# **Micromorphic Crystal Plasticity**

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#### The "microcurl" model

- Kinematics and balance equations
- Constitutive equations
- Internal stress arising from the model
- Internal constraint and strain gradient plasticity
- Linearized formulation

#### 2 Size effect in a two-phase single crystal laminate

- Boundary value problem
- Interface conditions
- Strain gradient plasticity as a limit case

- Hall–Petch effect
- Strain localization in ultra-fine grains

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# **Enhancing classical continuum mechanics**

Within the framework of generalized continuum mechanics, we introduce additional degrees of freedom

$$DOF = \{ \underline{\mathbf{u}}, \quad \hat{\boldsymbol{\chi}}^{p} \}$$

where  $\hat{\chi}^{\rm p}$  is a generally non compatible plastic microdeformation tensor.

In a first gradient theory, only the first gradients of the *DOF* intervene in the model

$$GRAD = \{ \mathbf{E} := \mathbf{1} + \mathbf{\underline{u}} \otimes \mathbf{\nabla}_{\mathbf{X}}, \quad \mathbf{\underline{K}} := \operatorname{Curl} \hat{\mathbf{\chi}}^{p} \}$$

In the context of crystal plasticity, only the curl part of the plastic microdeformation is considered, instead of its full gradient. The following definition of the Curl operator is adopted:

$$\mathbf{K} := \operatorname{Curl} \hat{\mathbf{\chi}}^{\boldsymbol{\rho}} := \frac{\partial \hat{\mathbf{\chi}}^{\boldsymbol{\rho}}}{\partial X_k} \times \underline{\mathbf{e}}_k, \quad K_{ij} := \epsilon_{jkl} \frac{\partial \hat{\chi}^{\boldsymbol{\rho}}_{ik}}{\partial X_l}$$

The method of virtual power is used to derive the balance and boundary conditions, following [Germain, 1973].

• Power density of **internal forces**; it is a linear form with respect to the velocity fields and their Eulerian gradients:

$$oldsymbol{
ho}^{(i)} = arphi: (\dot{\mathbf{u}} \otimes oldsymbol{
abla}_{\mathsf{x}}) + \mathbf{\underline{s}}: \dot{\hat{\chi}}^{
ho} + oldsymbol{\mathsf{M}}: \operatorname{curl} \dot{\hat{\chi}}^{
ho}, \quad orall \mathbf{\underline{x}} \in V$$

where the conjugate quantities are the Cauchy stress tensor  $\sigma$ , which is symmetric for objectivity reasons, the microstress tensor,  $\underline{s}$ , and the generalized couple stress tensor  $\underline{M}$ . The curl of the microdeformation rate is defined as

$$\operatorname{curl} \dot{\hat{\boldsymbol{\chi}}}^{\boldsymbol{\rho}} := \epsilon_{jkl} \frac{\partial \dot{\hat{\boldsymbol{\chi}}}_{ik}^{\boldsymbol{\rho}}}{\partial x_l} \underline{\mathbf{e}}_i \otimes \underline{\mathbf{e}}_j = \dot{\mathbf{K}} \cdot \mathbf{E}^{-1}$$

The method of virtual power is used to derive the balance and boundary conditions, following [Germain, 1973].

• Power density of contact forces;

$$p^{(c)} = \underline{\mathbf{t}} \cdot \underline{\dot{\mathbf{u}}} + \underline{\mathbf{m}} : \dot{\underline{\chi}}^{p}, \quad \forall \underline{\mathbf{x}} \in \partial V$$

where  $\underline{t}$  is the usual simple traction vector and  $\underset{\sim}{m}$  the double traction tensor.

The method of virtual power is used to derive the balance and boundary conditions, following [Germain, 1973].

• Application of the **principle of virtual power**, in the absence of volume forces and in the static case, for brevity:

$$-\int_D p^{(i)} dV + \int_{\partial D} p^{(c)} dS = 0$$

for all virtual fields  $\dot{\underline{u}}$  ,  $\dot{\hat{\chi}}^{p}$ , and any subdomain  $D \subset V.$ 

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• By application of Gauss divergence theorem, assuming sufficient regularity of the fields, this statement expands into:

$$\int_{V} \frac{\partial \sigma_{ij}}{\partial x_{j}} \dot{u}_{i} \, dV + \int_{V} \left( \epsilon_{kjl} \frac{\partial M_{ik}}{\partial x_{l}} - s_{ij} \right) \dot{\chi}_{ij}^{p} \, dV \\ + \int_{\partial V} \left( t_{i} - \sigma_{ij} n_{j} \right) \dot{u}_{i} \, dS + \int_{\partial V} \left( m_{ik} - \epsilon_{jkl} M_{ij} n_{l} \right) \dot{\chi}_{ik}^{p} \, dS = 0, \, \forall \dot{u}_{i}, \forall \dot{\chi}_{ij}^{p}$$

