A phase field model incorporating strain gradient plasticity

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Motivation

- *Need for* **(visco)plasticity**
  Microstructure evolution induce and is controlled by local elastic and plastic processes.
- *Need for* **continuum** *plasticity models*
  Discrete or phase field dislocation models are possible but for representative microstructures in metallurgy, continuum constitutive equations are preferable.
- *Need for* **size–dependent** *crystal plasticity models*
  In such microstructures, the plastic processes take place at the micron scale at which they are known to be size-dependent; **strain gradient plasticity** is required at this micro-level.

Plan

1. Phase field model accounting for size dependent plasticity
   - Phase-field model
   - Mechanical behaviour
   - Strain gradient plasticity model (Micromorphic approach)
   - Coupling between phase field and strain gradient plasticity
   - Phase field approach and "Homogenization"
2. Size effect in an elastoplastic laminate
   - Boundary value problem
   - Interface conditions
   - Plastic strain profiles
3. Application to creep in Nickel-base superalloys

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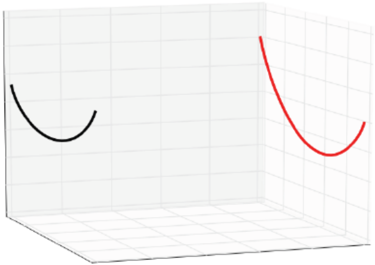
Phase-field model

Total free energy functional

$$F(\phi, \boldsymbol{\nabla}\phi, c) = \int_V f(\phi, \boldsymbol{\nabla}\phi, c)\, dv = \int_V \left(f_{\mathrm{ch}}(\phi, c) + \frac{\alpha}{2} |\nabla \phi|^2 \right) dv$$

Chemical energy density $f_{\mathrm{ch}}(c, \phi)$ (binary alloys, 2 phases α, β)



$$f_{\mathrm{ch}}(c, \phi) \;=\; {\color{blue} f_\alpha(c)} + \quad {\color{red} f_\beta(c)} \quad +$$

$$f_{\alpha,\beta}(c) = \frac{1}{2} k_{\alpha,\beta} (c - a_{\alpha,\beta})^2 + b_{\alpha,\beta}$$

Phase-field model

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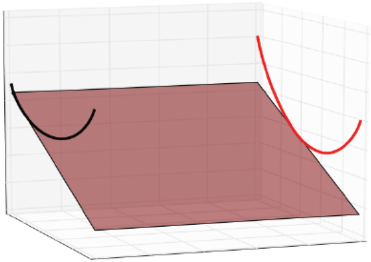

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$$f_{\alpha,\beta}(c) = \frac{1}{2} k_{\alpha,\beta} (c - a_{\alpha,\beta})^2 + b_{\alpha,\beta}$$

Phase-field model

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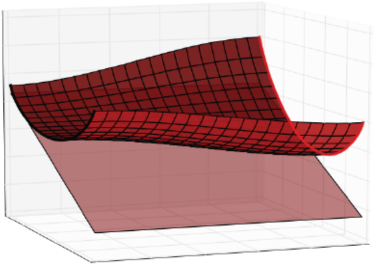
Chemical energy density $f_{\text{ch}}(c, \phi)$ (binary alloys, 2 phases α, β)



$$f_{\text{ch}}(c, \phi) \;=\; h(\phi)\; \color{blue}{f_\alpha(c)} \color{black}{+ (1 - h(\phi))}\; \color{red}{f_\beta(c)} \qquad \color{black}{+}$$

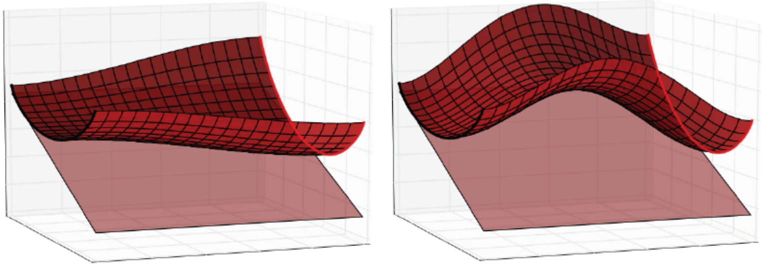
$$f_{\alpha,\beta}(c) = \frac{1}{2} k_{\alpha,\beta} (c - a_{\alpha,\beta})^2 + b_{\alpha,\beta} \text{ where } \; h(\phi) = \phi^2 (3 - 2\phi)$$

