

Plastic Spin, Gradients/Localization & Texture

[From Micro/Single Slip to Macro/Phenomenological Plasticity]

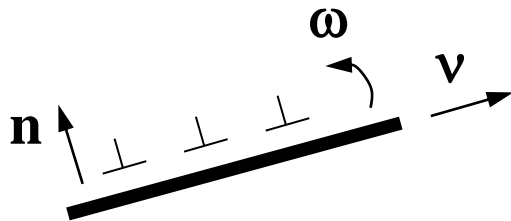
■ A Scale Invariance Argument

• *Momentum Balance for Dislocated State*

$$\operatorname{div} \mathbf{T}^D = \hat{\mathbf{f}}; \quad \mathbf{T}^D = \mathbf{S} - \mathbf{T}^L; \quad \operatorname{div} \mathbf{S} = 0$$

\mathbf{T}^D ...dislocation stress; $\hat{\mathbf{f}}$...dislocation-lattice interaction force

• *Yield Condition:* $f = \hat{\mathbf{f}} \cdot \mathbf{v} = 0$; $\hat{\mathbf{f}} = (\hat{\alpha} + \hat{\beta}j - \hat{\gamma}\tau^L) \mathbf{v}$, $\tau^L = \mathbf{T}^L \cdot \mathbf{M}$



$$\mathbf{M} = (\mathbf{v} \otimes \mathbf{n})_s, \quad \mathbf{\Omega} = (\mathbf{v} \otimes \mathbf{n})_a, \quad \dot{\mathbf{v}} = \boldsymbol{\omega} \mathbf{v}$$

$$\mathbf{D}^P = \dot{\gamma}^P \mathbf{M}, \quad \mathbf{W}^P = \dot{\gamma}^P \mathbf{\Omega}, \quad \mathbf{T}^D = t_m \mathbf{M} + t_n \mathbf{N}$$

$$\max \{ \operatorname{tr} \mathbf{T}^L \mathbf{D}^P \}; \quad \operatorname{tr} \mathbf{M} = 0, \quad \operatorname{tr} \mathbf{M}^2 = 1/2 \quad \Rightarrow \quad \mathbf{D}^P = \frac{\dot{\gamma}^P}{2\sqrt{J}} \mathbf{T}^{L'}; \quad J = \frac{1}{2} \operatorname{tr} (\mathbf{T}^{L'} \mathbf{T}^{L'})$$

$$\therefore \tau = \sqrt{J} = \kappa(\gamma^P)$$

• *Structure of Macroscopic Anisotropic Hardening Plasticity*

$$\mathbf{D}^p = \frac{\dot{\gamma}^p}{2\sqrt{J}}(\boldsymbol{\sigma}' - \boldsymbol{\alpha}'); \quad \dot{\boldsymbol{\alpha}} = \begin{pmatrix} \dot{t}_m & -\dot{t}_n t_m \\ \dot{\gamma}^p & t_n \dot{\gamma}^p \end{pmatrix} \mathbf{D}^p + \frac{\dot{t}_n}{t_n} \boldsymbol{\alpha}$$

$$\dot{\boldsymbol{\alpha}} = \dot{\boldsymbol{\alpha}} - \boldsymbol{\omega} \boldsymbol{\alpha} + \boldsymbol{\alpha} \boldsymbol{\omega}; \quad \boldsymbol{\omega} = \mathbf{W} - \mathbf{W}^p, \quad \mathbf{W}^p = -\frac{1}{t_n}(\boldsymbol{\alpha} \mathbf{D}^p - \mathbf{D}^p \boldsymbol{\alpha})$$

$$\dot{\gamma}^p = \frac{\dot{\boldsymbol{\sigma}}' \cdot (\boldsymbol{\sigma}' - \boldsymbol{\alpha}')}{\kappa(t'_m + 2\kappa')}; \quad \begin{cases} \dot{f} = 0 \dots \text{consistency condition} \\ f = \frac{1}{2}(\boldsymbol{\sigma}' - \boldsymbol{\alpha}') \cdot (\boldsymbol{\sigma}' - \boldsymbol{\alpha}') - \kappa^2 = 0 \dots \text{yield condition} \end{cases}$$

• *Example Models*

$$\mathbf{M1}: \dot{t}_m = c\dot{\gamma}^p; \quad \dot{t}_n = 0 \rightarrow \begin{cases} \dot{\boldsymbol{\alpha}} = c\mathbf{D}^p \\ \mathbf{W}^p = \zeta(\boldsymbol{\alpha} \mathbf{D}^p - \mathbf{D}^p \boldsymbol{\alpha}) \end{cases} \quad \dots \text{Prager}$$

$$\mathbf{M2}: \left. \begin{cases} \dot{t}_m = c\dot{\gamma}^p - \bar{c}\dot{\gamma}^p t_m \\ \dot{t}_n = -\bar{c}\dot{\gamma}^p t_n \end{cases} \right\} \rightarrow \begin{cases} \dot{\boldsymbol{\alpha}} = c\mathbf{D}^p - \bar{c}\dot{\gamma}^p \boldsymbol{\alpha} \\ \mathbf{W}^p = \zeta e^{\bar{c}\dot{\gamma}^p} (\boldsymbol{\alpha} \mathbf{D}^p - \mathbf{D}^p \boldsymbol{\alpha}) \end{cases} \quad \dots \text{Armstrong-Frederick}$$

- **Inhomogeneous Back Stress:** $\mathbf{T}^D = \boldsymbol{\alpha} + \mathbf{T}^{inh}$

- $\boldsymbol{\alpha}$ = homogeneous back stress ... as before

$$\mathbf{T}^{inh} = \hat{\mathbf{g}}(\mathbf{n}, \mathbf{v}, \nabla\gamma^p)$$

$$\approx \left[\mathbf{n} \otimes \nabla\gamma^p + (\nabla\gamma^p) \otimes \mathbf{n} \right] + \left[\mathbf{v} \otimes \nabla\gamma^p + (\nabla\gamma^p) \otimes \mathbf{v} \right]$$

$$\text{div}\mathbf{T}^{inh} \approx (\mathbf{n} + \mathbf{v})\nabla^2\gamma^p + (\mathbf{grad}^2\gamma^p)(\mathbf{n} + \mathbf{v})$$

$$(\text{div}\mathbf{T}^{inh}) \cdot \mathbf{v} \approx \nabla^2\gamma^p + \gamma_{,ij}^p (v_i v_j + v_i n_j)$$

- Integrate over all possible orientations of (\mathbf{n}, \mathbf{v})

$$(\text{div}\mathbf{T}^{inh}) \cdot \mathbf{v} \rightarrow \nabla^2\gamma^p$$

$$\therefore \tau = \kappa(\gamma^p) - \mathbf{c}\nabla^2\gamma^p$$

- **Same Procedure for Nanopolycrystals**

- Representative slip plane \rightarrow Representative planar GB

■ A Note on Consistency with Continuum Thermodynamics

Thermodynamics applied to gradient theories :

The theories of Aifantis and Fleck & Hutchinson and their generalization

[*J. Mech. Phys. Sol.* **57**, 405-421 (2009)]

M.E. Gurtin/Carnegie-Mellon & L. Anand/MIT

Abstract : We discuss the physical nature of flow rules for rate-independent (gradient) plasticity laid down by Aifantis and Fleck and Hutchinson. As central results we show that:

- the flow rule of Fleck and Hutchinson is incompatible with thermodynamics unless its nonlocal term is dropped.
- If the underlying theory is augmented by a general defect energy dependent on γ^p and $\nabla\gamma^p$, then compatibility with thermodynamics requires that its flow rule reduce to that of Aifantis.

Refs

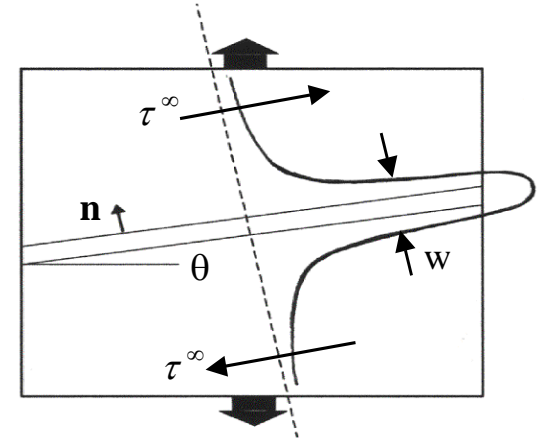
- E.C. Aifantis, On the microstructural origin of certain inelastic models, *Trans. ASME, J. Engng. Mat. Tech.* **106**, 326-330 (1984).
- E.C. Aifantis, The physics of plastic deformation, *Int. J. Plasticity* **3**, 211-247 (1987).
- N.A. Fleck and J.W. Hutchinson, A reformulation of strain gradient plasticity, *J. Mech. Phys. Solids* **49**, 2245-2271 (2001).