This leads to the two field equations of balance of momentum and generalized balance of moment of momentum:

$$\operatorname{div} \boldsymbol{\sigma} = \mathbf{0}, \quad \operatorname{curl} \mathbf{M} + \mathbf{s} = \mathbf{0}, \quad \forall \mathbf{x} \in V$$

and two boundary conditions

$$\underline{\mathbf{t}} = \underline{\boldsymbol{\sigma}} \cdot \underline{\mathbf{n}}, \quad \underline{\mathbf{m}} = \underline{\mathbf{M}} \cdot \underline{\underline{\boldsymbol{\epsilon}}} \cdot \underline{\mathbf{n}}, \quad \forall \underline{\mathbf{x}} \in \partial V$$

the index notation of the latter relation being  $m_{ij} = M_{ik} \epsilon_{kjl} n_l$ .

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# **State variables**

- The deformation gradient is decomposed into elastic and plastic parts in the form  $\label{eq:elastic} E = E \cdot P$
- The elastic strain is defined as

$$\begin{split} \mathbf{F} &= \mathbf{E} \cdot \mathbf{P} \\ \mathbf{E}^e &:= \frac{1}{2} (\mathbf{E}^T \cdot \mathbf{E} - \mathbf{1}) \end{split}$$

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- The microdeformation is linked to the plastic deformation via the introduction of a relative deformation measure defined as

$$\mathbf{e}^{p} := \mathbf{P}^{-1} \cdot \hat{\chi}^{p} - \mathbf{1}$$

It measures the departure of the microdeformation from the plastic deformation, which is associated with a cost in the free energy potential. When  $\underline{e}^{\rho} \equiv 0$ , the microdeformation coincides with plastic deformation.

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• The state variables are assumed to be the elastic strain, the relative deformation, the curl of microdeformation and some internal variables,  $\alpha$ :

$$STATE := \{ \mathbf{\underline{E}}^{e}, \quad \mathbf{\underline{e}}^{p}, \quad \mathbf{\underline{K}}, \quad \alpha \}$$

The specific Helmholtz free energy density,  $\psi$ , is a function of these variables. In this simple version of the model, the curl of microdeformation is assumed to contribute entirely to the stored energy.

 $\mathbf{E}^e := \frac{1}{2} (\mathbf{E}^T \cdot \mathbf{E} - \mathbf{1})$ 

# **Entropy principle**

The dissipation rate density is the difference:

$$D:=p^{(i)}-\rho\dot{\psi}\geq 0$$

which must be positive according to the second principle of thermodynamics. When the previous strain measures are introduced, the power density of internal forces takes the following form:

$$p^{(i)} = \boldsymbol{\varphi} : \dot{\mathbf{E}} \cdot \mathbf{E}^{-1} + \boldsymbol{\varphi} : \mathbf{E} \cdot \dot{\mathbf{P}} \cdot \mathbf{P}^{-1} \cdot \mathbf{E}^{-1} + \mathbf{s} : (\mathbf{P} \cdot \dot{\mathbf{e}}^{p} + \dot{\mathbf{P}} \cdot \mathbf{e}^{p}) + \mathbf{M} : \dot{\mathbf{K}} \cdot \mathbf{F}^{-1} = \frac{\rho}{\rho_{i}} \mathbf{n}^{e} : \dot{\mathbf{E}}^{e} + \frac{\rho}{\rho_{i}} \mathbf{n}^{M} : \dot{\mathbf{P}} \cdot \mathbf{P}^{-1} + \mathbf{s} : (\mathbf{P} \cdot \dot{\mathbf{e}}^{p} + \dot{\mathbf{P}} \cdot \mathbf{e}^{p}) + \mathbf{M} : \dot{\mathbf{K}} \cdot \mathbf{F}^{-1}$$

where  $\underline{\Pi}^e$  is the second Piola–Kirchhoff stress tensor with respect to the intermediate configuration and  $\underline{\Pi}^M$  is the Mandel stress tensor:

$$\Pi^{e} := J_{e} \mathbf{\underline{E}}^{-1} \cdot \underline{\sigma} \cdot \mathbf{\underline{E}}^{-T}, \quad \Pi^{M} := J_{e} \mathbf{\underline{E}}^{T} \cdot \underline{\sigma} \cdot \mathbf{\underline{E}}^{-T} = \mathbf{\underline{E}}^{T} \cdot \mathbf{\underline{E}} \cdot \Pi^{e}$$

