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*Title:* Crystal plasticity based constitutive laws for Be: effect of strain rate, twinning and texture on the mechanical response

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Khariton Readings, Sarov, Russia
March 14-18, 2011

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# Crystal plasticity based constitutive laws for Be: effect of strain rate, twinning and texture on the mechanical response

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Abstract

Because of its intrinsic anisotropy and variety of slip and twin modes, Beryllium displays a mechanical behavior that strongly depends upon texture, temperature and strain rate. As a consequence, accounting for crystal plasticity mechanisms and directionality is imperative for developing reliable constitutive laws for Be. In this presentation we describe a self-consistent polycrystal model and apply it to the prediction of internal stress of thermal origin, mechanical response of textured and non-textured Be, deforming in compression at strain rates ranging from $10^{-3}$ $s^{-1}$ to $10^{4}$ $s^{-1}$. We also discuss the possibility of measuring dislocation densities using the technique of Peak Shape Analysis.

To be presented at Khariton Readings, March 14-18, 2011, Sarov, Russia

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# Crystal plasticity based constitutive laws for Be: effect of strain rate, twinning and texture on the mechanical response

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# Visco-plastic grain model

Grain deformation is based on crystallographic shear on slip and twinning systems.

The shear-rate of each system *s* is given by a viscous (rate sensitive) law

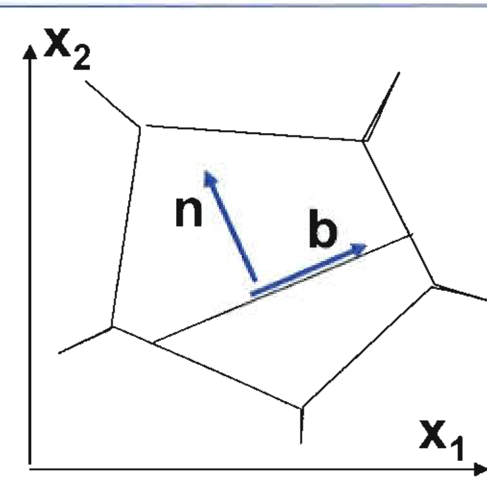
$$\dot{\gamma}^s = \dot{\gamma}_0 \left( \frac{\tau_{resolved}}{\tau^s} \right)^n = \dot{\gamma}_0 \left( \frac{m^s : \sigma}{\tau^s} \right)^n$$

The threshold stress describes the hardening of slip systems

The crystallographic shears determine crystal reorientation and texture evolution

The strain-rate of the grain is given by superposition of shear rates on all active systems

$$\dot{\varepsilon}'_{ij} = \sum_s \frac{n_i^s b_j^s + n_j^s b_i^s}{2} \dot{\gamma}^s = \sum_s m_{ij}^s \dot{\gamma}^s$$

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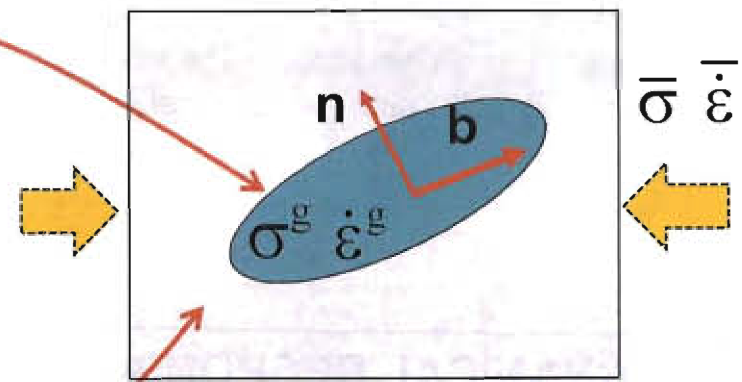
# Visco Plastic Self Consistent (VPSC) Polycrystal Model

- Each grain is a visco-plastic anisotropic ellipsoidal inclusion embedded in a visco-plastic anisotropic Homogeneous Effective Medium (HEM).

- Linearized constitutive response: $M^g$ and $\overline{M}$ → grain and effective medium compliance tensors

grain: $\dot{\varepsilon}^g_{ij} = \dot{\gamma}_o \sum_s m^s_{ij} \left( \frac{m^s : \sigma^g}{\tau^s} \right)^n = M^g_{ijkl}\sigma^g_{kl} + \dot{\varepsilon}^{og}_{ij}$

medium: $\dot{\overline{\varepsilon}}_{ij} = \overline{M}_{ijkl}\overline{\sigma}_{kl} + \dot{\overline{\varepsilon}}^o_{ij}$




Solve equilibrium equation for inclusion in homogeneous medium: $\sigma_{ij,j} = 0$

Eshelby result → stress and strain-rate are uniform inside the inclusion

…but different from the macroscopic stress and strain rate !

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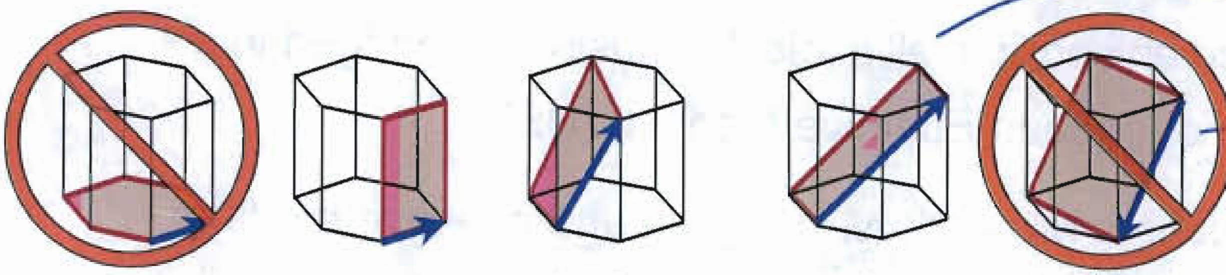
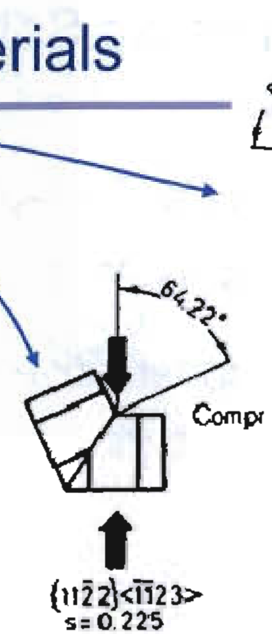
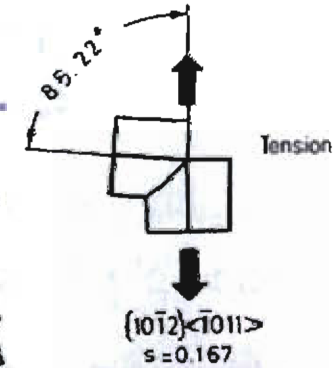
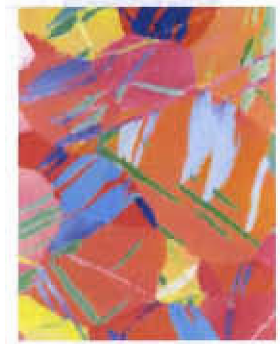
# Plasticity of hexagonal materials



| $(0001)\langle 11\bar{2}0\rangle$ | $(10\bar{1}0)\langle 11\bar{2}0\rangle$ | $(11\bar{2}2)\langle 11\bar{2}3\rangle$ | $(10\bar{1}2)\langle 10\bar{1}1\rangle$ | $(10\bar{1}1)\langle 10\bar{1}2\rangle$ |
|---|---|---|---|---|
| Basal slip | Prismatic slip | Pyramidal slip | Tensile twin | Compressive twin |





