Strain gradient and micromorphic plasticity

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- Mechanics of generalized continua
- 2 Strain gradient plasticity theory
 - Method of virtual power
 - Constitutive equations
 - Shearing of a laminate microstructure

3 Micromorphic plasticity theory

- Balance and constitutive equations
- Rate-independent plasticity
- Shearing of a laminate microstructure

4 Discussion

Notations

Cartesian basis

 $\underline{\mathbf{A}} = A_i \underline{\mathbf{e}}_i, \quad \underline{\mathbf{A}} = A_{ij} \underline{\mathbf{e}}_i \otimes \underline{\mathbf{e}}_j, \quad \underline{\underline{\mathbf{A}}} = \underline{\underline{\mathbf{A}}} = \underline{\underline{\mathbf{A}}} = A_{ijk} \underline{\mathbf{e}}_i \otimes \underline{\mathbf{e}}_j \otimes \underline{\mathbf{e}}_k$

tensor products

$$\underline{\mathbf{a}} \otimes \underline{\mathbf{b}} = a_i b_j \, \underline{\mathbf{e}}_i \otimes \underline{\mathbf{e}}_j, \quad \underbrace{\mathbf{A}}_{\sim} \otimes \underbrace{\mathbf{B}}_{\sim} = A_{ij} B_{kl} \, \underline{\mathbf{e}}_i \otimes \underline{\mathbf{e}}_j \otimes \underline{\mathbf{e}}_k \otimes \underline{\mathbf{e}}_l$$
$$\underbrace{\mathbf{A}}_{\sim} \boxtimes \underbrace{\mathbf{B}}_{\sim} = A_{ik} B_{jl} \, \underline{\mathbf{e}}_i \otimes \underline{\mathbf{e}}_j \otimes \underline{\mathbf{e}}_k \otimes \underline{\mathbf{e}}_l$$

contractions

$$\underline{\mathbf{A}} \cdot \underline{\mathbf{B}} = A_i B_i, \quad \underline{\mathbf{A}} : \underline{\mathbf{B}} = A_{ij} B_{ij}, \quad \underline{\mathbf{A}} : \underline{\mathbf{B}} = A_{ijk} B_{ijk}$$

nabla operators

$$\nabla_{x} = {}_{,i} \underline{\mathbf{e}}_{i}, \quad \nabla_{X} = {}_{,l} \underline{\mathbf{E}}_{l}$$
$$\underline{\mathbf{u}} \otimes \nabla = u_{i,j} \underline{\mathbf{e}}_{i} \otimes \underline{\mathbf{e}}_{j}, \quad \underline{\sigma} \cdot \nabla = \sigma_{ij,j} \underline{\mathbf{e}}_{i}$$

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Mechanics of generalized continua

Principle of local action: the stress state at a point <u>X</u> depends on variables defined at this point only [Truesdell, Toupin, 1960] [Truesdell, Noll, 1965]



Mechanics of generalized continua



Introduction

Mechanics of generalized continua

Simple material: A material is simple at the particle \underline{X} if and only if its response to deformations homogeneous in a neighborhood of \underline{X} determines uniquely its response to every deformation at \underline{X} . [Truesdell, Toupin, 1960] [Truesdell, Noll, 1965]

simple material Cauchy continuum (1823) (classical / Boltzmann) Cosserat (1909) <u>u</u>, R local medium of order a micromorphic action [Eringen, Mindlin 1964] non simple <u>u</u>, χ Continuous material second gradient [Mindlin, 1965] medium $F, F \otimes \nabla$ Medium of grade n gradient of internal variable [Maugin, 1990] \underline{u}, α nonlocal nonlocal theory: integral formulation [Eringen, 1972] action

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Power of internal forces

• Model variables according to a first gradient theory

$$MODEL = \{ \underline{\mathbf{v}}, \underline{\mathbf{v}} \otimes \boldsymbol{\nabla}, \dot{\boldsymbol{p}}, \boldsymbol{\nabla} \dot{\boldsymbol{p}} \}$$

velocity $\underline{\mathbf{v}}$ and cumulative plastic strain p are assumed to be independent degrees of freedom

- Virtual power of internal forces of a subdomain $\mathcal{D} \subset \mathcal{B}$ of the body

$$\mathcal{P}^{(i)}(\underline{\mathbf{v}}^*,\dot{p}^*) = \int_{\mathcal{D}} p^{(i)}(\underline{\mathbf{v}}^*,\dot{p}^*) \, dV$$

simple stress tensor $\underline{\sigma}$, generalized stresses *a* (unit MPa), <u>b</u> (unit MPa.mm), microforces according to [Gurtin, 2002]

• The virtual power density of internal forces is a linear form on the fields of virtual modeling variables

$$p^{(i)} = \mathbf{\sigma} : (\mathbf{v}^* \otimes \mathbf{\nabla}) + a \dot{p}^* + \mathbf{b} \cdot \mathbf{\nabla} \dot{p}^*$$

• The virtual power density of internal forces is invariant with respect to superimposed rigid body motion $\Rightarrow \sigma$ is symmetric [Germain, 1973a]

Power of contact forces

• Application of Gauss theorem to the power of internal forces

$$\int_{\mathcal{D}} p^{(i)} dV = \int_{\partial \mathcal{D}} \underline{\mathbf{v}}^* \cdot \underline{\boldsymbol{\sigma}} \cdot \underline{\mathbf{n}} \, dS + \int_{\partial \mathcal{D}} \dot{p}^* \underline{\mathbf{b}} \cdot \underline{\mathbf{n}} \, dS$$
$$- \int_{\mathcal{D}} \underline{\mathbf{v}}^* \cdot \underline{\boldsymbol{\sigma}} \cdot \nabla \, dV - \int_{\mathcal{D}} \dot{p}^* \left(\underline{\mathbf{b}} \cdot \nabla - a\right) dV$$