# **State laws**

On the other hand,

$$\rho\dot{\psi} = \rho\frac{\partial\psi}{\partial\underline{\mathsf{E}}^{\mathsf{e}}}: \dot{\underline{\mathsf{E}}}^{\mathsf{e}} + \rho\frac{\partial\psi}{\partial\underline{\mathsf{e}}^{\mathsf{p}}}: \dot{\underline{\mathsf{e}}}^{\mathsf{p}} + \rho\frac{\partial\psi}{\partial\underline{\mathsf{K}}}: \dot{\underline{\mathsf{K}}} + \rho\frac{\partial\psi}{\partial\alpha}\dot{\alpha}$$

We compute

$$J_{e}D = (\Pi^{e} - \rho_{i}\frac{\partial\psi}{\partial\mathbf{E}^{e}}) : \dot{\mathbf{E}}^{e} + (J_{e}\mathbf{P}^{T} \cdot \mathbf{s} - \rho_{i}\frac{\partial\psi}{\partial\mathbf{e}^{p}}) : \dot{\mathbf{e}}^{p}$$
$$+ (J_{e}\mathbf{M} \cdot \mathbf{F}^{-T} - \rho_{i}\frac{\partial\psi}{\partial\mathbf{K}}) : \dot{\mathbf{K}}$$
$$+ (\Pi^{M} + J_{e}\mathbf{s} \cdot \hat{\mathbf{\chi}}^{pT}) : \dot{\mathbf{P}} \cdot \mathbf{P}^{-1} - \rho_{i}\frac{\partial\psi}{\partial\alpha}\dot{\alpha} \ge 0$$

Assuming that the processes associated with  $\dot{\mathbf{E}}^{e}, \dot{\mathbf{e}}^{p}$  and  $\dot{\mathbf{K}}$  are non–dissipative, the state laws are obtained:

$$\mathbf{\Pi}^{e} = \rho_{i} \frac{\partial \psi}{\partial \mathbf{E}^{e}}, \quad \mathbf{s} = J_{e}^{-1} \mathbf{P}^{-T} \cdot \rho_{i} \frac{\partial \psi}{\partial \mathbf{e}^{p}}, \quad \mathbf{M} = J_{e}^{-1} \rho_{i} \frac{\partial \psi}{\partial \mathbf{K}} \cdot \mathbf{E}^{T}$$

# **Evolution laws**

The residual dissipation rate is

$$J_e D = (\prod^{M} + J_e \underline{\mathbf{s}} \cdot \hat{\underline{\chi}}^{pT}) : \dot{\underline{\mathbf{P}}} \cdot \underline{\underline{\mathbf{P}}}^{-1} - R\dot{\alpha} \ge 0, \quad \text{with} \quad R := \rho_i \frac{\partial \psi}{\partial \alpha}$$

At this stage, a dissipation potential, function of stress measures,  $\Omega(\boldsymbol{\mathcal{S}}, R)$ , is introduced in order to formulate the evolution equations for plastic flow and internal variables:

$$\dot{\mathbf{P}} \cdot \mathbf{P}^{-1} = \frac{\partial \Omega}{\partial \mathbf{S}}, \quad \text{with} \quad \mathbf{S} := \mathbf{\Pi}^M + J_e \mathbf{s} \cdot \hat{\mathbf{\chi}}^{pT}$$
 $\dot{\alpha} = -\frac{\partial \Omega}{\partial R}$ 

where R is the thermodynamic force associated with the internal variable  $\alpha$ , and  $\boldsymbol{\mathcal{S}}$  is the effective stress conjugate to plastic strain rate, the driving force for plastic flow.

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# Application to crystal plasticity

In the case of crystal plasticity, a **generalized Schmid law** is adopted for each slip system *s* in the form:

$$f^{s}(\boldsymbol{\mathcal{S}}, \tau_{c}^{s}) = |\boldsymbol{\mathcal{S}}: \boldsymbol{\mathbb{N}}^{s}| - \tau_{c}^{s} \geq 0, \quad \text{with} \quad \boldsymbol{\mathbb{N}}^{s} = \underline{I}^{s} \otimes \underline{\mathbf{n}}^{s}$$

for activation of slip system *s* with slip direction,  $\underline{I}^{s}$ , and normal to the slip plane,  $\underline{n}^{s}$ . We call  $\underline{N}^{s}$  the orientation tensor. The critical resolved shear stress is  $\tau_{c}^{s}$  which may be a function of *R* in the presence of isotropic hardening.