ACTIVE SYSTEMS IN BERYLLIUM

## MECHANICAL RESPONSE OF HEXAGONALS

- Several slip and twin modes with different temperature and rate dependencies
- Anisotropy of single crystal → difficult to deform along the c-axis
- Need to account for slip-slip and for slip-twin interactions
- Twinning activity affects texture, hardening and anisotropy

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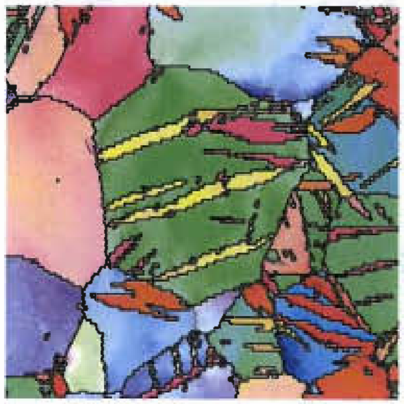
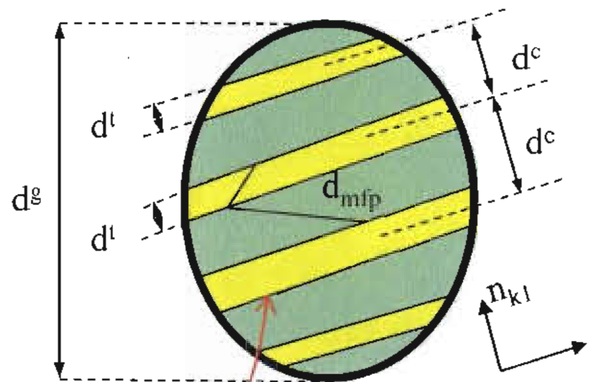
# Composite-Grain Twin Model






Treat grain as an evolving stack of twin-matrix layers on the plane of the predominant twin system.

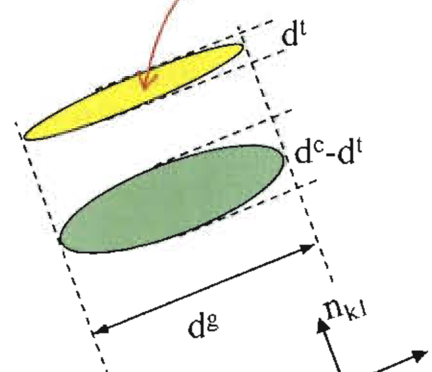
**COUPLED**

Continuity of stress and strain across the twin-matrix interface

$$\sigma_{13}^{parent} = \sigma_{13}^{twin}$$

$$\sigma_{23}^{parent} = \sigma_{23}^{twin}$$

$$\dot{\varepsilon}_{12}^{parent} = \dot{\varepsilon}_{12}^{twin}$$




**UNCOUPLED**

Separate treatment of parent and twin as ellipsoidal inclusions.

Account for ellipsoid orientation and thickness evolution with deformation


Proust & Tome, Acta Materialia **55** (2007) 2137
Proust et al, Int. J. of Plasticity **25** (2009) 861

## Rate Dependent Experiments Prompt Dislocation Based Hardening Model

(α = slip mode)

$$\frac{\partial \rho^{\alpha}}{\partial \gamma^{\alpha}} = \frac{\partial \rho^{\alpha}_{storage}}{\partial \gamma^{\alpha}} - \frac{\partial \rho^{\alpha}_{removed}}{\partial \gamma^{\alpha}} = k_1^{\alpha}\sqrt{\rho^{\alpha}} - k_2^{\alpha}(\dot{\varepsilon}, T)\rho^{\alpha}$$

$$\frac{\partial \rho^{\alpha}_{removed}}{\partial \gamma^{\alpha}} \rightarrow \left(1 - f^{\alpha}\right)\frac{\partial \rho^{\alpha}_{removed}}{\partial \gamma^{\alpha}}$$ **ANNIHILATION**

$$\frac{\partial \rho^{\alpha}_{removed}}{\partial \gamma^{\alpha}} \rightarrow f^{\alpha}\frac{\partial \rho^{\alpha}_{removed}}{\partial \gamma^{\alpha}}$$ **SUBSTRUCTURE** $\rho_{sub}$

- **Temperature and strain rate dependence enter in rate of annihilation.**

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# Dislocation-based constitutive law for HCP (temperature and rate dependent)

Dislocation densities in the slip systems (α = basal, prism or pyramidal) evolve with crystal shears via generation, annihilation (removal) and substructure build-up

$$d\rho^{\alpha}_{gener,forest} = k_1^{\alpha}\sqrt{\rho^{\alpha}_{forest}}\,d\gamma^{\alpha}$$ ⟵ Dislocation generation

$$d\rho^{\alpha}_{remov,forest} = k_2^{\alpha}(\dot{\varepsilon},T)\,\rho^{\alpha}_{forest}\,d\gamma^{\alpha}$$ ⟵ Dislocation annihilation

$$d\rho_{substructure} = \sum_{\alpha} f^{\alpha}(T)\,d\rho^{\alpha}_{remov,forest}$$ ⟵ Substructure formation

The threshold to propagate dislocations is related to the density via Taylor's law

$$\tau^{\alpha}_{slip} = b^{\alpha}\chi\mu\sqrt{\sum_{\alpha'} D^{\alpha\alpha'}\rho^{\alpha'}_{forest}}$$ ⟵ Forest hardening

$$\tau^{\beta}_{twin} = \mu\sum_{\alpha} C^{\beta\alpha} b^{\alpha} b^{\beta} \rho^{\alpha}$$ ⟵ Twin hardening by dislocations

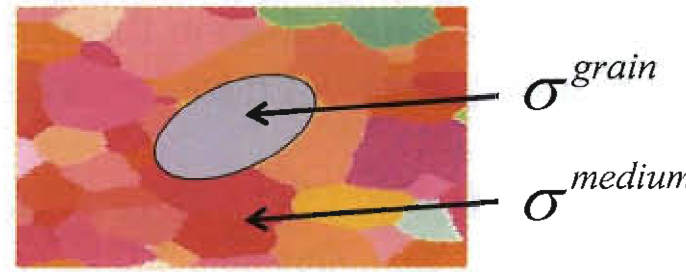
Beyerlein and Tomé, Int. J. Plast. **24** (2008) 867.

