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# Cosserat continuum modelling of grain size effects in metal polycrystals

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The global response of polycrystalline aggregates is investigated, in order to simulate grain size effects in IF ferritic steels. The mechanics of generalized continua is used to describe the studied phenomena. The polycrystal is regarded as a heterogeneous Cosserat medium, and the overall properties are estimated using a specific homogenization technique. To illustrate the capabilities of the model, some simple bidimensionnal computations are presented for different grain sizes. Afterwards tridimensionnal computations are shown in order to extract the global effect on the mechanical behaviour for grain sizes ranging from $5\mu m$ to $120\mu m$. The finite element response is harder for the smallest grain size, but the model still underestimate the grain size effect on the tensile response.



## 1 Introduction

Classical crystal plasticity models are available to derive the overall mechanical properties of polycrystals using efficient homogenization techniques. However, one important shortcoming of this classical approach is that they do not predict the grain size effect, well known in physical metallurgy.

In contrast, generalized continuum plasticity models provide an efficient way of describing the phenomena [1, 2]. The incompatibility of plastic deformation in a heterogeneously deforming crystal is at the origin of size effects. It is related to the concept of density of geometrically necessary dislocations [3]. The Cosserat model is available to introduce this notion. Indeed, this approach includes the gradient of the lattice rotation vector, namely the lattice curvature, which is related to the dislocation density tensor introduced by Nye [4].

The aim of the present work is to reproduce the grain size effect on the overall mechanical behaviour of IF ferritic steels. Polycrystalline aggregates will be computed using Cosserat crystal plasticity. The Cosserat crystal plasticity approach is presented in section 2. The main capabilities of the model are then shown with some simple bidimensionnal computations. Precise modelling of IF steels based on crystal plasticity at a fixed grain size can be found in [6]. The identification of the model parameters for IF steels requires the tridimensionnal simulations of section 3.

## 2 Cosserat crystal plasticity model

### 2.1 Balance and constitutive equations

The material is considered as a heterogeneous Cosserat continuum. The independent degrees of freedom are the displacement vector $u_i$ and the microrotation axial vector $\phi_i$. In the intermediate relaxed configuration, the vector $\phi_i$ describes the rotation of a triad of rigid directors, which corresponds to the lattice directions [2]. Within the small perturbation framework, the Cosserat deformation and curvature tensors are defined by :

$$e_{ij} = u_{i,j} + \epsilon_{ijk}\Phi_k \qquad \kappa_{ij} = \Phi_{i,j} \tag{1}$$

where $\epsilon_{ijk}$ is the permutation symbol. In the static case, the force and couple stress tensors associated with the previous deformation measures, must fulfill two balance equations [7]:

$$\sigma_{ij,j} + f_i = 0, \qquad \mu_{ij,j} - \epsilon_{ijk}\sigma_{jk} + c_i = 0 \tag{2}$$

$f_i$ and $c_i$ are respectively the volume forces and couples. The isotropic elasticity law involves the 2 Lamé constants and 4 additional moduli:

$$\sigma_{ij} = \lambda\delta_{ij}e^e_{kk} + 2\mu e^e_{(ij)} + 2\mu_c e^e_{\{ij\}} \qquad \mu_{ij} = \alpha\delta_{ij}\kappa^e_{kk} + 2\beta\kappa^e_{(ij)} + 2\gamma\kappa^e_{\{ij\}} \tag{3}$$

where $(ij)$ and $\{ij\}$ respectively denote the symmetric and skew-symmetric parts of the tensor. We assume that the elastic rotations are material rotations. The elastic strain tensor $e_{ij}$ is thus quasi-symmetric. The Cosserat microrotations should follows the lattice rotations. As the parameter $\mu_c$ controls the difference between the Cosserat microrotations and the lattice

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rotations, it is used as a penalty factor in the crystal plasticity formulation. A characteristic intrinsic length $l_e = \sqrt{\beta/\mu}$ can be defined. The Cosserat deformation measure and the torsion curvature tensor are decomposed into elastic and plastic parts :

$$\dot{e}_{ij} = \dot{e}^e_{ij} + \dot{e}^p_{ij}, \quad \dot{\kappa}_{ij} = \dot{\kappa}^e_{ij} + \dot{\kappa}^p_{ij} \tag{4}$$

