Lectures on:

Introduction to and fundamentals of discrete dislocations and dislocation dynamics. Theoretical concepts and computational methods

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Recent Advances in Multiscale Modeling of Materials Behavior

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Lawrence Livermore National Laboratory, T. Diaz de la Rubia (Division Director)
Sandia: Hughes
PNNL: Khaleel

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T. Ohashi,  Bi-crystals, thin films
Y. Tomita, K. Yashiro, Kobe Japan  Dislocations in N-Based superalloys

Max Victoria (PSI, Switzerland)  Irradiated materials
B. Singh (Riso National Lab, Denmark)  Damage and in irradiated materials

Major sponsors:
NSF, DOE, LANL, LLNL
Continuum Viscoplasticity

Momentum: \( \text{div } S = \rho \dot{\mathbf{v}} \)

Energy: \( \rho c_v \dot{T} = k \nabla^2 T + \mathbf{S} \dot{\varepsilon}^p \)

Hooke's Law: \( \mathbf{S} = \mathbf{C} : (\dot{\varepsilon} - \dot{\varepsilon}^p) \)

\( \dot{\mathbf{S}} = \dot{\mathbf{S}} - \omega \mathbf{S} + \mathbf{S} \omega \), \( \omega = \mathbf{W} - \mathbf{W}^p \)

Dislocation Dynamics

Equation of Motion

\[ m^*_i \ddot{\mathbf{v}}_i = - \sum_{\text{electron, phonon}} B \mathbf{v}_i + F_i \]

\[ F_i = F_{\text{Peirels}} + F_{\text{Disl-Disl}} + F_{\text{Self}} + F_{\text{External}} + F_{\text{Obstacle}} + F_{\text{Image}} + F_{\text{Osmotic}} + F_{\text{Thermal}} \]

\[ \dot{\varepsilon}^p = \sum_{i=1}^{N} \frac{-l_i \nu_{gi}}{2V} (n_i \otimes b_i + b_i \otimes n_i) \]

\[ W^p = \sum_{i=1}^{N} \frac{-l_i \nu_{gi}}{2V} (n_i \otimes b_i - b_i \otimes n_i) \]

Discrete systems

Basic physical laws and underlying mechanisms
Multiscale Plasticity Phenomena

- Dislocations shock-wave interaction
- Size effects:
  - Torsion / bending & Tension/compression
  - Particle size effect in MMC’s
  - Nanolaminates
- Dislocation Structures – Internal stresses
- Dislocations in Silicon Crystal Induced by Laser Shock Peening
- Hardening
- Statistical study of dispersion hardening by point-like obstacles
- Dislocation-particle interaction:
  - Irradiated materials;
  - superalloys,…
- Fracture: Dislocation – Crack Interaction, plastic zone
- Cyclic loading, fatigue, ..
- Dislocation threading and deformation in thin films
- Nano-Indentation
- Shear Banding,
Why study shocks?

- Reach unexplored strain and strain rate regions ➔ NEW MATERIALS SCIENCE!
- How do things deform and break when pushed/pulled really fast?
- How do materials behave under extreme conditions? (explosives, earth’s core, stars) *Not well understood*
- Can we can create better, novel materials? Yes (*but how/when?*)

New tool: National Ignition Facility (NIF)

Frost and Ashby Deformation map

http://www.llnl.gov/nif/
Shock recovery experiments

TEM: 0.25 mm slices are cut from the recovered sample

Dislocation density increases with pressure

$<134>$ Cu 205 J pulse

$P_{\text{max}}$ (GPa) ~50-25 ~25-15 ~8-2 ~2-0

Dislocation density increases with pressure
High Strain Rate Dislocation Dynamic Plasticity Simulations in FCC and BCC Metals

Velocity controlled B.C
Confined to move in the Z direction
Rigidly/free

Cu single crystal
Uniaxial strain. Periodic and free BCs are examined.
Initially few F-R sources were distributed of on the slip planes
Periodic and reflective BCs used in DD.