# Multiscale modeling

Visco Plastic (VPSC) and Elasto Plastic (EPSC) Polycrystal Aggregate Models

*VPSC → Lebensohn & Tome (1993); Proust et al (2009)*

*EPSC → Turner & Tome (1994); Clausen et al (2008)*

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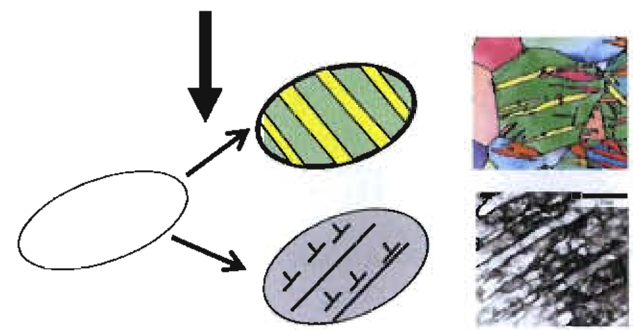
Composite Grain Model

*Proust et al. (2007)*

Dislocation-based Hardening Model

*Beyerlein & Tome (2008)*



↓

Shear rates & hardening for slip & twinning controlled by evolving Threshold Stress

$$\dot{\gamma}^s = \dot{\gamma}_0 \left( \frac{\tau_{resolved}}{\tau^s_{threshold}} \right)^n$$

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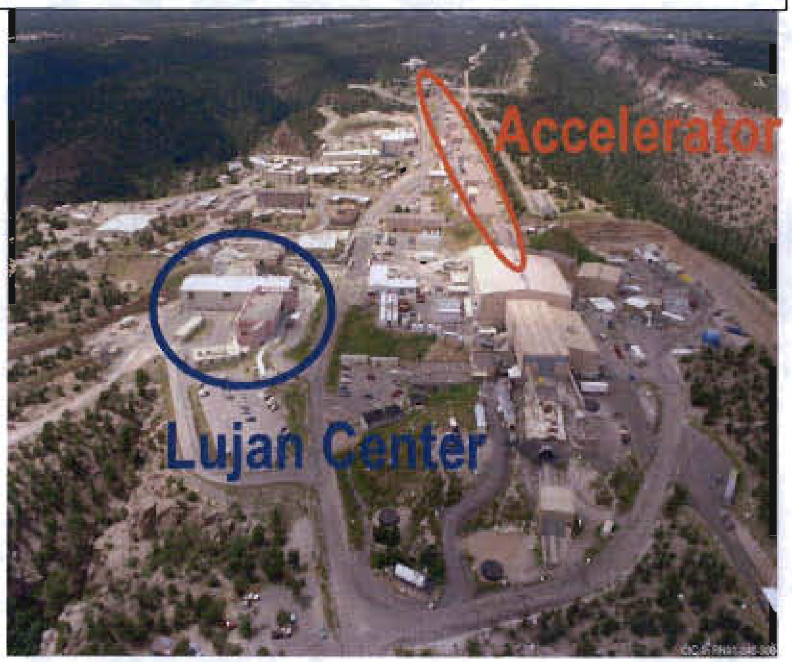
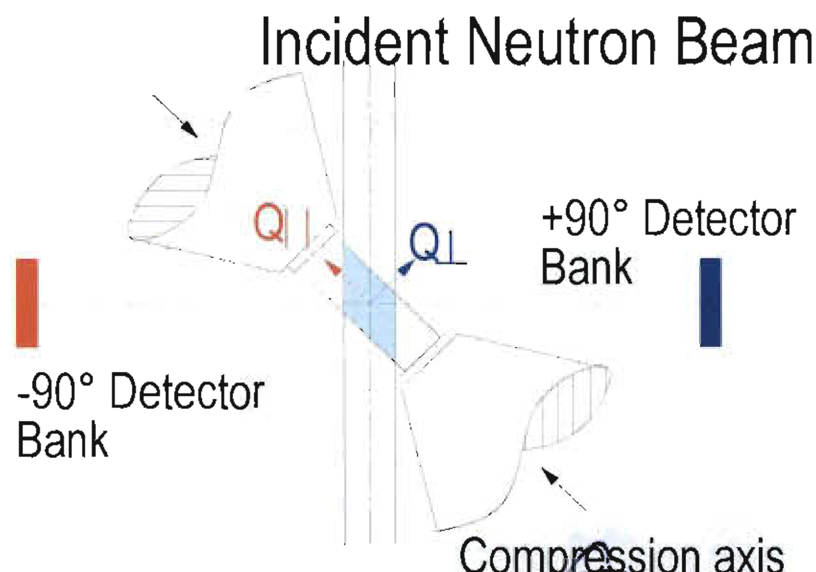
# Neutron diffraction facilities: a tool for 'in-situ' & 'in-bulk' stress measurements

SMARTS Diffractometer
LANSCE - LANL




- Crystal diffraction measures lattice spacing in the bulk
- Lattice spacing provides information about elastic strains
- Elastic strains are related to internal stress via Hooke's law
- Diffracting region: ~ 5mm

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## Modeling of Thermal and Mechanical Response of Be

- Use Elasto-Plastic Polycrystal model to calculate internal stress inside grains of non-textured Be.
  → Compare with neutron diffraction results

- Use Visco-Plastic Polycrystal model to calculate Stress-Strain response of rolled and non-textured Be.
  → Use an unique Single Crystal constitutive law, function of temperature and strain-rate

- Calculate dislocation densities using Peak Profile Analysis on neutron diffraction peaks

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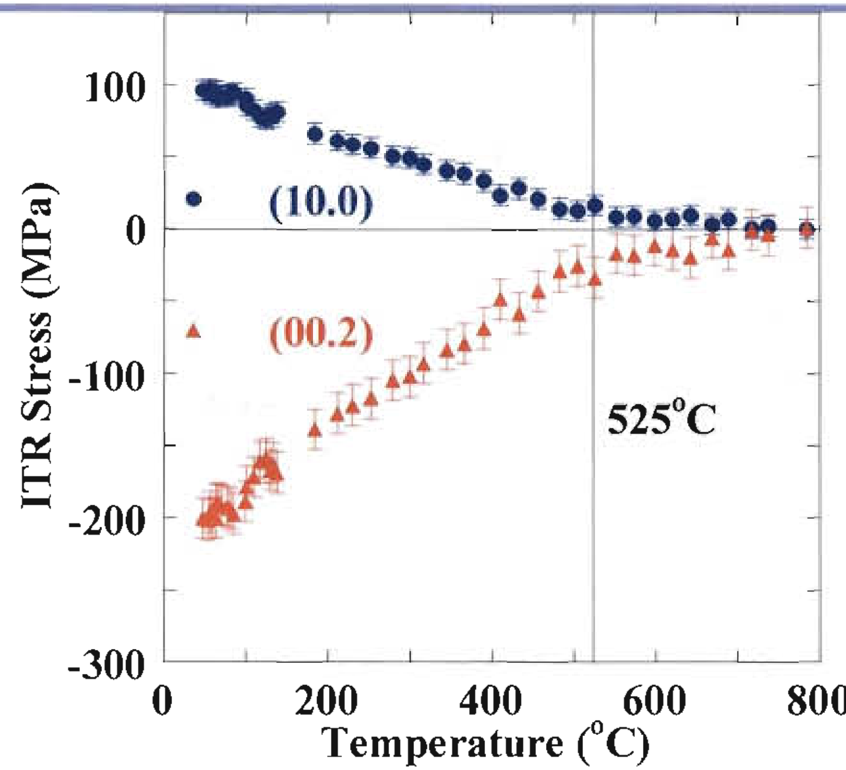
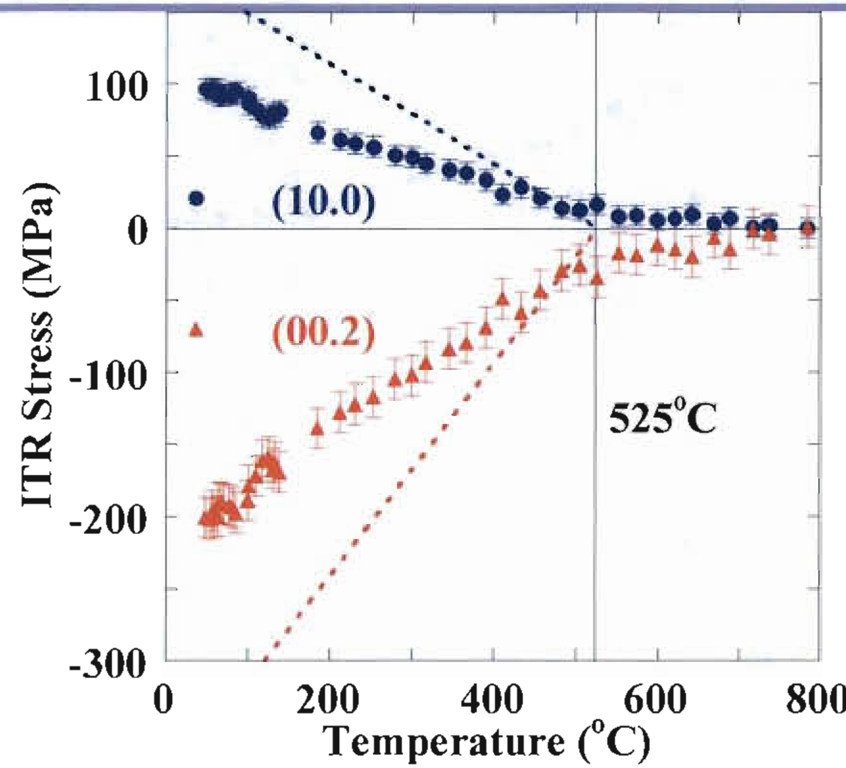
# Intergranular Thermal Residual Stresses in Beryllium are Significant.




