# Homogenization for Solid Polycrystals

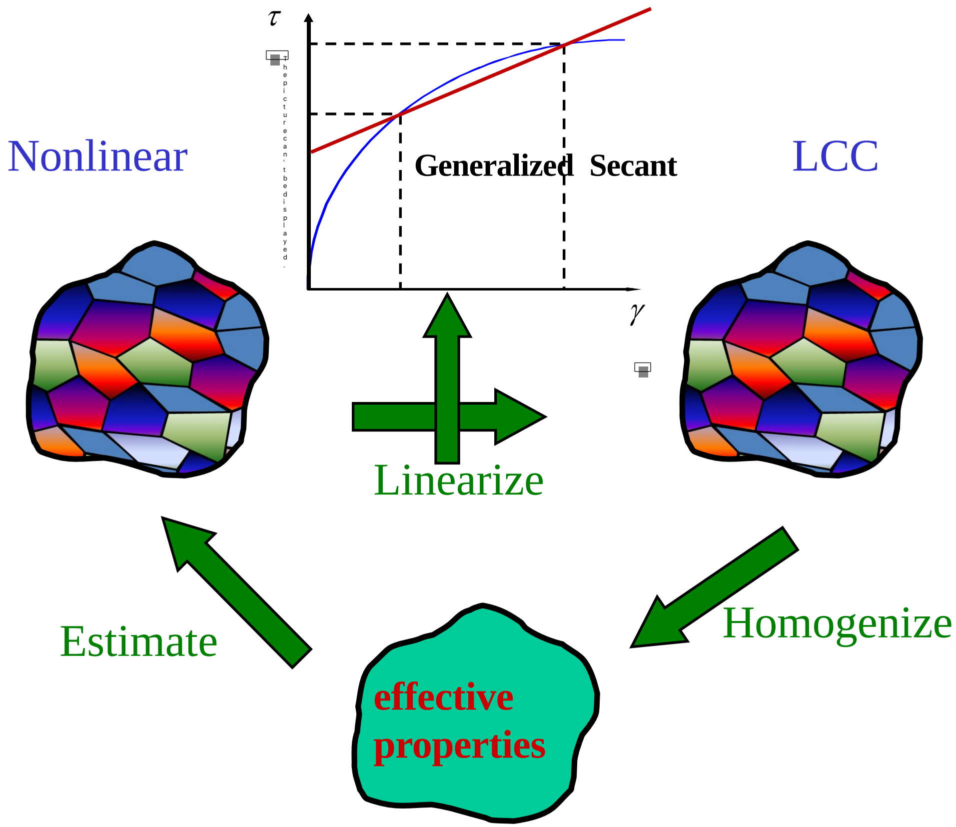
***INSTANTANEOUS RESPONSE***

- **Fully Optimized Second-Order (FOSO) variational method**

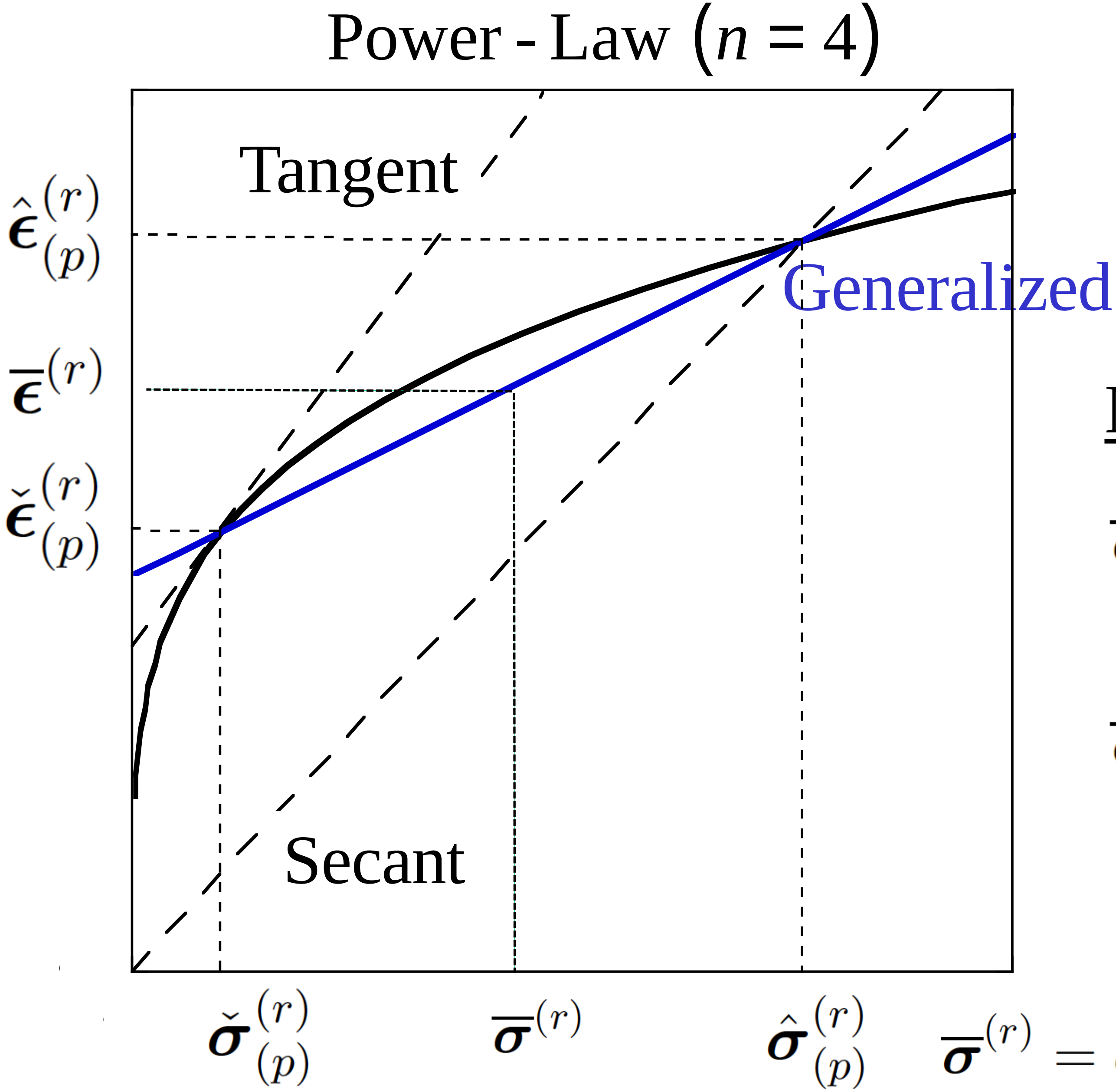
  Ponte Castañeda (2015) Proc. R. Soc. Lond. A

***MICROSTRUCTURE***

- **Grain shape**
- **Grain orientation**
- **Crystallographic texture**



# Generalized Secant Modulus




$$\overline{\boldsymbol{\sigma}}^{(r)} = \alpha^{(r)} \check{\boldsymbol{\sigma}}_{(p)}^{(r)} + \left(1 - \alpha^{(r)}\right) \hat{\boldsymbol{\sigma}}_{(p)}^{(r)}$$

