# Polycrystal Modeling of Precipitate Effects in Aluminum-Copper Alloys

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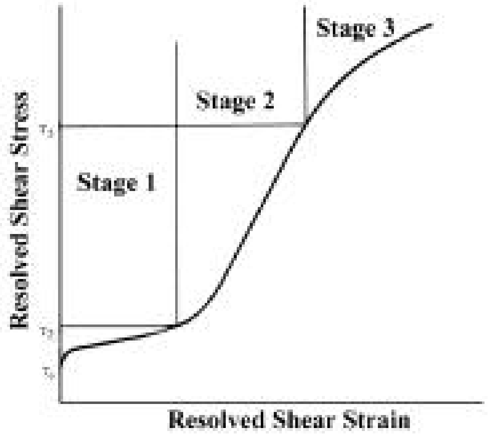
# Motivation

- 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

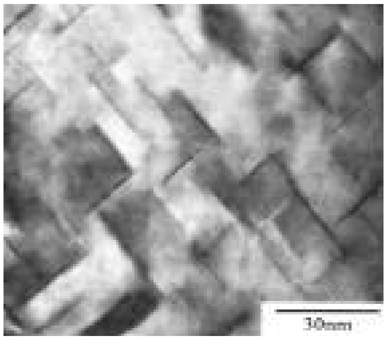
- Dislocation-dislocation interactions
- Flow stress exhibits a linear relationship with dislocation cell size. (Tabata, ‘73, ‘78, ‘82)
- Stage 1 - easy glide
  - At most 4 - 5 % shear strain
  - More pronounced for single slip orientations
- Stage 2 - linear hardening
  - Not well-defined at room temperature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

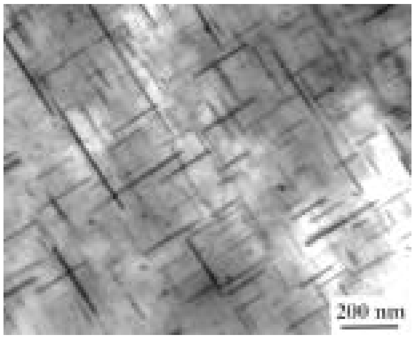


# Aluminum-Copper Alloys

- 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 $\theta''$ (Price and Kelly ‘64)
  - Higher yield stress than Al shearing of particles
  - Comparable work hardening rates and deformation to Al
- Semi-coherent - $\theta'$ ( P & K ‘64, Russell & Ashby ‘70)
  - High yield stress and high work hardening rates
- Incoherent particles - $\theta$ ( P & K ‘64, R & A ‘70)
  - Low initial yield stress
  - Highest rates of work hardening

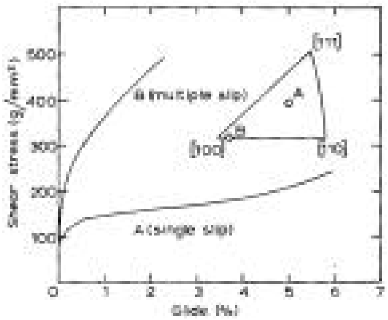
# Precipitate Development





# Precipitate Induced Anisotropy

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



Cupp & Chalmers, ‘54

- Solutionized and overaged structures have little influence.
- Peak-aged treatment large anisotropy effect.
- Soft orientations are strengthened more by θ' 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

$$\sigma = \underbrace{M\tau_m(1-f)}_{\text{matrix contribution}} + \underbrace{2\mu f\|\gamma\|\varepsilon^p}_{\text{precipitate contribution}}$$

# Plastic Inclusion

## (Hosford & Zeisloft, ‘72)

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

$$\sigma = \underbrace{M\tau_m(1 - f)}_{\text{matrix contribution}} + \underbrace{f\bar{\sigma}_{ppt}\bar{N}}_{\text{precipitate contribution}}$$