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$$\boldsymbol{\mathfrak{S}}: \boldsymbol{\mathbb{N}}^{s} = \boldsymbol{\tau}^{s} - \boldsymbol{x}^{s}, \quad \text{ with } \quad \boldsymbol{\tau}^{s} = \boldsymbol{\Pi}^{M}: \boldsymbol{\mathbb{N}}^{s} \quad \text{and } \quad \boldsymbol{x}^{s} = -\boldsymbol{\underline{s}} \cdot \boldsymbol{\hat{\chi}}^{pT}: \boldsymbol{\mathbb{N}}^{s}$$

The usual resolved shear stress is  $\tau^s$  whereas  $x^s$  can be interpreted as an internal stress or back-stress leading to kinematic hardening. [Steinmann, 1996] The back-stress component is induced by the microstress  $\underline{s}$  or, equivalently, by the curl of the generalized couple stress tensor,  $\underline{M}$ , via the balance equation

$$x^{s} = \operatorname{curl} \mathbf{M} \cdot \hat{\chi}^{pT} : \mathbf{N}^{s}$$

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for activation of slip system s with slip direction,  $\underline{\mathbf{I}}^{s}$ , and normal to the slip plane,  $\underline{\mathbf{n}}^{s}$ . The critical resolved shear stress is  $\tau_{c}^{s}$  which may be a function of R in the presence of isotropic hardening. The kinematics of plastic slip follows from the choice of a dissipation potential,  $\Omega(f^{s})$ , that depends on the stress variables through the yield function itself,  $f^{s}$ :

$$\dot{\mathsf{F}}^{p} \cdot \underbrace{\mathsf{F}}^{p-1} = \sum_{s=1}^{N} \frac{\partial \Omega}{\partial f^{s}} \frac{\partial f^{s}}{\partial \underline{\mathcal{S}}} = \sum_{s=1}^{N} \dot{\gamma}^{s} \underbrace{\mathsf{N}}^{s}, \quad \text{with} \quad \dot{\gamma}^{s} = \frac{\partial \Omega}{\partial f^{s}} \text{sign}(\underline{\mathcal{S}} : \underbrace{\mathsf{N}}^{s})$$

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# From micromorphic to strain gradient plasticity

If the following internal constraint is enforced:

$$\mathbf{e}^{\boldsymbol{
ho}} \equiv \mathsf{0} \quad \Longleftrightarrow \quad \hat{\chi}^{\boldsymbol{
ho}} \equiv \mathbf{P}_{\widetilde{\omega}}$$

the curl part of the plastic microdeformation is directly related to the dislocation density densor:

$$\mathsf{K} := \operatorname{Curl} \hat{\boldsymbol{\chi}}^{\boldsymbol{\rho}} \equiv \operatorname{Curl} \mathsf{P} = J_{\boldsymbol{\alpha}} \cdot \mathsf{F}^{-\boldsymbol{\tau}}$$

The *microcurl* theory reduces to strain gradient plasticity according to [Gurtin, 2002].

As a result the *microcurl* model incorporates, as wanted, a dependence of material behaviour on the dislocation density tensor.

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When deformations and rotations remain sufficiently small, the previous equations can be linearized as follows:

 $\mathbf{F} = \mathbf{1} + \mathbf{H} = \mathbf{1} + \mathbf{H}^{\mathbf{e}} + \mathbf{H}^{\mathbf{p}}, \quad \mathbf{H}^{\mathbf{e}} = \mathbf{\varepsilon}^{\mathbf{e}} + \boldsymbol{\omega}^{\mathbf{e}}, \quad \mathbf{H}^{\mathbf{p}} = \mathbf{\varepsilon}^{\mathbf{p}} + \boldsymbol{\omega}^{\mathbf{p}}$ 

where  $\underline{\varepsilon}^{e}, \underline{\omega}^{e}$  (resp.  $\underline{\varepsilon}^{p}, \underline{\omega}^{p}$ ) are practically equal to the symmetric and skew-symmetric parts of  $\underline{\mathsf{E}} - \underline{\mathsf{1}}$  (resp.  $\underline{\mathsf{P}} - \underline{\mathsf{1}}$ ). When microdeformation is small, the relative deformation is linearized as

$$\mathbf{e}^{
ho} = (\mathbf{1} + \mathbf{H}^{
ho})^{-1} \cdot (\mathbf{1} + \chi^{
ho}) - \mathbf{1} \simeq \chi^{
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$$\mathbf{\underline{e}}^{p} = (\mathbf{\underline{1}} + \mathbf{\underline{H}}^{p})^{-1} \cdot (\mathbf{\underline{1}} + \underline{\chi}^{p}) - \mathbf{\underline{1}} \simeq \underline{\chi}^{p} - \mathbf{\underline{H}}^{p}, \quad \text{with} \quad \underline{\chi}^{p} = \underline{\hat{\chi}}^{p} - \mathbf{\underline{1}}.$$

When linearized, the state laws become:

$$\underline{\sigma} = \rho \frac{\partial \psi}{\partial \underline{\varepsilon}^{e}}, \quad \underline{s} = \rho \frac{\partial \psi}{\partial \underline{e}^{p}}, \quad \underline{M} = \rho \frac{\partial \psi}{\partial \underline{K}}$$