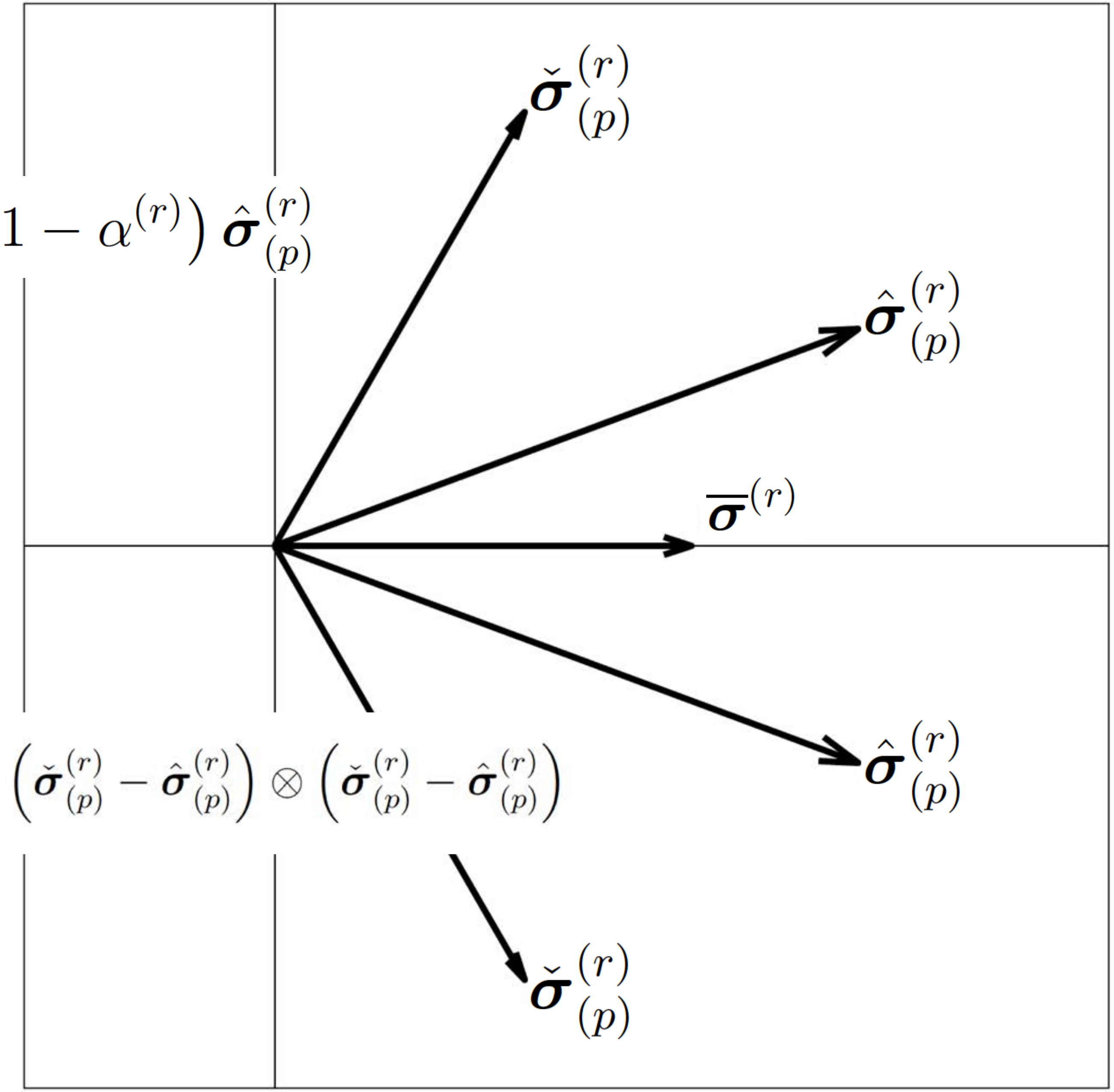
Note:

$$\overline{\boldsymbol{\epsilon}}^{(r)} = \mathbb{M}^{(r)} \overline{\boldsymbol{\sigma}}^{(r)} + \boldsymbol{\gamma}^{(r)}$$

$$\overline{\boldsymbol{\epsilon}}^{(r)} \neq \frac{\partial u^{(r)}\left(\overline{\boldsymbol{\sigma}}^{(r)}\right)}{\partial \boldsymbol{\sigma}}$$

