

Cosserat Modeling of Size Effects in Crystalline Solids

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ABSTRACT

The mechanics of generalized continua provides an efficient way of introducing intrinsic length scales into continuum models of materials. A Cosserat framework is presented here to describe the mechanical behavior of crystalline solids. The first application deals with the problem of the stress strain field at a crack tip in Cosserat single crystals. It is shown that the strain localization patterns developing at the crack tip differ from the classical picture : the Cosserat continuum acts as a bifurcation mode selector, whereby kink bands arising in the classical framework disappear in generalized single crystal plasticity. The problem of a Cosserat elastic inclusion embedded in an infinite matrix is then considered to show that the stress state inside the inclusion depends on its absolute size l_c . Two saturation regimes are observed : when the size R of the inclusion is much larger than a characteristic size of the medium, the classical Eshelby solution is recovered. When R is much smaller than the inclusion, a much higher stress is reached (for an inclusion stiffer than the matrix) that does not depend on the size any more. There is a transition regime for which the stress state is not homogeneous inside the inclusion. Similar regimes are obtained in the study of grain size effects in polycrystalline aggregates of Cosserat grains.

INTRODUCTION

The incompatibility of plastic deformation in heterogeneously deforming single crystals can be the origin of size effects in their mechanical behavior. It is related to the so-called dislocation density tensor α arising in the continuum theory of dislocations [1]. In contrast, classical crystal plasticity [2] relies on hardening variables related to the scalar densities of dislocation well-known in physical metallurgy. The question then is how to introduce α into a general constitutive framework. Two main ways have been traced. According to the first one, the dislocation density tensor is regarded as an additional non local internal variable [3]. The second one acknowledges the fact α is related, on the one hand, to the gradient of plastic deformation and therefore indirectly to the second gradient of the displacement. On the other hand, the dislocation density tensors is directly related to lattice curvature, namely the gradient of the lattice rotation vector. That is why the second class of models resorts to the mechanics of generalized of continua [4]. Generalized continua can be classified into three main groups. Higher grade media involve higher order gradients of the displacement field or of some internal variables. In higher order media, independent degrees of freedom are introduced in addition to the usual displacements. Fully non local media are characterized by an integral formulation of the constitutive equations [5]. In this work, attention is drawn

to the Cosserat continuum for which independent displacement \underline{u} and microrotation $\underline{\Phi}$ degrees of freedom are attributed to each material point. The vector $\underline{\Phi}$ describes the rotation of an underlying triad of rigid directors, here the crystal lattice directions in an intermediate stress–released configuration. Deformation and curvature tensors can be defined [8], so that there exist two associated stress tensors : the force-stress tensor $\underline{\sigma}$ and the couple-stress tensor $\underline{\mu}$. They are not necessarily symmetric. Two balance equations must be fulfilled, namely the balance of momentum and the balance of moment of momentum :

$$\sigma_{ij,j} = 0, \quad \mu_{ij,j} - \epsilon_{ijk}\sigma_{jk} = 0 \quad (1)$$

where volume forces and couples have been excluded for simplicity.

There have been at least two main attempts to deal with the single crystal as a generalized continuum : a Mindlin-type strain gradient theory [6,7] and a Cosserat model [8]. Both theories account for additional hardening due to lattice curvature. The slight differences concern the treatment of elastic curvature and the ability of the Cosserat continuum to account for non–symmetric stresses. This last possibility is not exploited in this work and only effects associated with lattice curvature are presented.

The whole constitutive framework of Cosserat single crystal plasticity is detailed in [8,10,11] and is not recalled here. It is based on a generalized Schmid law and the most important part of the model lies in the hardening rule :

$$\tau^s = \tau_0 + \sum_{i=1}^n H_{sr}(1 - e^{-b\gamma^r}) + H'\theta^s \quad (2)$$

where τ^s is the resolved shear stress on slip system s , τ_0 the initial critical resolved shear stress. Non–linear hardening is introduced as a function of cumulative slip γ^r on slip system r , H_{sr} being the interaction matrix accounting for latent and self–hardening. Additional hardening associated with lattice curvature θ^s/l_c is added, l_c being an intrinsic length scale. The consequences of the introduction of this non–classical term are investigated in three cases in the sequel. The first example deals with Cosserat plasticity in a single crystal. In the second one, only Cosserat elasticity is regarded. And the last one concerns aggregates of Cosserat single crystals.