The evolution equations read then:

$$\dot{\varepsilon}^{p} = \frac{\partial \Omega}{\partial (\sigma + \mathbf{s})}, \quad \dot{\alpha} = -\frac{\partial \Omega}{\partial R}$$

We adopt the most simple case of a quadratic free energy potential:

$$\rho\psi(\underline{\varepsilon}^{e},\underline{\mathbf{e}}^{p},\underline{\mathbf{K}}) = \frac{1}{2}\underline{\varepsilon}^{e}:\underline{\mathbf{C}}:\underline{\varepsilon}^{e} + \frac{1}{2}H_{\chi}\underline{\mathbf{e}}^{p}:\underline{\mathbf{e}}^{p} + \frac{1}{2}A\underline{\mathbf{K}}:\underline{\mathbf{K}}$$

The usual four-rank tensor of elastic moduli is denoted by  $\mathbf{C}_{\approx}$ . The higher order moduli have been limited to only two additional parameters:  $H_{\chi}$  (unit MPa) and A (unit MPa.mm<sup>2</sup>). It follows that:

Large values of  $H_{\chi}$  ensure that  $\underline{\mathbf{e}}^{p}$  remains small so that  $\underline{\chi}^{p}$  remains close to  $\underline{\mathbf{H}}^{p}$  and  $\underline{\mathbf{K}}$  is close to the dislocation density tensor:

$$\operatorname{curl} \chi^{\rho} \equiv \operatorname{curl} \overset{\mathsf{H}}{\underset{\sim}{\overset{\mathsf{P}}{=}}} = \overset{\mathsf{a}}{\underset{\sim}{\overset{\mathsf{curl}}{\overset{\mathsf{H}}{\underset{\sim}{=}}}}$$

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$$\underline{\sigma} = \underbrace{\mathbf{C}}_{\approx} : \underline{\varepsilon}^{e}, \quad \underline{\mathbf{s}} = H_{\chi} \underline{\mathbf{e}}^{p}, \quad \underline{\mathbf{M}} = A \underline{\mathbf{K}}$$

The yield condition for each slip system becomes:

$$f^s = |\tau^s - x^s| - \tau^s_c$$

with

$$x^{s} = -\underline{s}: \underbrace{\mathbf{P}}^{s} = (\operatorname{curl} \underline{\mathsf{M}}): \underbrace{\mathbf{P}}^{s} = A(\operatorname{curl} \operatorname{curl} \underline{\chi}^{p}): \underbrace{\mathsf{N}}^{s}$$

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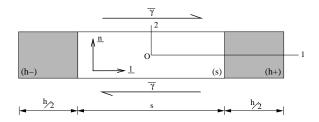
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The microstructure is composed of a hard elastic phase (h) and a soft elasto-plastic phase (s) where one slip system with slip direction normal to the interface between (h) and (s) is considered. A mean simple glide  $\bar{\gamma}$  is applied in the crystal slip direction of the phase (s). We consider displacement and microdeformation fields of the form:

$$u_1 = \bar{\gamma} x_2, \quad u_2(x_1), \quad u_3 = 0, \quad \chi_{12}^p(x_1), \quad \chi_{21}^p(x_1)$$

within the context of small deformation theory.

Size effect in a two-phase single crystal laminate

$$\begin{bmatrix} u_1 = \bar{\gamma}x_2, & u_2(x_1), & u_3 = 0, & \chi_{12}^p(x_1), & \chi_{21}^p(x_1) \end{bmatrix} \\ \begin{bmatrix} 0 & \bar{\gamma} & 0 \\ u_{2,1} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{H}^p \end{bmatrix} = \begin{bmatrix} 0 & \gamma & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{H}^e \end{bmatrix} = \begin{bmatrix} 0 & \bar{\gamma} - \gamma & 0 \\ u_{2,1} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \\ \begin{bmatrix} \chi^p \end{bmatrix} = \begin{bmatrix} 0 & \chi_{12}^p(x_1) & 0 \\ \chi_{21}^p(x_1) & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \operatorname{curl} \chi^p \end{bmatrix} = \begin{bmatrix} 0 & 0 & -\chi_{12,1}^p \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

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The resulting stress tensors are:

$$\begin{bmatrix} \sigma \end{bmatrix} = \mu \begin{bmatrix} 0 & \bar{\gamma} - \gamma + u_{2,1} & 0\\ \bar{\gamma} - \gamma + u_{2,1} & 0 & 0\\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} s \end{bmatrix} = -H_{\chi} \begin{bmatrix} 0 & \gamma - \chi_{12}^{p} & 0\\ -\chi_{21}^{p} & 0 & 0\\ 0 & 0 & 0 \end{bmatrix}$$
$$\begin{bmatrix} M \end{bmatrix} = \begin{bmatrix} 0 & 0 & -A\chi_{12,1}^{p}\\ 0 & 0 & 0\\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \operatorname{curl} \mathbf{M} \end{bmatrix} = \begin{bmatrix} 0 & -A\chi_{12,11}^{p} & 0\\ 0 & 0 & 0\\ 0 & 0 & 0 \end{bmatrix}$$

These forms of matrices are valid for both phases, except that  $\gamma \equiv 0$  in the hard elastic phase. Each phase possesses its own material parameters,  $H_{\chi}$  and A, the shear modulus,  $\mu$ , being assumed for simplicity to be identical in both phases.