# Generalized Secant Modulus

$$\overline{\boldsymbol{\sigma}}_L^{(r)} = \alpha^{(r)} \check{\boldsymbol{\sigma}}_{(p)}^{(r)} + \left(1 - \alpha^{(r)}\right) \hat{\boldsymbol{\sigma}}_{(p)}^{(r)}$$




$$\mathbb{C}_{\boldsymbol{\sigma}}^{(r)} = \alpha^{(r)}(1 - \alpha^{(r)}) \sum_{p=1}^{M} \beta_{(p)}^{(r)} \left(\check{\boldsymbol{\sigma}}_{(p)}^{(r)} - \hat{\boldsymbol{\sigma}}_{(p)}^{(r)}\right) \otimes \left(\check{\boldsymbol{\sigma}}_{(p)}^{(r)} - \hat{\boldsymbol{\sigma}}_{(p)}^{(r)}\right)$$

# Additional Properties

- The nonlinear estimate can be rewritten as

$$\widetilde{U}_N(\overline{\boldsymbol{\sigma}}) = \sum_{r=1}^{N} c^{(r)} \sum_{p=1}^{M} \beta_{(p)}^{(r)} \left[\alpha^{(r)} u^{(r)} \left(\check{\boldsymbol{\sigma}}_{(p)}^{(r)}\right) + \left(1-\alpha^{(r)}\right) u^{(r)} \left(\hat{\boldsymbol{\sigma}}_{(p)}^{(r)}\right)\right]$$

while the macroscopic stress-strain relation can be written as

$$\overline{\boldsymbol{\epsilon}} = \widetilde{\mathbb{M}}\,\overline{\boldsymbol{\sigma}} + \tilde{\boldsymbol{\gamma}}$$

- The field statistics can be written as

$$\overline{\boldsymbol{\sigma}}^{(r)} = \overline{\boldsymbol{\sigma}}_L^{(r)} \qquad \langle \boldsymbol{\sigma} \otimes \boldsymbol{\sigma} \rangle^{(r)} = \langle \boldsymbol{\sigma} \otimes \boldsymbol{\sigma} \rangle_L^{(r)}$$

$$\overline{\boldsymbol{\epsilon}}^{(r)} = \overline{\boldsymbol{\epsilon}}_L^{(r)} \qquad \langle \boldsymbol{\epsilon} \otimes \boldsymbol{\epsilon} \rangle^{(r)} = \langle \boldsymbol{\epsilon} \otimes \boldsymbol{\epsilon} \rangle_L^{(r)}$$