From James Cazamias and D. Lassila, plate impact exp.
Shock in Cu, $P_H=50$ GPa

Dislocation dynamics

Deformed shapes

MD by E. M. Bringa (LLNL)
The dislocation microstructure in copper crystal at 5.0 GPa peak pressure and 1.50 ns pulse duration for crystal oriented in (a) (001) (b) (011) (c) (111) and (d) subsequent events that lead to the activation of the cross slip mechanism.
Figure 4.9. Dislocation microstructure in copper (a) DD results (b) Laser shock experiment by Meyers et al (2003).
Figure 5.9. Contour plots of the effective plastic strain in copper (a) with slip rotation (b) no slip rotation.
\[ P = 3 \times 10^{-8} \rho_{\text{dis}}^{0.5889} \]

- Results from Murr
- Results from Meyers et al. (no dislocation motion)
- Results from Meyers et al. (with dislocation motion)
- Our calculations
- Power law curve fitting

\[ P(GPa) \]
\[ \rho_{\text{dis}}(1/m^2) \]

\[ \Delta T(K) \]

\[ P(GPa) \]

- DD
- MD (shock front)
Nanolaminates

F. Akasheh, Zbib, Hirth (WSU)
R. Hoagland, A. Misra (LANL)

Increased Strength with decreased layer thickness
Resistance to irradiation damage (Hoagland)

$h_{Cu}$: Cu layer thickness
$h_{Ni}$: Ni layer thickness
$h_t$: bilayer period
Background

**High performance multifunctional materials**

- Ultra high strength \((\text{GPa level})\)
- High ductility
- High fatigue resistance
- Irradiation damage resistance \((\text{preliminary results})\)
- Morphological stability

**Potential Applications**

- High performance/reliability components for MEMS and NEMS device
- Surface engineering: e.g. superior fatigue resistant coatings \((\text{Stoudt et al., 2003})\)

Courtesy, Los Alamos National Lab

- Average spacing between misfit dislocations is significantly higher than that predicted by theory
- Origin of multiplication
- Origin or work hardening

Length-Scale-Dependent Deformation Mechanisms in Nanolaminates

Deformation involves glide of single dislocations confined to individual layers

\[ \sigma \propto \ln\left( \frac{h}{b} \right) \]

Deformation assisted by mechanical advantage of pile-up

\[ \sigma \propto h^{-1/2} \]

Mathews & Blakeslee (1974)
Hirth & Feng (1990)
Hoagland and Misra (2000)…..
Dependence of strength on layer thickness

![Graph showing the dependence of strength on layer thickness](image)

Factors controlling the strength of coherent and semicoherent interfaces (Hoagland)

Coherency stresses due to lattice mismatch - $\sigma_{coh}$

Image (Koehler) stresses due to elastic modulus mismatch - $\sigma_K$

Crossing involves creation of a step (possibly faulted) on the interface and a change in stacking fault energy - $\sigma_S$ and $\sigma_{sf}$

Misfit dislocation core structure

Glide dislocations crossing a semicoherent interface must cut/interact with misfit dislocations

Cu/Ni mismatch strain=2.7%
coherency stress= 2.6 GPA
aCu=0.3615 nm
aNi=0.352 nm
<table>
<thead>
<tr>
<th>Mechanism</th>
<th>Illustrating Sketch</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Threading</td>
<td><img src="image1" alt="Threading Sketch" /></td>
<td>Sample simulation clip at: <a href="http://www.mme.wsu.edu/%E2%80%A6">www.mme.wsu.edu/…</a>.</td>
</tr>
<tr>
<td>Annihilation</td>
<td><img src="image2" alt="Annihilation Sketch" /></td>
<td>Sample simulation clip at:</td>
</tr>
<tr>
<td>Blockage</td>
<td><img src="image3" alt="Blockage Sketch" /></td>
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<tr>
<td>Cross slip</td>
<td><img src="image4" alt="Cross slip Sketch" /></td>
<td>Sample simulation clip at:</td>
</tr>
<tr>
<td>Nucleation of half loops</td>
<td><img src="image5" alt="Nucleation Sketch" /></td>
<td>Sample simulation clip at:</td>
</tr>
<tr>
<td>Formation of Lomer</td>
<td><img src="image6" alt="Lomer Formation Sketch" /></td>
<td>Sample simulation clip at:</td>
</tr>
</tbody>
</table>