■ A Note on Shear Band Widths/Spacings

● *Constitutive Eq.*

$$\mathbf{S}' = -p\mathbf{1} + 2\mu\mathbf{D} \quad ;$$

$$\mu = \frac{\tau}{\dot{\gamma}} \quad , \quad \begin{cases} \tau \equiv \sqrt{\frac{1}{2}\mathbf{S}' \cdot \mathbf{S}'} \\ \dot{\gamma} \equiv \sqrt{2\mathbf{D} \cdot \mathbf{D}} \end{cases} ; \quad \tau = \kappa(\gamma) - c\nabla^2\gamma$$

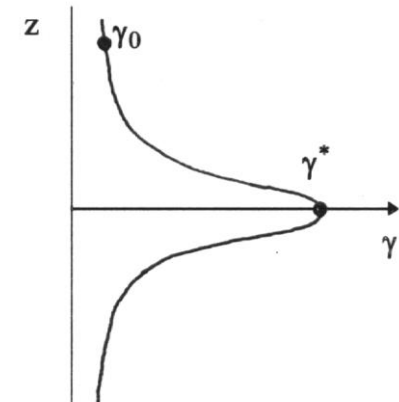
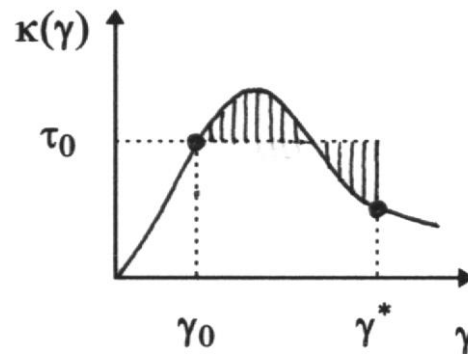


● *Linear Stability / SB Orientation*

$$\mathbf{v} = \mathbf{L}_\infty \mathbf{x} + \tilde{\mathbf{v}} e^{iqz + \omega t} ; \quad \omega > 0 \quad (\& \omega_{\max}) \quad \rightarrow \quad \theta_{cr} = \frac{\pi}{4} \quad \& \quad \begin{cases} h_{cr} = 0 \\ q_{cr} = 0 \end{cases}$$

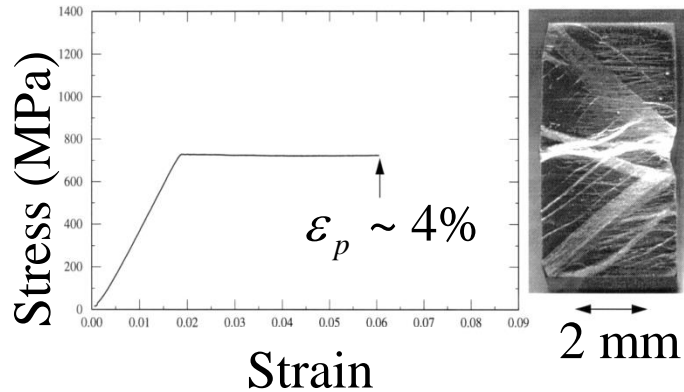
● *Nonlinear Solution / SB Thickness*

$$c\gamma_{zz} = \kappa(\gamma) - \tau^\infty$$

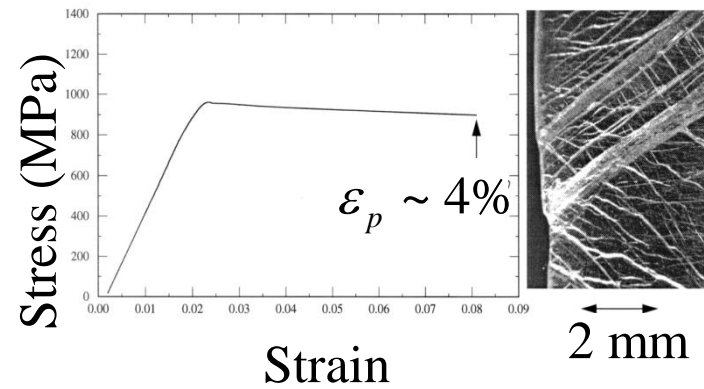


- **Multiple SBs in Bulk Nanostructured Fe-10% Cu Polycrystals**
 - *Compression tests*

$d \sim 1370 \text{ nm}$, $\sigma_y \sim 750 \text{ Mpa}$
angle $\sim 49^\circ$



$d \sim 540 \text{ nm}$, $\sigma_y \sim 960 \text{ MPa}$
angle $\sim 49^\circ$



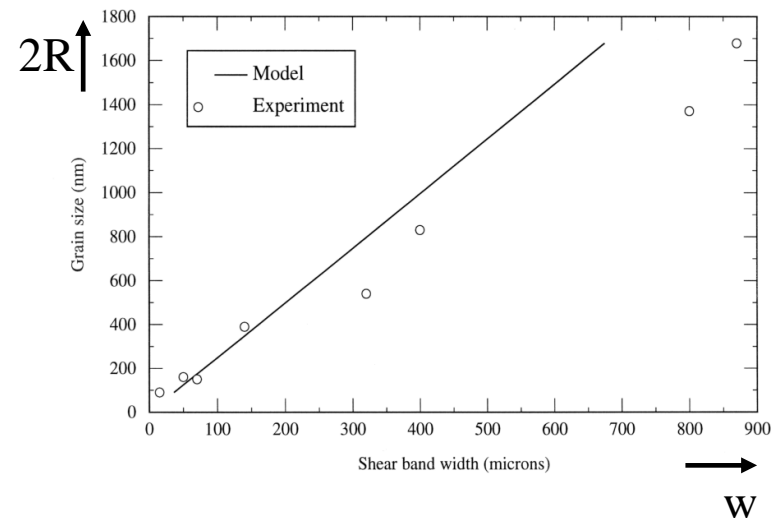
- *Shear band width analysis*

$$\tau = \kappa(\gamma) - c \nabla^2 \gamma$$

$$w \sim 0.4 \sqrt{c}$$

$$c \sim \frac{R^2}{10} (\beta + h)$$

$$\beta = \alpha G \frac{7 - 5\nu}{15(1 - \nu)}$$



■ A Note on Rotational Bands

Simple shear (no elastic deformation)

$$[\mathbf{D}] = [\mathbf{D}^p] = \frac{\dot{\gamma}^p}{2} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad [\mathbf{W}] = \frac{\dot{\gamma}^p}{2} \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

Armstrong-Frederick hardening rule

$$\dot{a}_m = c_1 \dot{\gamma}^p - c_2 \dot{\gamma}^p \alpha_m, \quad \dot{a}_n = -c_2 \dot{\gamma}^p \alpha_n$$

$$\Rightarrow \begin{cases} \dot{\alpha} = c_1 \mathbf{D}^p - c_2 \dot{\gamma}^p \alpha; & \dot{\alpha} = \dot{\alpha} - \omega \alpha + \alpha \omega \\ \mathbf{W}^p = \zeta e^{c_2 \gamma^p} (\alpha \mathbf{D}^p - \mathbf{D}^p \alpha); & \omega = \mathbf{W} - \mathbf{W}^p \end{cases}$$

