 & \gamma & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \lambda & 0 & 0 \\ 0 & \lambda & 0 \\ 0 & 0 & \lambda \end{pmatrix} \]
Phase transitions in Fe – Effect of shear

- Shear lowers bcc to hcp transition pressure.
- bcc to hcp transition path involves mixed states in the form of rank-1 and rank-3 laminates.
ECAP – Lamination

Evolution of microstructure
(sequential lamination)
(Sivakumar and Ortiz ‘03)

(Beyerlein et al ‘03)
Crystal plasticity – size effects

- Optimal scaling constructions for double slip, antiplane shear (Conti and Ortiz ’04)

\[ \tau_c \sim d^{-1/2} \]

\[ \tau_c \sim d^{-2/3} \]

Hall-Petch effect!

Shocked Ta
(Meyers et al ’95)

Laminate

Branching

LiF impact
(Meir and Clifton ’86)

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Subgrid microstructures - Lamination

- Sequential lamination supplies microstructures ‘on demand’ and is another example of concurrent multiscale computing
- Sub-grid microstructural information is recovered locally at the Gauss-point level
- But: Effective response is known explicitly in very few cases (e.g., nematic elastomers)
- Instead: Consider easy-to-generate special microstructures, such as sequential laminates
  - Off-line (Dolzmann ’99; Dolzmann & Walkington ’00)
  - Concurrently with the calculations (Aubry et al. ’03)
Summary and conclusions

- The multiscale modeling paradigm provides a systematic means of eliminating empiricism and uncertainty from material models.
- Present computing capacity is not sufficient to integrate entire multiscale hierarchies into large-scale engineering simulations.
- There remains a need for modeling at all lengthscales, including:
  - *subgrid models of microstructure (a la sequential lamination)*
  - *analytical methods, algorithms, for computing effective behavior, coarse graining*
  - *Kinetics, dynamics, rare events...*