Multiscale Materials Modeling

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Computer Simulation and Physical Testing of Complex Fracturing Processes
Symposium in honor of Prof. Anthony R. Ingraffea on his retirement
September 27, 2014
Fatigue and fracture in metal: from cracks in the rivet holes to voids in grains to dislocation and atomistic fracture

Cracking beneath a rivet
DISLOCATIONS AND MECHANICAL PROPERTY
• Large-scale atomistic simulation opens a new way to study \textit{mechanics of materials}.

\[ \sim 10^9 \text{ atoms} \quad \text{Nano-twinned Metal} \]

\[ 200,000 \times 40,000 \times 600\text{nm} \quad \text{Nanomedicine targets cancer, Scientific American, Feb 2009} \]

\[ \sim 10^{14} \text{ atoms} \]

• (Key features) mechanisms and properties are emerged directly from fundamental evolution of atoms.
ELASTIC DEFORMATION

1. Initial
2. Small load
3. Unload

Elastic means *reversible*!

David (C-S) Chen

Callister, 1997
PLASTIC DEFORMATION
(SHEAR and SLIP)

1. Initial

Plastic means **permanent**!

2. Small load

bonds stretch & planes shear

\[ \delta_{\text{elastic + plastic}} \]

3. Unload

planes still sheared

\[ \delta_{\text{plastic}} \]

\[ F \]

Callister, 1997
Dislocation and Plasticity

- Glide of dislocations results in slip, the most common manifestation of plastic deformation in crystalline solids.
Atomistic Simulation Environment

• Specimen samples
  – Contains $\sim 10^8$ atoms.

• Empirical interatomic potential: embedded atom method (EAM)

• Quasi-static, conjugate gradient (CG) minimization.

• LAMMPS: an open source molecular dynamics program.
**Dislocation Extraction From Burgers Circuit**

Nanoindentation: Dislocation Evolution
Dislocations Glide When $\tau > \tau_c$

Nanoindentation into Al(001)

Graph showing load vs. displacement for nanoindentation into Al(001), indicating glide at 5.75 Å.
Cross Slip of Screw Dislocations

Nanoindentation into Al(001)

Screw dislocation moves from one \{111\} slip plane to another.

Multiple cross glide
Lomer Lock Blocks Dislocations

Nanoindentation into Al(111)

Lomer lock: a strong barrier to dislocation glides.

Materials Strength ≡ restricted dislocation motion

5.85 Å
**Indentation Size Effect (Smaller is Stronger)**

Spherical indenter

Hardness increases when indenter radius decreases.

Gerberich et al. (2002), J of Applied Mechanics

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*Note: The diagram shows a plot of hardness (H) versus indentation size (a). The data points indicate that hardness increases as the indenter radius decreases.*
Indentation Size Effect: The Quest

- **(Imagine)** We push atoms into the underneath material.
- Atoms become extra planes of atoms (dislocations) in the original lattice.
- These dislocations are called geometrically necessary dislocations (GNDs).
- GNDs are believed to block other mobile dislocations thus contribute to hardening.
- The smaller indents, the higher **density** of GNDs, and thus stronger.
Repulsive Force Field for Indenters

\[ F_i = \varepsilon(r - r_i)^2 \] (Plimpton 1995).

- **Spherical Indenter**
  - Smooth transition from elastic to elastic-plastic contact

- **Berkovich Indenter**
  - Routinely used in nanoindentation tests

\[ r_i \]

\[ Fr \varepsilon = - \]
Hardness Calculation

\[ \text{Hardness} = \frac{P_{\text{Load}}}{A_{\text{contact}}} \]

![Graph showing the relationship between hardness and indentation depth.](image)
Hardness vs. Dislocation Evolution

Materials Strength ≡ restricted dislocation motion.
Hardness - Spherical
Quantify Density of Geometrically Necessary Dislocations ($\rho_g$)

