Polycrystal Modeling of Precipitate Effects in Aluminum-Copper Alloys

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Motivation

• Develop an accurate and physically-based model that can describe the mechanical behavior of a precipitation-hardened alloy over a range of heat treatments.
Aluminum

- Dislocation-dislocation interactions
- Flow stress exhibits a linear relationship with dislocation cell size. (Tabata, ‘73, ‘78, ‘82)
- Stage 1 - easy glide
  - At most 4 - 5 % shear strain
  - More pronounced for single slip orientations
- Stage 2 - linear hardening
  - Not well-defined at room temperature
  - More defined when T < room temperature
- Stage 3 - parabolic hardening
  - Observed at room temperature
  - Becomes more prominent as temperature increases
Aluminum-Copper Alloys

- Precipitate-dislocation interactions
  - Anisotropy on plastic flow behavior (Hosford & Zeislfot ‘72, Bate et al. ‘81, Barlat & Liu ‘98, Choi & Barlat ‘99)
  - Bauschinger effect (Abel & Ham ‘66, Moan & Embury ‘79, Wilson ‘65)
- Coherent particles - GP zones and θ" (Price and Kelly ‘64)
  - Higher yield stress than Al
  - Shearing of particles
  - Comparable work hardening rates and deformation to Al
- Semi-coherent - θ' (P & K ‘64, Russell & Ashby ‘70)
  - High yield stress and high work hardening rates
- Incoherent particles - θ (P & K ‘64, R & A ‘70)
  - Low initial yield stress
  - Highest rates of work hardening
Precipitate Development

*Sato & Takahashi, 1983*
Precipitate Induced Anisotropy

• Amount of anisotropy is dependent upon:
  – Aging treatment
  – Orientation of precipitates
  – Morphology of precipitates

• Solutionized and overaged structures have little influence.
• Peak-aged treatment large anisotropy effect.
• Soft orientations are strengthened more by $\theta'$ precipitates.
  – Correlates with observations of the Bauschinger effect (Moan & Embury '79)

Hosford and Zeisloft '72, Bate et al. '81, Barlat and Liu '98, Choi and Barlat '99
Polycrystal Plasticity

- Properties of polycrystalline aggregate treated as averages over all of the constituent grains.
  - Model the material at the single crystal level

- Different from macroscopic theories of plasticity
  - Does not consider the individual grains, sample treated as a whole

- Advantages
  - More physically-based approach to material modeling
  - Describe effects of initial texture and grain morphology
  - Predict texture changes during deformation
Modeling of Precipitate Effects

• Model precipitate-induced anisotropy of plastic flow

• Proposed methods for modeling aged material
  – Plastic inclusion - precipitates deform and rotate to maintain compatibility with the matrix (Hosford & Zeisloft, ‘72)
  – Elastic inclusion - precipitates considered as non-deforming particles (Bate et al., ‘81)
  – Combined isotropic-kinematic hardening law, based on elastic inclusion hypothesis (Barlat & Liu, ‘98)
  – ***Barlat equation***
  – Modify hardening matrix to include dislocation-precipitate interactions (Schmitt et al., ‘97)
Elastic Inclusion
(Bate et al., ‘81)

- Precipitates considered as non-deforming particles.
- Plastic properties of precipitates not involved as the dislocation bypass the precipitates
- Anisotropy arises from the long-range back stress built up during deformation
- \( \| \gamma \| \) dependent upon shape and orientation of precipitates

\[
\sigma = M \tau_m (1 - f) + 2\mu f \| \gamma \| \varepsilon^p
\]

matrix contribution precipitate contribution
Plastic Inclusion
(Hosford & Zeisloft, ‘72)

- Precipitates deform and rotate to maintain compatibility with the matrix
- Anisotropy arises from the relaxation of shear strains

\[ \sigma = M\tau_m (1 - f) + f\vec{\sigma}_{ppt}\vec{N} \]

- matrix contribution
- precipitate contribution
Limitations of Current Models

- Incorporating precipitate effects partially addressed
  - focus on only one aging treatment

- No incorporation of microstructural length scales

- Lack of physically-based hardening laws

- Limited incorporation into polycrystal models

- Few direct comparisons with experimental stress-strain results
Experimental Details

• Materials used:
  – Pure Al
  – Binary Al-Cu alloy with different aging treatments

• Compression tests
  – Single crystal and polycrystals
  – Different orientations for single crystals

• Transmission electron microscopy (TEM)
  – Investigate different deformation mechanisms, dislocation interactions, and evaluate precipitate spacing

• X-Ray Diffraction
  – Texture measurements
Orientations and Heat Treatments

- Single crystal orientations in the stereographic triangle

- Heat treatments used for single and polycrystals

<table>
<thead>
<tr>
<th>Aging Treatment</th>
<th>Single Crystal</th>
<th>Polycrystal</th>
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</thead>
<tbody>
<tr>
<td>Natural Aging</td>
<td>X</td>
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</tr>
<tr>
<td>190C, 3 hours</td>
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<td>X</td>
</tr>
<tr>
<td>190C, 10 hours</td>
<td>X</td>
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<tr>
<td>190C, 24 hours</td>
<td>X</td>
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</tr>
<tr>
<td>260C, 3 hours</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>260C, 5 hours</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>260C, 24 hours</td>
<td>X</td>
<td>X</td>
</tr>
</tbody>
</table>
TEM of Pure Aluminum