Phase-field model

Total free energy functional

$$F(\phi, \nabla\phi, c) = \int_V f(\phi, \nabla\phi, c)\, dv = \int_V \left(f_{\mathrm{ch}}(\phi, c) + \frac{\alpha}{2} |\nabla\phi|^2 \right) dv$$

Chemical energy density $f_{\mathrm{ch}}(c, \phi)$ (binary alloys, 2 phases α, β)



$$f_{\mathrm{ch}}(c, \phi) \;=\; h(\phi)\; f_\alpha(c) + (1 - h(\phi))\; f_\beta(c) \qquad + \qquad Wg(\phi)$$

$$f_{\alpha,\beta}(c) = \frac{1}{2} k_{\alpha,\beta}(c - a_{\alpha,\beta})^2 + b_{\alpha,\beta} \text{ where } \; h(\phi) = \phi^2(3 - 2\phi)$$

$$g(\phi) = \phi^2(1 - \phi)^2$$

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Mechanical behaviour

Specific free energy

$$f_{\mathrm{mech}}(\underset{\sim}{\varepsilon}^e, V) = f_e(\underset{\sim}{\varepsilon}^e) + f_p(V)$$

where V is the set of internal variables.

- Strain partition $\underset{\sim}{\varepsilon} = \underset{\sim}{\varepsilon}^e + \underset{\sim}{\varepsilon}^\star + \underset{\sim}{\varepsilon}^p$
- Elastic energy $f_e(\underset{\sim}{\varepsilon}^e) = \dfrac{1}{2}\underset{\sim}{\varepsilon}^e : \underset{\approx}{\mathbf{C}} : \underset{\sim}{\varepsilon}^e$
- Plasticity induced stored energy $f_p^k = \dfrac{1}{3}C_k \underset{\sim}{\alpha}_k : \underset{\sim}{\alpha}_k + \dfrac{1}{2} b_k Q_k r_k^2$
- Mechanical dissipation potential $\Omega(\underset{\sim}{\sigma}, A)$

A: set of thermodynamical forces associated with V

State laws

$$\underset{\sim}{\sigma} = \frac{\partial f_{\mathrm{mech}}}{\partial \underset{\sim}{\varepsilon}^e}$$

$$A = \frac{\partial f_{\mathrm{mech}}}{\partial V}$$

Complementary laws

$$\dot{\underset{\sim}{\varepsilon}}^p = \frac{\partial \Omega}{\partial \underset{\sim}{\sigma}}$$

$$\dot{V} = -\frac{\partial \Omega}{\partial A}$$

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Enhancing classical continuum mechanics

- Within the framework of generalized continuum mechanics, we introduce an additional degree of freedom

$$DOF = \{\underline{\mathbf{u}}\,, \quad p_\chi\},$$

where p_χ is a scalar *plastic micromorphic variable* [Eringen and Suhubi, 1964]

- The state variables are assumed to be the elastic strain, the accumulated plastic strain related to the isotropic hardening, the plastic micromorphic strain p_χ and its gradient:

$$STATE = \{\underset{\sim}{\varepsilon}^e, \quad p, \quad p_\chi, \quad \nabla p_\chi\}$$

- The specific Helmholtz free energy density, f_{mech}, is a function of these variables:

$$f_{\mathrm{mech}}(\underset{\sim}{\varepsilon}^e, p, p_\chi, \nabla p_\chi) = \frac{1}{2}\underset{\sim}{\varepsilon}^e : \underset{\approx}{\mathbf{C}} : \underset{\sim}{\varepsilon}^e + \frac{1}{2}Hp^2 + \frac{1}{2}H_\chi(p - p_\chi)^2 + \frac{1}{2}A\nabla p_\chi \cdot \nabla p_\chi$$