**Note**: These nice properties are a direct consequence of full optimality

Ponte Castañeda (2016) JMPS

# Random “Ellipsoidal” Granular Microstructure

- Orientation distribution function

I. Crystal lattice orientation

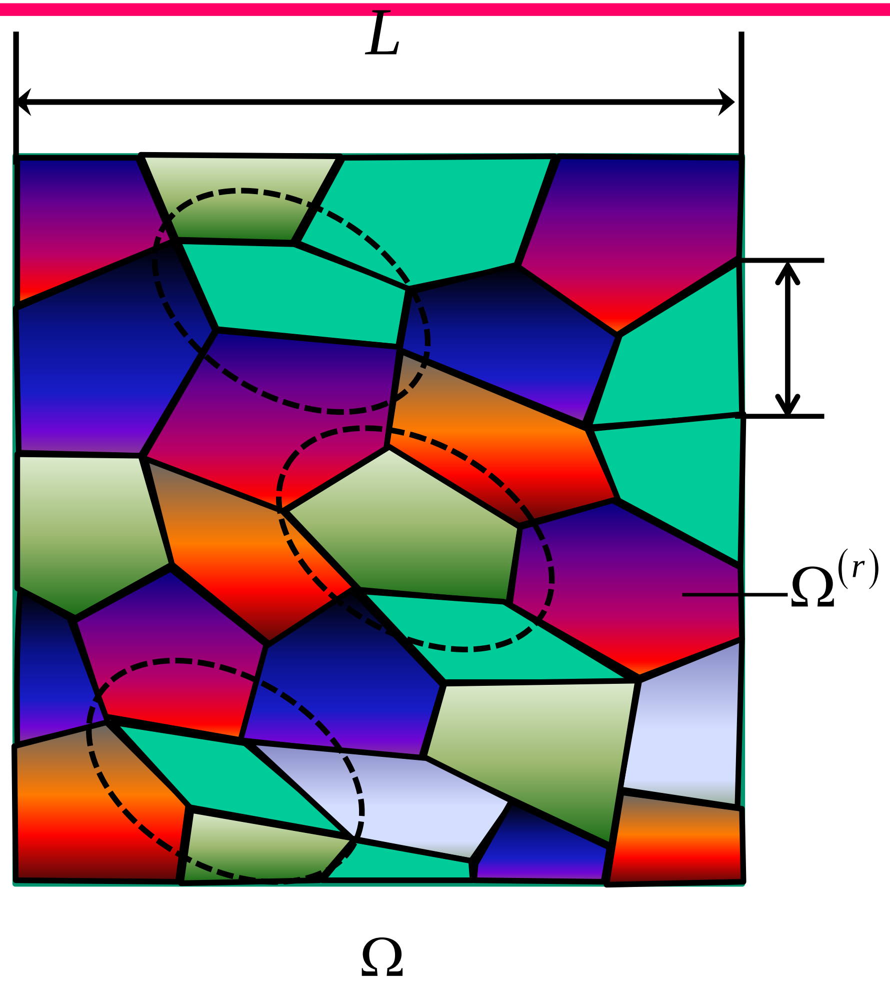
$$\mathbf{Q}^{(r)} \quad (r = 1, \cdots, N)$$

II. Volume fractions

$$c^{(r)} = \frac{\Omega^{(r)}}{\Omega} \quad (r = 1, \cdots, N)$$

- Two-point correlation function

$$p^{(rs)}(\mathbf{x}, \mathbf{x}') = p^{(rs)}(|\boldsymbol{Z}^{(g)}(\mathbf{x} - \mathbf{x}')|)$$