Plastic deformation is due to the activation of plastic slip $\gamma^s$ on slip system $s$ :

$$\dot{e}^p = \sum_{s=1}^{n} \dot{\gamma}^s P^s_{ij}, \quad \text{with} \quad P^s_{ij} = m^s_i n^s_j \tag{5}$$

where $m^s_i$ and $n^s_i$ respectively are the slip direction and the normal to the slip plane for slip systems $s$. For IF steels, the 24 slip systems $\{110\} < 111 >$ and $\{112\} < 111 >$ are retained [6]. In this work, only the plastic lattice bending is taken into account :

$$\dot{\kappa}^p_{ij} = \sum_{s=1}^{n} \left( \frac{\dot{\theta}^s_\perp}{l_p} Q^s_{ij} \right), \quad \text{with} \quad Q_{ij} = \epsilon_{ikl} n^s_k m^s_l m^s_k \tag{6}$$

It is represented for each slip system by the angle $\theta^s$ divided by a second characteristic length $l_p$. $Q_{ij}$ is the curvature orientation tensor corresponding to the contribution of edge dislocations. The set of equations is completed by the flow rules and hardening laws. Viscoplastic flow rules are adopted for both plastic slip and curvature :

$$\dot{\gamma}^s = \langle \frac{\mid \tau^s \mid - r^s}{k} \rangle^n \, \text{sign}\,(\tau^s), \quad \dot{\theta}^s = \langle \frac{\mid \nu^s \mid \, - l_p \, r^s_{c0}}{l_p \, k^s_c} \rangle^{n_c} \, \text{sign}\,(\nu^s) \tag{7}$$

where $\tau^s = \sigma_{ij} P^s_{ij}$ and $\nu^s = \mu_{ij} Q^s_{ij\perp}$ are respectively the resolved shear stress and the resolved couple stress. If the quantities in the angle brackets is positive, it denotes a non zero slip and plastic curvature rate. The most important part of the model lies in the hardening rule :

$$r^s = r_0 + Q \sum_{r=1}^{n} h^{sr}(1 - \exp(-bv^r)) + r^\perp, \quad v^s = \mid \dot{\gamma}^s \mid \tag{8}$$

where $r^s$ is the critical resolved shear stress on slip system $s$. $r_0$ is the initial critical resolved shear stress. Non linear hardening is introduced and the interaction matrix $h^{rs}$ represents a simplified version of the model used in [6]. An extra-hardening term $r^\perp$ associated with lattice curvature is added :

$$r^\perp \; = \; Q^G (\sum_{s=1}^{n} |\theta|)^{1/2} \tag{9}$$

Other extra-hardening laws are summarized and commented in [3]. This function of curvature angle $\theta$ is of purely phenomenological nature. In particular, Ashby [10] recommended that the effect of geometrically necessary dislocations associated with lattice curvature is more important at the very beginning of plastic flow. The additional hardening term proposed in this work is relevant because it induces a strong effect at incipient plasticity. The consequences of the introduction of this additional term is shown in the next paragraph.

### 2.2 Main capabilities of the Cosserat crystal plasticity model

Simple 2d computations are reported in this section to illustrate the different capabilities of the Cosserat crystal plasticity model. Finite element simulations results of the shearing of a 2d aggregate are shown on figure 1-(b) and 1-(c). The two computations are identical, the geometry and orientations of the grains are identical (figure 1-(a)), the value of the applied mean strain is the same, the whole difference is the absolute size introduced in the mesh which are respectively $120\mu m$ and $5\mu m$. Periodic homogenization is used [2]. It allows us to consider small representative volumes [2]

The bending modulus $\beta$, introduced by Kröner [8], affects significantly the spreading of the lattice curvature inside the grains. Physically, this term is related to the density of geometrically necessary dislocations and therefore to the lattice curvature angle over the corresponding intrinsic length $\theta^s/l_p$. Higher values of $\beta$ promote a larger spreading of lattice curvature for a given mean strain. Its influence has been captured and it plays an important role in the simulations of grain size effects. Non homogeneous deformation and lattice rotations in the polycrystal are due to the plastic strain incompatibilities between grains having different orientations. At the very beginning of intragranular plastic flow, the plastic strain is identical for both grain sizes, $120\mu m$ and $5\mu m$. The lattice rotation maps are also quasi identical for the simulations for the two different grain sizes. As a result, a large difference is shown in the norm of the lattice curvature tensor results on figure 1-(b). Lattice curvature is localized near the grain boundaries and it is significantly larger in the smaller grains. The curvature hardening rule (8) induces higher stress level in the small grains as it is shown on figure 1-(c).

| $E$ $(MPa)$ | $\nu$ | $k$ $(MPa.s^{1/n})$ | $n$ | $r_0$ $(MPa)$ | $Q$ $(MPa)$ | $b$ |
|---|---|---|---|---|---|---|
| 208000. | 0.3 | 3. | 10. | 29. | 39. | 16. |

| $\beta$ $(MPa.mm^2)$ | $r_{c0}$ $(MPa)$ | $Q^G$ $(MPa)$ | $l_p$ $(mm)$ | $k_c$ $(MPa.s^{1/n_c})$ | $n_c$ |
|---|---|---|---|---|---|
| 0.001 | 0.000001 | 15. | 1. | 0.01 | 1. |