- Intergranular stresses relax on time scale of measurement above 525C.
  - Zero strength temperature.
  - Important for modeling studies.

# Intergranular Thermal Residual Stresses in Beryllium are Significant.




- Upper bound model, assuming grain in rigid matrix over-predicts stresses by ~x2

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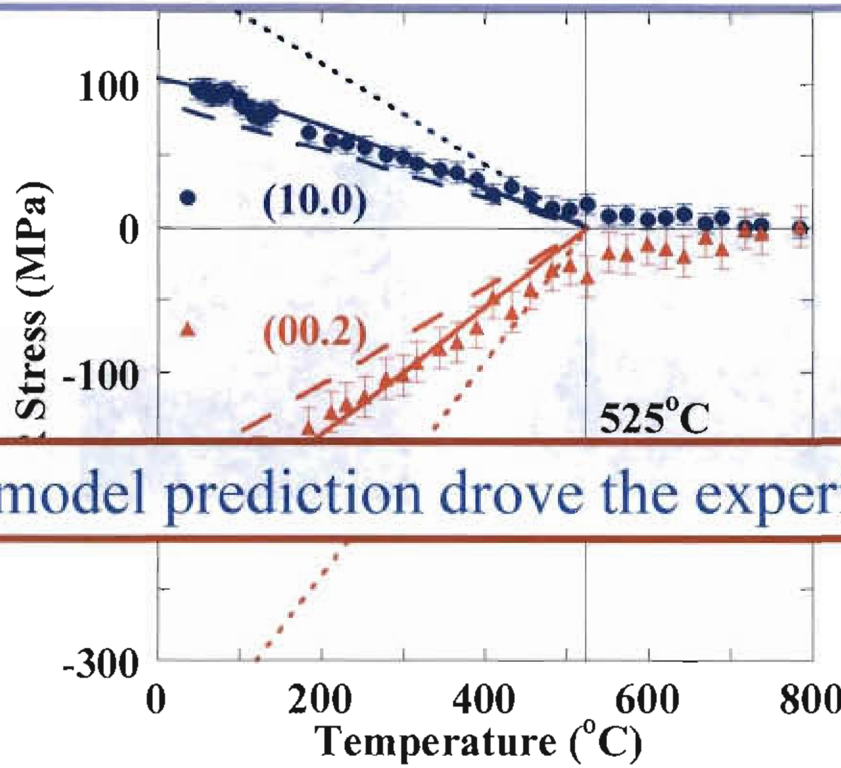
# Intergranular Thermal Residual Stresses in Beryllium are Significant.




In this case, model prediction drove the experimental path !

- Upper bound model, assuming grain in rigid matrix over-predicts stresses by ~x2.
- EPSC model with room temperature CTE's under-predicts stresses slightly.
- EPSC with temperature dependent CTE matches data well.

