Introduction on Crystal plasticity

강의명: 금속가공학특론 (AMB2004)

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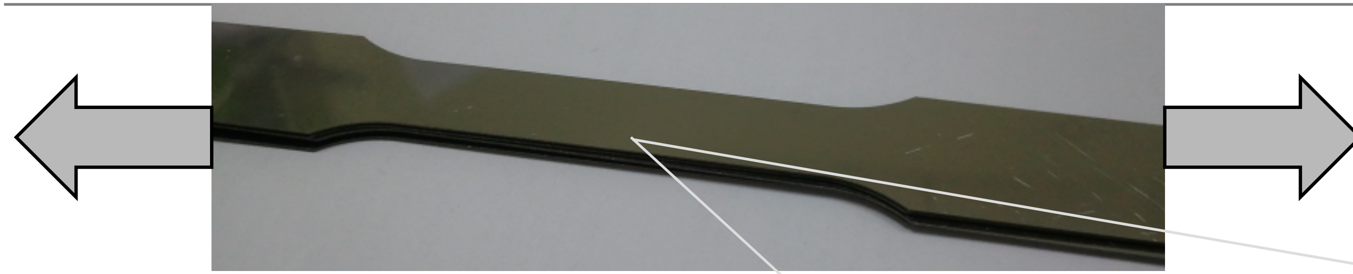
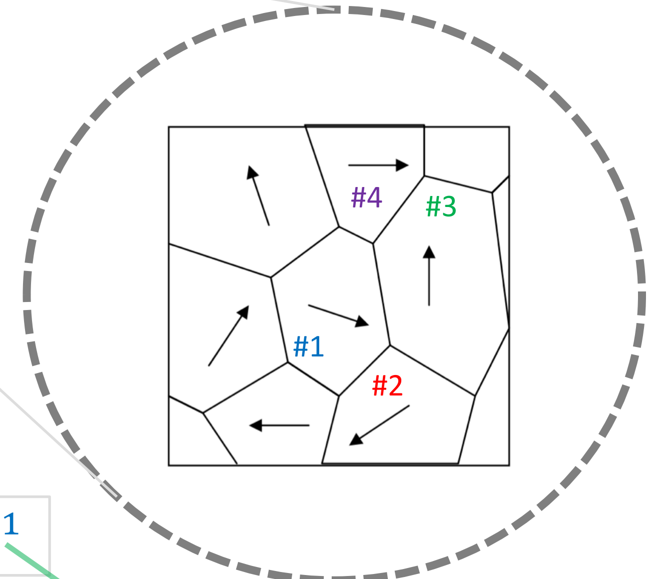
Mathematical treatment on polycrystal behavior



$$\bar{\boldsymbol{\sigma}} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \bar{\sigma}_{33} \end{bmatrix}$$



$$\bar{\boldsymbol{\varepsilon}} = \begin{bmatrix} ? & 0 & 0 \\ 0 & ? & 0 \\ 0 & 0 & \bar{\varepsilon}_{33} \end{bmatrix}$$

$$\boldsymbol{\varepsilon}^{\#1} = \bar{\boldsymbol{\varepsilon}} + \tilde{\boldsymbol{\varepsilon}}^{\#1}$$

$$\boldsymbol{\varepsilon}^{\#2} = \bar{\boldsymbol{\varepsilon}} + \tilde{\boldsymbol{\varepsilon}}^{\#2}$$

.
.
.

Local inhomogeneity should be influenced by orientation↑

$$\boldsymbol{\sigma}^{\#1} = \bar{\boldsymbol{\sigma}} + \tilde{\boldsymbol{\sigma}}^{\#1}$$

$$\boldsymbol{\sigma}^{\#2} = \bar{\boldsymbol{\sigma}} + \tilde{\boldsymbol{\sigma}}^{\#2}$$

.
.
.