# Limitations of Current Models

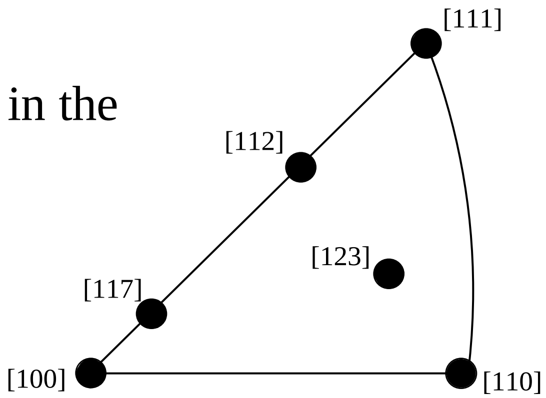
- Incorporating precipitate effects partially addressed
  - focus on only one aging treatment
- No incorporation of microstructural length scales
- Lack of physically-based hardening laws
- Limited incorporation into polycrystal models
- Few direct comparisons with experimental stress-strain results

# 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

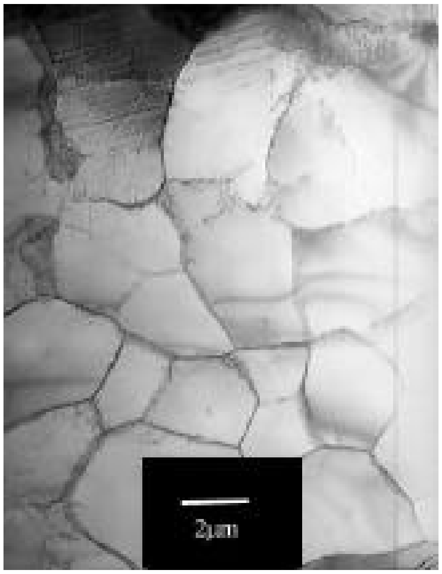
- Single crystal orientations in the stereographic triangle



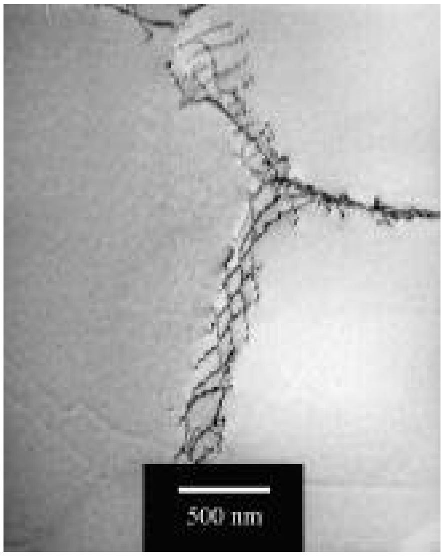
- Heat treatments used for single and polycrystals

| **Aging Treatment** | **Single Crystal** | **Polycrystal** |
|---|---|---|
| Natural Aging | X | X |
| 190C, 3 hours | X | X |
| 190C, 10 hours | X | X |
| 190C, 24 hours | X | X |
| 260C, 3 hours | X | X |
| 260C, 5 hours | X | X |
| 260C, 24 hours | X | X |