Total length of dislocation lines

$$\rho_g = \frac{l}{V}$$

plastic zone

plastic zone
Plastic Zone Calculations

\[
\alpha = \sqrt{\frac{A_{\text{contact}}}{\pi}}
\]

\[
r_p = \sqrt[3]{\left(\frac{2}{3} \pi a^3 + V_{\text{indenter, in}}\right)} \times \frac{3}{2\pi}
\]

\[
V_p = \frac{2}{3} \pi r_p^3 - V_{\text{indenter, in}}
\]
Hardness (Property) and GNDs (Mechanism)

Hardness

Indentation depth, Å

Hardness, GPa

ρG cm⁻²

Indentation depth, Å

0 5 10 15 20 25 30 35 40
0 5 10 15 20 25 30 35 40
0 0.005 0.01 0.015 0.02 0.025 0.03 0.035 10¹⁶

David (C-S) Chen

Civil Engineering, NTU
VOID NUCLEATION AND GROWTH
Ultra High Temperature Ceramics

Sintering process of $\text{ZrB}_2$

Microstructure of $\text{ZrB}_2$


ZrB$_2$-SiC Ceramic Composites

ZrB$_2$ is one of the material candidates for UHTC: high strength, low density and excellent thermal properties.

SiC content improves the flexure strength and toughness.
Modeling Intergranular Fracture

SEM image of ZrB$_2$-SiC composite at 1500°C CT test

creep zone
damage zone

$2a$
$2b$

$\Psi$
Micromechanics Model: Simple Grain

- Constitutive model of ceramic grain
  - Superposition of strain rate
    \[ \dot{\varepsilon}_{ij} = \dot{\varepsilon}_{ij}^e + \dot{\varepsilon}_{ij}^{cr} \]
  - Stress
    \[ \sigma_{ij}^{(m+1)} = D(\varepsilon_{ij}^{(m+1)} - \varepsilon_{ij}^{cr(m+1)}) \]
    \[ D = \frac{E}{(1+\nu)(1-2\nu)} \begin{bmatrix} 1-\nu & \nu & 0 \\ \nu & 1-\nu & 0 \\ 0 & 0 & 1-2\nu \end{bmatrix} \]

- Power law creep rate for a ceramic grain
  \[ \dot{\varepsilon}_{ij}^{cr} = \frac{3}{2\sigma_e} S_{ij} \dot{\varepsilon}_0 \exp\left(\frac{-Q}{RT}\right) \left(\frac{\sigma_e}{\sigma_0}\right)^n \]
Micromechanics Model: Grain Boundary

- Smeared out cohesive model for grain boundary

\[ 2n \quad V \quad u_b \quad \pi = \psi \quad h(a) \quad V = \psi \quad \psi \quad \sin \psi \quad \cos \psi \quad (1 + \cos \psi)^{-1} - \frac{1}{2} \cos \psi \quad \frac{V}{\pi b^2} \]

 Grain separation in normal direction can be expressed by

\[ u_n = \frac{V}{\pi b^2} \]

- a: cavity radius
- b: half cavity spacing
- \( V \): cavity volume
Micromechanics Model: Grain Boundary

- Normal separation rate
  \[ \dot{u}_n = \frac{\dot{V}}{\pi b^2} - \frac{2V\dot{b}}{\pi b^3} \]

- **Three ingredients** in normal separation rate at grain boundary
  - Cavity nucleation
  - Cavity growth enabled by atom diffusion
  - Cavity growth enabled by creep
Cavity Nucleation

- The change rate of void spacing
  \[
  \frac{\dot{b}}{b} = \frac{1}{2} (\dot{\varepsilon}_I + \dot{\varepsilon}_{II}) - \frac{1}{2} \frac{\dot{N}}{N}
  \]
  where \( \dot{\varepsilon}_I \) and \( \dot{\varepsilon}_{II} \) are the principal logarithmic strain rates at grain boundary