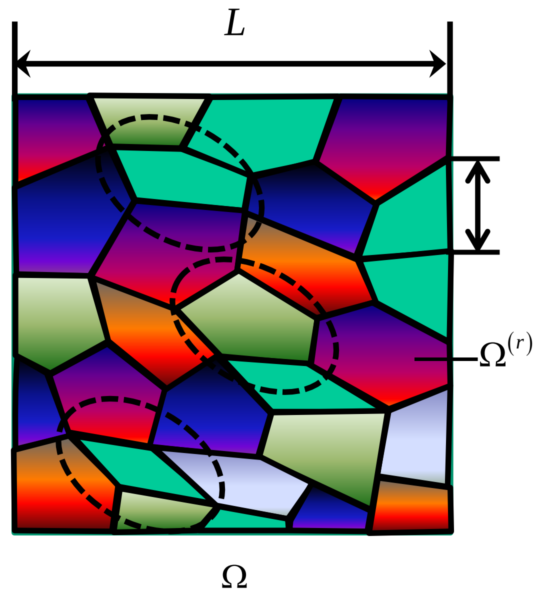


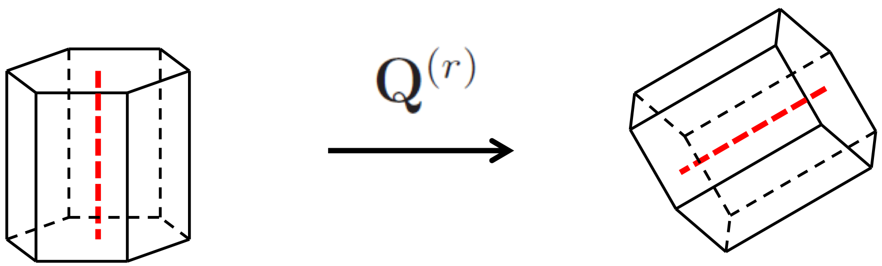

Willis (1977) JMPS

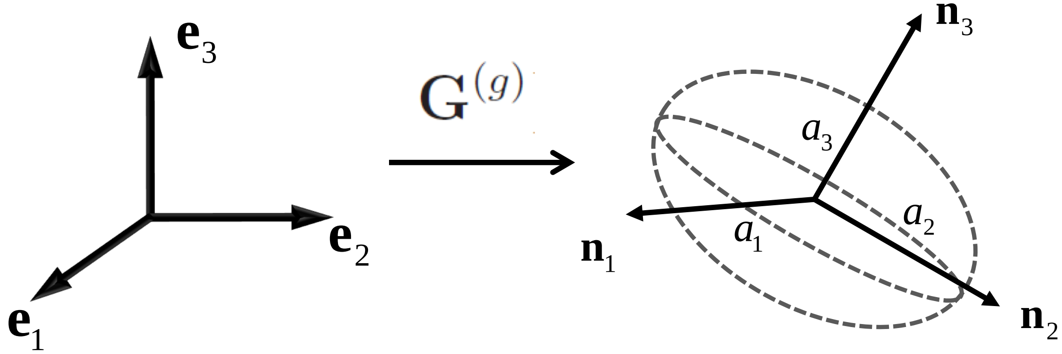
# Microstructural Variables

## Define the set of microstructural variables

$$\mathbf{s} \equiv \{\mathbf{Q}^{(r)}, w_1^{(g)}, w_2^{(g)}, \mathbf{G}^{(g)}\}$$



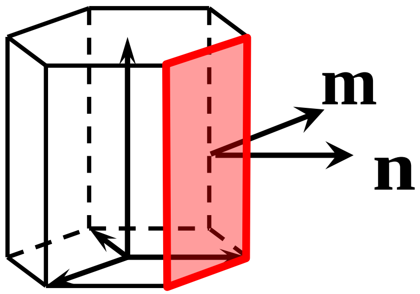




$$w_1^{(g)} = \frac{a_3}{a_1}$$

$$w_2^{(g)} = \frac{a_3}{a_2}$$

# Local Properties of the Single-Crystal Phases

- Viscoplastic flow potential




$$u^{(r)}(\boldsymbol{\sigma}) = \sum_{k=1}^{K} \phi^{(r)}_{(k)}(\tau^{(r)}_{(k)})$$

$$\tau^{(r)}_{(k)} = \boldsymbol{\sigma} \cdot \boldsymbol{\mu}^{(r)}_{(k)}, \quad \text{where} \quad \boldsymbol{\mu}^{(r)}_{(k)} = \frac{1}{2}\left(\mathbf{n}^{(r)}_{(k)} \otimes \mathbf{m}^{(r)}_{(k)} + \mathbf{m}^{(r)}_{(k)} \otimes \mathbf{n}^{(r)}_{(k)}\right).$$

- Eulerian strain rate: $\mathbf{D} = \dfrac{\partial u^{(r)}}{\partial \boldsymbol{\sigma}} = \displaystyle\sum_{k=1}^{K} \gamma^{(r)}_{(k)} \boldsymbol{\mu}^{(r)}_{(k)}, \quad \gamma^{(r)}_{(k)} = \phi^{(r)\prime}_{(k)}(\tau^{(r)}_{(k)})$

- Plastic spin: $\mathbf{W}_p = \dfrac{1}{2} \displaystyle\sum_{k=1}^{K} \gamma^{(r)}_{(k)} \left(\mathbf{m}^{(r)}_{(k)} \otimes \mathbf{n}^{(r)}_{(k)} - \mathbf{n}^{(r)}_{(k)} \otimes \mathbf{m}^{(r)}_{(k)}\right)$