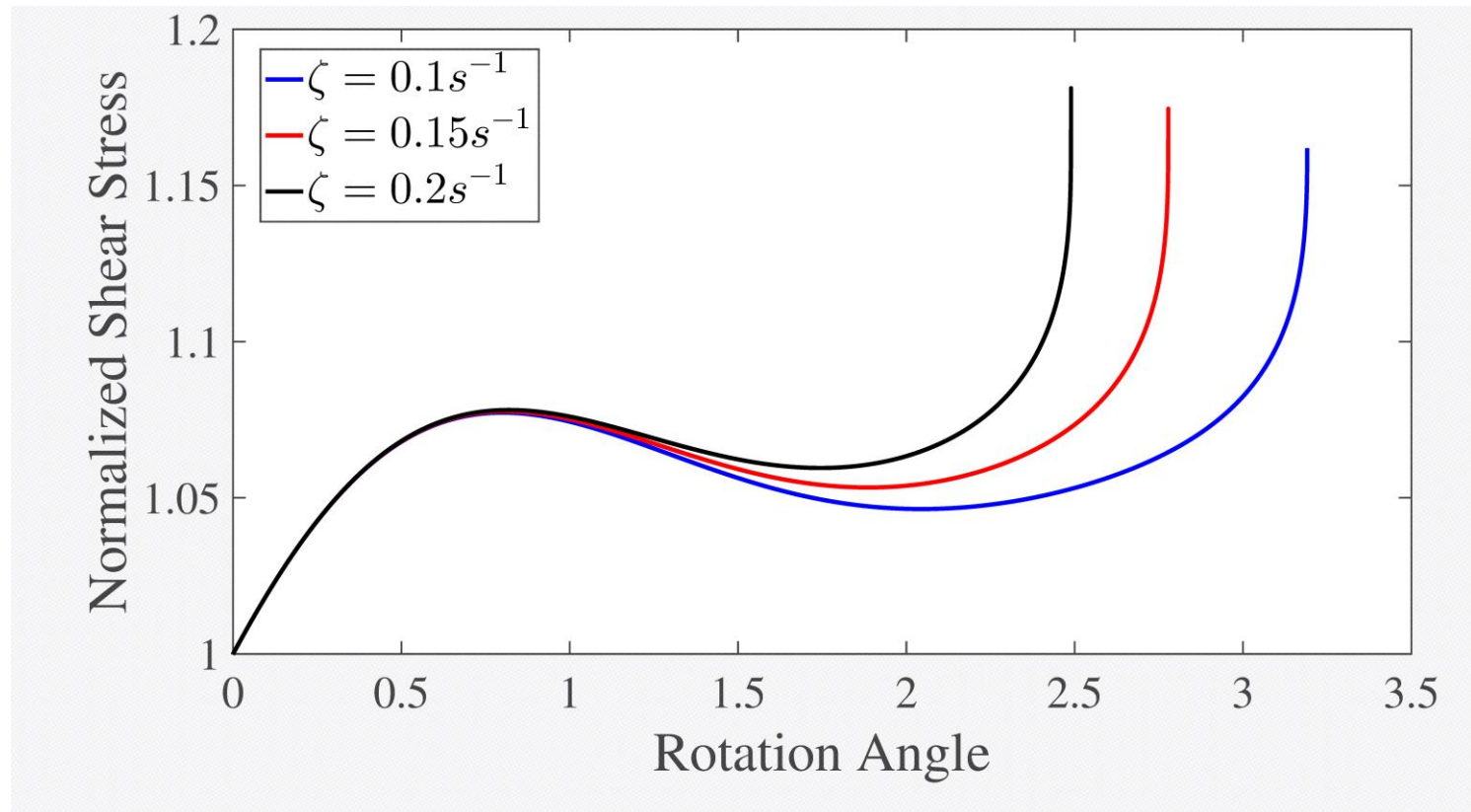
Flow rule

$$\mathbf{D}^p = \frac{\dot{\gamma}^p}{2\sqrt{J}} (\boldsymbol{\sigma}' - \boldsymbol{\alpha}') \Rightarrow \boldsymbol{\sigma} = \boldsymbol{\alpha}' + 2\mu \mathbf{D}^p - p\mathbf{1}; \quad \mu = \tau / \dot{\gamma}^p$$

- *Rotational Softening*

$$\theta = \int \frac{1}{2} \sqrt{\boldsymbol{\omega} \cdot \boldsymbol{\omega}} dt = \int \frac{1}{2} \sqrt{\text{tr}(\boldsymbol{\omega} \boldsymbol{\omega}^T)} dt \quad \dots \text{rotation angle in 2D}$$

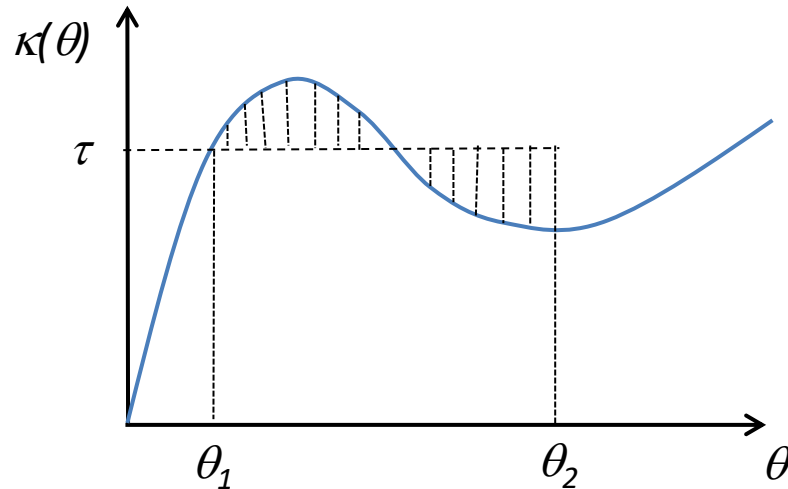
θ ... accumulative rotational variable (analogous to plastic strain γ)



• *Inhomogeneous Rotation / Gradient of θ*

$$\theta = \theta(z)$$

$$\tau = \kappa(\theta) - a\theta_{zz} - b\theta_z^2$$



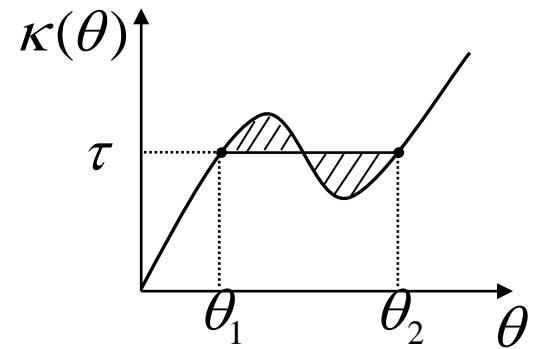
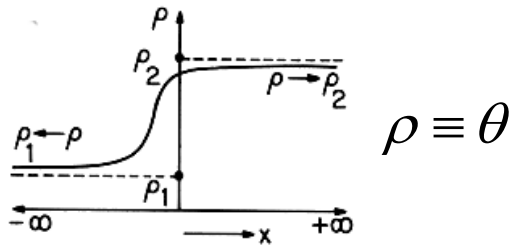
- *Analytical Solutions / Conditions for Existence*

$$\kappa(\theta_1) = \kappa(\theta_2) = \tau, \quad \int_{\theta_1}^{\theta_2} [\kappa(\theta) - \tau] \mathbf{E}(\theta) d\theta = 0; \quad \mathbf{E}(\theta) \equiv \frac{1}{a} \exp\left(2 \int \frac{b}{a} d\theta\right)$$

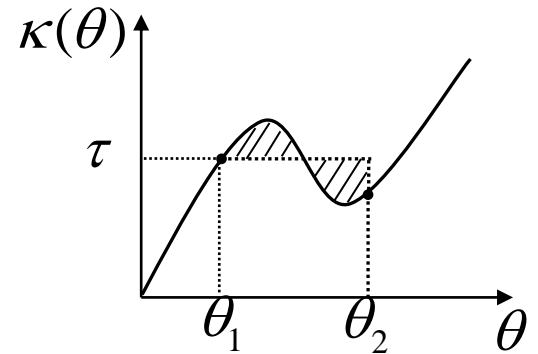
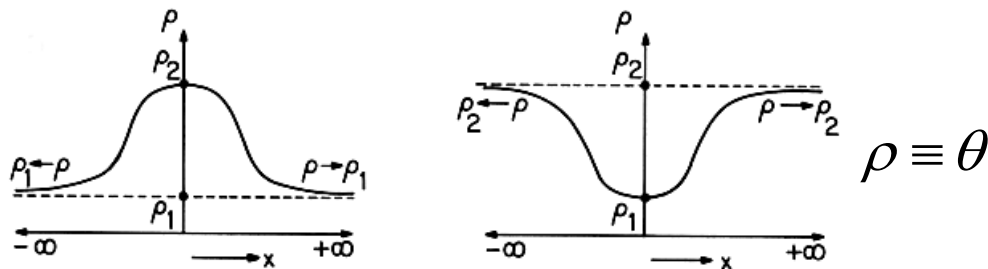
$$z = z_0 + \int_{\theta(z_0)}^{\theta(z)} \frac{d\theta}{\sqrt{2F(\theta)/G(\theta)}}; \quad F \equiv \int_{\theta_1}^{\theta} (\kappa(\theta) - \tau) \mathbf{E}(\theta) d\theta; \quad G \equiv \alpha \mathbf{E}(\theta)$$