The form of the previous boundary integral dictates the form of the

• power of contact forces acting on the boundary $\partial \mathcal{D}$ of the subdomain $\mathcal{D}\subset \mathcal{B}$

$$\mathcal{P}^{(c)}(\underline{\mathbf{v}}^{*},\dot{p}^{*}) = \int_{\partial \mathcal{D}} p^{(c)}(\underline{\mathbf{v}}^{*},\dot{p}^{*}) \, dS$$
$$p^{(c)}(\underline{\mathbf{v}}^{*},\dot{p}^{*}) = \underline{\mathbf{t}} \cdot \underline{\mathbf{v}}^{*} + a_{c}\dot{p}^{*}$$

simple traction $\underline{\mathbf{t}}$ (unit MPa), double traction a_c (unit MPa.mm)

Power of forces acting at a distance

$$\mathcal{P}^{(e)}(\underline{\mathbf{v}}^*, \dot{p}^*) = \int_{\mathcal{D}} p^{(e)}(\underline{\mathbf{v}}^*, \dot{p}^*) \, dV$$
$$p^{(e)}(\underline{\mathbf{v}}^*, \dot{p}^*) = \underline{\mathbf{f}} \cdot \underline{\mathbf{v}}^* + \underline{\mathbf{c}} : (\underline{\mathbf{v}}^* \otimes \nabla) + a_e \dot{p}^* + \underline{\mathbf{b}}_e \cdot \nabla \dot{p}^*$$
simple body forces $\underline{\mathbf{f}}$ (unit N.mm⁻³), double body forces $\underline{\mathbf{c}}$ and a_e (unit N.mm⁻²), triple body force $\underline{\mathbf{b}}_e$ (unit N.mm⁻¹)

$$\mathcal{P}^{(e)}(\underline{\mathbf{v}}^{*},\dot{p}^{*}) = \int_{\partial \mathcal{D}} \left(\underline{\mathbf{v}} \cdot \underline{\mathbf{c}} \cdot \underline{\mathbf{n}} + \dot{p}^{*} \underline{\mathbf{b}}_{e} \cdot \underline{\mathbf{n}} \right) dS$$
$$- \int_{\mathcal{D}} \left(\underline{\mathbf{v}}^{*} \cdot \left(\underline{\mathbf{c}} \cdot \nabla - \underline{\mathbf{f}} \right) dV + \dot{p}^{*} \left(\underline{\mathbf{b}}_{e} \cdot \nabla - a_{e} \right) \right) dV$$

Principle of virtual power

In the static case, $\forall \underline{v}^*, \forall \dot{p}^*, \forall \mathcal{D} \subset \mathcal{B}$,

$$\mathcal{P}^{(i)}(\underline{\mathbf{v}}^*,\dot{p}^*) = \mathcal{P}^{(c)}(\underline{\mathbf{v}}^*,\dot{p}^*) + \mathcal{P}^{(e)}(\underline{\mathbf{v}}^*,\dot{p}^*)$$

[Germain, 1973b]

Principle of virtual power

In the static case, $\forall \underline{v}^*, \forall \dot{p}^*, \forall \mathcal{D} \subset \mathcal{B}$,

$$\mathcal{P}^{(i)}(\underline{\mathbf{v}}^{*},\dot{p}^{*})=\mathcal{P}^{(c)}(\underline{\mathbf{v}}^{*},\dot{p}^{*})+\mathcal{P}^{(e)}(\underline{\mathbf{v}}^{*},\dot{p}^{*})$$

which leads to

$$\int_{\partial \mathcal{D}} \underline{\mathbf{v}}^* \cdot (\underline{\mathbf{t}} - (\underline{\sigma} - \underline{\mathbf{c}}) \cdot \underline{\mathbf{n}}) + \dot{p}^* (\mathbf{a}_c - (\underline{\mathbf{b}} - \underline{\mathbf{b}}^e) \cdot \underline{\mathbf{n}}) \, dS$$

$$+\int_{\mathcal{D}} \underline{\mathbf{v}}^* \cdot \left(\left(\underline{\boldsymbol{\sigma}} - \underline{\mathbf{c}} \right) \cdot \boldsymbol{\nabla} + \underline{\mathbf{f}} \right) + \dot{\boldsymbol{p}}^* \left(\left(\underline{\mathbf{b}} - \underline{\mathbf{b}}_e \right) \cdot \boldsymbol{\nabla} - \boldsymbol{a} + \boldsymbol{a}_e \right) dV = 0$$

cf. [Germain, 1973b, Forest and Sievert, 2003, Kirchner and Steinmann, 2005, Lazar and Maugin, 2007, Hirschberger et al., 2007]

Balance and boundary conditions

The application of the principle of virtual power leads to the

• balance of momentum equation (static case)

$$(\underline{\sigma} - \underline{c}) \cdot \nabla + \underline{f} = 0, \quad \forall \underline{x} \in \mathcal{B}$$

balance of generalized moment of momentum equation (static case)

$$(\underline{\mathbf{b}} - \underline{\mathbf{b}}_{e}) \cdot \boldsymbol{\nabla} - \boldsymbol{a} + \boldsymbol{a}_{e} = 0, \quad \forall \underline{\mathbf{x}} \in \mathcal{B}$$

• boundary conditions

$$(\underline{\sigma} - \underline{c}) \cdot \underline{\mathbf{n}} = \underline{\mathbf{t}}, \quad \forall \underline{\mathbf{x}} \in \partial \mathcal{B}$$
$$(\underline{\mathbf{b}} - \underline{\mathbf{b}}_{e}) \cdot \underline{\mathbf{n}} = a_{c}, \quad \forall \underline{\mathbf{x}} \in \partial \mathcal{B}$$