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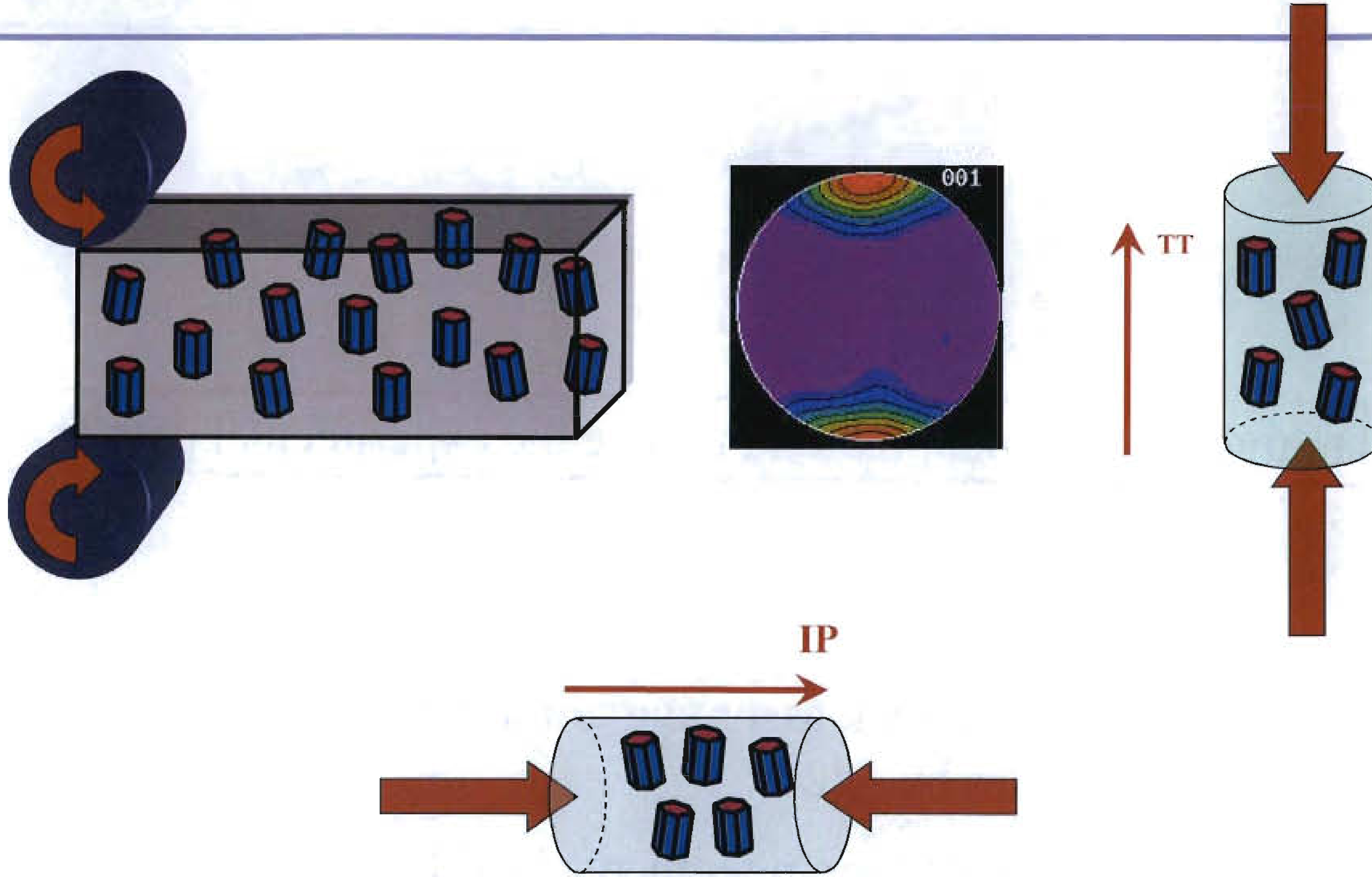
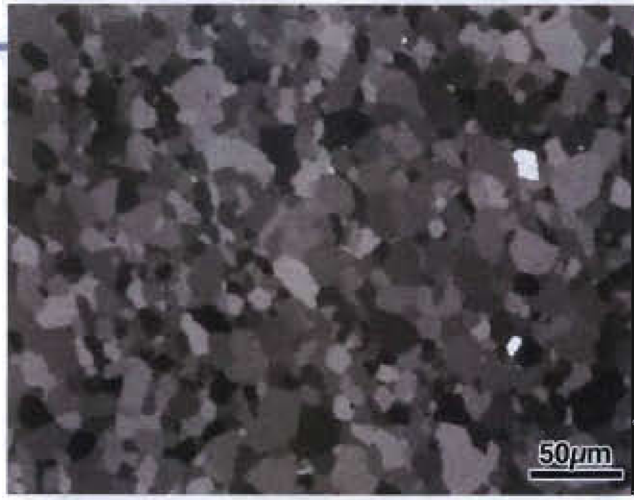
# Rolling of Beryllium Results in Strong Crystallographic Texture

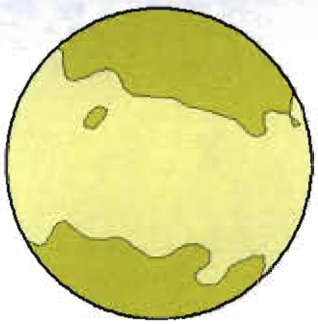


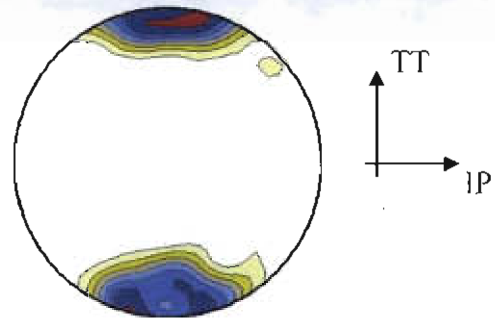

• **Orientation of crystals with respect to load axis is critical.**

## Rate and Temperature Dependent Deformation of Beryllium










- Hot-pressed (random texture) and rolled plate (strong texture) beryllium.
- In-plane (IP) and through-thickness (TT) compression of rolled plate.
  - Normal and parallel to dominant basal texture, respectively.
- Strain rates from 0.0001/sec to 5000/sec.

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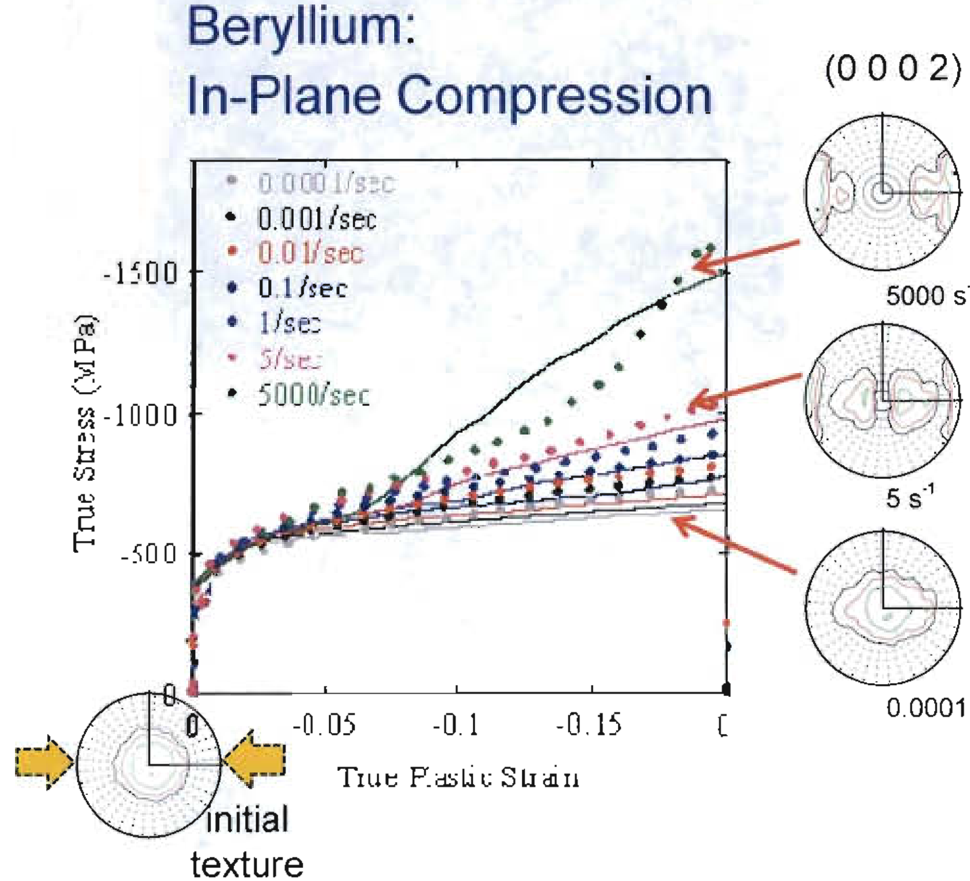
# Be: slip vs twinning competition




Rapid transition from dislocation-controlled to twin-controlled hardening as the temperature decreases (Zr) or as the strain rate increases (Be)