• Planar Rotational Bands / 1D Profiles

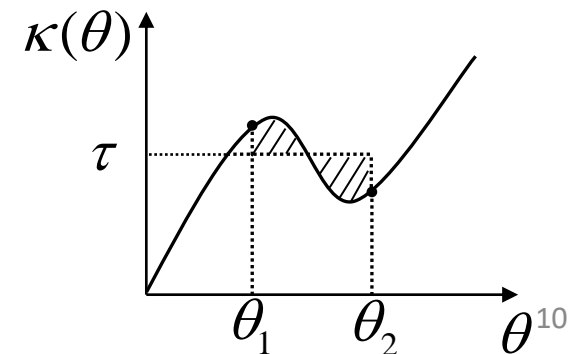
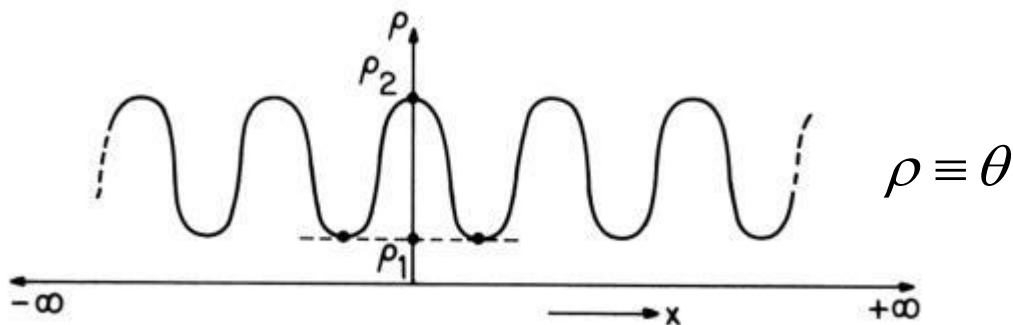
- Transitions $\theta \rightarrow \theta_{1,2}$ as $z \rightarrow \mp\infty$



- Reversals $\theta \rightarrow \theta_1$ as $z \rightarrow \mp\infty$



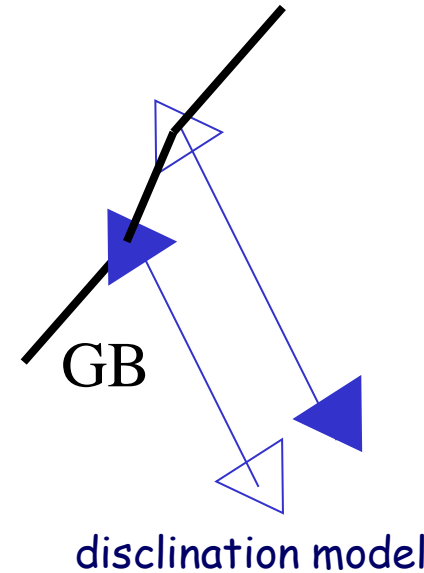
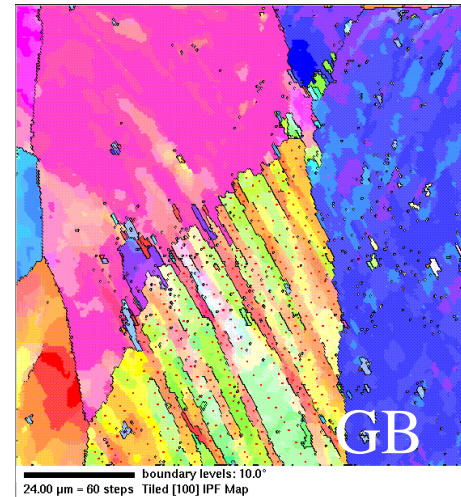
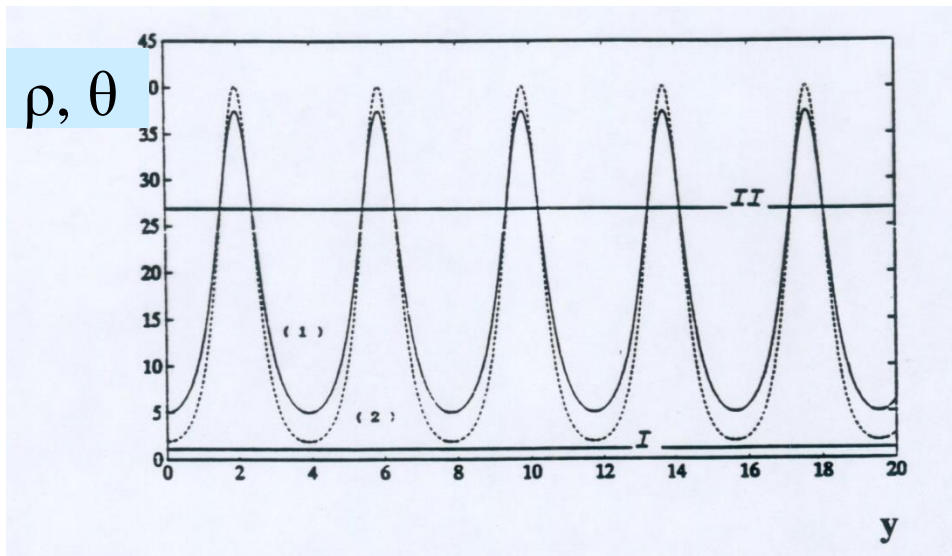
- Oscillations



Disclination-dislocation kinetics and patterning

$$\frac{\partial \rho}{\partial t} = F(\rho) - L(\theta)B\rho^2 - M\rho\theta + D\frac{\partial^2 \rho}{\partial x^2}; \quad \frac{\partial \theta}{\partial t} = -Q(\theta) + \mu M\rho\theta.$$

ρ - density of mobile dislocations; θ - density of immobile disclinations



The solution for reaction-kinetic equations
 [A.E.Romanov, E.C.Aifantis, Scripta Met. Mat. 29 (1993) 707]

EBSD orientation map image Al, 40% cold rolling [by L. Delannay]

■ Extension to Anisotropic Plastic Flow

- *Yield condition (Non-Schmid effects)*

$$\tau = \text{tr}(\mathbf{T}^L \mathbf{M}) = f(\gamma^p; \mathbf{M}, \mathbf{N}, \mathbf{A}_i)$$

- *Flow rule*

$$\mathbf{D}^p = \dot{\gamma}^p \mathbf{M}$$

- *Determination of M*

$$\max \left\{ \text{tr}(\mathbf{T}^L \mathbf{D}^p) \right\} \Bigg|_{\substack{\text{tr} \mathbf{M}=0, \text{tr} \mathbf{M}^2=1/2 \\ \text{tr} \mathbf{N}\mathbf{M}=0, \text{tr} \mathbf{N}^2=1, \tau=f}}$$

$$\Rightarrow \quad \mathbf{M} = \frac{1}{2l_2} \{ \mathbf{T}^{L'} \dot{\gamma}^p - 2l_5 \mathbf{P} \}, \quad \mathbf{P} = \frac{1}{2} \{ \mathbf{T}^{L'} - \mathbf{H}'_2 + 2\sqrt{J_{H_1}} \mathbf{N}' \}$$

$$\mathbf{H}'_1 = \frac{\partial f}{\partial \mathbf{N}}, \quad \mathbf{H}'_2 = \frac{\partial f}{\partial \mathbf{M}}, \quad J_{H_1} = \frac{1}{2} \text{tr}(\mathbf{H}'_1 \mathbf{H}'_1)$$

$$l_2, l_5: \begin{cases} J \dot{\gamma}^p - l_5 \text{tr}(\mathbf{P} \mathbf{T}^{L'}) = l_2 f(\gamma^p; \mathbf{M}, \mathbf{N}, \mathbf{A}_i) \\ l_2 = \left\{ J (\dot{\gamma}^p)^2 - 2l_5 \dot{\gamma}^p \text{tr}(\mathbf{P} \mathbf{T}^{L'}) + 2l_5 \text{tr}(\mathbf{P}^2) \right\}^{1/2} \end{cases}$$