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Continuum thermodynamics

• Enhance the local balance of energy and the entropy inequality

$$\rho \dot{\epsilon} = p^{(i)} - \operatorname{div} \mathbf{\underline{q}} + \rho r, \quad -\rho(\dot{\psi} + \eta \dot{T}) + p^{(i)} - \frac{\mathbf{\underline{q}}}{T} \cdot \nabla T \ge 0$$

• Decomposition of total strain

$$egin{aligned} & \underline{\mathbf{v}} = \dot{\underline{\mathbf{u}}} \,, \quad & \varepsilon = rac{1}{2} (\underline{\mathbf{u}} \otimes oldsymbol{
abla} + oldsymbol{
abla} \otimes \underline{\mathbf{v}} \,) \ & \varepsilon = arepsilon^e + arepsilon^p \end{aligned}$$

• Consider the constitutive functionals:

$$\begin{split} \psi &= \hat{\psi}(\underline{\varepsilon}^{e}, T, p, \alpha, \nabla p), \ \eta = \hat{\eta}(\underline{\varepsilon}^{e}, T, p, \alpha, \nabla p) \\ \underline{\sigma} &= \hat{\sigma}(\underline{\varepsilon}^{e}, T, p, \alpha, \nabla p) \\ a &= \hat{a}(\underline{\varepsilon}^{e}, T, p, \alpha, \nabla p), \quad \underline{\mathbf{b}} = \underline{\mathbf{\hat{b}}}(\underline{\varepsilon}^{e}, T, p, \alpha, \nabla p) \end{split}$$

State laws

Clausius–Duhem inequality (isothermal)

$$(\underline{\sigma} - \rho \frac{\partial \psi}{\partial \underline{\varepsilon}^{\mathbf{e}}}) : \underline{\dot{\varepsilon}}^{\mathbf{p}} + (\mathbf{a} - \rho \frac{\partial \psi}{\partial \mathbf{p}})\dot{\mathbf{p}} + (\underline{\mathbf{b}} - \rho \frac{\partial \psi}{\partial \boldsymbol{\nabla} \mathbf{p}}) \cdot \boldsymbol{\nabla} \dot{\mathbf{p}} + \underline{\sigma} : \underline{\dot{\varepsilon}}^{\mathbf{p}} - \rho \frac{\partial \psi}{\partial \alpha} \dot{\alpha} \ge \mathbf{0}$$

• Derive the state laws [Coleman and Noll, 1963]

 $\mathbf{g} = \rho \frac{\partial \hat{\psi}}{\partial \mathbf{r}^{e}}, \quad \mathbf{X} = \rho \frac{\partial \hat{\psi}}{\partial \alpha}, \quad \mathbf{R} = \frac{\partial \hat{\psi}}{\partial \mathbf{r}}, \quad \mathbf{b} = \frac{\partial \hat{\psi}}{\partial \mathbf{\nabla} \mathbf{r}}$

• Residual dissipation

$$D^{res} = {\mathbf \sigma}: \dot{\mathbf \varepsilon}^p + (\mathbf a - R) \dot{\mathbf p} - X \dot{lpha} \geq 0$$

Flow rule and evolution law

• Introduce an equivalent stress measure σ_{eq} such that

$$\underline{\sigma}: \dot{\underline{\varepsilon}}^{p} = \sigma_{eq}\dot{p}$$

which defines the cumulative plastic strain rate \dot{p}

$$D^{res} = (\sigma_{eq} + a - R)\dot{p} - X\dot{lpha} \ge 0$$

• Introduce the viscoplastic potential $\Omega(\sigma_{eq} + a - R, X)$ such that

$$\dot{\varepsilon}^{p} = \frac{\partial \Omega}{\partial (\sigma_{eq} + a - R)}, \quad \dot{\alpha} = -\frac{\partial \Omega}{\partial X}$$

 $\boldsymbol{\Omega}$ convex with respect to the first, concave with respect to the second variable for positive dissipation

• Rate-independent case; introduce the yield function

$$f(\mathbf{\sigma}, \mathbf{a}, \mathbf{R}) = \sigma_{eq} - \mathbf{R}_0 - \mathbf{R} + \mathbf{a}$$

where R_0 is the initial yield stress

$$\underline{\dot{\varepsilon}}^{p} = \dot{p} \frac{\partial f}{\partial \sigma}, \quad \sigma_{eq} = \underline{\sigma} : \frac{\partial f}{\partial \alpha}$$

Strain gradient plasticity theory

Specific constitutive equations

• Free energy function

$$\rho\psi(\boldsymbol{\varepsilon}^{e},\boldsymbol{p},\boldsymbol{\nabla}\boldsymbol{p}) = \frac{1}{2}\boldsymbol{\varepsilon}^{e}: \boldsymbol{\Lambda}: \boldsymbol{\varepsilon}^{e} + \frac{1}{2}H\boldsymbol{p}^{2} + \frac{1}{2}\boldsymbol{\nabla}\boldsymbol{p}\cdot\boldsymbol{\Lambda}: \boldsymbol{\nabla}\boldsymbol{p}$$

State laws

$$\underline{\sigma} = \underset{\approx}{\mathbf{\Lambda}} : \underline{\varepsilon}^{e}, \quad R = Hp, \quad \underline{\mathbf{b}} = \underline{\mathbf{A}} \cdot \boldsymbol{\nabla}p$$

• Balance of generalized momentum (homogeneous material)

$$a = \operatorname{div} \underline{\mathbf{b}} = \operatorname{div} \left(\underbrace{\mathbf{A}}_{\sim} \cdot \nabla p \right) = \underbrace{\mathbf{A}}_{\sim} : \left(\nabla \otimes \nabla p \right)$$