**Table 1** (a) Classical parameters used in the computations (b) Specific Cosserat parameters used in the computations

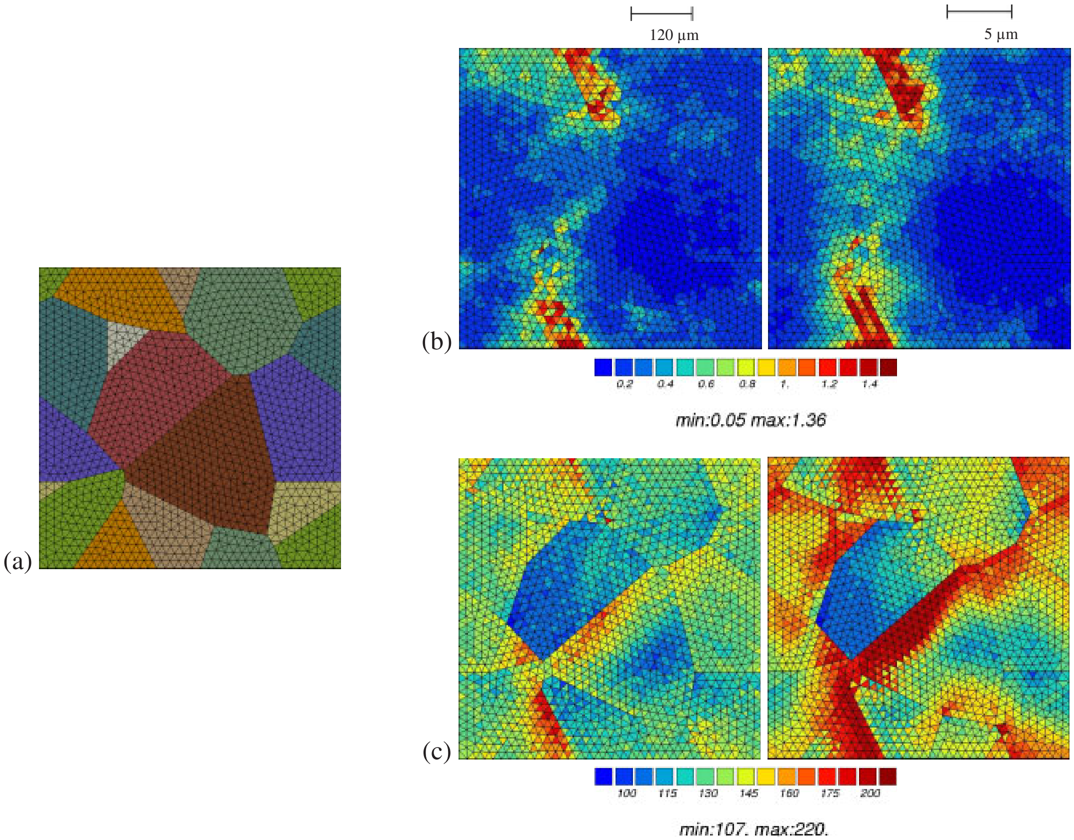


**Fig. 1** Finite element simulations of the shear deformation of the 2D aggregates of figure 1 with different grain sizes: (a) mesh of the grains (b) norm of the plastic curvature tensor (unit $mm^{-1}$); (c) Von Mises equivalent stress fields (unit $MPa$). The geometry of the grains is the same for both computations but the absolute size of the aggregates differ. Geometrical and kinematical periodicity conditions are imposed.

## 3 Tridimensionnal finite element analysis of IF ferritic steels

Tridimensionnal simulations are necessary to reproduce quantitatively the experimental results of grain size effects on the overall mechanical properties of a polycrystal. For that purpose, a mean tensile strain equal to $10\%$ is applied on a periodic aggregate containing 10 grains (figure 2-a). Each grain has a random crystallographic orientation. The polycrystal is regarded as a heterogeneous Cosserat medium. A specific homogenization procedure is developed in order to estimate the resulting properties of the representative volume. The considered material is a IF ferritic steel for which material parameters are given in table 1. The essential additional parameter is the term $r^{\perp}$ in the relation (8), function of plastic lattice curvature. Its value, given in table 1-(b), has been fixed to evidence the induced grain size effect.