Micromorphic approach to gradient plasticity

- State laws

$$\underset{\sim}{\sigma} = \frac{\partial f_{\mathrm{mech}}}{\partial \underset{\sim}{\varepsilon}^e} = \underset{\approx}{\mathbf{C}} : \underset{\sim}{\varepsilon}^e, \qquad R = \frac{\partial f_{\mathrm{mech}}}{\partial p} = Hp + H_\chi (p - p_\chi)$$

$$a = \frac{\partial f_{\mathrm{mech}}}{\partial p_\chi} = -H_\chi (p - p_\chi), \qquad \underline{\mathbf{b}} = \frac{\partial f_{\mathrm{mech}}}{\partial \boldsymbol{\nabla} p_\chi} = A \boldsymbol{\nabla} p$$

- Generalized balance equation (from the principle of virtual power)

$$a = \mathrm{div}\, \underline{\mathbf{b}} \quad \Longrightarrow \quad p_\chi - \frac{A}{H_\chi} \boldsymbol{\nabla}^2 p_\chi = p$$

- Yield function $\qquad g(\underset{\sim}{\sigma}, R) = \sigma_{eq} - R_0 - R = 0$ under plastic loading:

$$\sigma_{eq} = R_0 + R = R_0 + Hp + H_\chi (p - p_\chi) = R_0 + Hp - A \boldsymbol{\nabla}^2 p_\chi$$

- Flow and evolution rules

$$\dot{\underset{\sim}{\varepsilon}}^p = \dot{\lambda} \frac{\partial g}{\partial \underset{\sim}{\sigma}}, \quad \dot{p} = -\dot{\lambda} \frac{\partial g}{\partial R} = \dot{\lambda}$$

Aifantis model is retrieved when the constraint $p \equiv p_\chi$ is enforced [Aifantis, 1987]

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Mechanical phase-field coupling

Total free energy functional:

$$\begin{aligned} F &= \int_V f(\phi, \nabla\phi, c, \underset{\sim}{\varepsilon}^e, V_k, p_\chi, \nabla p_\chi)\, dv \\ &= \int_V \left(f_{\mathrm{ch}}(\phi, c) + f_{\mathrm{mech}}(\phi, c, \underset{\sim}{\varepsilon}^e, V_k, p_\chi, \nabla p_\chi) + \frac{\alpha}{2}|\nabla\phi|^2 \right) dv \end{aligned}$$

Mechanical free energy contribution

$$f_{\mathrm{mech}}(\phi, c, \underset{\sim}{\varepsilon}^e, V_k, p_\chi) = f_e(\phi, c, \underset{\sim}{\varepsilon}^e) + f_p(\phi, c, V_k, p_\chi, \nabla p_\chi)$$

Mechanical dissipation potential

$$\Omega(\phi, c, \underset{\sim}{\sigma}, A_k)$$

Mechanical phase-field coupling: field equations

- Local static mechanical equilibrium

$$\boldsymbol{\nabla}.\,\underset{\sim}{\boldsymbol{\sigma}} = \boldsymbol{\nabla}.\left(\frac{\partial f}{\partial \underset{\sim}{\boldsymbol{\varepsilon}}^{e}}\right) = 0$$

- Generalized balance equation

$$a = \boldsymbol{\nabla}.\underline{\mathbf{b}} \quad \Longrightarrow \quad p_\chi - \frac{A}{H_\chi}\boldsymbol{\nabla}^2 p_\chi = p$$

- Balance of mass

$$\dot{c} + \boldsymbol{\nabla}.\,\underline{\mathbf{J}} = \dot{c} - \boldsymbol{\nabla}.\left[L(\phi)\left(\boldsymbol{\nabla}\frac{\partial f}{\partial c}\right)\right] = 0$$

- Evolution equation of order parameter (Cahn/Allen, Landau/Ginzburg equation)

$$-\beta\dot{\phi} - \frac{\partial f}{\partial \phi} + \boldsymbol{\nabla}.\,\frac{\partial f}{\partial \boldsymbol{\nabla}\phi} = 0$$

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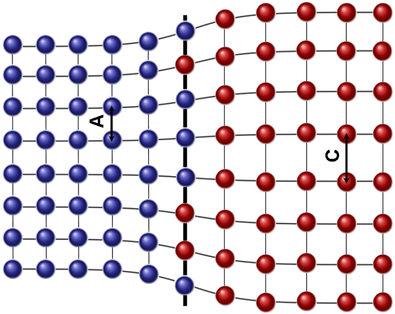
Phase field approach and "Homogenization"