■ Classes of Yield Behavior

• *Vertex type:* $\tau = \zeta \operatorname{tr}(\dot{\mathbf{T}}^L \mathbf{M}) + \kappa(\gamma^p)$

$$\mathbf{D}^p = \frac{\dot{\gamma}^p}{2\lambda} \{ \mathbf{T}^{L'} - \bar{\lambda} (\mathbf{T}^{L'} - \zeta \dot{\mathbf{T}}^{L'}) \}$$

$$\lambda = \sqrt{(2I_2 J - I_1^2) / (2I_2 - \kappa^2)}, \quad \bar{\lambda} = (I_1 - \lambda \kappa) / 2I_2$$

$$I_1 = \operatorname{tr}(\mathbf{T}^{L'} \mathbf{P}), \quad I_2 = \operatorname{tr}(\mathbf{P}^2), \quad \mathbf{P} = \frac{1}{2} (\mathbf{T}^{L'} - \zeta \dot{\mathbf{T}}^{L'})$$

$$\dot{\gamma}^p = \frac{\dot{\mathbf{P}} \cdot (\mathbf{T}^{L'} - 2\bar{\lambda} \mathbf{P})}{\lambda \kappa'}$$

• *Transversely isotropic:* $\tau = \zeta(\gamma^p) \operatorname{tr}(\mathbf{A} \mathbf{M}) + \kappa(\gamma^p), \quad \mathbf{A} = \mathbf{a} \otimes \mathbf{a}$

$$\mathbf{D}^p = \frac{\dot{\gamma}^p}{2\lambda} \{ \mathbf{T}^{L'} - \bar{\lambda} (\mathbf{T}^{L'} - \zeta \mathbf{A}') \}$$

$$I_1 = \operatorname{tr}(\mathbf{T}^{L'} \mathbf{P}), \quad I_2 = \operatorname{tr}(\mathbf{P}^2), \quad \mathbf{P} = \frac{1}{2} (\mathbf{T}^{L'} - \zeta \mathbf{A}')$$

$$\dot{\gamma}^p = \left\langle \frac{(\mathbf{T}^{L'} - 2\bar{\lambda} \mathbf{P}) \cdot \dot{\boldsymbol{\sigma}}'}{(2h + a'_m) \lambda + \zeta' \mathbf{A} \cdot (\mathbf{T}^{L'} - 2\bar{\lambda} \mathbf{P})} \right\rangle$$

■ Extension to Double Slip

• *Plastic Stretching*

$$\mathbf{D}^P = \dot{\gamma}_1^P \mathbf{M}_1 + \dot{\gamma}_2^P \mathbf{M}_2, \quad \mathbf{M}_i = (\mathbf{v}^{(i)} \otimes \mathbf{n}^{(i)})_S, \quad (i=1,2)$$

Determination of \mathbf{M}_i ($\mathbf{T}^D = \boldsymbol{\alpha} = \mathbf{O}$)

$$\max \left\{ \text{tr}(\boldsymbol{\sigma} \mathbf{D}^P) \right\} \Big|_{\mathbf{M}_1}, \quad \text{tr} \mathbf{M}_1 = 0, \quad \text{tr} \mathbf{M}_1^2 = \frac{1}{2}$$

$$\max \left\{ \text{tr}(\dot{\boldsymbol{\sigma}} \mathbf{D}^P) \right\} \Big|_{\mathbf{M}_2}, \quad \text{tr} \mathbf{M}_2 = 0, \quad \text{tr} \mathbf{M}_2^2 = \frac{1}{2}$$

$$\Rightarrow \mathbf{M}_1 = \frac{1}{2\sqrt{J}} \boldsymbol{\sigma}', \quad \mathbf{M}_2 = \frac{1}{2\sqrt{I}} \dot{\boldsymbol{\sigma}}'; \quad J = \frac{1}{2} \text{tr}(\boldsymbol{\sigma}'^2), \quad I = \frac{1}{2} \text{tr}(\dot{\boldsymbol{\sigma}}'^2)$$

$$\therefore \mathbf{D}^P = \frac{\dot{\gamma}_1^P}{2\sqrt{J}} \boldsymbol{\sigma}' + \frac{\dot{\gamma}_2^P}{2\sqrt{I}} \dot{\boldsymbol{\sigma}}'$$

- *Plastic Spin*

$$\mathbf{W}^P = \dot{\gamma}_1^P \boldsymbol{\Omega}_1 + \dot{\gamma}_2^P \boldsymbol{\Omega}_2, \quad \boldsymbol{\Omega}_i = (\mathbf{v}^{(i)} \otimes \mathbf{n}^{(i)})_A, \quad (i=1,2)$$

Determination of $\boldsymbol{\Omega}_i$

$$\max \left\{ \text{tr}(\dot{\boldsymbol{\sigma}} \mathbf{D}^P) \right\}, \quad \text{tr} \boldsymbol{\Omega}_1 = \text{tr} \boldsymbol{\Omega}_2 = 0, \quad \text{tr} \boldsymbol{\Omega}_1^2 = \text{tr} \boldsymbol{\Omega}_2^2 = -\frac{1}{2}$$

$$\Rightarrow \mathbf{W}^P = -\frac{1}{a_\omega} (\boldsymbol{\sigma} \mathbf{D}^P - \mathbf{D}^P \boldsymbol{\sigma}); \quad a_\omega = \frac{1}{\dot{\gamma}^P} \sqrt{-2 \text{tr}(\boldsymbol{\sigma} \mathbf{D}^P - \mathbf{D}^P \boldsymbol{\sigma})^2}$$

$$\dot{\gamma}^P = \dot{\gamma}_1^P + \dot{\gamma}_2^P$$

- *Yield Conditions*

$$\tau_i = \text{tr}(\boldsymbol{\sigma} \mathbf{M}_i) = \kappa(\gamma_i^P)$$

- *Consistency Conditions ($\dot{\tau}_i = 0$)*

$$\dot{\gamma}_1^P = \frac{\boldsymbol{\sigma}' \cdot \dot{\boldsymbol{\sigma}}'}{2\kappa\kappa'} \quad ; \quad \dot{\gamma}_2^P = \frac{2I\ddot{J} - \dot{I}\dot{J}}{2\kappa'I\sqrt{I}}$$

■ Extension to Stress Space Description

$$\mathbf{T}^{L'} = 2\tau\mathbf{M}, \quad \tau = \sqrt{J} = \sqrt{\frac{1}{2}\text{tr}(\mathbf{T}^{L'}\mathbf{T}^{L'})}; \quad \mathbf{T}^D = a_m\mathbf{M} + a_n\mathbf{N}$$

• *Micro – Micro Transition*

$$\max \left\{ \text{tr}(\mathbf{T}^L \mathbf{D}^P) \right\} \Big|_{\text{tr} \mathbf{M}=0, \text{tr} \mathbf{M}^2=1/2}$$

$$\Rightarrow \dot{\gamma}^P = \sqrt{2\mathbf{D}^P \cdot \mathbf{D}^P}, \quad \mathbf{M} = \frac{1}{\dot{\gamma}^P} \mathbf{D}^P, \quad \mathbf{D}^P = \frac{\dot{\gamma}^P}{2\sqrt{J}} \mathbf{T}^{L'}$$

$$\text{Evolution of Back Stress: } \dot{\boldsymbol{\alpha}}' = \left(\frac{\dot{a}_m a_n - a_m \dot{a}_n}{2\dot{\tau} a_n + \dot{a}_m a_n - a_m \dot{a}_n} \right) \dot{\boldsymbol{\sigma}}' + \frac{2\dot{\tau} \dot{a}_n}{2\dot{\tau} a_n + \dot{a}_m a_n - a_m \dot{a}_n} \boldsymbol{\alpha}'$$

$$\mathbf{W}^P = -\frac{1}{a_n} (\boldsymbol{\sigma}' \mathbf{D}^P - \mathbf{D}^P \boldsymbol{\sigma}')$$