- Yield function $f(\sigma, R, a) = J_2(\sigma) R_0 Hp + a$
- Consistency condition; p is solution of a p.d.e.

$$(H + \frac{\partial f}{\partial \underline{\sigma}} : \bigwedge_{\approx} : \frac{\partial f}{\partial \underline{\sigma}})\dot{p} + \bigwedge_{\approx} : (\boldsymbol{\nabla} \otimes \boldsymbol{\nabla}\dot{p}) = \frac{\partial f}{\partial \underline{\sigma}} : \bigwedge_{\approx} : \dot{\underline{\xi}}$$

• Isotropic case + von Mises : Aifantis model [Aifantis, 1987]

$$\mathbf{A} = c^2 \mathbf{1}, \quad \sigma_{eq} = R_0 + Hp - c^2 \Delta p$$

Strain gradient plasticity theory

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Laminate microstructure under shear



Aifantis material in the white (soft) phase, purely elastic gray (hard) phase

• Form of the solution for imposed mean shear $\bar{\gamma}$

$$u_1 = \bar{\gamma} x_2, \quad u_2(x_1) = u(x_1), \quad u_3 = 0$$

unknown periodic functions $u(x_1), p(x_1)$

• Deformation gradient and strain

$$[\nabla \underline{\mathbf{u}}] = \begin{bmatrix} 0 & \bar{\gamma} & 0 \\ u_{,1} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \begin{bmatrix} \varepsilon \\ \varepsilon \end{bmatrix} = \begin{bmatrix} 0 & \frac{1}{2}(\bar{\gamma} + u_{,1}) & 0 \\ \frac{1}{2}(\bar{\gamma} + u_{,1}) & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

Strain gradient plasticity theory

Laminate microstructure under shear



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$$[\mathbf{\nabla}\underline{\mathbf{u}}] = \begin{bmatrix} 0 & \bar{\gamma} & 0\\ u_{,1} & 0 & 0\\ 0 & 0 & 0 \end{bmatrix}, \quad [\varepsilon] = \begin{bmatrix} 0 & \frac{1}{2}(\bar{\gamma} + u_{,1}) & 0\\ \frac{1}{2}(\bar{\gamma} + u_{,1}) & 0 & 0\\ 0 & 0 & 0 \end{bmatrix}$$

Resolution of the b.v.p.

Let us consider homogeneous isotropic elasticity and no hardening in the plastic phase for simplicity

- Equilibrium: homogeneous shear stress σ_{12} throughout the laminate
- Displacement in the hard phase

$$\sigma_{12} = \mu(\bar{\gamma} + u^h_{,1}) \implies u^h_{,1} = \mathcal{C}, \quad u^h = \mathcal{C}x_1 + \mathcal{D}$$

• Plastic strain in the soft phase

$$\dot{\varepsilon}^{p} = \frac{3}{2}\dot{p}\frac{\mathbf{s}}{J_{2}(\boldsymbol{\sigma})}, \quad \dot{\varepsilon}^{p} = \frac{\sqrt{3}}{2}\dot{p}(\mathbf{e}_{1}\otimes\mathbf{e}_{2} + \mathbf{e}_{2}\otimes\mathbf{e}_{1})$$

from the yield condition we get

$$\sigma_{12} = \mu(\bar{\gamma} + u_{,1}^h) \implies u_{,1}^h = C, \quad u^h = C x_1 + D$$

so that the plastic strain is parabolic

$$p = \frac{\alpha}{x_1^2} - \frac{s^2}{4})$$

• Continuity of plastic strain at the interface

 $p(\pm s/2) = 0$

Resolution of the b.v.p.

• Displacement in the soft phase

$$\sigma_{12} = \mu(\bar{\gamma} + u_{,1}^s - \sqrt{3}p) \implies u_{,1}^s = C + \sqrt{3}p$$
$$u^s = (C - \alpha\sqrt{3}\frac{s^2}{4})x_1 + \alpha\frac{\sqrt{3}}{3}x_1^3$$

Interface conditions

• Displacement continuity at $x_1 = \pm s/2$

$$u^{s}(\frac{s}{2}) = u^{h}(\frac{s}{2}) \implies -\sqrt{3}\alpha \frac{s^{3}}{12} = D$$

• Displacement periodicity at $x_1 = -s/2$ and $x_1 = s/2 + h$

$$u^{s}(-\frac{s}{2}) = u^{h}(\frac{s}{2}+h) \implies \sqrt{3\alpha}\frac{s^{3}}{12} = CI + D$$

• Continuity of the stress vector at $x_1 = \pm s/2$

$$R_0 - 2c\alpha = \mu\sqrt{3}(\bar{\gamma} + \mathbf{C})$$

The wanted constants are deduced from the previous equations

$$C = rac{R_0 - \sqrt{3}\mu\bar{\gamma}}{\sqrt{3}\mu + rac{12cl}{\sqrt{3}s^3}}, \quad D = -Crac{l}{2}, \quad lpha = -rac{12}{\sqrt{3}}rac{D}{s^3}$$

Plastic strain profile in the channel



• Characteristic length: $l_c = \sqrt{c/\mu} = 0.4 \ \mu$ m, leading to strong size effects in the micron range and below

Plastic strain profile in the channel



The higher order stress b₁ = 2cα experiences a jump at the interface s = ±s/2:

$$b_1(rac{s^+}{2}) - b_1(rac{s^-}{2}) = 0 - clpha s, \quad [\![b_1]\!](rac{s}{2}) = -clpha s$$