# TEM of Pure Aluminum

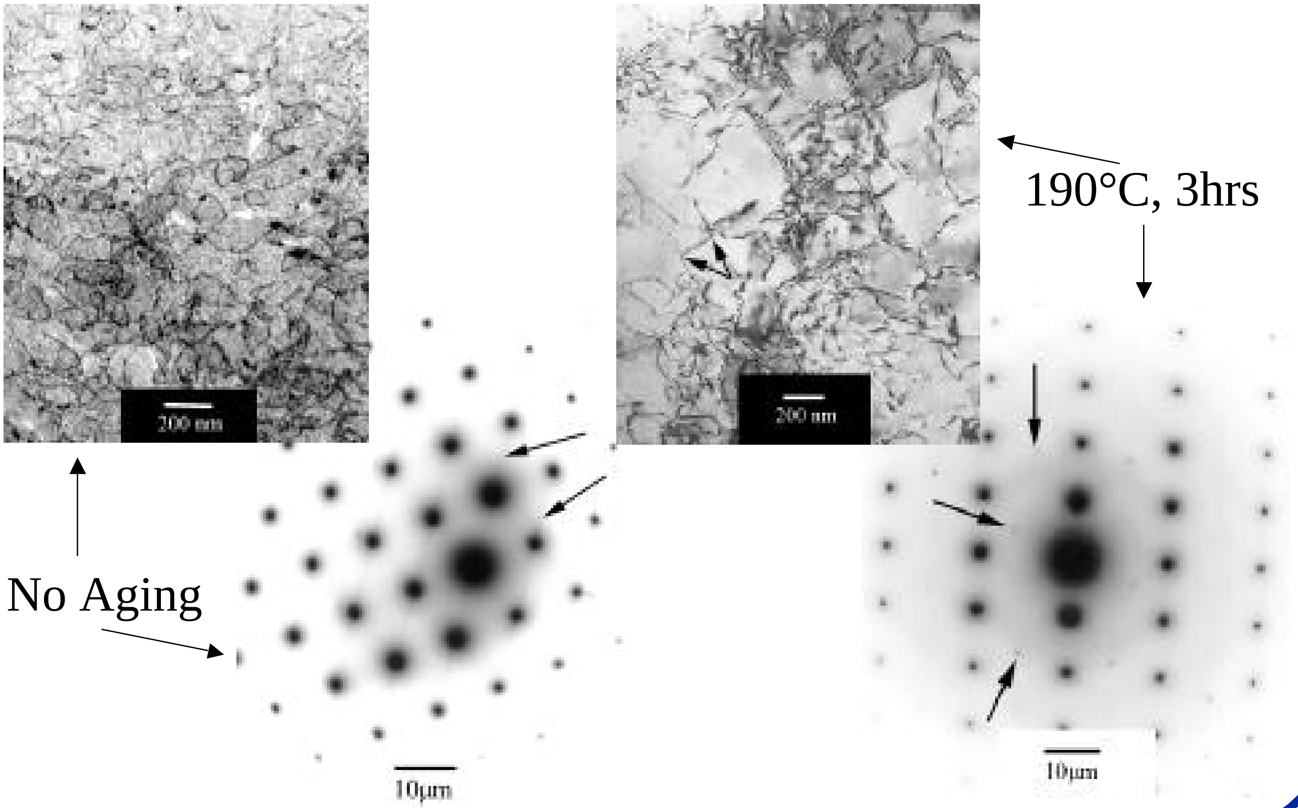


Subgrains



Subgrain boundary

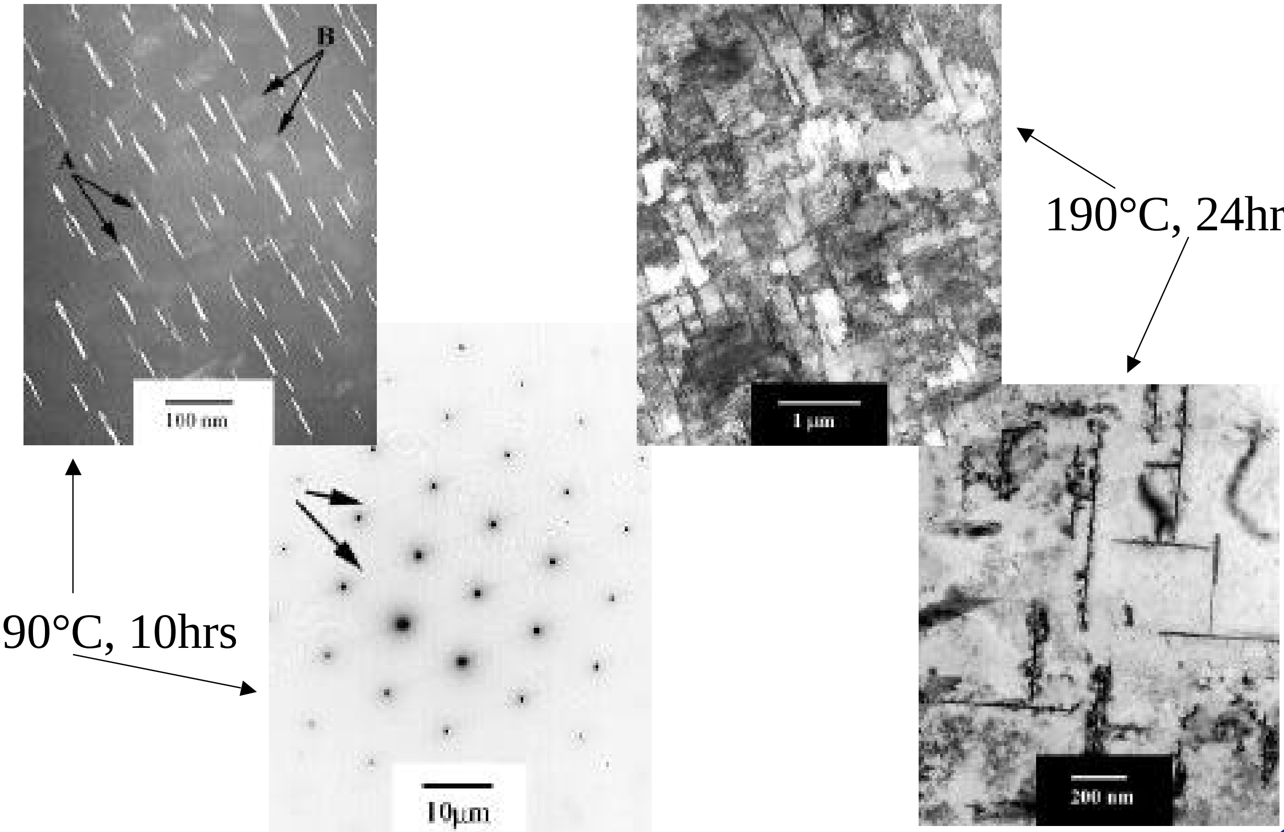
# TEM of Al-Cu, No Aging & 190°C 3hrs



190°C, 3hrs

No Aging

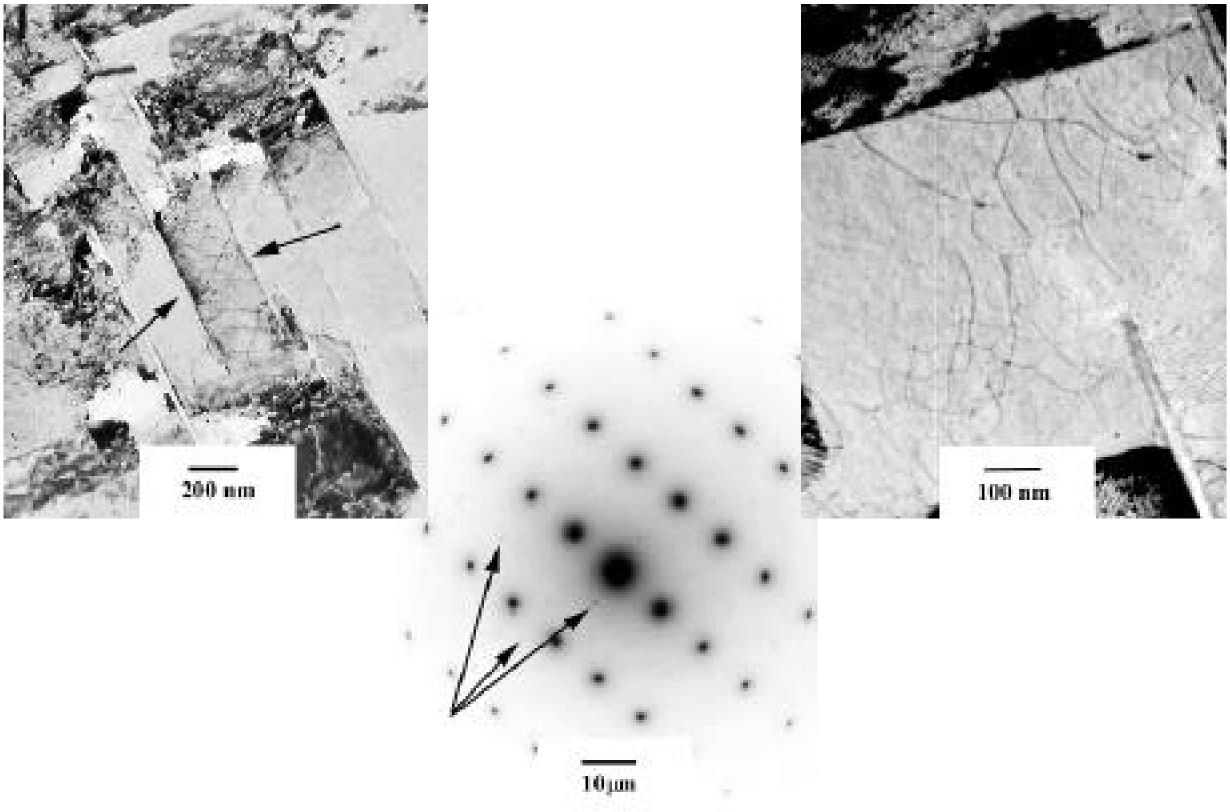