Two approaches for introducing linear and nonlinear mechanical constitutive equations into the standard phase field model:

1. Standard Khachaturyan–like Model

- The material behaviour is described by a unified set of constitutive equations.
- Each material parameter is interpolated between the limit values known for each phase. [Wang and Khachaturyan, 1995]



$$\underset{\sim}{\varepsilon}^{\star} = \phi\, \underset{\sim}{\varepsilon}^{\star}_{\alpha} + (1-\phi)\, \underset{\sim}{\varepsilon}^{\star}_{\beta}$$

$$\underset{\approx}{\mathbf{C}}(\phi, c) = \phi\, \underset{\approx}{\mathbf{C}}_{\alpha}(c) + (1-\phi)\, \underset{\approx}{\mathbf{C}}_{\beta}(c)$$

Elastic energy $f_e(\underset{\sim}{\varepsilon}^e, \phi, c)$:

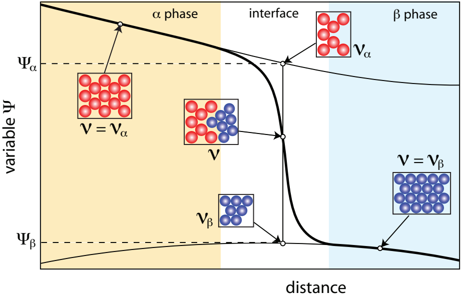
$$f_e(\phi, c, \underset{\sim}{\varepsilon}^e) = \frac{1}{2}\, \underset{\sim}{\varepsilon}^e : \underset{\approx}{\mathbf{C}}(\phi, c) : \underset{\sim}{\varepsilon}^e$$

Phase field approach and "Homogenization"

Two approaches for introducing linear and nonlinear mechanical constitutive equations into the standard phase field model:

2. Homogenization Approach

- One distinct set of constitutive equations is attributed to each individual phase k at any material point.



$$\underset{\sim}{\sigma} = \phi\, \underset{\sim}{\sigma}_\alpha + (1-\phi)\, \underset{\sim}{\sigma}_\beta$$

$$\underset{\sim}{\varepsilon} = \phi\, \underset{\sim}{\varepsilon}_\alpha + (1-\phi)\, \underset{\sim}{\varepsilon}_\beta$$

Elastic energy $f(\underset{\sim}{\varepsilon}^e, \phi, c)$:

$$f_e(\phi, c, \underset{\sim}{\varepsilon}^e) = \phi\, f_{e\alpha}(c) + (1-\phi)\, f_{e\beta}(c)$$

Phase field approach and "Homogenization"

2. Homogenization Approach

- Voigt/Taylor model
  [Ammar et al., 2009b, Ammar et al., 2011]

$$\boxed{\begin{array}{l} \underset{\sim}{\varepsilon}_\alpha = \underset{\sim}{\varepsilon}_\beta = \underset{\sim}{\varepsilon} \\ \underset{\sim}{\boldsymbol{\sigma}} = \phi\, \underset{\sim}{\boldsymbol{\sigma}}_\alpha + (1-\phi)\, \underset{\sim}{\boldsymbol{\sigma}}_\beta \end{array}}$$

- Effective elasticity tensor

$$\underset{\approx}{\mathbf{C}} = \phi\, \underset{\approx}{\mathbf{C}}_\alpha + (1-\phi)\underset{\approx}{\mathbf{C}}_\beta$$

- Plastic strain and eigenstrain:

$$\underset{\sim}{\varepsilon}^\star = \underset{\approx}{\mathbf{C}}^{-1} : (\phi \underset{\approx}{\mathbf{C}}_\alpha : \underset{\sim}{\varepsilon}^\star_\alpha + (1-\phi)\underset{\approx}{\mathbf{C}}_\beta : \underset{\sim}{\varepsilon}^\star_\beta)$$
$$\underset{\sim}{\varepsilon}^p = \underset{\approx}{\mathbf{C}}^{-1} : (\phi \underset{\approx}{\mathbf{C}}_\alpha : \underset{\sim}{\varepsilon}^p_\alpha + (1-\phi)\underset{\approx}{\mathbf{C}}_\beta : \underset{\sim}{\varepsilon}^p_\beta)$$

