VISION: Predict Microstructure-Sensitive Cyclic $S - e$ Curves!

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Prepared by ANSI Std Z39-18
OUTLINE

Microstructure Effects Within Grains (g+g)
Using DD SIMULATIONS (S.Rao, T.A.Parthasarathy, D.M.Dimiduk, P.M.Hazzledine)

• PROGRESS : Established a Working Model / Methodology
• CURRENT FOCUS : Connectivity (“Handshakes”)

Using FEM (Y-S Choi, T.A.Parthasarathy, D.M.Dimiduk)

• Unit Cell Model : Identified Key Issues – Refinements

Grain-Grain Interaction
• Polycrystal Model : Using DD results

Grain-Defect Interaction
Discrete Dislocation (DD) Simulations

Random Distribution of Cubes in a box

Spatial Distribution Varies with Plane of Sectioning

(111) Sections
**DD : Established 2D Methodology (Low T athermal)**

<table>
<thead>
<tr>
<th>Model</th>
<th>Findings: Parametric Studies</th>
<th>Issues</th>
</tr>
</thead>
<tbody>
<tr>
<td>Precipitate Hardening</td>
<td>Differs from Analytical Model (Reppich)</td>
<td>Other Models?</td>
</tr>
<tr>
<td></td>
<td>Size &amp; $V_f$ Dep. Reasonable (Expt.)</td>
<td>Scatter, ~10% Thresholding</td>
</tr>
<tr>
<td></td>
<td>Real Microstructure Simulated</td>
<td></td>
</tr>
<tr>
<td></td>
<td>APB Energy: Primary Factor</td>
<td>Measure/Calc.</td>
</tr>
<tr>
<td></td>
<td>Friction Stress in $g$ Significant</td>
<td>Measure?</td>
</tr>
<tr>
<td></td>
<td>Coherency, Curvature: Negligible</td>
<td></td>
</tr>
<tr>
<td>Multi-Slip WH</td>
<td>3D with cross-slip (Comp. Limited)</td>
<td>Parallel Proc. (CHSSI, AFOSR)</td>
</tr>
</tbody>
</table>

*Need “Handshakes” to Meet AIM Goals*
**DD : Current Focus - Connectivity (“Handshakes”)**

- Phase Field Simulations
- TEM
- Pollock-type Model
- FEM Polycrystal Simulations
- Discrete Dislocation Simulations
- Rapid Plug-in?
- APB
- Parameters
- CRSS, \( \hat{g}_o \)
- Saturation, \( \hat{g}_s \)
- Work-hardening, \( A^{ab} \)
- TEM
- Representative Microstructure
- SEM
- Discrete Dislocation Simulations
- Calibration Validation
- Advance Fidelity Of Representation
- Micro Tests
- Atomistic Simulations

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AFRL
**DD : Current Focus - Connectivity (“Handshakes”)**

- **Phase Field Simulations**
- **TEM**
- **Pollock-type Model**
- **FEM Polycrystal Simulations**
- **APB**
- **Discrete Dislocation Simulations**
- **SEM**
- **Micro Tests**
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- **Polycrystal**
- **Simulations**
- **Rapid Plug-in?**
- **Representative Microstructure**
- **CRSS, \( \hat{g}_o \)**
- **Saturation, \( \hat{g}_s \)**
- **Work-hardening, \( A^{ab} \)**
- **Advance Fidelity Of Representation**
- **Calibration Validation**
- **Advance Fidelity Of Representation**

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DD Parametric Studies

Fit's to Parametric Studies ⇒ Pollock-type Model
**Pollock-type Model: (derived from DD results)**

$$\text{CRSS} = \min \left\{ (A_1 + A_2 G_{APB}) + \right.$$  

$$+ (C_1 - C_2 G_{APB} + C_3 G_{APB}^2 - C_4 G_{APB}^3) \frac{C}{0.3} \right\}$$

$$+ \left\{ F \left\{ [P_1 + P_2 t_g' + P_3 t_g'^2], \left[M_1 t_g^{M2}\right] \right\} \right.$$  

$$\left. + f_{g'} \left(t_{0g'} + k_{g'} d_{g'}^{-0.5}\right) \right\}$$

$$S_Y = (1 - f_{g'}) \left\{ M \left( \text{CRSS} \right) + k_{g+g'} d_{g+g'}^{-0.5} \right\} + f_{g'} \left(t_{0g'} + k_{g'} d_{g'}^{-0.5}\right)$$
Data from Pollock’s slides