# TEM of Al-Cu, 190°C 10hrs & 24 hrs



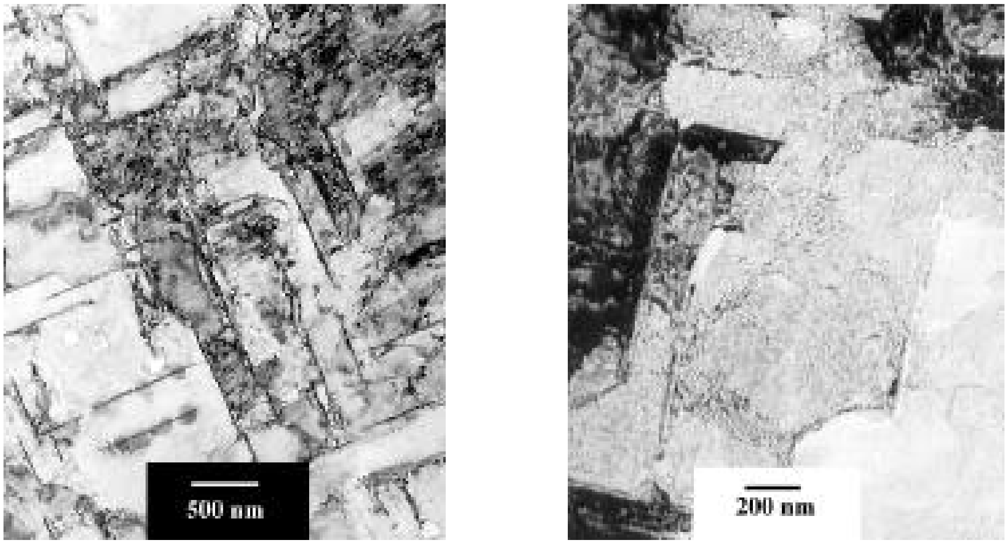
190°C, 24hrs

190°C, 10hrs

# TEM of Al-Cu, 260°C 3hrs



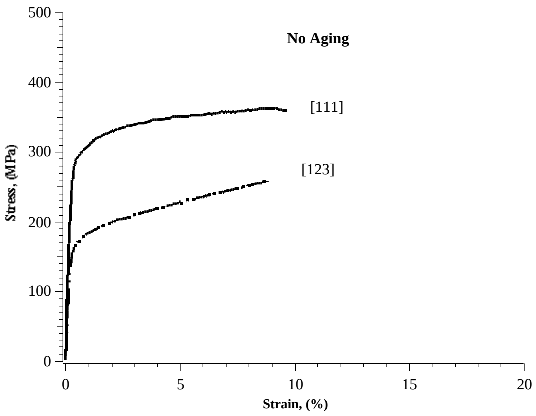
# TEM of Al-Cu, 260°C 24hrs

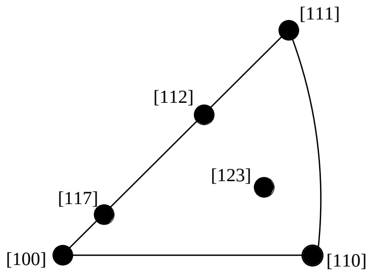