Strain gradient plasticity theory

Overall size effect

• Macroscopic stress strain relation

$$\frac{\sigma_{12}}{\mu} = \frac{1}{\mu f s^2 + 4c} \left(\frac{\sqrt{3}}{3} f s^2 R_0 + 4c\bar{\gamma} \right)$$

bilinear response depending explicitly on channel size s

• Macroscopic stress vs mean plastic strain;

$$\bar{p} = \frac{1}{l} \int_{-s/2}^{s/2} p(x_1) dx_1 \implies \sqrt{3}\bar{p} = f\bar{\gamma} - C(1-f) - f\frac{\sigma_{12}}{\mu}$$
$$\sigma_{12} = \frac{R_0}{\sqrt{3}} + \frac{4\sqrt{3}c}{f^3l^2}\bar{p}$$

- Limit cases
 - \star thick channels: size independent threshold $\sigma_{12}={\it R}_0/\sqrt{3}$
 - \star thin films: scaling law $\sigma_{12}/\bar{\it p}\sim 1/{\it I}^2$
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General scalar microstrain gradient plasticity

• Classical and generalized plasticity

 $DOF = \{\underline{\mathbf{u}}, p_{\chi}\} \quad STATE = \{\underline{\varepsilon}^{e}, p, \alpha, p_{\chi}, \nabla p_{\chi}\}$ scalar plastic microstrain variable p_{χ}

• Enhanced power of internal forces and extra balance equation $p^{(i)} = \boldsymbol{\sigma} : \boldsymbol{\dot{\varepsilon}} + \boldsymbol{a} \ \dot{\boldsymbol{p}}_{\chi} + \boldsymbol{\underline{b}} \cdot \boldsymbol{\nabla} \ \dot{\boldsymbol{p}}_{\chi}, \quad p^{(c)} = \boldsymbol{\underline{t}} \cdot \boldsymbol{\underline{\dot{u}}} + \boldsymbol{a}^c \ \dot{\boldsymbol{p}}_{\chi}$ $\operatorname{div} \boldsymbol{\underline{b}} - \boldsymbol{a} = \boldsymbol{0}, \quad \forall \boldsymbol{\underline{x}} \in \Omega, \quad \boldsymbol{\underline{b}} \cdot \boldsymbol{\underline{n}} = \boldsymbol{a}^c, \quad \forall \boldsymbol{\underline{x}} \in \partial \Omega$

General scalar microstrain gradient plasticity

• State laws

$$\begin{split} \boldsymbol{\varepsilon} &= \boldsymbol{\varepsilon}^{\mathbf{e}} + \boldsymbol{\varepsilon}^{\mathbf{p}} \\ \boldsymbol{\sigma} &= \rho \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}^{\mathbf{e}}}, \quad \boldsymbol{R} = \rho \frac{\partial \psi}{\partial \boldsymbol{p}}, \quad \boldsymbol{X} = \rho \frac{\partial \psi}{\partial \alpha} \\ \boldsymbol{a} &= \rho \frac{\partial \psi}{\partial \boldsymbol{p}_{\chi}} + \boldsymbol{a}^{\mathbf{v}}, \quad \underline{\mathbf{b}} = \rho \frac{\partial \psi}{\partial \boldsymbol{\nabla} \boldsymbol{p}_{\chi}} \end{split}$$

• Evolution laws $D^{res} = \sigma : \dot{\varepsilon}^p + (a^v - R)\dot{p} - X\dot{\alpha} \ge 0$

$$\dot{\varepsilon}^{p} = \dot{\lambda} \frac{\partial f}{\partial \sigma}, \quad \dot{p} = -\dot{\lambda} \frac{\partial f}{\partial R}, \quad \dot{\alpha} = -\dot{\lambda} \frac{\partial f}{\partial X}$$

[Forest, 2009]

Explicit constitutive equations

• Quadratic free energy potential

$$\rho\psi(\boldsymbol{\varepsilon}^{e},\boldsymbol{p},\boldsymbol{p}_{\chi},\boldsymbol{\nabla}\boldsymbol{p}_{\chi}) = \frac{1}{2}\boldsymbol{\varepsilon}^{e}: \boldsymbol{\wedge} : \boldsymbol{\varepsilon}^{e} + \frac{1}{2}H\boldsymbol{p}^{2} + \frac{1}{2}H\boldsymbol{\chi}(\boldsymbol{p}-\boldsymbol{p}_{\chi})^{2} + \frac{1}{2}\boldsymbol{\nabla}\boldsymbol{p}_{\chi}.\boldsymbol{\wedge} :\boldsymbol{\nabla}\boldsymbol{p}_{\chi}$$

[Forest, 2009, Dimitrijevic and Hackl, 2011]

• Constitutive equations

$$\underline{\sigma} = \underline{\Lambda}_{\approx} : \underline{\varepsilon}^{e}, \ a = -H_{\chi}(p - p_{\chi}), \ \underline{\mathbf{b}} = \underline{\mathbf{A}} \cdot \boldsymbol{\nabla} p_{\chi}, \ R = (H + H_{\chi})p - H_{\chi}p_{\chi}$$

Substitution of constitutive into extra balance equations

$$p_{\chi} - rac{1}{H_{\chi}} \operatorname{div}\left(\mathbf{A} \cdot \nabla p_{\chi}\right) = p$$

Homogeneous and isotropic materials

 $\mathbf{A} = A\mathbf{1}$

$$p_{\chi} - \frac{A}{H_{\chi}} \Delta p_{\chi} = p$$
, b.c. $\underline{\mathbf{b}} \cdot \underline{\mathbf{n}} = A \nabla p_{\chi} \cdot \underline{\mathbf{n}} = a^{2}$

same p.d.e. as in the *implicit gradient–enhanced* elastoplasticity with $a^c = 0$ [Engelen et al., 2003]