Local inhomogeneity should be influenced by orientation↑

Some classical models

- Sachs (or more correctly static model; often is assumed for Schmid factor estimations)
  - $\tilde{\boldsymbol{\sigma}} = 0$ regardless of orientation
  - Which leads to $\boldsymbol{\sigma} = \bar{\boldsymbol{\sigma}}$
  - Then, one could obtain $\boldsymbol{\varepsilon}$ from constitutive law (Linear Hooke's law $\boldsymbol{\varepsilon} = \mathbb{M}:\boldsymbol{\sigma}$)
  - Summing up $\sum_{\text{grain}}^{\text{n\# grain}} \boldsymbol{\varepsilon}^{\text{grain}} \ (= \langle \boldsymbol{\varepsilon} \rangle)$
  - But it turns out $\langle \boldsymbol{\varepsilon} \rangle \neq \bar{\boldsymbol{\varepsilon}}$ (compatibility is not satisfied; $\langle \boldsymbol{\sigma} \rangle = \bar{\boldsymbol{\sigma}}$ is naturally satisfied.
- Taylor model
  - $\tilde{\boldsymbol{\varepsilon}} = 0$ regardless of orientation
  - Which leads to $\boldsymbol{\varepsilon} = \bar{\boldsymbol{\varepsilon}}$
  - Then, one could obtain $\boldsymbol{\sigma}$ from constitutive law ($\boldsymbol{\sigma} = \mathbb{C}:\boldsymbol{\varepsilon}$)
  - Summing up $\sum_{\text{grain}}^{\text{n \# grain}} \boldsymbol{\varepsilon}^{\text{grain}} \ (= \langle \boldsymbol{\varepsilon} \rangle)$
  - But it turns out $\langle \boldsymbol{\varepsilon} \rangle \neq \bar{\boldsymbol{\varepsilon}}$ (compatibility is not satisfied; $\langle \boldsymbol{\sigma} \rangle = \bar{\boldsymbol{\sigma}}$ is naturally satisfied.

Self-consistent approach

- Self-consistent approach
  - $\tilde{\boldsymbol{\varepsilon}} \neq 0$ and $\tilde{\boldsymbol{\sigma}} \neq 0$, both of which are usually determined by following
    - the Eshelby approach ($\tilde{\boldsymbol{\varepsilon}} = \widetilde{\mathbb{M}}: \tilde{\boldsymbol{\sigma}}$)
    - $\widetilde{\mathbb{M}} = (\mathbb{I} - \mathbb{S})^{-\mathbf{1}}: \mathbb{S}: \overline{\mathbb{M}}$ where $\mathbb{S}$ is the Eshelby tensor
  - Both strain compatibility and force equilibrium are simultaneously satisfied

- Important contributions

- G. I. Taylor (1938)
  - Upper bound
- Sachs (1928) – Static model
  - Lower bound
- Kröner (1958) – self-consistent scheme for elasticity
- R. Hill's self-consistent scheme (1965) – elastoplastic
- Molinari et al. (1987) – Anisotropic inclusion embedded in isotropic HEM
- Carlos Tomé and Ricardo Lebensohn (1993) – anisotropic inclusion in anisotropy HEM

Self-consistent estimation of macroscopic properties

Self-consistent estimation

$\tilde{\boldsymbol{\varepsilon}} \neq 0$ and $\tilde{\boldsymbol{\sigma}} \neq 0$, which is usually determined following

the Eshelby approach ($\tilde{\boldsymbol{\varepsilon}} = \widetilde{\mathbb{M}}:\tilde{\boldsymbol{\sigma}}$)

$\widetilde{\mathbb{M}} = (\mathbb{I} - \mathbb{S})^{-\mathbf{1}}:\mathbb{S}:\overline{\mathbb{M}}$ where $\mathbb{S}$ is the Eshelby tensor

At the same time, compatibility and force equilibrium are simultaneously satisfied

Elastic self-consistent estimation

$\boldsymbol{\sigma} = \mathbb{C}:\boldsymbol{\varepsilon}$ for various grains in various orientations

$\overline{\boldsymbol{\sigma}} = \overline{\mathbb{C}}:\overline{\boldsymbol{\varepsilon}}$ for polycrystal consisting of such grains.

$\mathbb{C} = \mathbb{M}^{-\mathbf{1}}$

$\overline{\mathbb{C}} = \overline{\mathbb{M}}^{-\mathbf{1}}$

Anisotropic elasticity (Hooke-Cauchy law)

For polycrystals consisting of single crystal in various orientations?