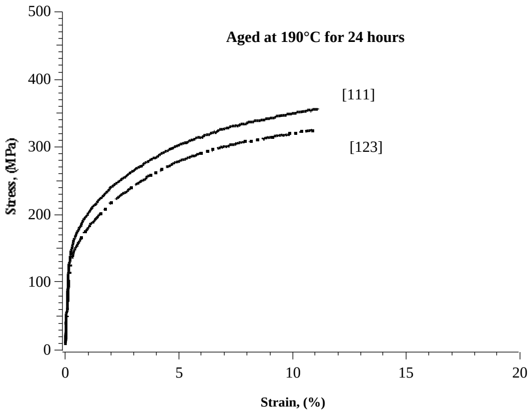
# Summary of TEM Results

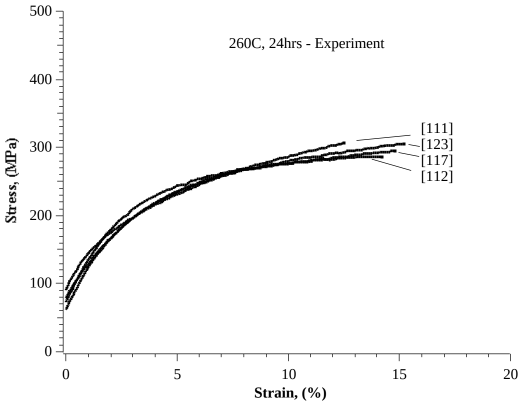
- Dislocations form subgrains in pure aluminum
- Small, incoherent precipitates present for all heat treatments
  - very little impact on stress-strain behavior, not homogeneously distributed
- Presence of coherent GP zones
  - no artificial aging
- Well-developed θ' precipitates
  - 190°C  for 10 hrs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