### Exp.
- **Coh %**
  - 0.1
  - 0.0125
- **Vf-Total**
  - 0.544
- **Vf-t**
  - 0.01
  - 0.006
- **Size-t**
  - 0.334
  - 0.12
  - 0.04175
  - 0.015
- **Vf-s**
  - 0.2
- **Size-s**
  - 1.7
- **Vf-p**
  - 3.82
- **Size-p**
  - 100
  - 50
- **d_{(GH)}**
  - 6
- **sol-g**
  - 50
- **sol-g’**
  - 6

### Fit Par.
- **APB**
  - 360
  - 40.00
- **M**
  - 3
- **k_{O}**
  - 500

### Schirra (IN100)
- YS (ksi) = 66.3 + 6.43 x ASTM Grain Size #
- + .89 x % Cooling g’
- - 114.5 x cooling g’ size (in microns)
Data from Pollock on IN100 (PWA 1100 - ver.3)

YS (ksi) = 66.3 + 6.43 x ASTM Grain Size + .89 x % Cooling - 114.5 x cooling g' size (in micron)

<table>
<thead>
<tr>
<th>Exp.</th>
<th>oh %</th>
<th>Vf-Total</th>
<th>Vf-t</th>
<th>Size-t</th>
<th>Vf-s</th>
<th>Size-s</th>
<th>Vf-p</th>
<th>Size-p</th>
<th>d_{g-g'}</th>
<th>sol-g</th>
<th>sol-g'</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.1</td>
<td>0.6</td>
<td>0.06</td>
<td>0.002</td>
<td>0.34</td>
<td>0.17</td>
<td>0.2</td>
<td>1.2</td>
<td>4.1</td>
<td>100</td>
<td>50</td>
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<tr>
<td></td>
<td>0.0125</td>
<td></td>
<td></td>
<td></td>
<td>0.0425</td>
<td>0.02125</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Fit Par.</th>
<th>APB</th>
<th>M</th>
<th>k_g</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>360</td>
<td>3</td>
<td>450</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Coherency</th>
</tr>
</thead>
<tbody>
<tr>
<td>3/21/03 - Santa Fe</td>
</tr>
</tbody>
</table>
Rene 88 - 1200 F Data (from Pollock’s slides)

Data from Pollock’s slides

<table>
<thead>
<tr>
<th>Coh %</th>
<th>Experimental Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>d (g') (um)</td>
</tr>
<tr>
<td>0.1478</td>
<td>0.2321</td>
</tr>
<tr>
<td>0.1636</td>
<td>0.322</td>
</tr>
<tr>
<td>0.1489</td>
<td>0.32487</td>
</tr>
<tr>
<td>0.1669</td>
<td>0.3346</td>
</tr>
<tr>
<td>0.2738</td>
<td>0.1322</td>
</tr>
<tr>
<td>0.3865</td>
<td>0.2708</td>
</tr>
<tr>
<td>0.2477</td>
<td>0.2416</td>
</tr>
<tr>
<td>0.39</td>
<td>0.2771</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>APB</th>
<th>M</th>
<th>k_q</th>
</tr>
</thead>
<tbody>
<tr>
<td>240</td>
<td>3</td>
<td>500</td>
</tr>
</tbody>
</table>

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**DD: Current Focus - Connectivity (“Handshakes”)**

- Phase Field Simulations
- Representative Microstructure
- TEM
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- Micro Tests
- Atomistic Simulations

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SEM Image -> CRSS

<table>
<thead>
<tr>
<th>Bore</th>
<th>Rim</th>
<th>Web</th>
</tr>
</thead>
<tbody>
<tr>
<td>t = 275 MPa</td>
<td>t = 275 MPa</td>
<td>t = 265 MPa</td>
</tr>
</tbody>
</table>