Can we relate $\mathbb{E}$ of each individual grains to $\overline{\mathbb{E}}$?

Can we obtain $\overline{\mathbb{E}}$ that satisfies

$$\overline{\boldsymbol{\varepsilon}} = \overline{\mathbb{E}}:\overline{\boldsymbol{\sigma}}$$

which can be a function of $\mathbb{E}$ of grains in various orientation while satisfying

$\boldsymbol{\varepsilon} = \mathbb{E}:\boldsymbol{\sigma}$ and $\langle\boldsymbol{\varepsilon}\rangle = \overline{\mathbb{E}}:\langle\boldsymbol{\sigma}\rangle$, and $\langle\boldsymbol{\varepsilon}\rangle = \overline{\boldsymbol{\varepsilon}}$, $\langle\boldsymbol{\sigma}\rangle = \overline{\boldsymbol{\sigma}}$?

That's corresponding to finding self-consistent $\overline{\mathbb{E}}$ that represents the polycrystal.

Self-consistent estimation of macroscopic properties

Self-consistent estimation

$\tilde{\boldsymbol{\varepsilon}} \neq 0$ and $\tilde{\boldsymbol{\sigma}} \neq 0$, which is usually determined following

the Eshelby approach ($\tilde{\boldsymbol{\varepsilon}} = \widetilde{\mathbb{M}} : \tilde{\boldsymbol{\sigma}}$)

$\widetilde{\mathbb{M}} = (\mathbb{I} - \mathbb{S})^{-\mathbf{1}} : \mathbb{S} : \overline{\mathbb{M}}$ where $\mathbb{S}$ is the Eshelby tensor

At the same time, compatibility and force equilibrium are simultaneously satisfied

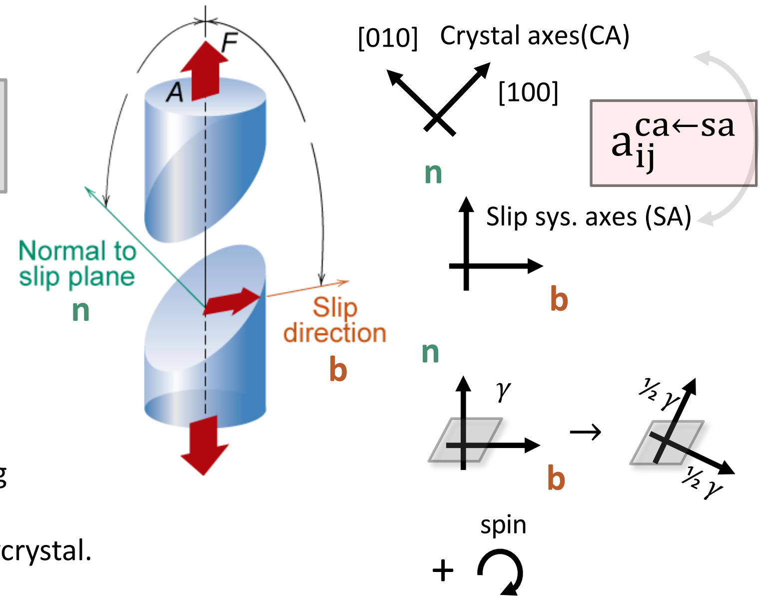
Visco-Plastic self-consistent estimation

$\boldsymbol{\sigma} = \mathbb{C}^{\mathrm{vp}} : \dot{\boldsymbol{\varepsilon}}$ for various grains in various orientations

$\bar{\boldsymbol{\sigma}} = \bar{\mathbb{C}}^{\mathrm{vp}} : \bar{\dot{\boldsymbol{\varepsilon}}}$ for polycrystal consisting of such grains.

Viscous plastic deformation should be accommodated by disl. slips

anisotropic viscous fluid
(Newtonian fluid's law)



For polycrystals consisting of single crystal in various orientations?

Can we related $\mathbb{C}^{vp}$ of each individual grains to $\bar{\mathbb{C}}^{vp}$?