Size effect in a two-phase single crystal laminate

The balance equation,  $\underline{s} = -\text{curl} \underbrace{\mathsf{M}}_{\sim}$ , gives  $\chi_{21}^{p} = 0$  and the plastic slip:

$$\gamma = \chi_{12}^{p} - \frac{A}{H_{\chi}}\chi_{12,11}^{p}$$

In the soft phase, the plasticity criterion stipulates that

$$\sigma_{12} + \mathbf{s}_{12} = \tau_c + H \gamma_{cum}$$

where H is a linear hardening modulus considered in this phase. We obtain the second order differential equation for the microdeformation variable in the soft phase,  $\chi_{12}^{ps}$ ,

$$\frac{1}{\omega^{s_2}}\chi_{12,11}^{ps} - \chi_{12}^{ps} = \frac{\tau_c - \sigma_{12}}{H}, \quad \text{with} \quad \omega^s = \sqrt{\frac{H_{\chi}^s H}{A^s \left(H_{\chi}^s + H\right)}}$$

where  $1/\omega^{\rm s}$  is the characteristic length of the soft phase for this boundary value problem.

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- Strain gradient plasticity as a limit case

- Hall–Petch effect
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The force stress balance equation requires  $\sigma_{12}$  to be uniform. It follows that the non-homogeneous part of the differential equation is constant and then the hyperbolic profile of  $\chi_{12}^{ps}$  takes the form:

 $\chi_{12}^{\rm ps} = C^{\rm s} \cosh\left(\omega^{\rm s} x\right) + D$ 

where  $C^s$  and D are constants to be determined. Symmetry conditions  $(\chi_{12}^{ps}(-s/2) = \chi_{12}^{ps}(s/2))$  have been taken into account. In the elastic phase, where the plastic slip vanishes, an hyperbolic profile of the microdeformation variable,  $\chi_{12}^{ph}$ , is also obtained:

$$\chi_{12}^{ph} = C^h \cosh\left(\omega^h \left(x \pm \frac{s+h}{2}\right)\right), \quad \text{with} \quad \omega^h = \sqrt{\frac{H_{\chi}^h}{A^h}}$$

where, again,  $C^h$  is a constant to be determined and symmetry conditions have been taken into account. It is remarkable that the plastic microvariable,  $\chi_{12}^{ph}$ , does not vanish in the elastic phase, close to the interfaces, although no plastic deformation takes place.

## Simple shear of a two-phase laminate

The coefficients  $C^s$ , D and  $C^h$  can be identified using the interface and periodicity conditions:

• Continuity of  $\chi_{12}^p$  at  $x = \pm s/2$ :

$$C^{s} \cosh\left(\omega^{s} \frac{s}{2}\right) + D = C^{h} \cosh\left(\omega^{h} \frac{h}{2}\right)$$
(1)

• Continuity of the double traction,  $m_{12} = -M_{13}$  at  $x = \pm s/2$ :

$$A^{s}\omega^{s}C^{s}\sinh\left(\omega^{s}\frac{s}{2}\right) = -A^{h}\omega^{h}C^{h}\sinh\left(\omega^{h}\frac{h}{2}\right)$$
(2)

## Simple shear of a two-phase laminate

• Periodicity of displacement component *u*<sub>2</sub>. We have the constant stress component

$$\sigma_{12} = \mu(\bar{\gamma} - \gamma + u_{2,1})$$

whose value is obtained from the plasticity criterion in the soft phase:

$$\sigma_{12} = \tau_c + H\gamma_{cum} - A^s \chi_{12,11}^{ps}$$

$$u_{2,1}^{s} = \frac{\sigma_{12}}{\mu} - \bar{\gamma} + \gamma = \frac{\tau_{c}}{\mu} - \bar{\gamma} + \frac{A^{s} \omega^{s2} C^{s}}{H} \cosh\left(\omega^{s} x\right) + \frac{H + \mu}{\mu} D$$

in the soft phase and

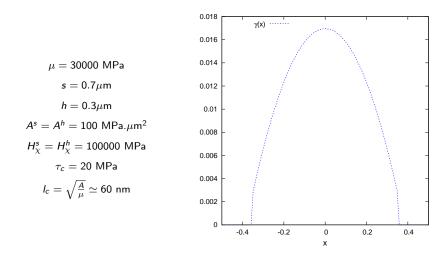
$$u_{2,1}^h = \frac{\sigma_{12}}{\mu} - \bar{\gamma} = \frac{\tau_c}{\mu} - \bar{\gamma} + \frac{H}{\mu}D$$