# Precipitate-Induced Anisotropy

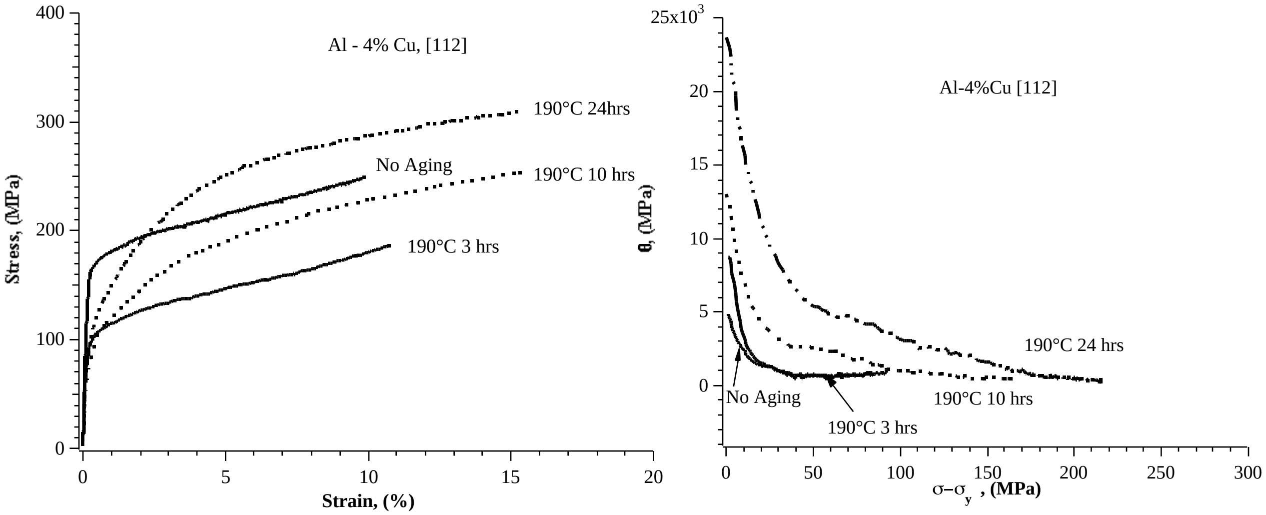








# The Role of Aging on Strain Hardening Behavior



# 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 Δt.
- Convergence is achieved when self-consistency is met.

$$\left|\left\langle \sigma'^{(n)} \right\rangle - \Sigma' \right| < error$$

$$\left\langle \left| \sigma'^{(n)} - \sigma'^{(n-1)} \right| \right\rangle < error$$

- Final step: calculate reorientation of grain due to slip.

# Hardening with Precipitates

- Start with dislocation evolution equation

$$\dot{\rho} = \sum_k \left[ \frac{K_o}{db} + k_1\sqrt{\rho} - k_2\rho \right] \left|\dot{\gamma}_k\right|$$

Geometric storage term due to boundaries / obstacles

Statistical storage of dislocations

Dynamic recovery of dislocations

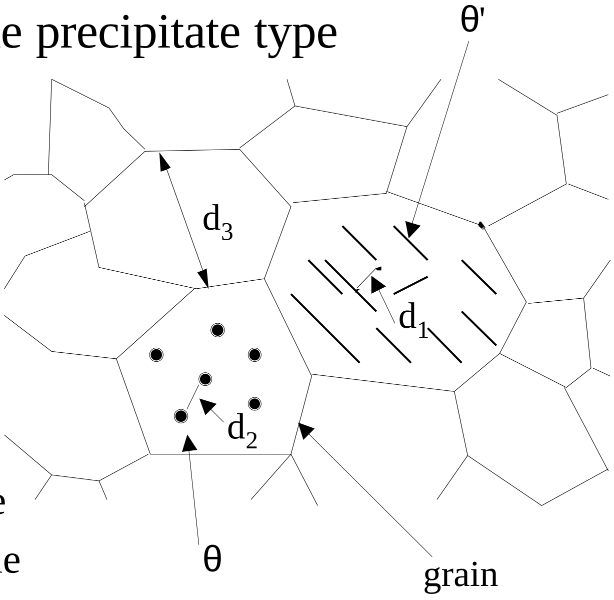
- Combine with the Bailey-Hirsch relationship for flow stress.

$$\tau = \tau_o + \alpha\mu b\sqrt{\rho}$$

# Proposed Hardening Law

- Single crystal formulation - one precipitate type

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



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

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

# Incorporation of Precipitate-Induced Anisotropy

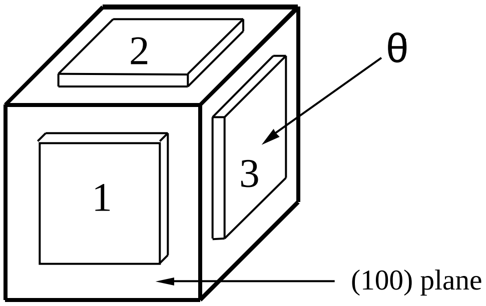
$$\dot{\tau} = \left[\frac{\alpha^2\mu^2 b}{2\left(\tau-\tau_o\right)}\left(W\frac{K_{01}}{d_1}+\frac{K_{02}}{d_2}\right)+\theta_o\left(\frac{\tau_s-\tau}{\tau_s-\tau_o}\right)\right]\sum_k\left|\dot{\gamma}^k\right|$$