Can we obtain $\bar{\mathbb{C}}$ that satisfies

$$\bar{\dot{\boldsymbol{\varepsilon}}} = \bar{\mathbb{C}}^{vp} : \bar{\boldsymbol{\sigma}}$$

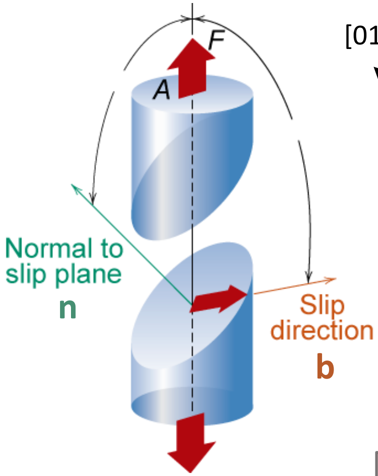
which can be a function of $\mathbb{E}$ of grains in various orientation while satisfying

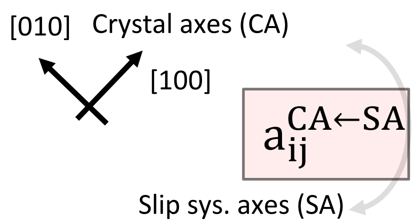
$\dot{\boldsymbol{\varepsilon}} = \bar{\mathbb{C}}^{vp} : \boldsymbol{\sigma}$ and $\langle \dot{\boldsymbol{\varepsilon}} \rangle = \bar{\mathbb{C}}^{vp} : \langle \boldsymbol{\sigma} \rangle$, and $\langle \dot{\boldsymbol{\varepsilon}} \rangle = \bar{\dot{\boldsymbol{\varepsilon}}}$, $\langle \boldsymbol{\sigma} \rangle = \bar{\boldsymbol{\sigma}}$?

That's corresponding to finding self-consistent $\bar{\mathbb{C}}^{vp}$ that represents the polycrystal.

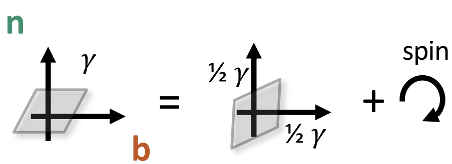
Crystal deformation by disl. slip

Viscous plastic deformation should be accommodated by disl. slips





$$a_{ij}^{CA\leftarrow SA}$$



$$\varepsilon_{ij}^{SA} = \begin{bmatrix} 0 & \frac{1}{2}\gamma & 0 \\ \frac{1}{2}\gamma & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$a_{ij}^{CA\leftarrow SA} = \begin{bmatrix} b_1 & n_1 & t_1 \\ b_2 & n_2 & t_2 \\ b_3 & n_3 & t_3 \end{bmatrix} \text{ where } \mathbf{t} = \mathbf{b}\times\mathbf{n}$$

$$\varepsilon_{ij}^{CA} = a_{ik}^{CA\leftarrow SA} a_{jl}^{CA\leftarrow SA} \varepsilon_{kl}^{SA}$$

2nd order tensor transformation rule

Among 9 components of ε_{kl}^{SA}, only ε_{12}^{SA} and ε_{21}^{SA} non-zero: (k=1,l=2) or (k=2,k=1)

$$\varepsilon_{ij}^{CA} = a_{i1}^{CA\leftarrow SA} a_{j2}^{CA\leftarrow SA} \varepsilon_{12}^{SA} + a_{i2}^{CA\leftarrow SA} a_{j1}^{CA\leftarrow SA} \varepsilon_{21}^{SA}$$

$$\varepsilon_{ij}^{CA} = b_i n_j \frac{1}{2}\gamma + n_i b_j \frac{1}{2}\gamma$$

$$\varepsilon_{ij}^{CA} = \frac{1}{2}(b_i n_j + b_j n_i)\gamma$$

$\varepsilon_{ij}^{CA} = \mathbb{m}_{ij}\gamma$ **where** $\mathbb{m}_{ij} = \frac{1}{2}(b_i n_j + b_j n_i)$

This is for a single slip system.

$$\varepsilon_{ij}^{CA} = \sum_{s}^{\text{N of slip systems.}} \mathbb{m}_{ij}^{s}\gamma^{s}$$

$$\dot{\varepsilon}_{ij}^{CA} = \sum_{s}^{\text{N of slip systems.}} \mathbb{m}_{ij}^{s}\dot{\gamma}^{s}$$

Time derivative form.