- Reuss approach: see [Steinbach and Apel, 2006]

Elastoplastic phase field coupling

Total free energy functional:

$$f(\phi, \nabla\phi, c, \underset{\sim}{\varepsilon}^{e}, V_\alpha, V_\beta) = f_{\mathrm{ch}}(\phi, c) + f_e(\phi, c, \underset{\sim}{\varepsilon}^{e}) + f_p(\phi, V_\alpha, V_\beta) + \frac{\alpha}{2}|\nabla\phi|^2$$

Plastic free energy density $f_p(\phi, V_\alpha, V_\beta)$:

$$f_p = \phi\, f_\alpha^p(\phi, p_\alpha, p_{\chi\alpha}, \nabla p_{\chi\alpha}) + (1-\phi) f_\beta^p(\phi, p_\beta, p_{\chi\beta}, \nabla p_{\chi\beta})$$

$$\text{where} \quad f_k^p = \frac{1}{2} H_k p_k^2 + \frac{1}{2} H_{\chi k}(p_k - p_{\chi k})^2 + \frac{1}{2} A_k \nabla p_{\chi k} . \nabla p_{\chi k} \quad \text{with} \quad k = \{\alpha, \beta\}$$

Dissipation potential Ω :

$$\Omega = \phi\Omega_\alpha(A_\alpha) + (1-\phi)\Omega_\beta(A_\beta)$$

$A_{\alpha,\beta}$: are the set of thermodynamic forces.

Classical Von Mises yield function $g_{\alpha,\beta}$:

$$g_{\alpha,\beta} = \sigma^{\mathrm{eq}}_{\alpha,\beta} - R_{\alpha,\beta}$$

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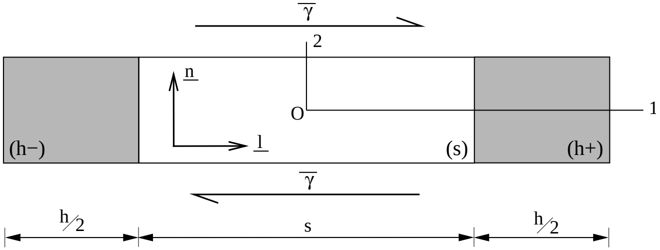
Simple shear of a two–phase laminate



The microstructure is composed of a hard elastic phase (h) and a soft elasto–plastic isotropic phase (s). A mean simple shear $\bar{\gamma}$ is applied to the unit cell with periodicity constraints.

Simple shear of a two–phase laminate

The displacement and micromorphic strain take the form the form:

$$\underline{\mathbf{u}}\,(x_1, x_2) = \begin{cases} u_1 = \bar{\gamma} x_2 \\ u_2 = u_2(x_1) \\ u_3 = 0 \end{cases}$$

The strain, stress and plastic strain fields read:

$$\underset{\sim}{\varepsilon} = \frac{1}{2}\begin{bmatrix} 0 & \bar{\gamma} + u_{2,1} & 0 \\ \bar{\gamma} + u_{2,1} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \underset{\sim}{\varepsilon}^p = \frac{3}{2} p \frac{\underset{\sim}{\mathbf{s}}}{J_2} = \frac{\sqrt{3}}{2} p \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad J_2 = \sqrt{3}\sigma_{12}$$

$$\underset{\sim}{\boldsymbol{\sigma}} = \begin{bmatrix} 0 & \sigma_{12} & 0 \\ \sigma_{12} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} = 2\mu(\underset{\sim}{\varepsilon} - \underset{\sim}{\varepsilon}^p)$$

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

Simple shear of a two–phase laminate

$$u_2(x_1) = \bar{\gamma}, \qquad p_\chi(x_1)$$

The plasticity criterion in the soft phase:

$$\begin{aligned} g(\sigma, R) &= \sqrt{3}\sigma_{12} - R_0 - R = 0 \\ &= \sqrt{3}\sigma_{12} - R_0 - Hp - H_\chi(p - p_\chi) = 0 \end{aligned}$$

$$\frac{\partial g(\sigma, R)}{\partial x_1} = 0 = (H + H_\chi)\frac{\partial p}{\partial x_1} - H_\chi \frac{\partial p_\chi}{\partial x_1}$$