# Effective Properties for the LCC: Self-Consistent Estimates

- Local Properties of the LCC $\quad \mathbf{D} = \mathbb{M}^{(r)}\boldsymbol{\sigma} + \boldsymbol{\eta}^{(r)}$

$$\mathbb{M}^{(r)} = \sum_{k=1}^{K} \frac{1}{2\mu_{(k)}^{(r)}} \boldsymbol{\mu}_{(k)}^{(r)} \otimes \boldsymbol{\mu}_{(k)}^{(r)}, \quad \text{and} \quad \boldsymbol{\eta}^{(r)} = \sum_{k=1}^{K} \eta_{(k)}^{(r)}\, \boldsymbol{\mu}_{(k)}^{(r)}$$

- Effective Stress Potential

$$\widetilde{u}_L(\overline{\boldsymbol{\sigma}}) = \frac{1}{2}\overline{\boldsymbol{\sigma}} \cdot \widetilde{\mathbb{M}}\overline{\boldsymbol{\sigma}} + \widetilde{\boldsymbol{\eta}} \cdot \overline{\boldsymbol{\sigma}} + \frac{1}{2}\widetilde{g}.$$

- Effective constitutive relation

$$\overline{\mathbf{D}}_L = \frac{\partial \widetilde{u}_L}{\partial \overline{\boldsymbol{\sigma}}}(\overline{\boldsymbol{\sigma}}) = \widetilde{\mathbb{M}}\overline{\boldsymbol{\sigma}} + \widetilde{\boldsymbol{\eta}}$$

- Effective compliance tensor

$$\widetilde{\mathbb{M}} = \left\{ \sum_{r=1}^{N} c^{(r)} \left[\mathbb{M}^{(r)} + \widetilde{\mathbb{M}}^*\right]^{-1} \right\}^{-1} - \widetilde{\mathbb{M}}^*, \qquad \widetilde{\mathbb{M}}^* = \widetilde{\mathbb{Q}}^{-1} - \widetilde{\mathbb{M}},$$

- Effective eigenstrain rate

$$\widetilde{\boldsymbol{\eta}} = \sum_{r=1}^{N} c^{(r)} \left(\mathbb{B}^{(r)}\right)^T \boldsymbol{\eta}^{(r)}$$

- Effective potential at zero stress

$$\widetilde{g} = \sum_{r=1}^{N} c^{(r)} \boldsymbol{\eta}^{(r)} \cdot \mathbf{b}^{(r)}$$

Willis (1977) JMPS

# Self-Consistent Estimates: Field Statistics in the LCC

- First and second moments of stress

$$\overline{\boldsymbol{\sigma}}_L^{(r)} = \mathbb{B}^{(r)}\overline{\boldsymbol{\sigma}} + \mathbf{b}^{(r)}, \quad \langle \boldsymbol{\sigma} \otimes \boldsymbol{\sigma} \rangle_L^{(r)} = \frac{2}{c^{(r)}} \frac{\partial \widetilde{u}_L}{\partial \mathbb{M}^{(r)}}$$

- First and second moments of the resolved shear stress

$$\overline{\tau}_{(k)}^{(r)} = \overline{\boldsymbol{\sigma}}_L^{(r)} \cdot \boldsymbol{\mu}_{(k)}^{(r)}, \quad \overline{\overline{\tau}}_{(k)}^{(r)} = \boldsymbol{\mu}_{(k)}^{(r)} \cdot \langle \boldsymbol{\sigma} \otimes \boldsymbol{\sigma} \rangle_L^{(r)} \boldsymbol{\mu}_{(k)}^{(r)}$$

- First moment of the strain rate and spin

$$\overline{\mathbf{D}}_L^{(r)} = \mathbb{M}^{(r)}\overline{\boldsymbol{\sigma}}_L^{(r)} + \boldsymbol{\eta}^{(r)}, \quad \overline{\mathbf{W}}_L^{(r)} = \overline{\mathbf{W}} - \mathbb{R}\mathbb{P}^{-1}\left(\overline{\mathbf{D}} - \overline{\mathbf{D}}_L^{(r)}\right)$$

etc.

Liu & Ponte Castañeda (2004) JMPS