Rate-sensitive formula

$$\dot{\varepsilon}_{ij}^{CA} = \sum_{s}^{\text{N of slip systems.}} \mathbb{m}_{ij}^{s} \dot{\gamma}^{s}$$

$$(\dot{\gamma}^{s})^{m} \propto \tau_{RSS}^{s} \rightarrow \frac{\dot{\gamma}^{s}}{\dot{\gamma}_{\circ}} = \left(\frac{\tau_{RSS}^{s}}{\tau_{\circ}^{s}}\right)^{1/m} = \left(\frac{\boldsymbol{\sigma} \cdot \mathbf{n}^{s} \cdot \mathbf{b}^{s}}{\tau_{\circ}^{s}}\right)^{1/m} = \left(\frac{\boldsymbol{\sigma} : \mathbb{m}^{s}}{\tau_{\circ}^{s}}\right)^{1/m}$$

m: SRS

τ_{RSS}^{s}: Resolved shear stress on slip system s

$\mathbb{m}^{s}$: Schmid tensor

$$\dot{\varepsilon}_{ij}^{CA} = \sum_{s}^{\text{N of slip systems.}} \mathbb{m}_{ij}^{s} \left(\frac{\boldsymbol{\sigma} : \mathbb{m}^{s}}{\tau_{\circ}^{s}}\right)^{1/m}$$

Recall

$$\mathbb{m}_{ij}^{s} = \frac{1}{2}\left(b_i^s n_j^s + b_j^s n_i^s\right)$$

$$\mathbb{q}_{ij}^{s} = \frac{1}{2}\left(b_i^s n_j^s - b_j^s n_i^s\right)$$

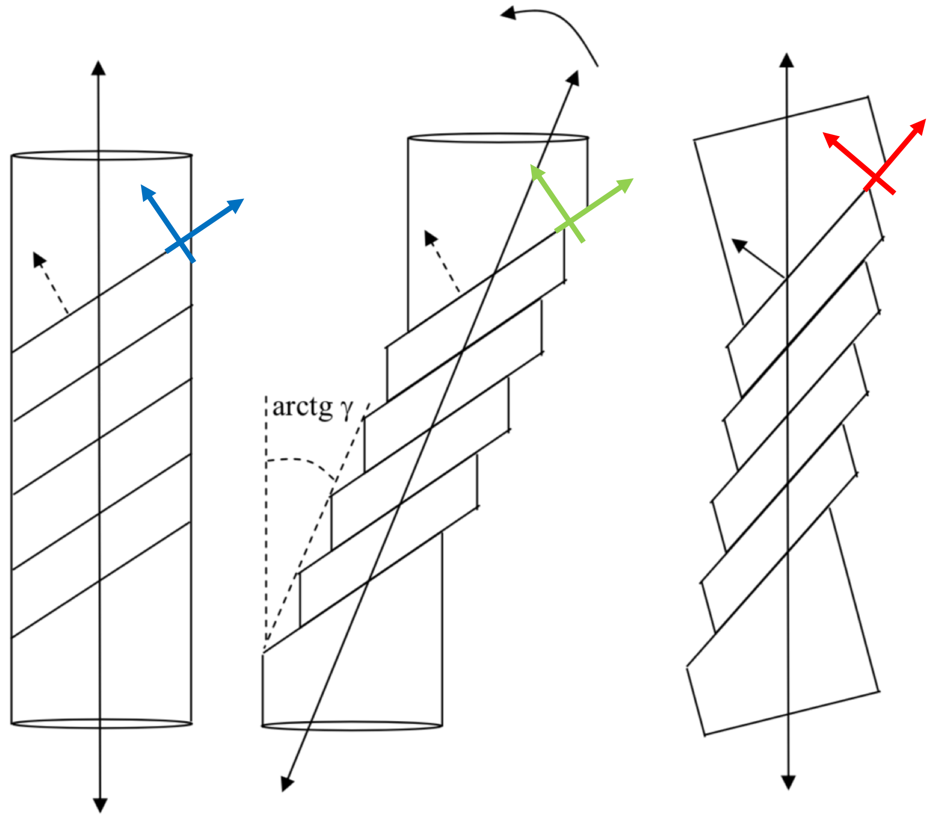
$$\mathbf{L} = \dot{\boldsymbol{\varepsilon}} + \dot{\boldsymbol{\omega}} = \sum_{s} \mathbb{m}^{s} \dot{\gamma}^{s} + \sum_{s} \mathbb{q}^{s} \dot{\gamma}^{s}$$