Sisneros et al, Mats. Sc. and Engng. **A527** (2010) 5181

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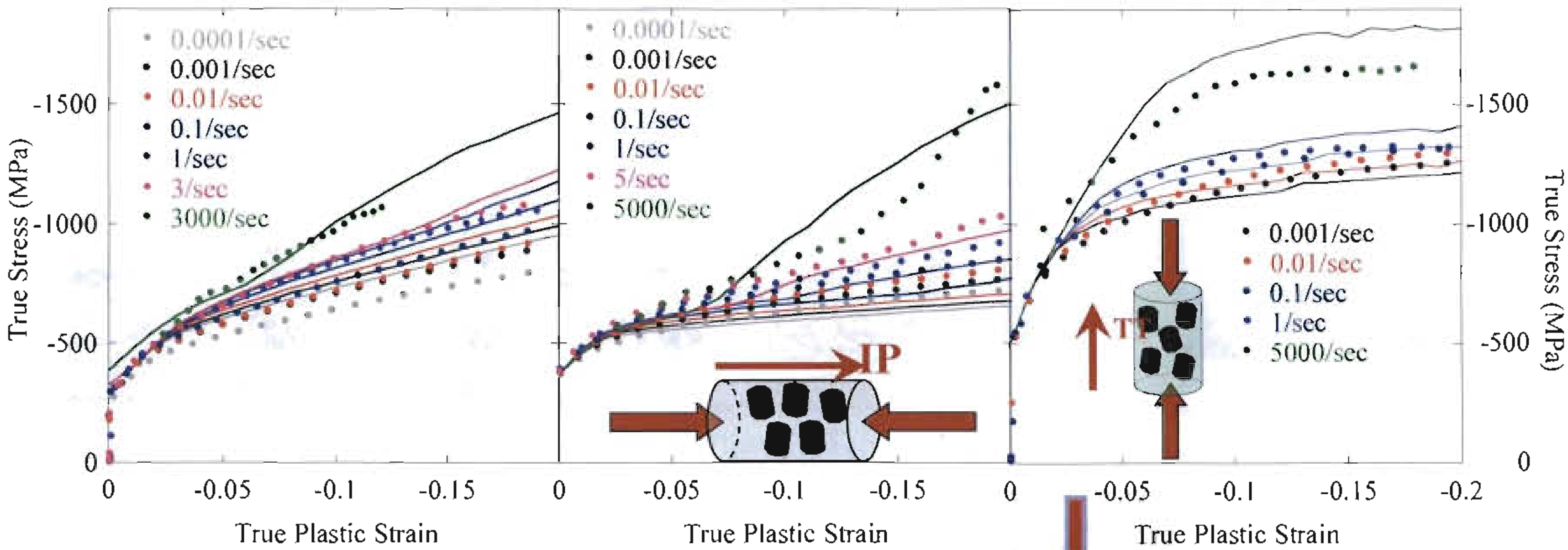
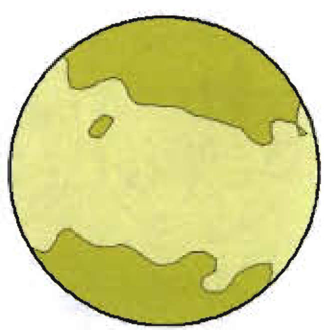
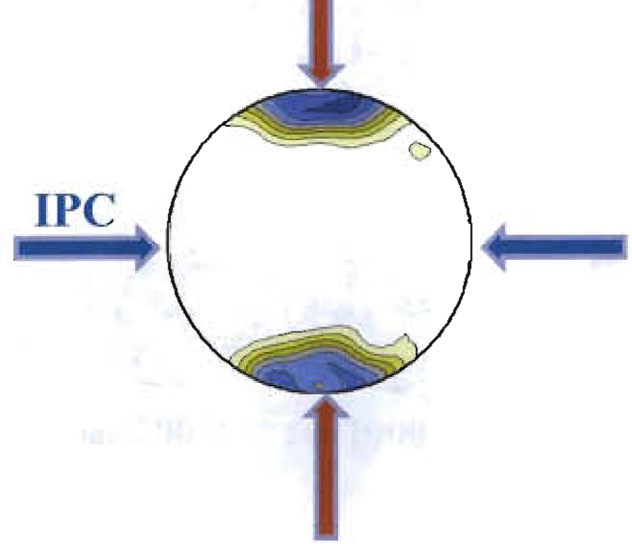
# Dislocation Based Hardening Law Allows Us to Predict Rate Dependent Flow curve



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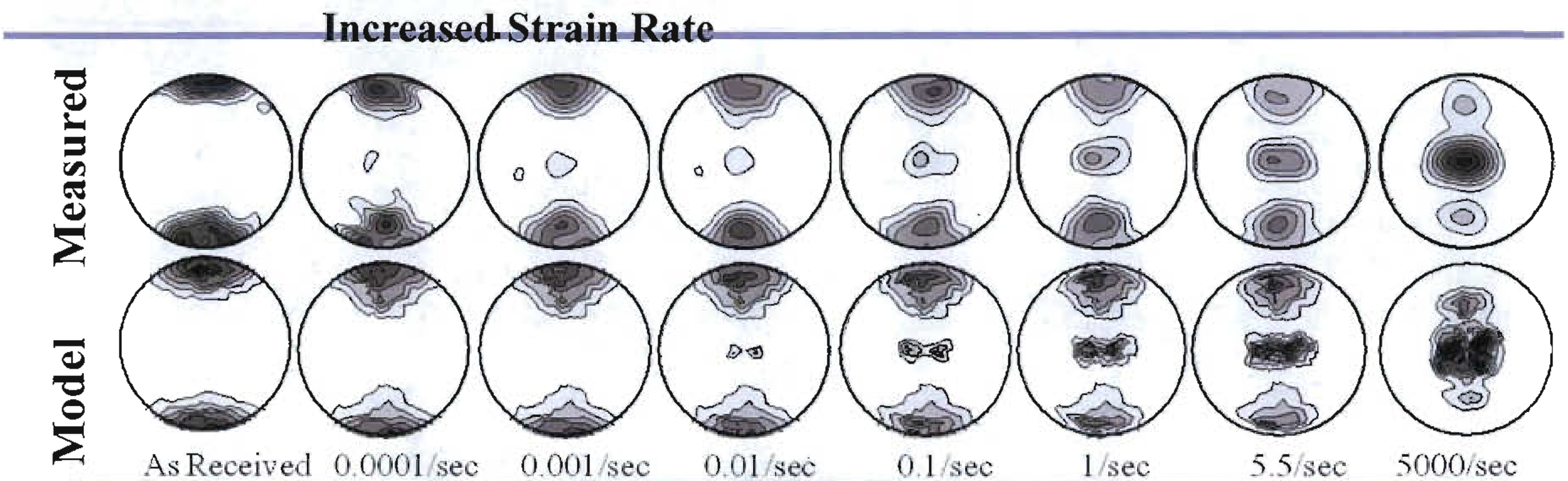
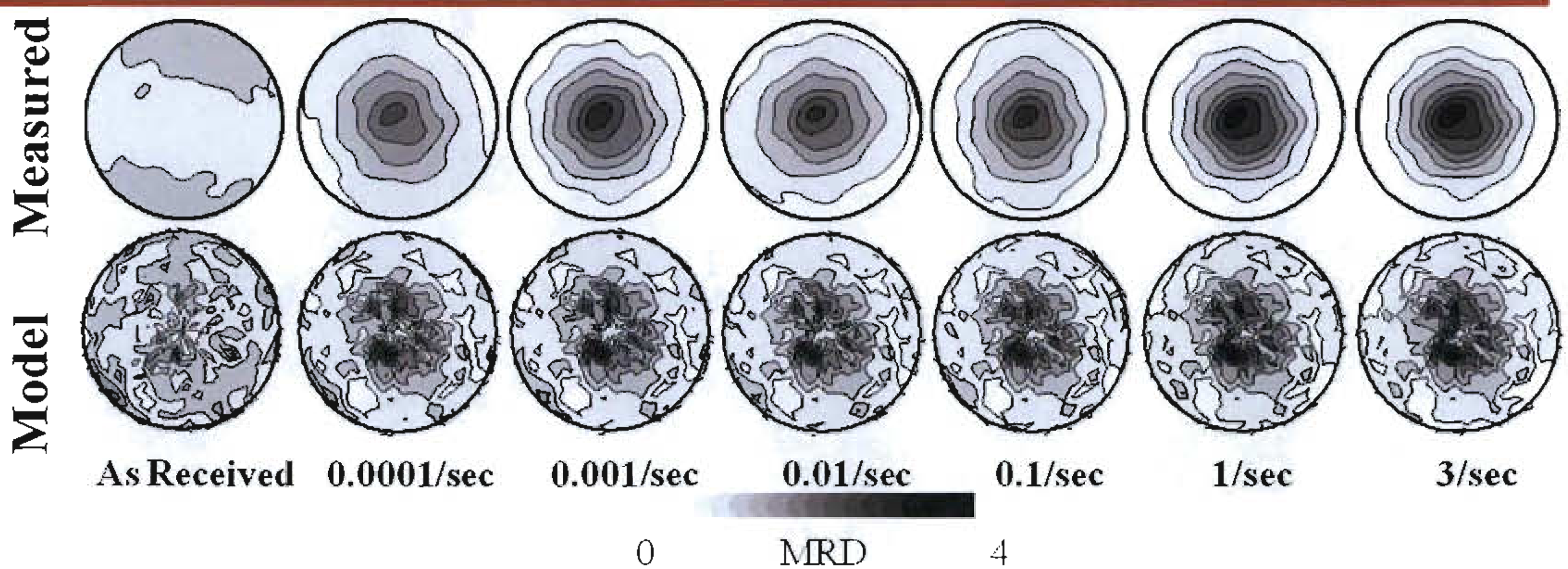
# Dislocation Based Hardening Law Allows Us to Predict Rate Dependent Texture