STRAIN LOCALIZATION PHENOMENA AT A CRACK TIP

The asymptotic stress-strain field at a stationary crack tip in elastic-ideally plastic f.c.c. and b.c.c. single crystals, as determined by Rice *et al.* [9], turns out to be locally constant within angular sectors. It involves shear displacement discontinuities at sector boundaries, that can be interpreted as strain localization bands. The numerical analysis of the same problem using finite strain crystal elastoplasticity in [2] reveals that the condition of constant stress state in each sector must be relieved because of possible local unloading, but also that the strain localization patterns pertain. Two types of deformation bands exist in single crystals undergoing single slip : slip bands lying in the slip plane of the locally activated slip system, or kink bands lying in a plane normal to the slip direction of the slip system [10]. The formation of a kink band is associated with the development of strong lattice rotation gradients at its boundary and may therefore be precluded if the model incorporates additional hardening due to lattice curvature [10]. An example is given in this section but a more thorough analysis of application of generalized crystal plasticity at the crack tip can be found in [12].

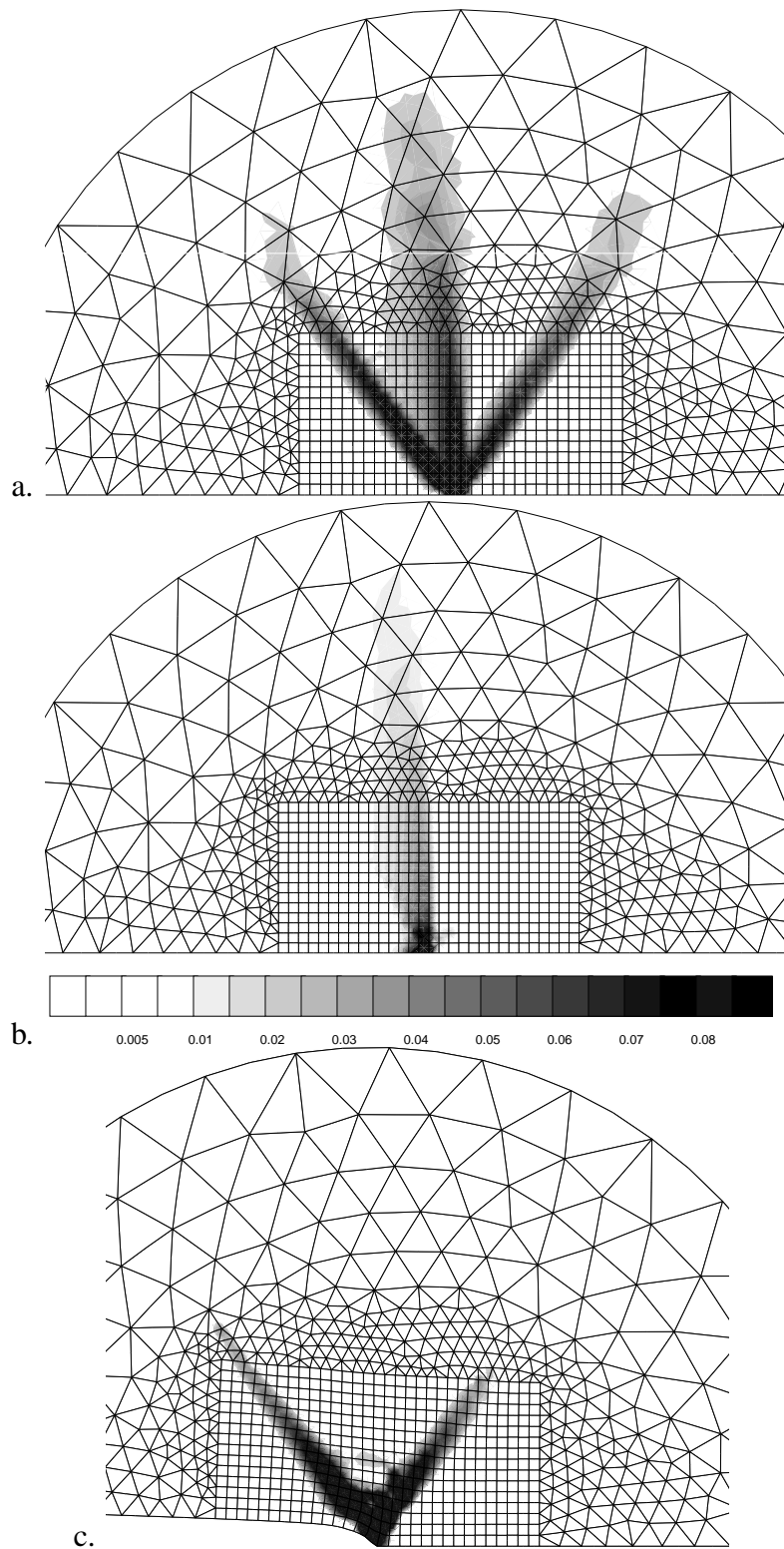


Figure 1. Strain localization phenomena at the crack tip of a f.c.c. single crystalline CT specimen with vertical orientation [001] and horizontal one [110] : equivalent plastic strain (a), lattice rotation (b) in the classical case. The picture (c) gives the equivalent plastic strain distribution when the Cosserat continuum is used : the vertical kink band has disappeared.