The balance equation for micromorphic variable:

$$a = \mathrm{div}\,\underline{\mathbf{b}} \quad \Rightarrow \quad A\frac{\partial^2 p_\chi}{\partial x_1^2} = H_\chi(p - p_\chi)$$

We obtain the following differential equation for the micromorphic variable in both phases:

$$\frac{\partial^3 p_\chi}{\partial x_1^3} - \omega^{s2}\frac{\partial p_\chi}{\partial x_1} = 0 \qquad \text{where} \qquad \omega^s = \sqrt{\frac{H_\chi H}{A\,(H_\chi + H)}}$$

where H is a linear hardening modulus and $1/\omega^s$ is the characteristic length of the soft phase for this boundary value problem.

Simple shear of a two–phase laminate

From the differential equation, the hyperbolic profile of p_χ takes the form:

$$p_\chi = \alpha \cosh(\omega x) + \beta$$

Symmetry conditions ($p_\chi(-s/2) = p_\chi(s/2)$) have been taken into account.

Elastic phase: In the elastic phase, where the plastic slip vanishes, an hyperbolic profile of the micromorph variable, p_χ^h, is obtained:

$$p_\chi^h = \alpha^h \cosh\left(\omega^h (x \pm \frac{(s+h)}{2})\right), \quad \text{with} \quad \omega^h = \sqrt{\frac{H}{A^e}}$$

Plastic phase

$$p_\chi^s = \alpha^s \cosh(\omega^s x) + \beta^s, \quad \text{with} \quad \omega^s = \sqrt{\frac{H H_\chi^h}{A^h \left(H + H_\chi^h\right)}}$$

where, again, α^h, α^s and β^s are constants to be determined. It is remarkable that the plastic microvariable, p_χ, does not vanish in the elastic phase, close to the interfaces, although no plastic deformation takes place.

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Simple shear of a two–phase laminate

The coefficients α^h, α^s and β^s can be identified using the interface and periodicity conditions:

- Continuity of p_χ at $x = \pm s/2$:

$$\alpha^h \cosh\left(\omega^h \frac{h}{2}\right) = \alpha^s \cosh\left(\omega^s \frac{s}{2}\right) + \beta^p$$

- Continuity of the double traction ($\underline{\mathbf{b}}\,.\underline{\mathbf{n}} = A\,\boldsymbol{\nabla} p_\chi.\underline{\mathbf{n}}$) at $x = \pm s/2$:

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

Simple shear of a two–phase laminate

Periodicity of displacement component u_2.
We have the constant stress component

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

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

$$f(\sigma, R) = \sqrt{3}\sigma_{12} - R_0 - Hp - H_\chi(p - p_\chi) = 0$$

$$u^s_{2,1} = \left(\frac{R_0}{\sqrt{3}\mu} + \left(\sqrt{3} + \frac{H}{\sqrt{3}\mu} \right) \beta^s + \alpha^s \frac{\sqrt{3}H^h_\chi}{(H + H^h_\chi)} \cosh\left(\omega^s x\right) - \bar{\gamma} \right)$$

The average of the fluctuation on the whole structure:

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

must vanish for periodicity reasons.

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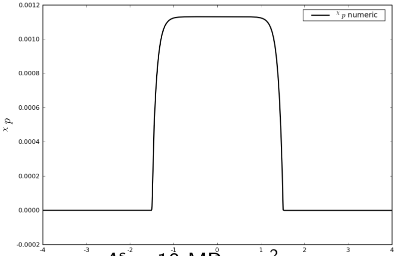
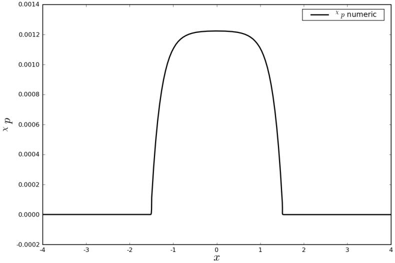
Plastic micromorphic strain and plastic slip