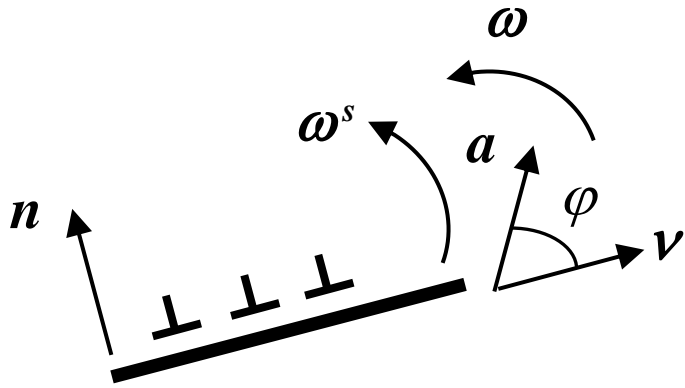
$$\mathbf{M1:} \quad \dot{a}_m = \frac{2\mu_1}{1-\mu_1} \dot{\tau}, \quad a_n = \text{const.} \quad \Rightarrow \quad \dot{\boldsymbol{\alpha}}' = \mu_1 \dot{\boldsymbol{\sigma}}' \quad \dots \text{Phillips' rule}$$

$$\mathbf{M2:} \quad \dot{a}_m = \frac{2\mu_1}{1-\mu_1} \dot{\tau} - \frac{\mu_2 \dot{\boldsymbol{\varepsilon}}}{1-\mu_1} a_m, \quad \dot{a}_n = -\frac{\mu_2 \dot{\boldsymbol{\varepsilon}}}{1-\mu_1} a_n \quad \Rightarrow \quad \dot{\boldsymbol{\alpha}}' = \mu_1 \dot{\boldsymbol{\sigma}}' - \mu_2 \dot{\boldsymbol{\varepsilon}} \boldsymbol{\alpha}'$$

... Extension of Phillips' rule

■ Extension to Textured Polycrystals

• Texture vector



$$\mathbf{a} = (\cos \varphi)\mathbf{v} + (\sin \varphi)\mathbf{n}$$

$$\dot{\mathbf{a}} = \boldsymbol{\omega}\mathbf{a}, \quad \dot{\mathbf{n}} = \boldsymbol{\omega}_s\mathbf{n}, \quad \dot{\mathbf{v}} = \boldsymbol{\omega}_s\mathbf{v}$$

$$\mathbf{M} = (\mathbf{v} \otimes \mathbf{n})_s = \frac{1}{2}(\mathbf{b} \otimes \mathbf{b} - \mathbf{a} \otimes \mathbf{a}) \sin 2\varphi + (\mathbf{a} \otimes \mathbf{b})_s \cos 2\varphi$$

$$\boldsymbol{\Omega} = (\mathbf{v} \otimes \mathbf{n})_a = (\mathbf{a} \otimes \mathbf{b})_a$$

$$\mathbf{b} = (-\sin \varphi)\mathbf{v} + (\cos \varphi)\mathbf{n}$$

$$\Rightarrow \boldsymbol{\omega} = \boldsymbol{\omega}^s - \mathbf{W}^t; \quad \mathbf{W}^t = 2\dot{\varphi}\boldsymbol{\Omega}$$

- Kinematics**

$$\mathbf{D}^p = \dot{\gamma}^p \mathbf{M}, \quad \mathbf{W}^p = \dot{\gamma}^p \mathbf{\Omega}, \quad \mathbf{T}^D = t_m \mathbf{M} + t_n \mathbf{N} \quad \dots \text{as before}$$

But now, two independent spins for polycrystalline aggregate: ω^s, ω

$$\mathbf{F} = \mathbf{R} \mathbf{R}_t \mathbf{F}^p, \quad \omega = \dot{\mathbf{R}} \mathbf{R}^T, \quad \mathbf{W}^t = \mathbf{R} \dot{\mathbf{R}}_t \mathbf{R}_t^T \mathbf{R}^T$$

$$\mathbf{W}^p = \left(\mathbf{R} \mathbf{R}_t \dot{\mathbf{F}}^p \mathbf{F}^{p-1} \mathbf{R}_t^T \mathbf{R}^T \right)_a, \quad \mathbf{D}^p = \left(\mathbf{R} \mathbf{R}_t \dot{\mathbf{F}}^p \mathbf{F}^{p-1} \mathbf{R}_t^T \mathbf{R}^T \right)_s$$

$$\therefore \omega = \underbrace{\mathbf{W} - \mathbf{W}^p}_{\omega^s} - \mathbf{W}^t$$

$$\mathbf{W}^p = \lambda (\mathbf{A} \mathbf{D}^p - \mathbf{D}^p \mathbf{A}), \quad \mathbf{W}^t = 2\lambda \frac{d\varphi}{d\gamma^p} (\mathbf{A} \mathbf{D}^p - \mathbf{D}^p \mathbf{A});$$

$$\lambda = \sec 2\varphi, \quad \mathbf{A} = \mathbf{a} \otimes \mathbf{a}$$

• Geometry of Polycrystalline Aggregate

Orientation Distribution Function (ODF): The probability of a grain being oriented along \mathbf{a} at time t is defined by ODF $\psi(\mathbf{a}, t)$

Conservation Law

$$\frac{d}{dt} \oint \psi(\mathbf{a}, t) d\mathbf{a} = 0 \quad \Rightarrow \quad \frac{\partial \psi}{\partial t} + \frac{\partial}{\partial a_i} (\dot{a}_i \psi) = 0$$

- $\psi(\theta, \phi; t) = \psi(\pi + \theta, \pi - \phi; t), \quad \oint \psi(\mathbf{a}, t) d\mathbf{a} = 1$
- $\psi(\theta; 0) = 1 / \pi \dots (2D), \quad \psi(\theta, \phi; 0) = 1 / 4\pi \dots (3D)$

General Solution (Dihn and Armstrong, 1984)

$$\dot{\mathbf{a}} = (\mathbf{L}\mathbf{A} - \mathbf{A}\mathbf{L})\mathbf{a} \quad \rightarrow \quad \mathbf{a} = \frac{\mathbf{F}\mathbf{a}_0}{\left(\mathbf{F}^T \mathbf{F} \cdot \mathbf{a}_0 \otimes \mathbf{a}_0\right)^{1/2}}$$

$$\Rightarrow \begin{cases} \psi(\mathbf{a}, t) = \frac{1}{\pi} \left[\mathbf{F}^{-T} \mathbf{F}^{-1} \cdot \mathbf{A} \right]^{-1} & \dots (2D) \\ \psi(\mathbf{a}, t) = \frac{1}{4\pi} \left[\mathbf{F}^{-T} \mathbf{F}^{-1} \cdot \mathbf{A} \right]^{-3/2} & \dots (3D) \end{cases}$$

- **Geometry of Continuum (*Oriented Continuum*)**

Fourier series (2D) or spherical harmonics (3D) expansion (*Gelfand, et al., 1963*)

$$\psi(\mathbf{a}, t) = \frac{1}{4\pi} (1 + b_2 B_{ij} a_i a_j + b_4 C_{ijkl} a_i a_j a_k a_l + \dots)$$

$$b_2 = \frac{5}{4} \binom{4}{2}, \quad b_4 = \frac{9}{16} \binom{8}{4}$$

$B_{ij} = \oint a_i a_j \psi(\mathbf{a}, t) d\mathbf{a}$...2nd order orientation tensor (2nd moment)

$C_{ijkl} = \oint a_i a_j a_k a_l \psi(\mathbf{a}, t) d\mathbf{a}$...4th order orientation tensor (4th moment)

• Micro – Macro Transition

This involves two successive steps

- *First step: single slip \rightarrow crystallite level*

Scale invariance argument and maximization procedure ... as before

$$\mathbf{D}^p = \frac{\dot{\gamma}^p}{2\kappa(\gamma^p)} \mathbf{T}^{L'} ; \quad \dot{\mathbf{T}}^D = \begin{pmatrix} \dot{t}_m & -\dot{t}_n t_m \\ \dot{\gamma}^p & t_n \dot{\gamma}^p \end{pmatrix} \mathbf{D}^p + \frac{\dot{t}_n}{t_n} \mathbf{T}^D$$

$$\dot{\mathbf{T}}^D = \dot{\mathbf{T}}^D - \boldsymbol{\omega}^s \mathbf{T}^D + \mathbf{T}^D \boldsymbol{\omega}^s ; \quad \boldsymbol{\omega}^s = \mathbf{W} - \mathbf{W}^p$$

$$\mathbf{W}^p = -\frac{1}{t_n} (\mathbf{T}^D \mathbf{D}^p - \mathbf{D}^p \mathbf{T}^D)$$