- Cavity density of undefomed grain boundary
  \[
  N = \frac{1}{\pi b^2}
  \]
Cavity Nucleation Rule

- Cavity density rate

\[ \dot{N} = F_n \left( \frac{\sigma_n}{\Sigma_0} \right)^2 \dot{\varepsilon}_e^C \]

- **\( F_n \)** is material parameter,
- **\( \sigma_n \)** is normal traction,
- **\( \Sigma_0 \)** is a normalized factor,
- and **\( \dot{\varepsilon}_e^C \)** is the effective strain which is the average value of adjacent grains.
Cavity Growth

- Cavity growth from diffusion
- Cavity growth from creep

\[
\dot{V}_1 = 4\pi D \frac{\sigma_n}{\ln\left(\frac{1}{f}\right) - \frac{1}{2}(3-f)(1-f)}
\]

where

\[
f = \max\left\{\left(\frac{a}{b}\right)^2, \left(\frac{a}{a + 1.5L}\right)^2\right\}
\]

and

\[
L = \left[D \frac{\sigma_e}{\dot{\varepsilon}_e^c}\right]^{\frac{1}{3}}
\]

\[
\dot{V}_2 = \begin{cases}
\pm 2\pi \dot{\varepsilon}_e^c a^3 h(\psi) \left[\alpha_n \left|\frac{\sigma_m}{\sigma_e}\right| + \beta_n\right]^n, & \text{for } \pm \frac{\sigma_m}{\sigma_e} > 1 \\
2\pi \dot{\varepsilon}_e^c a^3 h(\psi) \left[\alpha_n + \beta_n\right]^n \frac{\sigma_m}{\sigma_e}, & \text{for } \left|\frac{\sigma_m}{\sigma_e}\right| < 1
\end{cases}
\]

where \(\sigma_e\) and \(\sigma_m\) are the average effective stress and mean stress from adjacent grains; and

\[
\alpha_n = \frac{3}{2n}, \quad \beta_n = \frac{(n-1)(n + 0.4319)}{n^2}
\]
Intergranular Fracture: Experimental Observation

- SiC acts as microstructure anchors and some lead to cavitation but not all.
- SiC remains near constant shape (relatively high rigidity)
- Cavitation is only observed at high temperature region (above 1500°C)
- About 5% cavitation is found at ZrB$_2$-SiC grain boundary and the rotation angle is less than 3°

Micrograph at the tension side after creep test at 1700°C
Polycrystalline Model

ZrB$_2$-SiC composite w/ Grain boundary elements

MATLAB image processing

*.py (Python script)

MATLAB parser

ABAQUS
Comparison of Strain Rate

- Simulation results show a significant variation when cavitation nucleation was assigned.
- Simulation with nucleation allowed at ZrB$_2$-SiC interface show a great agreement with experiment data.
Grain Rotation

(a) Without nucleation

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(b) With nucleation @ ZS grain boundary

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scale 100 times. Nucleation occurs at ZS grain boundary as softening.
Tensile Stress Contour

without nucleation

nucleation at ZrB$_2$-SiC

Severe stress concentration at ZrB$_2$-SiC grain boundary when nucleation is not allowed.
Fatigue and fracture in metal: from cracks in the rivet holes to voids in grains to dislocation and atomistic fracture.
“Crystals are like people, it is the defects in them which tend to make them interesting!”
- Colin Humphreys
From Tony, 1991.12

DAVID (Chuin-Shan) CHEN !!!

THIS IS A PUBLIC THANK YOU FOR BEING AN OUTSTANDING TA IN CE 673

STUDENTS AND PROFESSOR ALIKE APPLAUD YOU FOR YOUR KNOWLEDGE, CARING, AND ACCESSIBILITY.
Driven and Determine
Achieving one’s dream in the most Gracious Manner
Braving all Obstacles with Confidence and
Emerged as a Glorious Winner