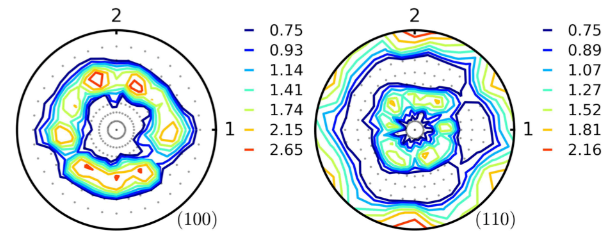
Grain spin rate

$$\boldsymbol{\sigma} \cdot \mathbf{n}^{s} \cdot \mathbf{b}^{s} = \sigma_{ij} n_i b_j = \frac{1}{2}\sigma_{ij}\left(b_i n_j + b_j n_i\right) = \frac{1}{2}\sigma_{ji}\left(b_i n_j + b_j n_i\right)$$

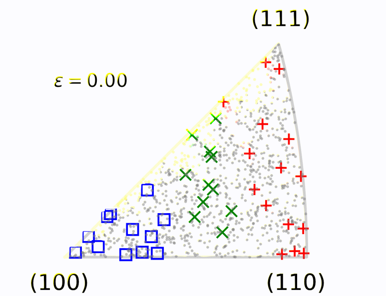
If $\boldsymbol{\sigma}$ is symmetric; meaning $\sigma_{ij} = \sigma_{ji}$

Slip and Lattice rotations





+RBR (BC)
+Inclusion spin



Dislocation slip is a simple shear deformation; which involves
a) pure shear, b) spin (lattice rotation)

$$\mathbf{L}^s = \begin{bmatrix} 0 & \dot{\gamma}^s & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\dot{\boldsymbol{\varepsilon}}^s = \frac{1}{2}\left[\boldsymbol{L}^s + (\boldsymbol{L}^s)^T\right]$$

$$\dot{\boldsymbol{\omega}}^s = \frac{1}{2}\left[\boldsymbol{L}^s - (\boldsymbol{L}^s)^T\right]$$

Polycrystal aggregate

- The polycrystalline aggregate is represented by a statistical population of ***discrete orientations.***

Intragranular fluctuation (inhomogeneity) is discarded in VPSC
- See full-field crystal plasticity models (FFT, FEM …)

VPSC input texture file

```
Tue Jun 25 18:07:54 2013
Current texture file was made by cmb.py
contact: youngung.jeong@gmail.com
 B 2000
   63.2250082     57.1281552      4.3953561   1.3825509e-04
  116.7749918    122.8718448   -175.6046439   1.3825509e-04
  -63.2250082    122.8718448   -175.6046439   1.3825509e-04
 -116.7749918     57.1281552      4.3953561   1.3825509e-04
   14.9941829     86.2185766     51.6090972   2.4673198e-04
  165.0058171     93.7814234   -128.3909028   2.4673198e-04
  -14.9941829     93.7814234   -128.3909028   2.4673198e-04
 -165.0058171     86.2185766     51.6090972   2.4673198e-04
   34.9540018     73.9669201     69.3593877   6.5328445e-04
  145.0459982    106.0330799   -110.6406123   6.5328445e-04
  -34.9540018    106.0330799   -110.6406123   6.5328445e-04
 -145.0459982     73.9669201     69.3593877   6.5328445e-04
   13.6175819     25.0736041     54.9601498   5.3392363e-04
```

(Often) Dummy lines

Orientation notation (B: Bunge), # of Grains

Discrete orientation represents each grain (inclusion): 3 Euler angles followed by weight

Macroscopic properties in VPSC follow from 'weighted' average of individual grains

$$\bar{\varepsilon}_{ij} = \sum_{g}^{2000} f^{g} \varepsilon_{ij}^{g} = \langle \varepsilon_{ij} \rangle$$