In this case, the experiment drove the model development.

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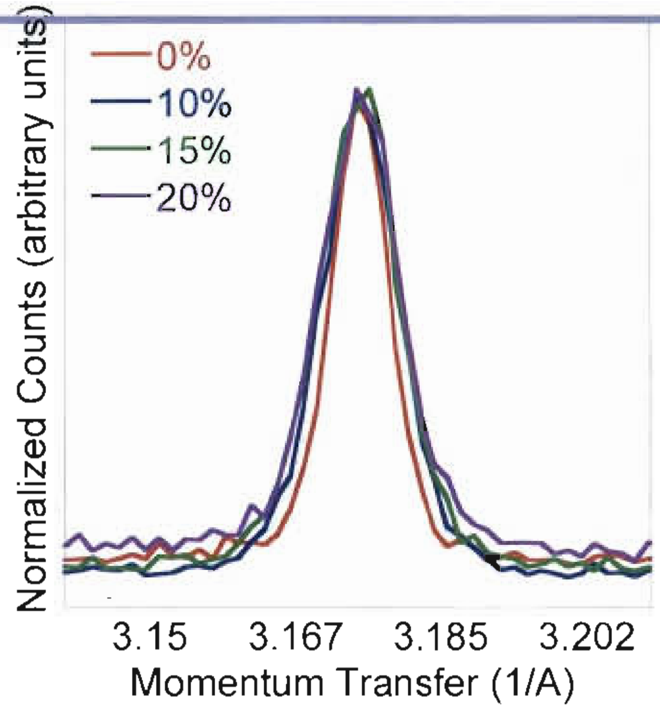
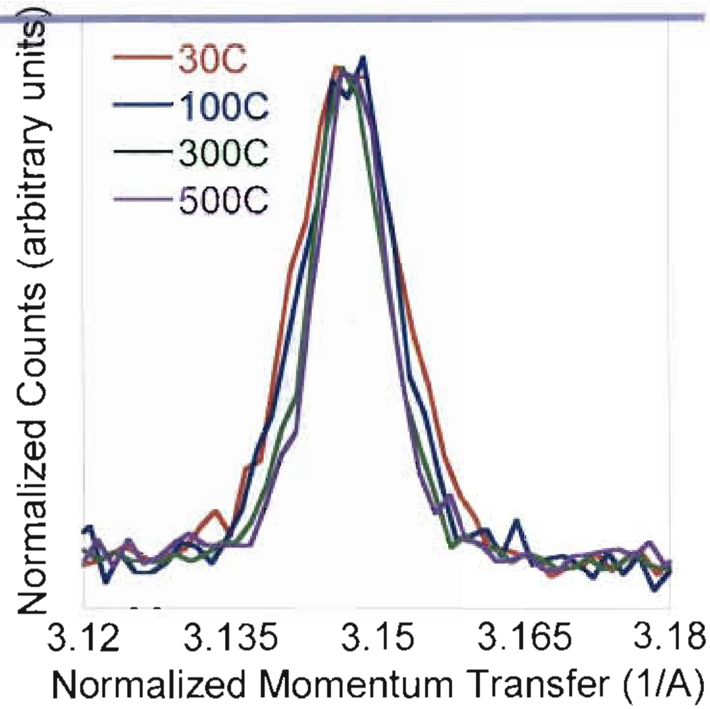
## Ability to Calculate Dislocations Drives Us To Measure Dislocations




- **Diffraction peak breadth is related to the dislocation density.**
- **Completed in-situ measurements of peak breadth during deformation and subsequent annealing.**
- **Qualitatively, breadth increases with plastic deformation, decreases with annealing.**