- *Second step: crystallite \rightarrow macroscopic level*

(Taylor's argument and the following average procedure)

□ Average Stress

$$\boldsymbol{\sigma}' = \oint \mathbf{K} \mathbf{S}' \psi(\mathbf{a}, t) d\mathbf{a} ; \quad \boldsymbol{\alpha}' = \oint \mathbf{K} \mathbf{T}^{D'} \psi(\mathbf{a}, t) d\mathbf{a}$$

\mathbf{K} ...4th order texture tensor: $K_{ijkl} = K_{jikl} = K_{ijlk} = K_{klij}$

$$K_{ijkl} = k_1 a_i a_j a_k a_l + k_2 (a_i a_j \delta_{kl} + a_k a_l \delta_{ij}) + k_3 (a_i a_k \delta_{jl} + a_i a_l \delta_{jk} \\ + a_j a_k \delta_{il} + a_j a_l \delta_{ik}) + k_4 \delta_{ij} \delta_{kl} + k_5 (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk})$$

Incompressibility: $K_{ijkk} = 0 \Rightarrow$

$$k_1 + 2k_2 + 4k_3 = 0, \quad k_2 + 2k_4 + 2k_5 = 0 \quad \dots(2D)$$

$$k_1 + 3k_2 + 4k_3 = 0, \quad k_2 + 3k_4 + 2k_5 = 0 \quad \dots(3D)$$

Note: $k_1 = k_2 = 0, k_5 = 1/2 \Rightarrow \boldsymbol{\sigma}' = \oint \mathbf{S}' \psi(\mathbf{a}, t) d\mathbf{a}$

i.e. conventional “averaging” formula

□ Flow Rule

Average Procedure and Taylor's Assumption ($\mathbf{D}^p = \bar{\mathbf{D}}^p$) \Rightarrow

$$\bar{\mathbf{D}}^p = \frac{\dot{\gamma}^p}{2\kappa(\bar{\gamma}^p)} \langle \mathbf{K} \rangle^{-1} (\boldsymbol{\sigma}' - \boldsymbol{\alpha}')$$

$$\begin{aligned} \langle \mathbf{K} \rangle_{ijkl} = & k_1 \mathbf{C}_{ijkl} + k_2 (B_{ij} \delta_{kl} + B_{kl} \delta_{ij}) + k_3 (B_{ik} \delta_{jl} + B_{il} \delta_{jk} \\ & + B_{jk} \delta_{il} + B_{jl} \delta_{ik}) + k_4 \delta_{ij} \delta_{kl} + k_5 (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) \end{aligned}$$

□ Evolution Equation of Back Stress

Average Procedure and Taylor's Assumption ($\mathbf{D}^p = \bar{\mathbf{D}}^p$) \Rightarrow

$$\dot{\boldsymbol{\alpha}}' = \left(\frac{\dot{t}_m}{\dot{\gamma}^p} - \frac{\dot{t}_n t_m}{t_n \dot{\gamma}^p} \right) \langle \mathbf{K} \rangle \bar{\mathbf{D}}^p + \frac{\dot{t}_n}{t_n} \boldsymbol{\alpha}'$$

$$\dot{\boldsymbol{\alpha}}' = \dot{\boldsymbol{\alpha}} - \bar{\omega}^s \boldsymbol{\alpha} + \boldsymbol{\alpha} \bar{\omega}^s ; \quad \bar{\omega}^s = \mathbf{W} - \bar{\mathbf{W}}^p, \quad \bar{\mathbf{W}}^p = -\frac{1}{t_n} (\boldsymbol{\alpha}' \bar{\mathbf{D}}^p - \bar{\mathbf{D}}^p \boldsymbol{\alpha}')$$

Note: Scale invariance argument and Taylor's assumption was used to obtain $\bar{\mathbf{W}}^p$

□ Yield Condition

$$\left\{ \frac{1}{2} \text{tr}(\langle \mathbf{K} \rangle^{-1} (\boldsymbol{\sigma}' - \boldsymbol{\alpha}')^2) \right\}^{1/2} = \kappa(\bar{\gamma}^p)$$

□ Consistency Condition

$$\dot{\bar{\gamma}}^p = \frac{1}{2\kappa' \kappa} \overline{\langle \mathbf{K} \rangle^{-1} (\boldsymbol{\sigma}' - \boldsymbol{\alpha}') \cdot \langle \mathbf{K} \rangle^{-1} (\boldsymbol{\sigma}' - \boldsymbol{\alpha}')}$$

$$\overset{\square}{\boldsymbol{\sigma}}' = \dot{\boldsymbol{\sigma}}' - \bar{\omega} \boldsymbol{\sigma}' + \boldsymbol{\sigma}' \bar{\omega}; \quad \bar{\omega} = \mathbf{W} - \bar{\mathbf{W}}^p - \bar{\mathbf{W}}^t$$

□ Texture Spin

$$\bar{\mathbf{w}}^t = \oint \Lambda \mathbf{w}^t \psi(\mathbf{a}, t) d\mathbf{a}; \quad \bar{W}_{ij}^t = -\varepsilon_{ijk} \bar{W}_k^t$$

2nd order texture tensor: $\Lambda_{ij} = \Lambda_1 a_i a_j + \Lambda_2 \delta_{ij} \Rightarrow (\bar{\lambda} = \lambda \Lambda_2)$

$$\therefore \bar{\mathbf{W}}^t = \bar{\lambda} (\mathbf{B} \bar{\mathbf{D}}^p - \bar{\mathbf{D}}^p \mathbf{B})$$

• *Structure of Texture Plasticity*

$$\mathbf{D}^p = \frac{\dot{\gamma}^p}{2\kappa(\gamma^p)} \langle \mathbf{K} \rangle^{-1} (\boldsymbol{\sigma}' - \boldsymbol{\alpha}')$$

$$\begin{aligned} \langle \mathbf{K} \rangle_{ijkl} = & k_1 C_{ijkl} + k_2 (B_{ij} \delta_{kl} + B_{kl} \delta_{ij}) + k_3 (B_{ik} \delta_{jl} + B_{il} \delta_{jk} \\ & + B_{jk} \delta_{il} + B_{jl} \delta_{ik}) + k_4 \delta_{ij} \delta_{kl} + k_5 (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) \end{aligned}$$

$$\dot{\boldsymbol{\alpha}}' = \left(\frac{\dot{t}_m}{\dot{\gamma}^p} - \frac{\dot{t}_n t_m}{t_n \dot{\gamma}^p} \right) \langle \mathbf{K} \rangle \mathbf{D}^p + \frac{\dot{t}_n}{t_n} \boldsymbol{\alpha}', \quad \mathbf{W}^p = -\frac{1}{t_n} (\boldsymbol{\alpha}' \mathbf{D}^p - \mathbf{D}^p \boldsymbol{\alpha}')$$

$$\dot{\boldsymbol{\alpha}}' = \dot{\boldsymbol{\alpha}} - \boldsymbol{\omega}^s \boldsymbol{\alpha} + \boldsymbol{\alpha} \boldsymbol{\omega}^s; \quad \boldsymbol{\omega}^s = \mathbf{W} - \mathbf{W}^p$$

$$\left\{ \frac{1}{2} \text{tr}(\langle \mathbf{K} \rangle^{-1} (\boldsymbol{\sigma}' - \boldsymbol{\alpha}'))^2 \right\}^{1/2} = \kappa(\bar{\gamma}^p),$$