Table 1. Examples of significant individual dislocation mechanisms in confined layers.
Deformation physics: dislocation interactions

strained layer in an infinite elastic medium:

*Step over them/ go through to neighboring layer*
Deformation physics: other factors

- Type and density of INTERFACES and dislocation interface interactions:
  - Opaque interfaces
- Dislocation interactions
- Anisotropy
- Image (Koehler) forces
- Layer thickness
- Lattice parameter mismatch
- Chemical forces
Problem Setup

Short-range interactions enabled (the physical scenario)
Orthogonal Interaction: structure prediction

DD simulation

Experiment, Misra et al., 2002
Orthogonal Interactions- Strength

Orthogonal dislocation interactions comparison

Layer thickness (nm)

Resolved channeling stress (GPa)

- Free threading
- Interfacial dipole
- Cu/Ni exp., Misra 2002
- Single interfacial dislocation
Parallel dislocation interactions in nanoscale strained layers

- Based on the view that deformation proceeds by successive single-dislocation pileups (dipoles)
- Single dipoles and arrays
- Collinear vs inclined Burgers vector
Semi-analytical energetic model

Slip plane view

Slip plane edge-on view
threading dislocation, \( b_{\text{threader}}: a/2 \)

"infinite" interfacial array; Collinear Burgers;

\[ b_{\text{array}} = b_{\text{threader}} = a/2[0\,-1\,-1] \]

\[ \tau \text{ (GPa)} \]

\[ \lambda/h \]

"infinite" interfacial array; Inclined Burgers

\[ b_{\text{array}} = a/2[1\,-1\,0]; b_{\text{threader}} = a/2[0\,-1\,-1] \]

\[ \tau \text{ (GPa)} \]

\[ \lambda/h \]
Threading next to a single interfacial dipole;

Effect of $b_{dipole}$; $h$: 6.4nm; $b_{threader} = a/2[0\overline{1}-1\overline{1}]$
Implications of parallel dislocation interactions

\[ \tilde{b} : a/2 [1 \bar{1} 0] \]

\[ b : a/2 [0 \bar{1} 1] \]

\[ n: (\bar{1} \bar{1} 1) \]

- \[ b \] or -\[ \tilde{b} \]
- \[ b \] or -\[ \tilde{b} \]

Cu, Nb

30 nm
Strengthening due to parallel interactions

Inclined Burgers; $b_{\text{threader}} = a/2[0\bar{1}1]$  

Collinear Burgers vectors; $b_{\text{threader}} = a/2[0\bar{1}1]$  

$$\sigma(h,l) = c_1 \mu \frac{\ln(h/b)}{h/b} + c_2 \mu \frac{b}{l}$$
Collective Dislocation Simulations

- Incorporate all complex interactions
- Natural evolution of system
- Two phases:
  - Relaxation
  - Loading
Relaxation Models

- Ni/Cu: Four layers
- Periodic Boundaries
- Biaxial coherency stress: 2.6 GPa
- Procedure: run till dislocation activity ceases
Relaxation:
\( h \ 25.6 \text{ nm} \); \( r6 \)
Relaxation- conclusions

• A cross slip-based mechanism for multiplication was identified
• Multiple pileups observed in 25 nm and thicker
Loading: Biaxial stretching with constant strain rate

- Ni/Cu: Four layers
- Periodic Boundaries
- constant strain rate
- Biaxial loading
h 12.8 nm; r6; loading
Large scale simulations: strength v.s. h

large scale simulation- comparison

- Free threading
- Cu/Ni exp., Misra 2002
- Large scale simul.