Link to Aifantis strain gradient plasticity

• Yield function

$$f(\sigma, R) = \sigma_{eq} - R_0 - R$$

• Hardening law

$$R = \frac{\partial \psi}{\partial p} = (H + H_{\chi})p - H_{\chi}p_{\chi}$$

• Under plastic loading

$$\sigma_{eq} = R_0 + Hp_{\chi} - A(1 + \frac{H}{H_{\chi}})\Delta p_{\chi}$$

compare with Aifantis model [Aifantis, 1987]

$$\sigma_{eq} = R_0 + R(p) - c^2 \Delta p$$

The equivalence is obtained for $H_{\chi} = \infty$ (internal constraint):

$$p_{\chi} \simeq p, \quad A = c^2$$

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Consistency condition

Consistency condition

$$\dot{f} = \frac{\partial f}{\partial \varphi} : \dot{\varphi} + \frac{\partial f}{\partial R} \dot{R}$$

$$= \frac{\partial \sigma_{eq}}{\partial \sigma} : \bigwedge_{\approx} : (\dot{\xi} - \dot{\xi}^{p}) - \frac{\partial R}{\partial p} \dot{p} - \frac{\partial R}{\partial p_{\chi}} \dot{p}_{\chi} = 0$$

Plastic multiplier

$$\dot{p} = \frac{\underbrace{\mathbb{N}} : \bigwedge_{\approx} : \dot{\underline{e}} - \frac{\partial R}{\partial p_{\chi}} \dot{p}_{\chi}}{\underbrace{\mathbb{N}} : \bigwedge_{\approx} : \underbrace{\mathbb{N}} + \frac{\partial R}{\partial p}}, \quad \text{with} \quad \underbrace{\mathbb{N}} = \frac{\partial \sigma_{eq}}{\partial \underline{\sigma}}$$

where $\dot{\varepsilon}$ and \dot{p}_{χ} are controllable variable.

• Even though the yield condition can be written as a partial differential equation, there is no need for a variational formulation of the consistency condition contrary to [Mühlhaus and Aifantis, 1991, Liebe et al., 2001]. There is no need for a plastic front tracking technique. The plastic microstrain p_{χ} and the generalized traction $\underline{\mathbf{b}} \cdot \underline{\mathbf{n}}$ are continuous across the elastic/plastic domain.

Thermal effects

• For temperature dependent parameters

$$a = \operatorname{div} \underline{\mathbf{b}} = \operatorname{div} (A \nabla p_{\chi}) = A \Delta p_{\chi} + \frac{\partial A}{\partial T} \nabla T \cdot \nabla p_{\chi}$$
$$p_{\chi} - \frac{A}{H_{\chi}} \Delta p_{\chi} - \frac{1}{H_{\chi}} \frac{\partial A}{\partial T} \nabla T \cdot \nabla p_{\chi} = p$$

• Consistency condition

$$\dot{p} = \frac{\underbrace{\aleph}: \bigwedge_{\approx}: (\dot{\varepsilon} - \dot{\varepsilon}^{th}) - \frac{\partial R}{\partial p_{\chi}} \dot{p}_{\chi} - \frac{\partial R}{\partial T} \dot{T}}{\underbrace{\aleph}: \bigwedge_{\approx}: \aleph + \frac{\partial R}{\partial p}}$$

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Laminate microstructure under shear

Unit cell of a periodic two-phase laminate l = s + h $0 \longrightarrow 1$ s h

Micromorphic material in the white (soft) phase, purely elastic micromorphic gray (hard) phase

• Form of the solution for impose mean shear $\bar{\gamma}$

$$u_1 = \bar{\gamma} x_2, \ u_2(x_1) = u(x_1), \ u_3 = 0$$

unknown periodic functions $u(x_1), p(x_1), p_{\chi}(x_1)$

• Deformation gradient and strain

$$[\mathbf{\nabla}\underline{\mathbf{u}}] = \begin{bmatrix} 0 & \bar{\gamma} & 0\\ u_{,1} & 0 & 0\\ 0 & 0 & 0 \end{bmatrix}, \quad [\varepsilon] = \begin{bmatrix} 0 & \frac{1}{2}(\bar{\gamma} + u_{,1}) & 0\\ \frac{1}{2}(\bar{\gamma} + u_{,1}) & 0 & 0\\ 0 & 0 & 0 \end{bmatrix}$$

Micromorphic plasticity theory

Resolution of the b.v.p.

Let us consider homogeneous isotropic elasticity, homogeneous $H_{\!\chi}$ and no hardening in the plastic phase for simplicity

• The shear stress is uniform throughout the laminate and takes the value

$$\sqrt{3}\sigma_{12} = R_0 + R = R_0 + H_{\chi}(p - p_{\chi}) = R_0 - Ap_{\chi,11}$$

 Derivation of the previous equations with respect to x₁ shows that p_{χ,111} = 0 which leads to the parabolic profile of the micro-plastic deformation in the soft phase

$$p_{\chi}(x) = \frac{\alpha x^2 + \beta}{2}, \quad \forall |x| \leq \frac{s}{2}$$

Note that

$$\sqrt{3}\sigma_{12} = R_0 - 2A\alpha$$

• The parabolic plastic strain profile follows

$$p = \frac{\alpha x^2 + \beta}{H_{\chi}} - \frac{2A}{H_{\chi}}$$

Resolution of the b.v.p.