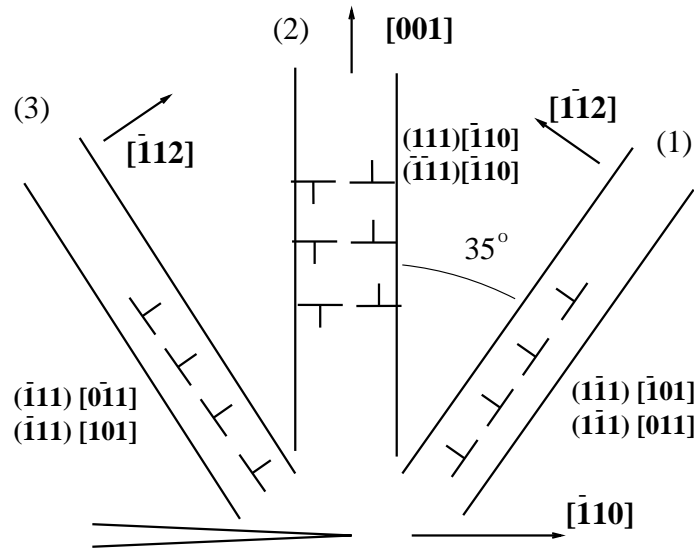


Figure 2. Interpretation of the strain localization pattern at the crack tip of a single crystal CT specimen : (1) and (3) are effective slip bands, (2) is an effective kink band.

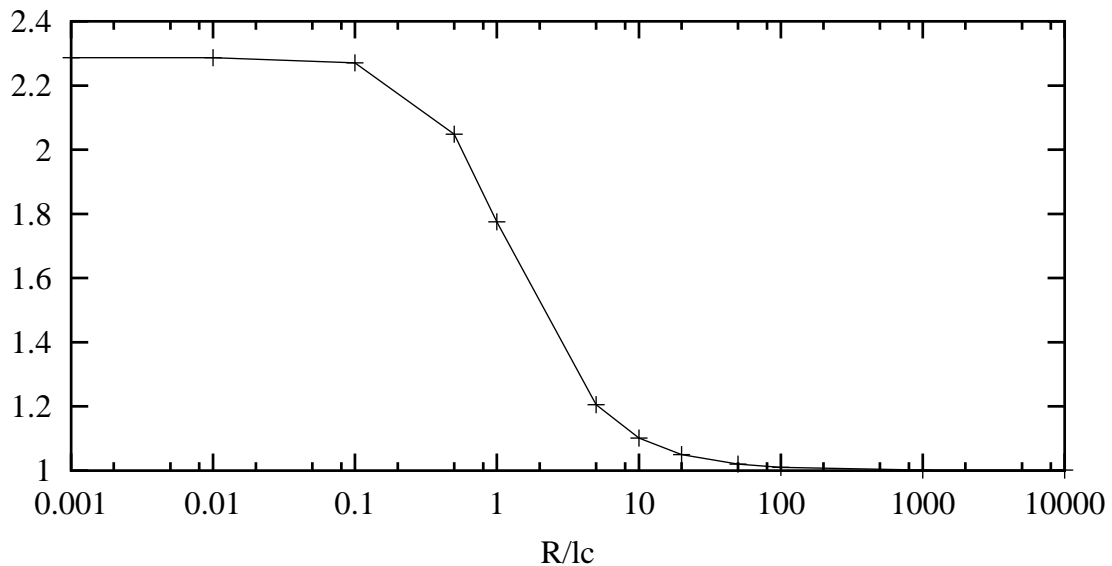


Figure 3. Ratio of the mean stress in an heterogeneous inclusion over the classical Eshelby result as a function of R/l_c .

Discrete models based on dislocation dynamics also lead to strongly localized dislocation distributions near the crack tip and to the progressive formation of the predicted sectors, but kink bands do not seem to form [13]. A single crystal CT specimen is considered here and its deformation is computed with the finite element method using firstly classical multiplicative single crystal plasticity. A ideal plastic f.c.c. crystal with 12 octahedral slip is computed under plane strain conditions. Three localization bands are observed at the crack tip (figure 1) : two intense slip bands and one kink band are obtained, as explained on figures 1 and 2. The application of Cosserat extra hardening leads to the disappearance of the kink band as shown figure 1c. The physical relevance

of this result cannot be definitively assessed, because there are only scarce detailed experimental analysis of the crack tip field in a single crystal.