![Bore Image](image1)
![Rim Image](image2)
![Web Image](image3)
Current Focus - Connectivity (“Handshakes”)
Atomistic Simulations -> Refinements of DD

DD Neglects Core Effects

Atomistics Include Core Effects

APB Energy
Critical Parameter

CSF, Core Effects Important?
(Cross-slip within $g'$)
Atomistics Simulation Validation Results

- EAM Potential with APB=140, CSF=120, SF(Ni)=60

- FLAT INTERFACE:

  Atomistics
  - Stress for first partial to enter: \((CSF-SF)/b\)
  - Stress for second partial to enter: \((APB)/b\)
  - No diffuse core effect

\[\text{DD} \quad \text{Max Stress} = \text{Stress for 1}^{\text{st}} \text{Disln entry} = (APB)/b\]

\[\Rightarrow \text{APB Energy Sufficient, if APB} \quad (CSF-SF)\]
DD : Current Focus - Connectivity (“Handshakes”)

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- \( gg \) Images
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- Atomic Simulations
- Advance Fidelity Of Representation

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$D^D \to FEM$ Handoffs

\[ g^a (r^b) = n b \sqrt{A^{ab} r^b} \]
**DD -> FEM Handoffs**

Forest Obstacle Model (Franciosi, 1985)

\[
\dot{g}^a = \dot{g}_o + mb \sqrt{\ddot{a}} A^{ab} r^b
\]

Initial Hardness = CRSS

\[
\dot{g}^# = \frac{h^2 mb}{2(\dot{g} - \dot{g}_o)} k_o \ddot{a} l^a g^# + q \ddot{a} g^#
\]

\[q = q_o \frac{\dot{g}_s - \dot{g}}{\dot{g}_s - \dot{g}_o}
\]

Strengthening interaction coefficients
Microstructure Effects Within Grains (g→g)
Using DD SIMULATIONS (S.Rao, T.A.Parthasarathy, D.M.Dimiduk, P.M.Hazzledine)

- PROGRESS: Established a Working Model / Methodology
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- Unit Cell Model: Identified Key Issues – Refinements

Grain-Grain Interaction
- Polycrystal Model: Using DD results

Grain-Defect Interaction
FEM : Unit Cell Model (Single Grain)

- Evaluated Unit Cell Approach using A-B Formalism
  - Yield Point -> determined by geometrical constraint 
    (different mechanism than DD)
  - W-H beyond Yield -> strain-gradient term dominant

- Refinement : Relaxation of Elastic $\mathcal{G}$ (using DD results)
FE Simulation of (g+g') : Unit Cell Approach


\[
\# = \#_0 \text{sgn}(t^a) \hat{t}^a |t^a|^{1/m} \quad \text{with} \quad \# = \frac{h^2 m^b}{2(\hat{g} - \hat{g}_o)} k_o \ddot{a} |l^a| \quad \text{Only } l^a \text{ (GND) contribution to slip resistance.}
\]
Effect of Strain-Gradient Parameter: $k_o$

Experimental data (from Busso / ALSTOM, 1998)

$S_{[001]}$ (Pa)

$\sigma_{[001]}$

$\hat{g}_o = 60 \text{MPa}, m = 0.03, \mu = 0.001$

Elastic-Plastic Transition

No Evolution of Slip Resistance
Effect of $\hat{g}_o$

$\hat{g}_o = 374 \text{ MPa}, k_o = 2$

$\hat{g}_o = 60 \text{ MPa}, k_o = 2$

Experimental data (from Busso / ALSTOM, 1998)

$\hat{g}_t + \Delta t = \hat{g}_t + \Delta t \hat{g}_t$
**Length Scale Effects**: \( g \) Size, \( V_f \)

- Constant \( g \)-ppt. \( V_f = 68\% \)
- Change \( g \)-size (g channel width)

![Graph 1](image1)

- Constant \( g \)-size = 0.52 \( \text{m} \)
- Change \( g \)-\( V_f \) (g channel width)

![Graph 2](image2)

\[ \hat{g}_o = 60 \text{ MPa}, m = 0.03, \hat{\rho}_o = 0.001, k_o = 5 \times 10^{-5} \]
Effect of $g_0$ 3D Geometry