Anisotropy weighting factor

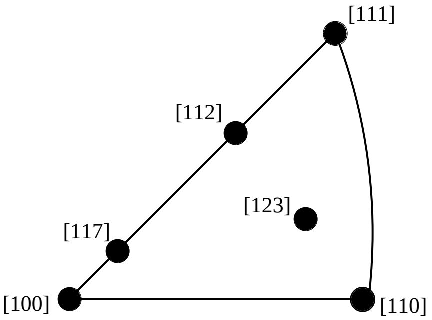
# Total Weighting Factors

$$W_{pt} = \tfrac{1}{3}\left(W_{p1} + W_{p2} + W_{p3}\right)$$

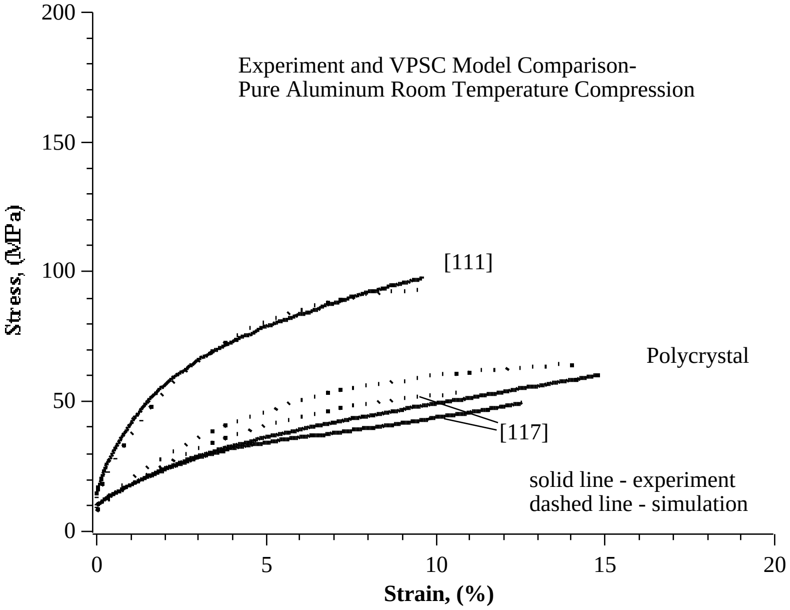
$$W_{et} = \tfrac{1}{3}\left(W_{e1} + W_{e2} + W_{e3}\right)$$



| **Compression Axis Direction** | $\mathbf{W_{plastic}}$ | $\mathbf{W_{elastic}}$ |
|---|---|---|
| [111] | 0.5774 | 0.3330 |
| [123] | 0.6900 | 0.4583 |
| [117] | 0.9611 | 0.7762 |
| [112] | 0.7016 | 0.4583 |
| [100] | 1.0000 | 0.8330 |
| Polycrystal | 0.7711 | 0.4688 |



# Model Simulations



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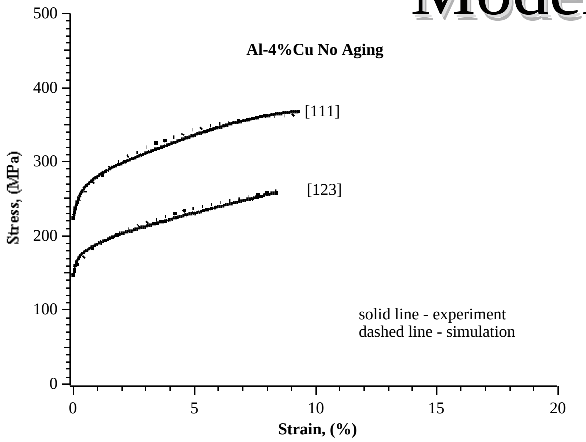

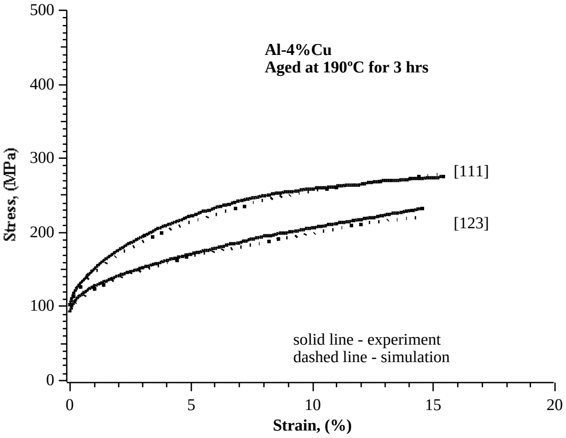

# Modeling Summary

- 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