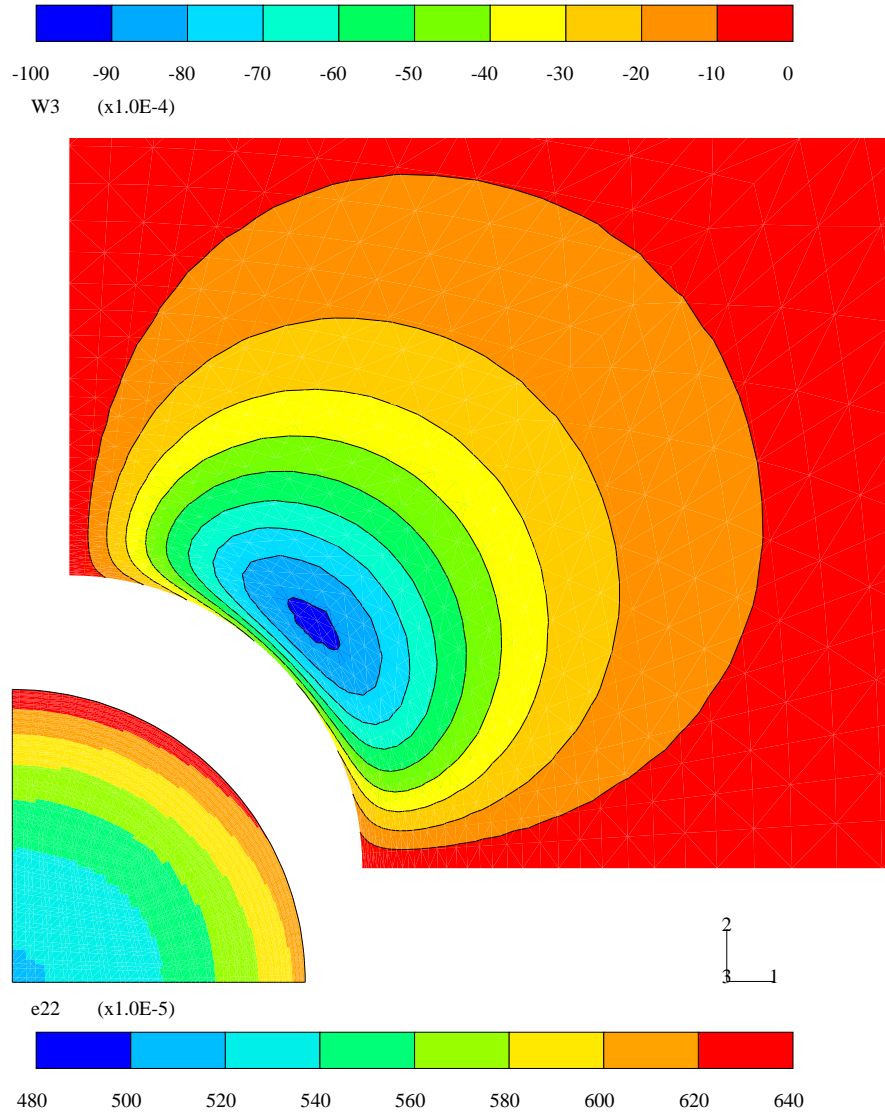


Figure 4. Deformation field in an heterogeneous elastic inclusion and microrotation field in the matrix submitted to tension; the deformation field is non-homogeneous inside the inclusion contrary to the classical case.

HETEROGENEOUS COSSERAT INCLUSION IN AN INFINITE MATRIX

The extension of the classical Eshelbian inclusion problem to the Cosserat framework may well be of the major importance to design homogenization techniques being able to account for absolute size effects in heterogeneous materials. Some aspects of the Eshelby inclusion problem have been reported in [14]. Let us consider a Cosserat elastic inclusion having elastic properties $(E^I, \nu^I, \mu_c^I, l_c^I)$ embedded in an infinite matrix endowed with different moduli (E, ν, μ_c, l_c) . Furthermore the matrix is loaded at infinity and a tensile test is considered (axisymmetric case).

For a given set of Cosserat elastic parameters for the inclusion and the matrix, the influence of the inclusion size R on the mean stress within the inclusion has been investigated and the results are presented on figure 3. For a large ratio R/l_c , the solution tends towards the classical one. For lower ratios, in the case of an inclusion more rigid than the matrix, higher values of the mean stress are reached. Again, the stress tends to an asymptotic value for ever decreasing inclusion sizes. Note that in our example, the stress in the tiny inclusion is more than twice as large as in the big one. In the transition domain, generalized stresses and deformations are non-homogeneous within the inclusion, as seen on figure 4, and contrary to the classical case. The typical curve with two saturation plateaus of figure 3 shows that the characteristic length of the Cosserat medium acts as a resolution parameter (as in microscopy). When the geometry interacts with this length scale, size effects will be observed.