in the hard phase. The average on the whole structure,

$$\int_{-(s+h)/2}^{(s+h)/2} u_{2,1} \, dx = 0$$

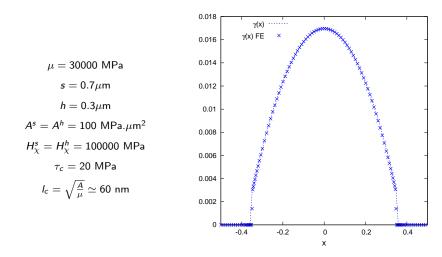
must vanish for periodicity reasons and gives

$$\left(\frac{\tau_c}{\mu} - \bar{\gamma}\right)(s+h) + \frac{2A^s\omega^s C^s}{H}\sinh\left(\omega^s \frac{s}{2}\right) + \frac{H(s+h) + \mu s}{\mu}D = 0 \quad (3)$$



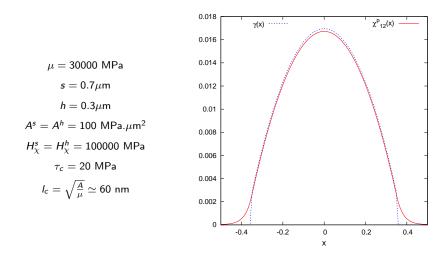
#### Size effect in a two-phase single crystal laminate

39/54



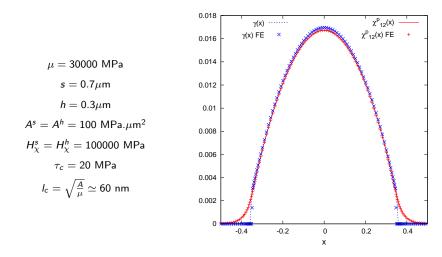
#### Size effect in a two-phase single crystal laminate

39/54



#### Size effect in a two-phase single crystal laminate

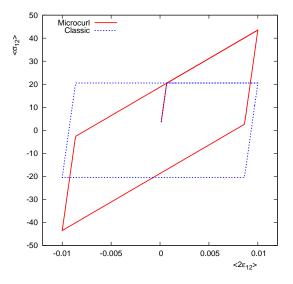
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#### Size effect in a two-phase single crystal laminate

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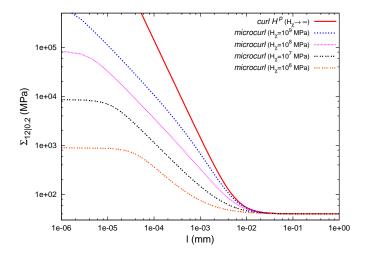
## **Overall cyclic response**



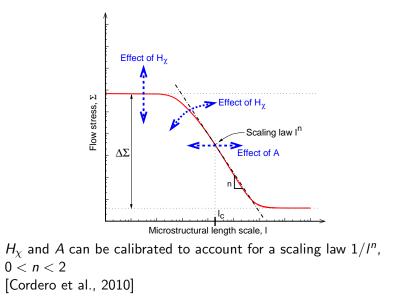
#### Size effect in a two-phase single crystal laminate

40/54

## **Size effects**



## **Size effects**



# Plan

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## 2 Size effect in a two-phase single crystal laminate

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## 3 Grain size effect in polycrystalline aggregates

- Hall–Petch effect
- Strain localization in ultra-fine grains

## Strain gradient plasticity as a limit case

• Size effect according to SGP

$$\lim_{H_{\chi}\to\infty}\Sigma_{12}=\tau_{c}+\frac{12A^{s}\langle\gamma\rangle}{f_{s}^{s}l^{2}}$$

physical meaning of a  $1/l^2$  scaling law?

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# Boundary value problem for micromorphic crystals

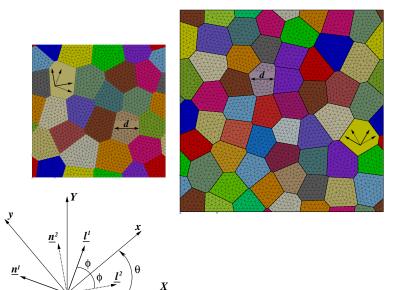
- Shear test
- Periodic grains with random orientations
- Periodic mesh
- Periodic boundary conditions: <u>u</u>(x) = <u>E</u>.<u>x</u> + <u>v</u>(x), <u>v</u> periodic <u>x</u><sup>p</sup>(x) periodic
- 2 slip systems / grain
- The grain size *d* is ranging from tens of nanometers to hundreds of microns.