Resolved channeling stress (GPa) vs. Layer thickness (nm)
Summary and conclusions

- DD analysis proved to be a valuable tool for the analysis of mechanisms and strength in nanoscale multilayered metallic (NMM) composites
- Neither orthogonal not parallel interactions can be representative of the behavior of NMM composites
- Collective dislocation simulations better capture the behavior of real systems- More verification and validation is needed
Dislocation Crack Interaction: Heterogeneous Deformation

The crack is located at the right side of the bottom of the specimen as can be deduced from the figures. The crack length is one third of specimen width. The bottom surface of the specimen (the un-cracked portion) and the left and right sides of the specimen are assumed to be symmetric boundaries. The crystal orientation is depicted in the figure with the x, y and z-axes being in the (110), (-110) and (001) directions respectively. Initial dislocation loops (Frank-Read sources) are distributed randomly in the crystal on two slip planes. The initial dislocation density is $10^{12}$ m/m$^3$. The upper surface of the specimen is displaced a constant distance such that the overall macroscopic strain is 1.67 % (stress relaxation condition). This orientation induces initially double slip deformation, but as the simulation proceeds, some of the dislocations segment cross-slip and multi-slip deformation prevails. The DD simulations is performed in parallel with the finite element analysis which corrects for boundary tractions, image stresses from the surfaces of the crack, and computes the heterogeneous stress field.
Dynamics of dislocations around a mode I crack.

Loading conditions: Tension-compression with average strain amplitude of 1.7%
**Quasi-Static Analysis:**

Dislocation Dynamics with Finite element simulation with NO inertia effects in the equation of linear momentum

>>>>>Quasi-static Stress distribution

SEE Clip: Stress-wave-DD-Crack-Static.avi
Stress-wave-DD-Crack-Static

**Dynamic Analysis:**

Dislocation Dynamics with Finite element simulation with inertia effects in the equation of linear momentum

>>>>>propagation of stress-waves

SEE Clip: Stress-wave-DD-Crack-Dynamics.avi
Stress-wave-DD-Crack-Dynamics
Quasi-static analysis

Dynamic analysis

- Dislocation pileup near boundary
- Crack
- Region of low stress
- Boundary of stress discontinuity
- Region of low stress
- Crack
Quasi-static analysis

Dynamic analysis

Evolution of dislocations

Double click to view movies
Dislocation density versus simulation time
Quasi-static analysis

Dynamic analysis

Stress contours (s23)
Quasi-static analysis

Dynamic analysis

Contour of increase in temperature

Max increase = 3 K

Max increase = 21 K
Quasi-static analysis

Dynamic analysis

Effective plastic strain
Loading condition:

Tension-compression step displacement function of the upper surface.

Analyses:

1) Dislocation dynamics coupled with finite element with No inertia effects, i.e. the inertia term in the momentum equation is zero >> Static analysis, therefore the stress distribution is stationary.

2) Dislocation dynamics coupled with finite element with inertia effects, > dynamic analysis >> stress wave propagation >> Magnification of stress amplitudes when the stress is suddenly reversed.

Main observations:

1) Dislocation multiplication in the dynamic case is higher.

2) Dislocations pile up at the boundary of "elastic discontinuity" i.e. where the stress jumps from high values around the crack tip to almost zero in a region behind the crack tip.

2) The density of the pileup in the dynamic case is much higher. If we associate this pileup with crack nucleation, then this would indicate that micocracks would initiate in that region? It would be interesting to check against experiments of Mode I crack under creep-fatigue then look at the cracked surface to see if we have "kinking" of the crack, and/or presence of microcracks in the bulk around the crack, this we could do with our new CT facility!