GRAIN SIZE EFFECTS IN POLYCRYSTALS

Efficient homogenization techniques are available to derive the overall mechanical properties of polycrystals, starting from the knowledge of single crystal constitutive equations and the texture (orientation distribution function). They also provide an estimation of the mean stress and strain of the grains having a same given orientation. However, two major shortcomings of these now classical approaches must be recalled. Firstly, they do not provide the stress concentration inside the grains that are relevant for damage prediction, and therefore strongly underestimate the intergranular and intragranular stress-strain heterogeneity [11,15]. Secondly, the effective properties deduced from classical homogenization theories do not depend on the absolute size of heterogeneities but only on their volume fraction and, at best, on the morphology of the constituents. In contrast, it is well-known in experimental metallurgy, that microstructures can be optimized for the desired overall nonlinear properties by varying the size of inclusions or grains.

That is why polycrystalline aggregates have been considered containing a detailed description of grain morphology and intragranular fields. A volume element with up to 1000 grains has been computed in [15] to show the tremendous dispersion of stress and strain. The grains of a polycrystal are regarded as three-dimensional Voronoi polyhedra, and the finite element mesh is fine enough to get a converged solution of the field inside each grain. This requires parallel computing as explained in [15]. This approach has been used in classical crystal plasticity but also using Cosserat crystal plasticity so as to introduce an actual scale in the computation. Small periodic aggregates have been computed in [11] to derive a grain size effect for f.c.c. crystals.

A larger but not periodic volume element is considered here containing 50 Cosserat grains, the mesh remaining small enough to allow a sequential computation. A crystal orientation is attributed to each grain in a random way. The displacement in direction z is prescribed at the bottom and top faces of the aggregates to simulate a tensile test. Six computations are reported here with the same set of material parameters, the same number and morphology of grains and the same mesh. The only difference is the absolute size of the cube edge length d which will vary from $10\mu\text{m}$ to 10mm . Due to the Cosserat hardening effect (2), a different overall curve $\Sigma_{zz} = \langle \sigma_{zz} \rangle$ vs. $E_{zz} = \langle \varepsilon_{zz} \rangle$ is obtained in each case as show on figure 7. The considered material is an alloyed zinc polycrystal for which material parameters are available from [16]. The only essential additional parameter is H' which has been arbitrarily fixed to evidence the induced size effects. Two slip system families must be taken into account : the 3 basal slip systems with a low initial critical resolved shear stress, and the 6 pyramidal Π_2 slip systems with a ten times higher initial threshold.