- $E=70000~{
  m MPa}$ u=0.3
- $A = 0.01 \mathrm{MPa.mm^2}$  $H_\chi = 10^6 \mathrm{MPa}$

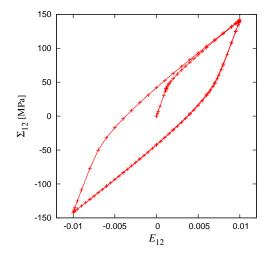
Intrinsic length scale:  $l_c = \sqrt{\frac{A}{H_{\chi}}} = 0.1 \mu m$ 

# Boundary value problem for micromorphic crystals



Grain size effect in polycrystalline aggregates

## Boundary value problem for micromorphic crystals



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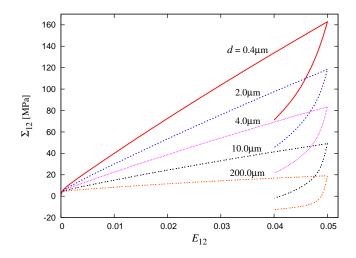
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- Boundary value problem
- Interface conditions
- Strain gradient plasticity as a limit case

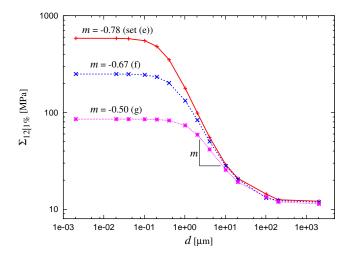
# Grain size effect in polycrystalline aggregates

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- Strain localization in ultra-fine grains

## **Grain size effect**



## Grain size effect



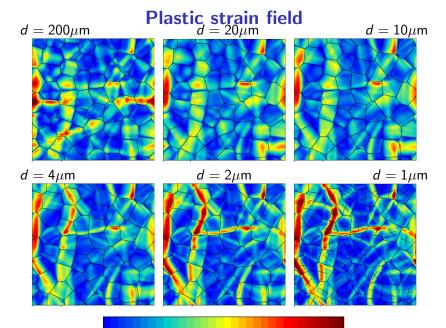
# Plan

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- Kinematics and balance equations
- Constitutive equations
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# Grain size effect in polycrystalline aggregates Hall–Petch effect

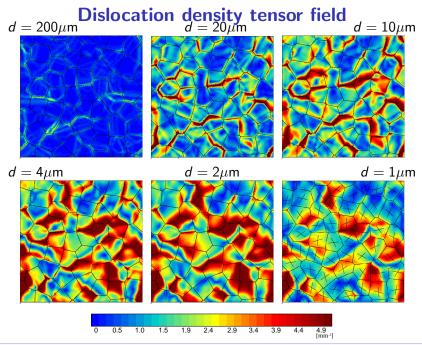
• Strain localization in ultra-fine grains



0 0.004 0.008 0.012 0.015 0.019 0.023 0.027 0.031 0.035 0.039

#### Grain size effect in polycrystalline aggregates

#### 53/54



Grain size effect in polycrystalline aggregates

Cordero N.M., Gaubert A., Forest S., Busso E., Gallerneau F., and Kruch S. (2010).

Size effects in generalised continuum crystal plasticity for two-phase laminates.

Journal of the Mechanics and Physics of Solids, vol. 58, pp 1963–1994.



Forest S. (2009).

The micromorphic approach for gradient elasticity, viscoplasticity and damage.

ASCE Journal of Engineering Mechanics, vol. 135, pp 117–131.

Forest S. and Sievert R. (2003). Elastoviscoplastic constitutive frameworks for generalized continua.

Acta Mechanica, vol. 160, pp 71-111.

Forest S. and Sievert R. (2006). Nonlinear microstrain theories.

International Journal of Solids and Structures, vol. 43, pp 7224–7245.

Germain P. (1973).

*The method of virtual power in continuum mechanics. Part 2 : Microstructure.* 

SIAM J. Appl. Math., vol. 25, pp 556–575.

Gurtin M.E. (2002).

A gradient theory of single–crystal viscoplasticity that accounts for geometrically necessary dislocations. Journal of the Mechanics and Physics of Solids, vol. 50, pp 5–32.

Gurtin M.E. and Anand L. (2009).
 Thermodynamics applied to gradient theories involving the accumulated plastic strain: The theories of Aifantis and Fleck & Hutchinson and their generalization.
 Journal of the Mechanics and Physics of Solids, vol. 57, pp 405–421.

Sedláček R. and Forest S. (2000).

Non-local plasticity at microscale : A dislocation-based model and a Cosserat model.

physica status solidi (b), vol. 221, pp 583-596.

Steinmann P. (1996).

Views on multiplicative elastoplasticity and the continuum theory of dislocations.

International Journal of Engineering Science, vol. 34, pp 1717–1735.