Four computations are reported here with the same set of material parameters, the same number and morphology of grains, the same orientations of the grains and the same mesh density. The only difference is the absolute size of the cube which corresponds to different polycrystals with grain sizes varying from $5\mu m$ to $120\mu m$. The additional hardening introduced in equation 8 allows a strong effect of extra hardening. A different overall curve $\Sigma = \langle\sigma\rangle$ vs. $E = \langle\varepsilon\rangle$ is obtained in each case as it is shown on figure 3. As expected, the finite element response is harder for the small grain sizes. When the grain size increases, the difference between the responses becomes less and less significant. The effect on the mechanical response saturates when the grain size is close to $120\mu m$ (the large grain polycrystal behaviour). Nevertheless, the prediction of the overall properties of ferritic steel polycrystals including grains size effects is still underestimated (figure 3. In particular, the values of the yield stress is too low for the predicted responses in comparison with the experimental results.

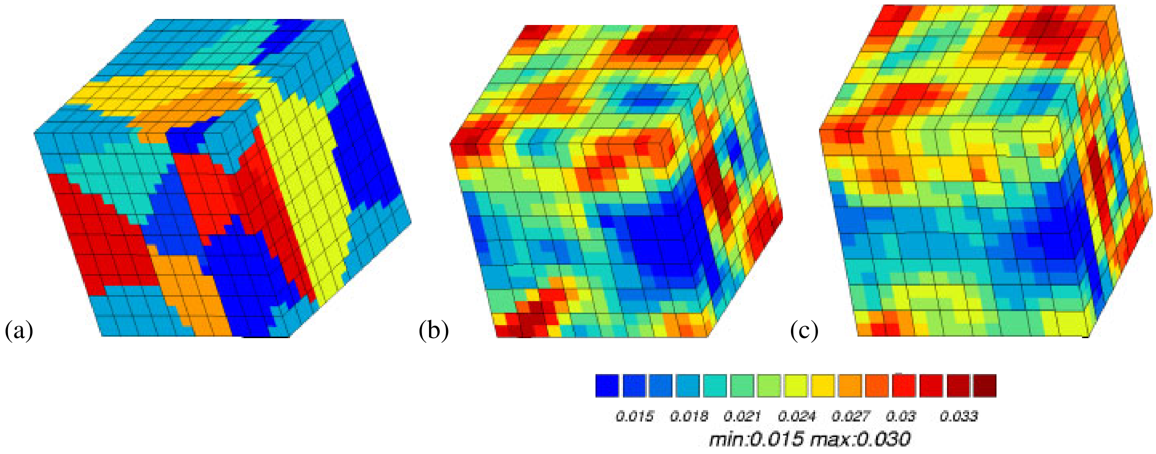


**Fig. 2** Finite element simulations of the tensile test of tridimensionnal aggregates containing 10 grains : (a) mesh of the grains (b) and (c) maps of the equivalent plastic strain (unit MPa) after $0.075\%$ mean strain and for a grain size respectively equal to $120\mu m$ and $5\mu m$. Geometricaly an kinematicaly boundary conditions are imposed.

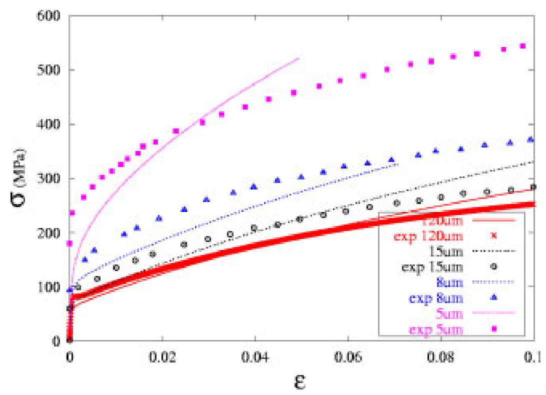


**Fig. 3** grain size effect in ferritic steel : experimental and simulated results

## 4 Conclusions and prospects

Finite element computations of ferritic polycrystalline aggregates are performed in a Cosserat framework. The illustration of the model capabilities through some simple 2d computations shows the influence of the spreading of lattice curvature inside grains at the very beginning of plastic flow. The most important part of the model lies in the extra-term in the hardening rule. The introduction of this non classical term induces higher stress levels for the small grain size. The grain size effect on the mechanical response is successfully captured for a large spectrum of different grain sizes. But it has been observed that the mechanical response is still underestimated by this approach. The agreement, in comparison with the tensile experimental results, is good from a qualitative point of view. More elaborate extra-hardening laws are necessary to reach better quantitative agreement. Finally, the influence of too coarse meshes or lattice curvature spreading must be investigated.

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