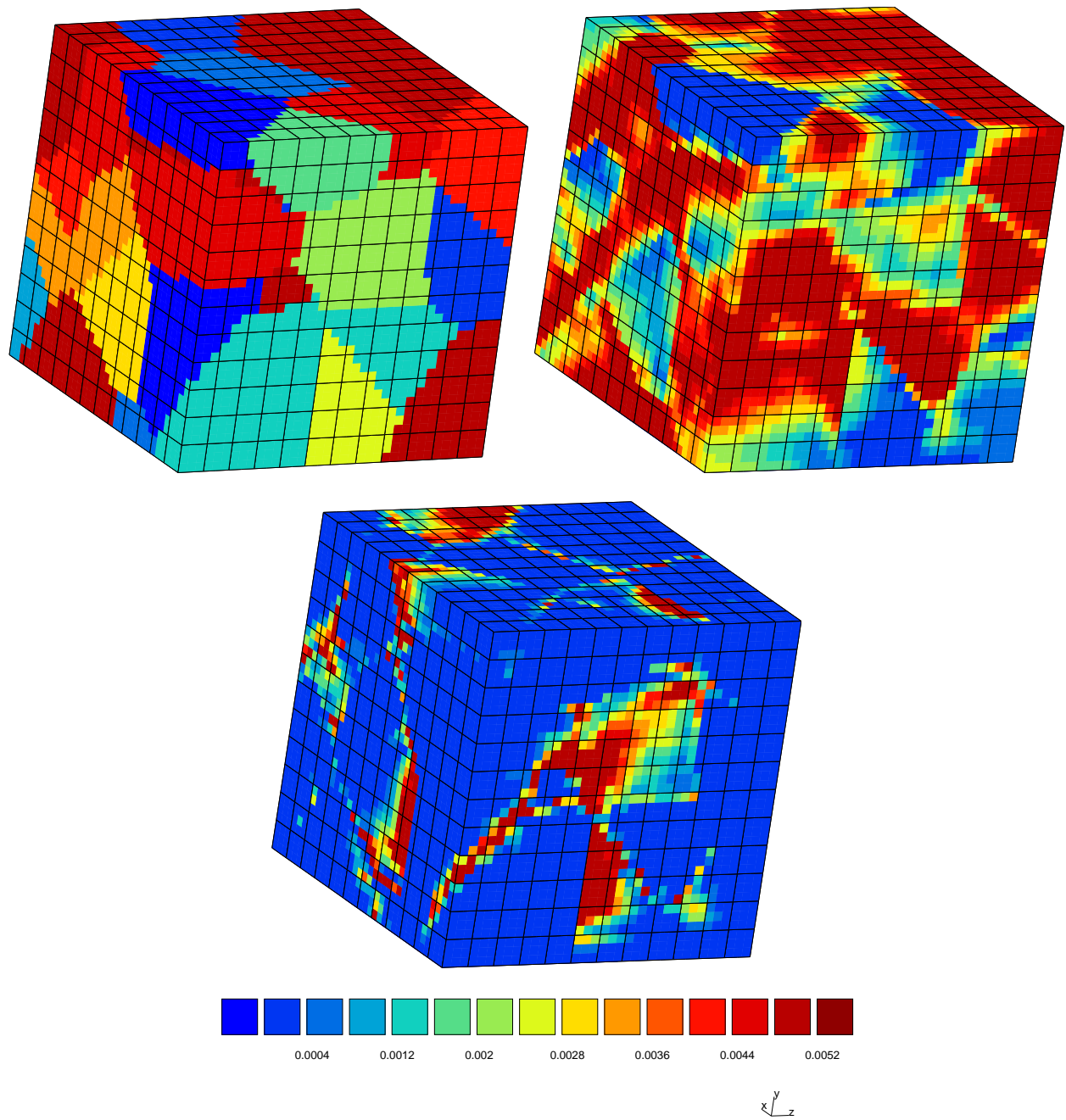


Figure 5. *Tension of a 50-grain zinc aggregate : morphology and map of cumulated basal slip (top) and cumulated pyramidal Π_2 slip (bottom).*

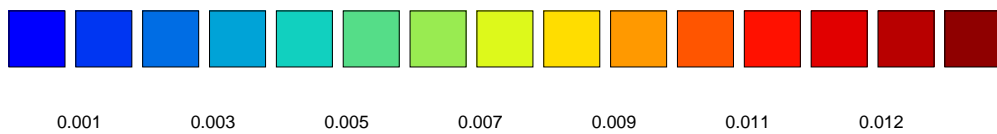
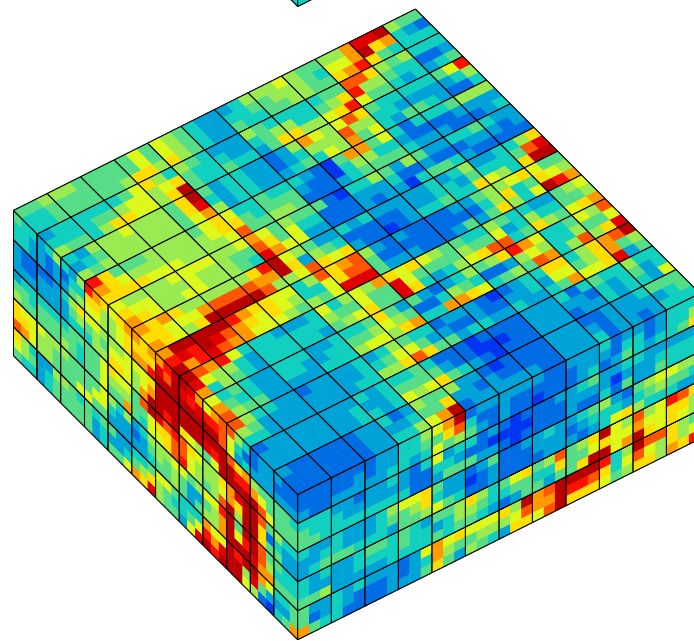
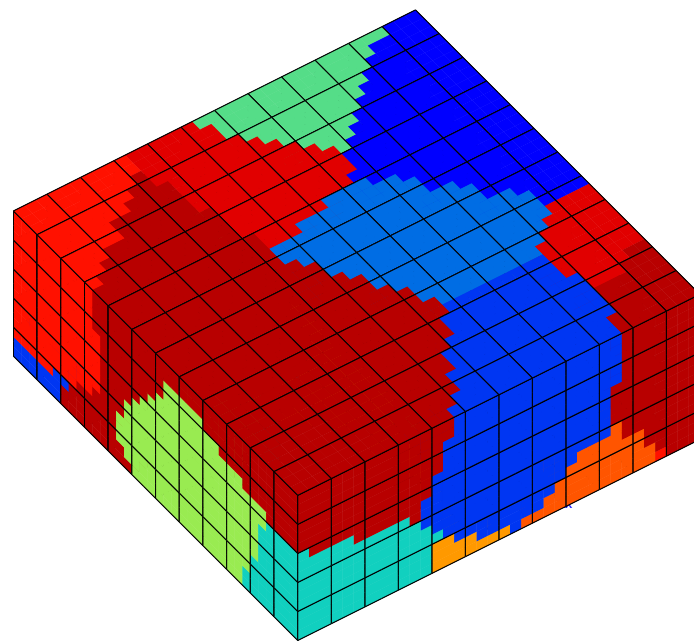