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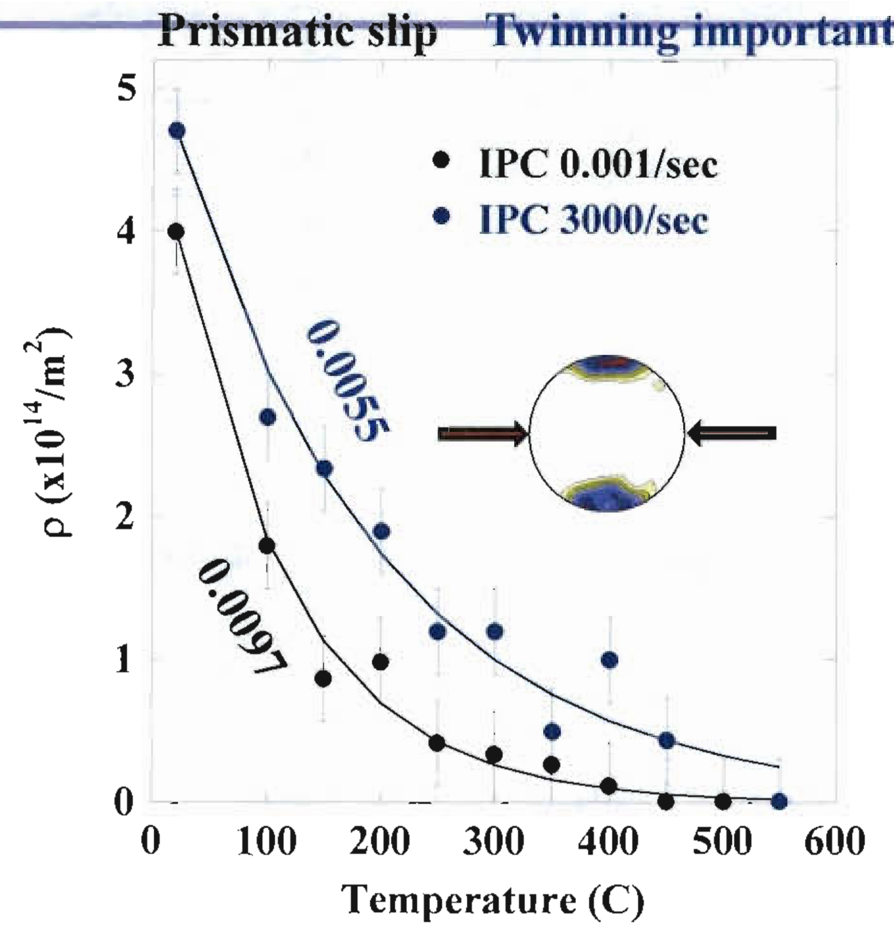
# Rate of Recovery Appears Dependent on Deformation Conditions




These experiments are now pushing the model development.

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# Summary and Conclusions

Polycrystal models are based on crystallinity.

Account for slip and twin systems and their interactions explicitly

Macroscopic anisotropic response is a combined result of: crystal anisotropy, microstructure inside crystal, and texture

Thermal, elastic and plastic regimes can be modeled

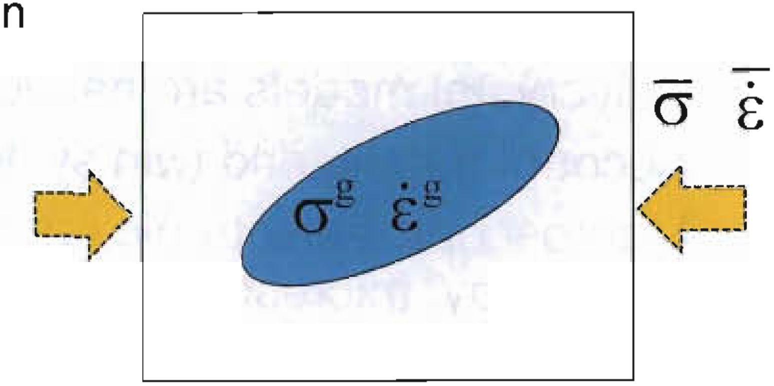
Stress-strain response (of grains and PX) can be predicted

Texture evolution (anisaotropy evolution) can be predicted

Dislocation density evolution can be predicted

## VPSC model → interaction equation, shape effects

Solving stress equilibrium equation for the VP inclusion embedded in the VP medium leads to the interaction equation




$$(\dot{\varepsilon}^g_{ij} - \bar{\dot{\varepsilon}}_{ij}) = -\tilde{M}_{ijkl}\,(\sigma^g_{kl} - \bar{\sigma}_{kl})$$

where $\tilde{M}_{ijkl} = (I\text{-}S)^{-1}_{ijmn}\, S_{mnpq}\, \bar{M}_{pqkl}$

and $S(\bar{M})$ is the Eshelby tensor

- $\bar{M}$ large → medium very compliant → $\sigma^g_{kl} = \bar{\sigma}_{kl}$ → lower bound Sachs
- $\bar{M}$ small → medium very stiff → $\dot{\varepsilon}^g_{ij} = \bar{\dot{\varepsilon}}_{ij}$ → upper bound Taylor
- $\tilde{M}$ components are a mix of small and large → relaxed constraints
- **self-consistent cases** → intermediate → secant, affine, tangent

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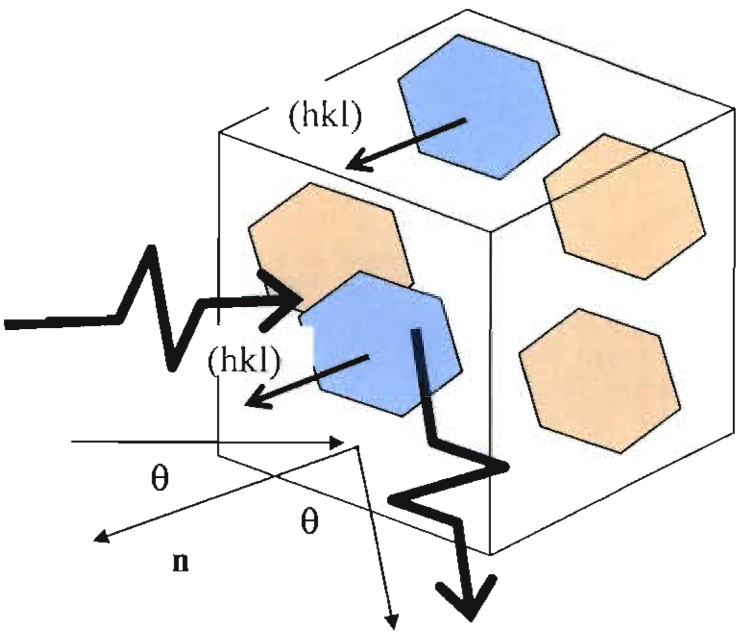
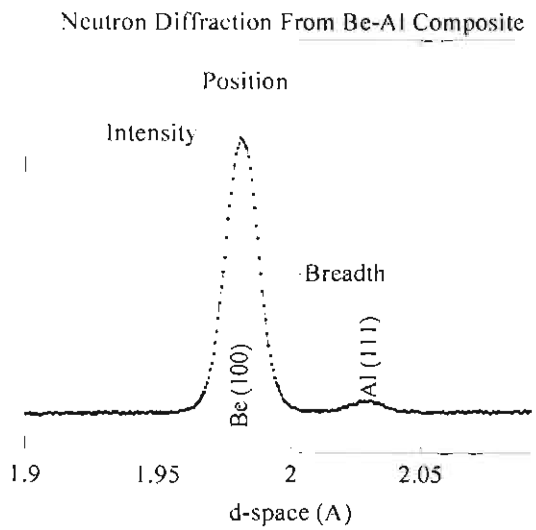
# Neutron & X-ray diffraction measurements of internal strains




Subset of diffracting grains with plane (hkl) perpendicular to the diffraction vector **n** .

The plane spacing $d^{hkl}$ is given by the Bragg diffraction condition: $d^{hkl} \sin\theta = n\lambda$

The difference between stressed and unstressed lattice parameters gives the elastic strain perpendicular to the plane (hkl)

$$\varepsilon^{hkl} = \frac{d^{hkl} - d_o^{hkl}}{d_o^{hkl}}$$

Peak shift → elastic strains → internal stress

Peak intensity → volume fraction of grains → texture

Peak width → elastic strain fluctuations → dislocation density