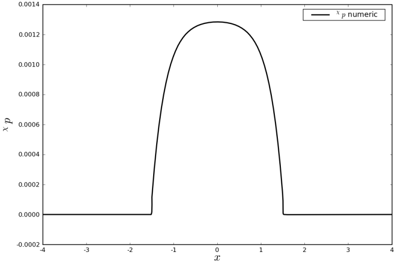
<u>Numerical values:</u>
$\mu = 27000$ MPa, $s = 3\mu$m
$h = 5\mu$m
$A^h = 10$ MPa.μm^2,
$H^s_\chi = H^h_\chi = 500000$ MPa
$\bar{\gamma} = 0.001$
FE implementation
[Ammar et al., 2009a]



$A^s = 10$ MPa.μm^2



$A^s = 50$ MPa.μm^2



$A^s = 100$ MPa.μm^2

Plastic micromorphic strain and plastic slip

<u>Numerical values:</u>
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$A^h = 10$ MPa.μm^2,
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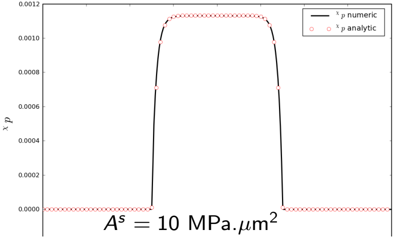
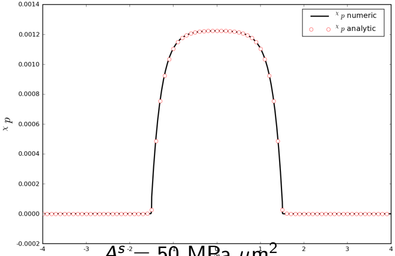
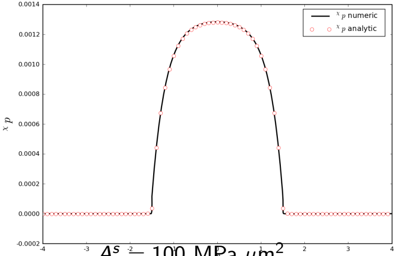


$A^s = 10$ MPa.μm^2



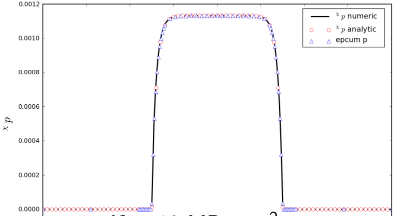
$A^s = 50$ MPa.μm^2



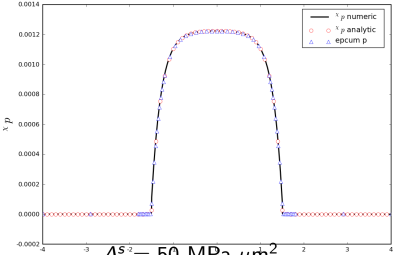
$A^s = 100$ MPa.μm^2

Plastic micromorphic strain and plastic slip

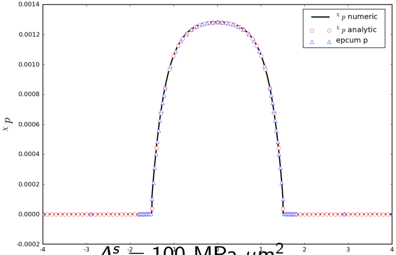
<u>Numerical values:</u>
$\mu = 27000$ MPa, $s = 3\mu$m
$h = 5\mu$m
$A^h = 10$ MPa.μm^2,
$H^s_\chi = H^h_\chi = 500000$ MPa
$\bar{\gamma} = 0.001$
FE implementation
[Ammar et al., 2009a]



$A^s = 10$ MPa.μm^2



$A^s = 50$ MPa.μm^2



$A^s = 100$ MPa.μm^2

Plan

1. Phase field model accounting for size dependent plasticity
   - Phase-field model
   - Mechanical behaviour
   - Strain gradient plasticity model (Micromorphic approach)
   - Coupling between phase field and strain gradient plasticity
   - Phase field approach and "Homogenization"
2. Size effect in an elastoplastic laminate
   - Boundary value problem
   - Interface conditions
   - Plastic strain profiles
3. Application to creep in Nickel-base superalloys