Figure 6. *Slice of a zinc aggregate (top) and corresponding equivalent lattice curvature field.*

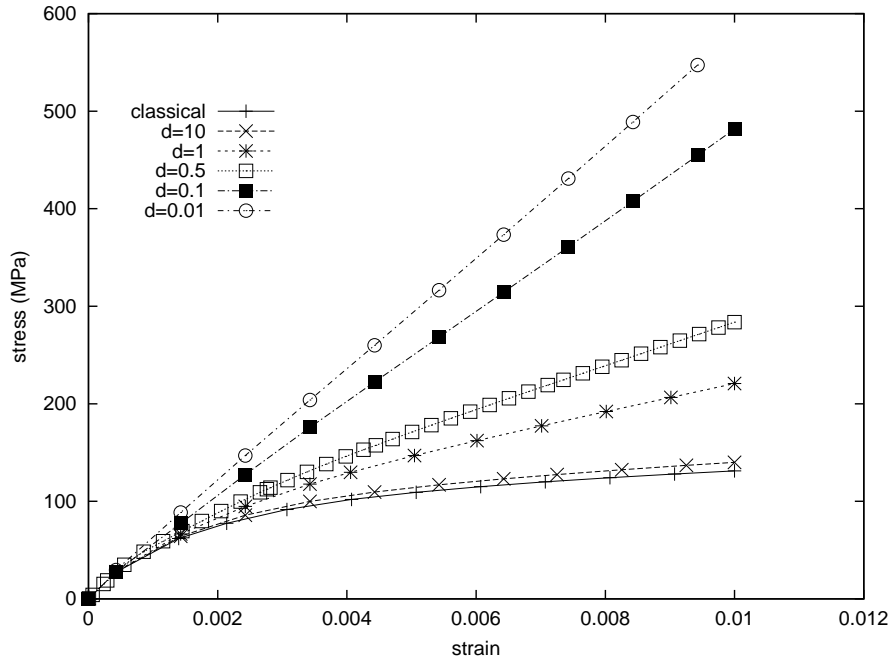


Figure 7. Mean stress–strain curves for the same 50-grain zinc aggregates but different absolute sizes d of the cube.

Figure 5 shows the grain distribution in the aggregate and that basal slip is predominantly activated in the grains. In contrast, pyramidal slip exclusively develops at the grain boundaries where basal slip alone cannot accommodate plastic incompatibilities between neighbouring grains. A map of a norm of the lattice curvature tensor in a slice of the sample is given in figure 6, showing that plastic curvature preferentially develops near the grain boundaries. This confirms the fact mentioned in [11] that lattice rotation tends to be relatively homogeneous in the core of the grains and is disturbed near the boundary. The curves of figure 7 shows that when the grains are very large, there is no difference between the computation using classical crystal plasticity and the Cosserat case. In contrast, when the grain size decreases, the response becomes more and more elastic. Figure 8 gives the same overall stress–strain curves but after removing the overall elastic deformation from the total one. This enables us to plot the difference between the mean axial stress Σ reached by the aggregate for each grain size at a given mean strain $E = 0.1\%$, minus the corresponding strain for the classical size-insensitive case, as a function of the grain size (figure 9). Three regimes appear in a similar way as for the inclusion problem (figure 3) : for very small and very large grains, a slope of approximately $-1/2$ is observed, whereas the transition regime is characterized by a slope of approximately -1 .