A new feature of the model is that the microplastic strain p_{χ} does not vanish in general in the hard phase, whereas p does:

$$p_{\chi} - \frac{A^h}{H_{\chi}} \Delta p_{\chi} = 0$$

$$p_{\chi}^{h} = \frac{\alpha_{h}}{\cosh \omega_{h}} (x - \frac{l}{2}), \quad \frac{s}{2} \le x \le \frac{s}{2} + h, \quad \text{with} \quad \omega_{h}^{2} = \frac{H_{\chi}}{A_{h}}$$

the p_{χ}^{h} profile is of hyperbolic nature

Interface conditions

• Continuity of micro-plastic deformation at x = s/2:

$$\alpha \frac{s^2}{4} + \beta = \alpha_h \cosh \omega_h \frac{h}{2}$$

• Continuity of the generalized stress component *b*₁:

$$A\alpha s = -A_h \alpha_h \omega_h \sinh \omega_h \frac{h}{2}$$

Interface conditions

The displacement in the plastic and elastic phases can be expressed as

$$u^{s} = \alpha \frac{x^{3}}{\sqrt{3}} + \left(\sqrt{3}\beta - \bar{\gamma} + \frac{R_{0}}{\sqrt{3}\mu} - 2A\alpha(\frac{1}{\sqrt{3}\mu} + \frac{\sqrt{3}}{H_{\chi}})\right) \times u^{h} = \left(\frac{1}{\sqrt{3}\mu}(R_{0} - 2A\alpha) - \bar{\gamma}\right) \times + C$$

They are used to exploit two additional interface conditions

 Continuity of the displacement at x = s/2: u^s(s/2) = u^h(s/2)

$$lpha rac{s^3}{8\sqrt{3}\mu} + \sqrt{3}(eta - rac{2Alpha}{H_\chi})rac{s}{2} = C$$

• Periodicity of the displacement component $u^{s}(-s/2) = u^{h}(s/2 + h)$

$$-(\frac{\sigma_{12}}{\mu}-\bar{\gamma})I+\sqrt{3}(\beta+\frac{2A\alpha}{H_{\chi}})\frac{s}{2}-\alpha\frac{s^{3}}{8\sqrt{3}}=C$$

Plastic strain profiles in the channel



μ (MPa)	$R_0~({ m MPa})$	H_χ (MPa)	A (MPa.mm ²)	f	/ (μm)	$ar{\gamma}$
30000	20	50000	0.005	0.7	10	0.01

Overall size effect

The scaling law results from the expression of the overall stress σ_{12} as a function of the mean plastic strain over the unit cell:

$$\bar{p} = \frac{1}{I} \int_{-\frac{s}{2}}^{\frac{s}{2}} (\alpha x^2 + \beta - \frac{2A\alpha}{H_{\chi}}) \, dx = \frac{\beta}{I} f \left(1 - \frac{1}{L^2} \left(\frac{s^2}{12} - \frac{2A}{H_{\chi}} \right) \right)$$

with $L^2 = \frac{s^2}{4} + \frac{A}{A_h} \frac{s}{\omega_h} \operatorname{cotanh}(\omega_h \frac{h}{2}) = -\frac{\beta}{\alpha}$. The uniform stress component can now be expressed as a function of the volume fraction f of the soft phase and of the unit cell size I:

$$\sqrt{3}\sigma_{12} = R_0 + \frac{2A}{f} \frac{\bar{p}}{\frac{f^2 l^2}{6} + \frac{2A}{H_{\chi}} + \frac{A}{A_h} \frac{fl}{\omega_h} \operatorname{cotanh}\left(\omega_h \frac{h}{2}\right)}$$

displaying a size-dependent overall linear hardening

Scaling laws

Two limit cases naturally arise

- Internal constraint $H_{\chi} \to \infty$ for which the strain gradient plasticity model is retrieved
- Unit cell size $I \rightarrow 0$ leads to saturation stress

$$\sqrt{3}\sigma_{12} - R_0 \sim H_{\chi} \frac{1-f}{f}\bar{p}$$



Micromorphic plasticity theory

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Main comments

- The choice of quadratic potentials with respect to strain gradients leads to the existence of a size dependent overall linear hardening modulus in a laminate microstructure
- The corresponding scaling law according to Aifantis strain gradient plasticity (one new material parameter) is $1/l^2$
- In contrast the micromorphic model (two new material parameters) leads to a saturation at nano-scales
- Physical metallurgy hints rather at scaling laws of the Orowan (1/l) or Hall-Petch $(1/\sqrt{l})$ types

Needed improvements

• Improve constitutive equations; for instance

$$\rho\psi(\boldsymbol{\nabla}\boldsymbol{p}) = \sqrt{\boldsymbol{\nabla}\boldsymbol{p}\cdot\boldsymbol{A}\cdot\boldsymbol{\nabla}\boldsymbol{p}}$$

[Conti and Ortiz, 2005, Okumura et al., 2007]

- Add higher order dissipative parts [Forest, 2009, Anand et al., 2012]
- Enhance interface conditions [Gurtin and Needleman, 2005, Acharya, 2007, Gurtin and Anand, 2008]

Extension to crystal plasticity

 In crystal plasticity, the relevant variable is not the gradient of the cumulative plastic strain but rather the dislocation density tensor

$$\underline{\mathsf{\Gamma}} = -\mathrm{curl}\,\underline{\mathsf{H}}^{\rho}, \quad \underline{\mathsf{H}} = \underline{\mathsf{u}}\,\otimes \boldsymbol{\nabla} = \underline{\mathsf{H}}^{e} + \underline{\mathsf{H}}^{\rho}$$

[Cermelli and Gurtin, 2001, Svendsen, 2002] but no effects in laminates...

- A strain gradient and a micromorphic theory can be designed based on the introduction of the dislocation density tensor in the free energy function [Aslan et al., 2011]
- Similar effects arise in laminate microstructures but the overall linear hardening is of kinematic nature

 $x = \operatorname{curl}\operatorname{curl} \underline{\mathsf{H}}^{p} : \underline{\mathbf{m}} \otimes \underline{\mathbf{n}}$

[Cordero et al., 2010, Cottura et al., 2012]

 Hall-Petch related size effects can be predicted in polycrystals based on full field simulations [Forest et al., 2000, Bayley et al., 2007, Neff et al., 2009, Bargmann et al., 2010, Cordero et al., 2012, Wulfinghoff and Boehlke, 2012]

• Constitutive equations are still unrealistic...