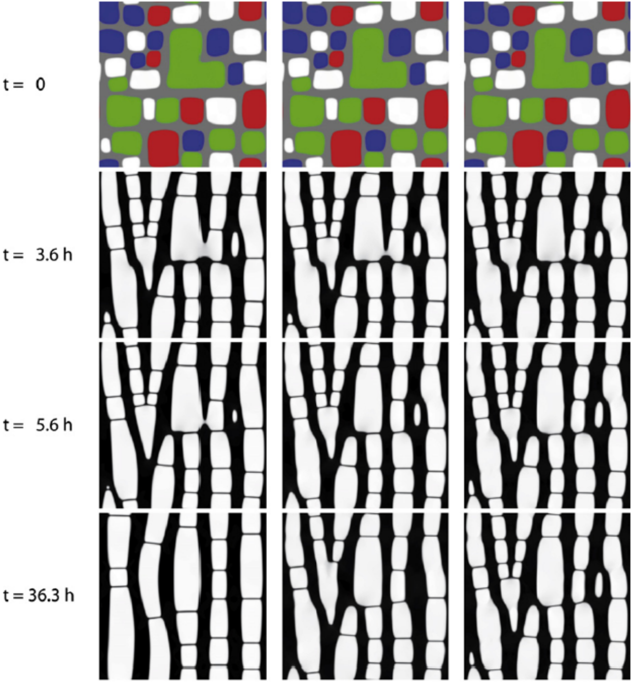
Application to microstructure evolution in Ni-based superalloys

Cooperation M. Cottura, Y. Le Bouar, A. Finel (ONERA-LEM)

creep test along [100] (150 MPa)

- *left:* elastic PFM
- *middle:* strain gradient viscoplastic PFM
- *right:* standard elastoviscoplastic PFM

[Cottura et al. JMPS 2012]



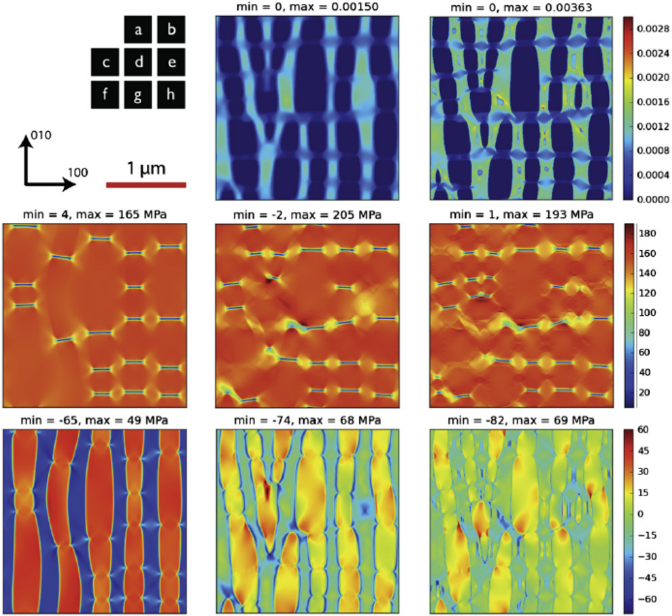
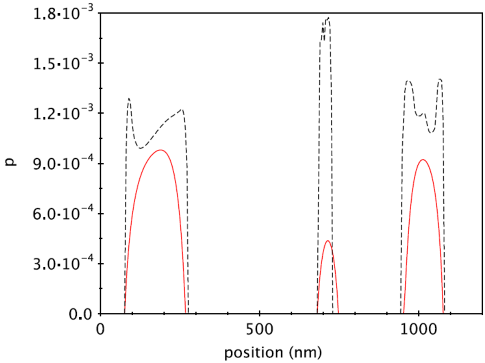


Fig. 6. Plastic and elastic fields obtained at t=36.3 h in the elastic model (first column), in the elasto-viscoplastic model including size effect (middle column) and in the elasto-viscoplastic model where $\bar{\xi}=0$ (last column). The first row is the cumulative plastic strain field p and the second and third rows are the stress components σ_{11} and σ_{22}, respectively. The nomenclature of the images is indicated in the upper left corner.

Application to microstructure evolution in Ni-based superalloys



[Cottura et al., JMPS, 2012]

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