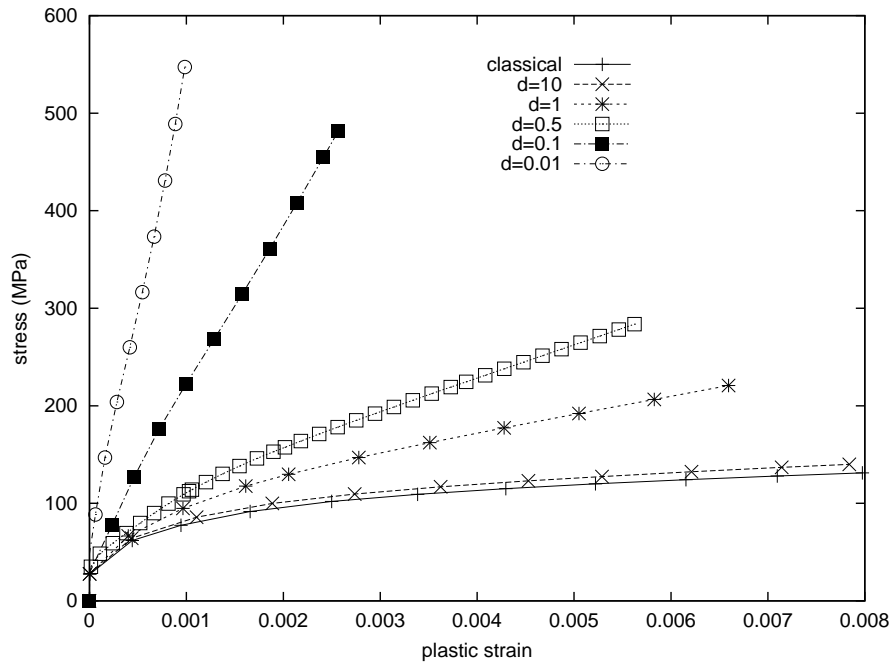


Figure 8. Mean stress–plastic strain curves corresponding to the overall curves of figure 7.

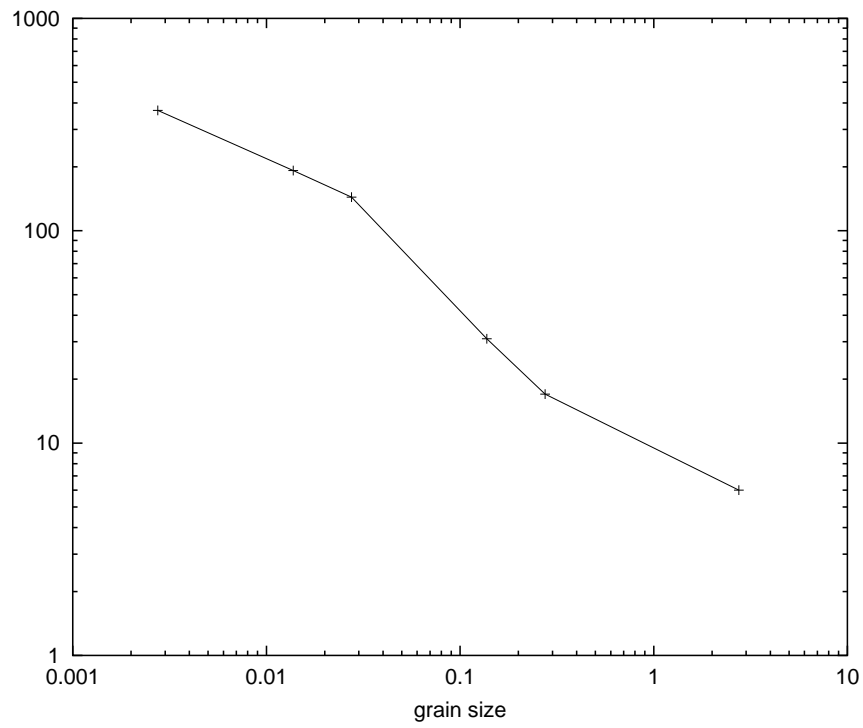


Figure 9. $\Sigma - \Sigma_0$ for a plastic strain of 0.1% as a function of grain size, Σ_0 being the stress reached by the classical solution.

CONCLUSION AND PROSPECTS

The proposed Cosserat framework to model size-dependent crystal plasticity is based on the introduction of additional hardening proportional to lattice curvature. Physically more relevant constitutive equations should be proposed. In particular, the reference [17] indicates that the effect of so-called geometrically necessary dislocations associated with lattice curvature is more important at the beginning of plastic flow, so that a nonlinear additional hardening term with possible saturation would be better. In particular, this would affect the initial yield stress of polycrystalline aggregates and not subsequent hardening, contrary to the result of figure 7.

Generalized crystal plasticity has been shown to strongly affect the stress-strain field at a crack tip in an ideally plastic single crystal. In particular, strain localization bands of kink type are significantly weakened or even precluded. Experimental investigations are necessary to assess the physical relevance of the result but some experimental results and discrete dislocations models seem to confirm this feature of crystal plasticity.

The prediction of the overall properties of polycrystals including grain size effects are possible using Cosserat crystal plasticity and corresponding homogenization techniques [18]. The promising results on small polycrystal volume element presented here for hexagonal crystal structures must be confirmed by more intensive computations involving more grains and much finer meshes. Parallel computing will play a major rôle in the future investigations.

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