Acharya A. (2007).

Jump condition for GND evolution as a constraint on slip transmission at grain boundaries.

Philosophical Magazine, vol. 87, pp 1349–1359.

- Aifantis E.C. (1987).
 The physics of plastic deformation.
 International Journal of Plasticity, vol. 3, pp 211–248.

Anand L., Aslan O., and Chester S.A. (2012). A large-deformation gradient theory for elastic-plastic materials: Strain softening and regularization of shear bands. International Journal of Plasticity, vol. 30–31, pp 116–143.

Aslan O., Cordero N. M., Gaubert A., and Forest S. (2011). *Micromorphic approach to single crystal plasticity and damage*. International Journal of Engineering Science, vol. 49, pp 1311–1325.



Bargmann S., Ekh M., Runesson K., and Svendsen B. (2010).

Modeling of polycrystals with gradient crystal plasticity: A comparison of strategies. Philosophical Magazine, vol. 90, pp 1263–1288.

Bayley C.J., Brekelmans W.A.M., and Geers M.G.D. (2007). A three-dimensional dislocation field crystal plasticity approach applied to miniaturized structures. Philosophical Magazine, vol. 87, pp 1361–1378.

- Cermelli P. and Gurtin M.E. (2001).
 On the characterization of geometrically necessary dislocations in finite plasticity.
 Journal of the Mechanics and Physics of Solids, vol. 49, pp 1539–1568.
 - Coleman B.D. and Noll W. (1963).

The thermodynamics of elastic materials with heat conduction and viscosity.

Arch. Rational Mech. and Anal., vol. 13, pp 167-178.

Conti S. and Ortiz M. (2005).

Dislocation Microstructures and the Effective Behavior of Single Crystals. Arch. Rational Mech. Anal., vol. 176, pp 103–147.

 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.

Cordero N. M., Forest S., and Busso E. P. (2012). Generalised continuum modelling of grain size effects in polycrystals.

Comptes Rendus Mécanique, vol. 340, pp 261–274.

 Cottura M., Le Bouar Y., Finel A., Appolaire B., Ammar K., and Forest S. (2012).
 A phase field model incorporating strain gradient viscoplasticity: application to rafting in Ni-base superalloys. Journal of the Mechanics and Physics of Solids, vol. 60, pp 1243–1256.

- Dimitrijevic B.J. and Hackl K. (2011).
 A regularization framework for damageplasticity models via gradient enhancement of the free energy.
 Int. J. Numer. Meth. Biomed. Engng., vol. 27, pp 1199–1210.
- Engelen R.A.B., Geers M.G.D., and Baaijens F.P.T. (2003).
 Nonlocal implicit gradient-enhanced elasto-plasticity for the modelling of softening behaviour.
 International Journal of Plasticity, vol. 19, pp 403–433.

Forest S. (2009).

The micromorphic approach for gradient elasticity, viscoplasticity and damage.

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

Forest S., Barbe F., and Cailletaud G. (2000). Cosserat Modelling of Size Effects in the Mechanical Behaviour of Polycrystals and Multiphase Materials.

International Journal of Solids and Structures, vol. 37, pp 7105–7126.

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

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

Germain P. (1973a).

La méthode des puissances virtuelles en mécanique des milieux continus, première partie : théorie du second gradient. J. de Mécanique, vol. 12, pp 235–274.

- Germain P. (1973b).

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. (2008).

Nanocrystalline grain boundaries that slip and separate: A gradient theory that accounts for grain-boundary stress and conditions at a triple-junction.

Journal of the Mechanics and Physics of Solids, vol. 56, pp 184–199.

- Gurtin M.E. and Needleman A. (2005). Boundary conditions in small-deformation, single-crystal plasticity that account for the Burgers vector. Journal of the Mechanics and Physics of Solids, vol. 53, pp 1-31.
- Hirschberger C.B., Kuhl E., and Steinmann P. (2007).
 On deformational and configurational mechanics of micromorphic hyperelasticity - Theory and computation.
 Computer Methods in Applied Mechanics and Engineering, vol. 196, pp 4027–4044.

Kirchner N. and Steinmann P. (2005). A unifying treatise on variational principles for gradient and micromorphic continua. Philosophical Magazine, vol. 85, pp 3875–3895.

- Lazar M. and Maugin G. A. (2007).
 On microcontinuum field theories: the Eshelby stress tensor and incompatibility conditions.
 Philosophical Magazine, vol. 87, pp 3853–3870.
- Liebe T., Steinmann P., and Benallal A. (2001).
 Theoretical and computational aspects of a thermodynamically consistent framework for geometrically linear gradient damage.
 Comp. Methods Appli. Mech. Engng, vol. 190, pp 6555–6576.
- Mühlhaus H.B. and Aifantis E.C. (1991).
 A variational principle for gradient plasticity.
 Int. J. Solids Structures, vol. 28, pp 845–857.
- Neff P., Sydow A., and Wieners C. (2009).

Numerical approximation of incremental infinitesimal gradient plasticity.

International Journal for Numerical Methods in Engineering, vol. 77, pp 414–436.

Okumura D., Higashi Y., Sumida K., and Ohno N. (2007).
 A homogenization theory of strain gradient single crystal plasticity and its finite element discretization.
 International Journal of Plasticity, vol. 23, pp 1148–1166.

Svendsen B. (2002).

Continuum thermodynamic models for crystal plasticity including the effects of geometrically-necessary dislocations. J. Mech. Phys. Solids, vol. 50, pp 1297–1329.

Wulfinghoff S. and Boehlke T. (2012). Equivalent plastic strain gradient enhancement of single crystal plasticity: theory and numerics. Proceedings of the Royal Society A, vol. 468, pp 2682–2703.