- Elastic $g_0$ + Elasto-viscoplastic $g$
- $g_0 = 60 \text{MPa}, m = 0.03, g_0^f = 0.001, k_0 = 0$ for Viscoplasticity
Effect of $g_i$ 3D Geometry

- Elastic $g_i$ + Elasto-viscoplastic $g$
- $\hat{g}_o = 60\text{MPa}$, $m = 0.03$, $\dot{\gamma}_0 = 0.001$, $k_o = 0$ for Viscoplasticity

Graphs showing the stress-strain relationship for $g$, $g_i$, and $g_i + g$.
The onset of softening accompanied by the massive shears localized along the edges and the corners in the \( g_g \) interfaces.

- Break down of geometric (kinematic) constraints
- Need to compare with experimental observations at this particular T-range.

\[ V_f = 68\%, \ g_{\text{size}} = 0.52 \, \text{nm} \]
\[ \hat{g}_o = 60 \, \text{MPa}, \ m = 0.03 \]
\[ \hat{g}_o = 0.001, \ k_o = 5 \times 10^{-5} \]
**FEM : Unit Cell Model (Single Grain)**

- Evaluated Unit Cell Approach using A-B Formalism
  - Yield Point \(\rightarrow\) determined by geometrical constraint
  - captures \(V_f\) Effect
  - W-H beyond Yield \(\rightarrow\) strain-gradient term dominant
    - captures size effect during work-hardening

- **Refinement : Allow Plasticity in \(\gamma\) (using DD results)**
  - DD captures APB cutting,
  - FEM captures Geometrical Constraint effect and Work Hardening
OUTLINE

Microstructure Effects Within Grains (\(g \leftrightarrow g\))
Using DD SIMULATIONS  (S.Rao, T.A.Parthasarathy, D.M.Dimiduk, P.M.Hazzledine)

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- Polycrystal Model : Using DD results

Grain-Defect Interaction
FEM : Polycrystal Model

• FY 2003 Goal : Combine DD with FEM to Build 1\textsuperscript{st} gen. \((\mathfrak{q}\mathfrak{g})\) Polycrystal model
  
  – Wigner-Seitz Cell (Beaudoin) – (144 grains, 12 el/gr)
  – Use DD results for \(g_0\) and \(A_{ij}\)
  – A-B model for Strain-gradient Terms

• Beyond FY 2003
  
  – Build/Borrow \(\mathfrak{g}\) const. Law to Model IN100 type alloy
  – Real Image 3D Polycrystal Models
    • Adaptive Meshing of Realistic Microstructures
Building Bridges: Inputs for Pollock-type Model

\[ s_y(C_i, T, \epsilon, \delta, \ldots) = \]

**Needs Development Within Atomistics**

\[ f_g \frac{T_o}{C T} \frac{dc}{dC_i} \frac{C_i}{C} + Mf_i \frac{G_{APB}}{b} \]

**Obtain by Dislocation Kinetics Simulation**

\[ M \frac{4}{\rho^{1.5}} \frac{T_L}{bd_s} \sqrt{f(1 - f_p)} \frac{\rho d_s g}{2T_L} - \frac{1}{\rho} \]

- **strong coupling**

\[ M \frac{G}{2b} \sqrt{2bd_s f(1 - f_p)} \frac{4}{\rho^{1.5}} - \frac{Gf(1 - f_p)\alpha}{2b} \]

- **weak coupling**

**Obtain by FEM Simulation of Grain Distribution Effects**

\[ + (1 - f_p) k_y \frac{1}{\sqrt{d_g}} + f_p \frac{\dot{\epsilon}}{\epsilon} (T)_{Ni,Al} + \frac{\dot{\alpha}}{\epsilon} \frac{dc}{dC_i} C_i \frac{\alpha}{\epsilon} + f_p k_y \frac{1}{\sqrt{d_g}} \]

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Building Bridges ...

TO

- Inputs for Pollock-type Model 3-6 mo.
- Fatigue Models (McDowell,..) 1-2 yrs

FROM

- Constitutive Laws (Parks, Cuitino/Ortiz, ..) 3-6 mo.
- 3D Voronoi Meshing (Parks, Gosh, ..) 3-6 mo.