Subgrains

Subgrain boundary
TEM of Al-Cu, No Aging & 190°C 3hrs

No Aging

190°C, 3hrs
TEM of Al-Cu, 190°C 10hrs & 24 hrs

190°C, 10hrs

190°C, 24hrs
TEM of Al-Cu, 260°C 3hrs
TEM of Al-Cu, 260°C 24hrs
Summary of TEM Results

- Dislocations form subgrains in pure aluminum
- Small, incoherent precipitates present for all heat treatments
  - very little impact on stress-strain behavior, not homogeneously distributed
- Presence of coherent GP zones
  - no artificial aging
- Well-developed $\theta'$ precipitates
  - $190^\circ C$ for 10 hrs & 24 hrs
  - $260^\circ C$ for 3 hrs, 5 hrs, & 24 hrs
- Dislocation networks develop in channels between the $\theta'$ precipitates.
Precipitate-Induced Anisotropy

No Aging

Aged at 190°C for 24 hours

260°C, 24hrs - Experiment

Strain, (%) vs. Stress (MPa)
The Role of Aging on Strain Hardening Behavior
VPSC Polycrystal Model*

• Develop constitutive equations to relate stress and strain rate.
  – Single crystal and polycrystal level

• Couple constitutive laws via Eshelby’s equivalent inclusion method.
  – Interaction equation

• Utilize self-consistent method to solve for compliances.

* Lebensohn and Tomé, ‘93
Self-Consistent Formulation

• To derive interaction equation, assumed that visco-plastic moduli are known.
• HEM describes average behavior of polycrystal aggregate.

• Relationship between single crystal and polycrystal compliances.

where
Execution of VPSC Polycrystal Model

• Iterative procedure to determine:
  – Stress in each grain
  – Grain’s compliance tensor
  – Polycrystal compliance tensor

• Incremental deformation by imposing during $\Delta t$.

• Convergence is achieved when self-consistency is met.

\[
\left| \sigma^{(n)} - \Sigma \right| < \text{error}
\]

\[
\left| \sigma^{(n)} - \sigma^{(n-1)} \right| < \text{error}
\]

• Final step: calculate reorientation of grain due to slip.
Hardening with Precipitates

- Start with dislocation evolution equation

\[ \dot{\rho} = \sum_k \left[ \frac{K_o}{db} + k_1 \sqrt{\rho} - k_2 \rho \right] f_k \]

Geometric storage term due to boundaries / obstacles
Dynamic recovery of dislocations
Statistical storage of dislocations

- Combine with the Bailey-Hirsch relationship for flow stress.

\[ \tau = \tau_o + \alpha \mu b \sqrt{\rho} \]
Proposed Hardening Law

- Single crystal formulation - one precipitate type

\[ \dot{\tau} = \left[ \frac{K_o \alpha^2 \mu^2 b}{2(\tau - \tau_o)} d \right] + \theta_o \left( \frac{\tau_s - \tau}{\tau_s - \tau_o} \right) \sum_k \dot{\gamma}^k \]

- Polycrystal formulation
  - More than one type of precipitate
  - Incorporate grain size length scale

\[ \dot{\tau} = \left[ \frac{\alpha^2 \mu^2 b}{2(\tau - \tau_o)} \left( \frac{K_{01}}{d_1} + \frac{K_{02}}{d_2} + \frac{K_{03}}{d_3} \right) \right] + \theta_o \left( \frac{\tau_s - \tau}{\tau_s - \tau_o} \right) \sum_k \dot{\gamma}^k \]
Incorporation of Precipitate-Induced Anisotropy

\[ \dot{\tau} = \left[ \frac{\alpha^2 \mu^2 b}{2(\tau - \tau_o)} \left( W \frac{K_{01}}{d_1} + \frac{K_{02}}{d_2} \right) + \theta o \left( \frac{\tau_s - \tau}{\tau_s - \tau_o} \right) \right] \sum_k |\gamma^k| \]

Anisotropy weighting factor
Total Weighting Factors

\[ W_{pt} = \frac{1}{3}(W_{p1} + W_{p2} + W_{p3}) \]
\[ W_{et} = \frac{1}{3}(W_{e1} + W_{e2} + W_{e3}) \]

<table>
<thead>
<tr>
<th>Compression Axis Direction</th>
<th>( W_{\text{plastic}} )</th>
<th>( W_{\text{elastic}} )</th>
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</thead>
<tbody>
<tr>
<td>[111]</td>
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<tr>
<td>Polycrystal</td>
<td>0.7711</td>
<td>0.4688</td>
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</tbody>
</table>

(100) plane
Experiment and VPSC Model Comparison
Pure Aluminum Room Temperature Compression

- Solid line - experiment
- Dashed line - simulation

Polycrystal

Strain, (%)
Model Simulations

Al-4% Cu No Aging

- Solid line: Experiment
- Dashed line: Simulation

Al-4% Cu Aged at 190ºC for 3 hrs

- Solid line: Experiment
- Dashed line: Simulation
Modeling Summary

• Precipitate-induced anisotropy described accurately by both elastic and plastic inclusion weighting factors
  – elastic inclusion more physically accurate
• Hardening parameters determined from single crystal experiments resulted in accurate prediction of polycrystalline results.

• Physically-based hardening law developed
  – incorporated microstructural length scales
  – applicable over a range of heat treatments