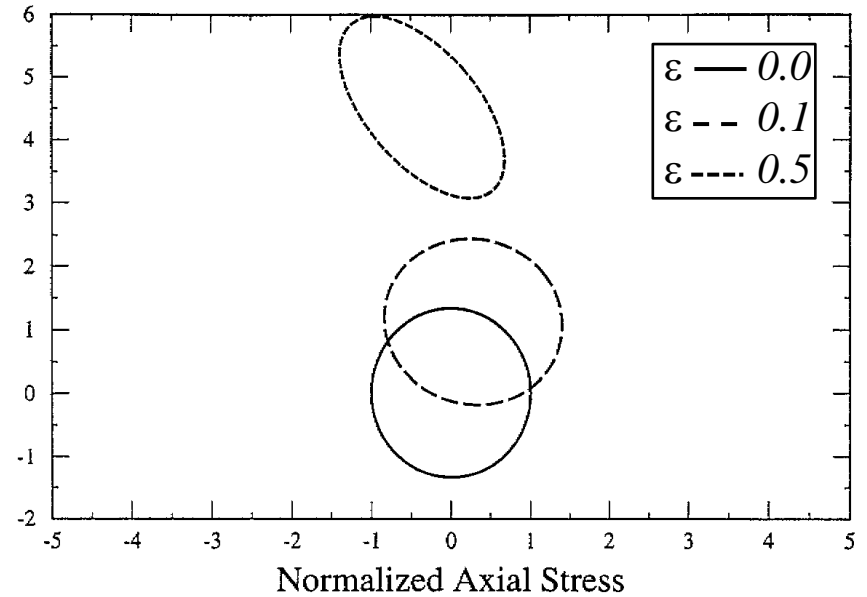
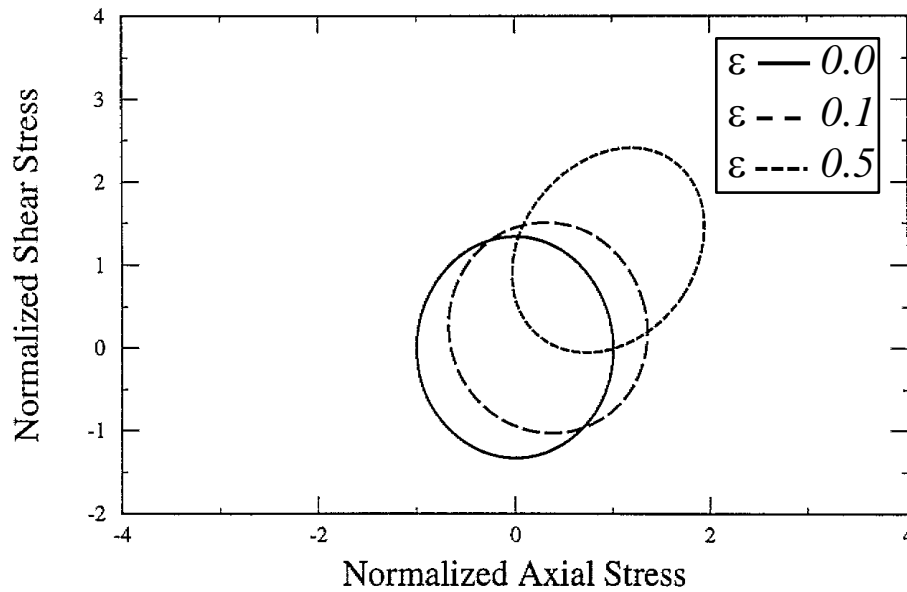
$$\dot{\bar{\gamma}}^p = \frac{1}{2\kappa' \kappa} \overline{\langle \mathbf{K} \rangle^{-1} (\boldsymbol{\sigma}' - \boldsymbol{\alpha}') \cdot \langle \mathbf{K} \rangle^{-1} (\boldsymbol{\sigma}' - \boldsymbol{\alpha}')}$$

$$\overline{\boldsymbol{\sigma}}' = \dot{\boldsymbol{\sigma}}' - \bar{\boldsymbol{\omega}} \boldsymbol{\sigma}' + \boldsymbol{\sigma}' \bar{\boldsymbol{\omega}}; \quad \bar{\boldsymbol{\omega}} = \mathbf{W} - \bar{\mathbf{W}}^p - \bar{\mathbf{W}}^t; \quad \mathbf{W}^t = \bar{\lambda} (\mathbf{B} \mathbf{D}^p - \mathbf{D}^p \mathbf{B})$$

• *Tension – Torsion Example*

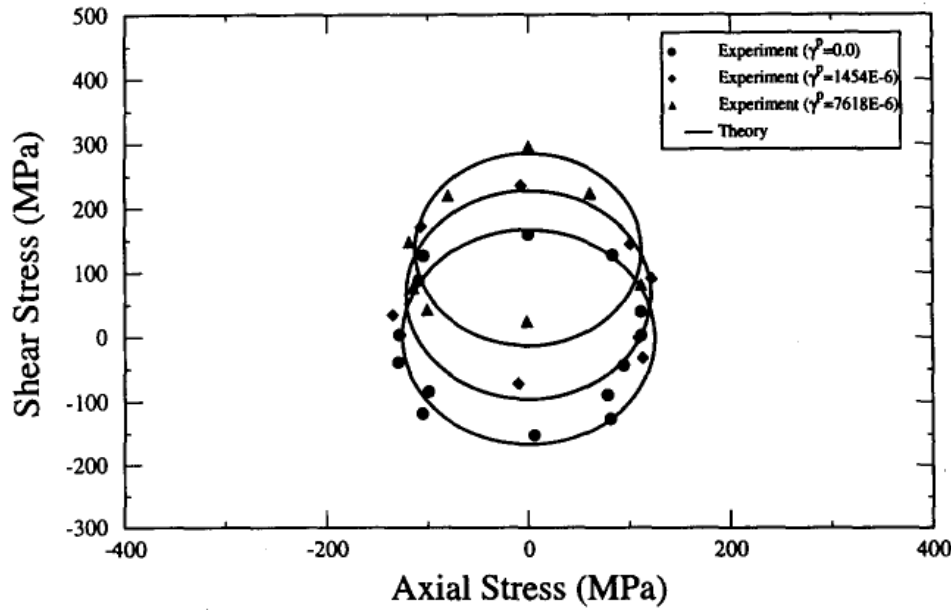
$$[\mathbf{D}] = \frac{1}{2} \begin{bmatrix} -\dot{\varepsilon} & \dot{\gamma} & 0 \\ \dot{\gamma} & 2\dot{\varepsilon} & 0 \\ 0 & 0 & -\dot{\varepsilon} \end{bmatrix},$$

$$[\mathbf{W}] = \frac{\dot{\gamma}}{2} \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

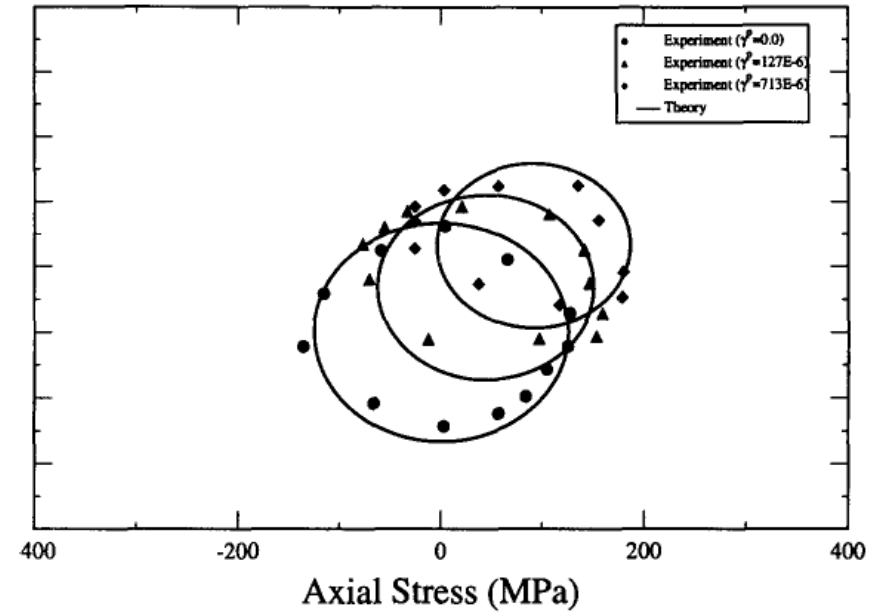


Evolution of yield surface in tension-torsion deformation for $\frac{\dot{\gamma}}{\dot{\varepsilon}} = 1$ and 5

• Comparison with Experimental Data



Evolution of yield surface of 304 stainless steel in torsion



Evolution of yield surface of 304 stainless steel in tension-torsion