FE approach of the plasticity of 3D polycrystals subjected to cyclic loading

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Abstract :

The Finite Elements method is used to compute the volume average responses of 3D multicrystals in elasticity and elastoplasticity: the cubic domain of computation is divided into Voronoi polyhedra that constitute the grains and discretized either regularly into $n^3$ brick elements or freely into tetrahedral elements. As the apparent (volume average) properties of multicrystals differ from one to the other, all the more as there are few grains, the determination of the effective properties of the polycrystalline medium can be completed by ensemble average over random multicrystals of a same size. After the analysis of the validity of ergodicity in the case of simple uniaxial tests with mixed boundary conditions, the configurations of modelling which are appropriate for investigations on elastoplasticity are determined and applications are performed for cases of cyclic loading.

Key-words :

crystalline plasticity, finite elements, cyclic loading

1 Introduction

The determination of the effective properties of a polycrystalline medium has been the subject of extensive studies for the last decades. Simplest approaches are based on assumptions of uniformity of strain or stress and provide respectively first order upper and lower bounds of the properties. In a second category, one finds the classical 1-site homogenization modelling that take into account the volume fraction of each class of heterogeneity, a class being distinguished between the other by its crystallographic orientation. In a third category, more accurate information concerning the distribution of the heterogeneities is considered. For example in n-sites homogenization modellings, each heterogeneity is no more supposed to interact with a homogeneous medium as in 1-site modelling: the nature of the neighbouring heterogeneities is also taken into account. However the heterogeneity is still considered to be an ellipsoidal inclusion. That is what confers to the Finite Elements method the potential for more physically based modelling as compared to n-sites homogenization modellings: the microstructure of a polycrystal can be represented by Voronoi polyhedra corresponding quite well to the morphology of a polycrystalline medium.

Such an approach has been extensively used in recent years and has laid an important groundwork (Barbe et al. (2001a,b); Diard et al. (2005); Zhegadi et al. (2006b,a)). The rigorous determination of the size of a Representative Volume Element has been made concerning elastic properties of bi-phase material (Kanit et al. (2003)) and polycrystalline aggregates (Nygards (2003)). In both works, the effective properties have been determined from computations on volumes very large as compared to the size of the structural heterogeneities (a volume that one may call a poly-crystal if the volume of study is extracted from a crystalline medium) as well as from ensemble averaging over small volumes (such volumes are then called multi-crystals in the case of a crystalline medium). The results with this latter method have shown that the
ergodicity hypothesis could apply rather well to elastic polycrystalline media, the accordance to this hypothesis depending on the kind of boundary conditions applied to the FE volumes.

This study proceeds in two steps: first we apply the method based on ensemble averaging over FE multicrystals to elastoplasticity (so as it has been done in Zhegadi et al. (2006a) for nearly 3D polycrystals); two types of mesh are used: mapped meshes where sets of identical brick elements are meant to represent Voronoi polyhedra and free meshes where sets of tetrahedral elements adopt the frontiers of Voronoi polyhedra. At second, from the analysis conducted in the first step, we deduce configurations of computation which are the most efficient for the study of polycrystalline plasticity and ratchetting. This second point is motivated by the fact that most phenomenological constitutive modellings, though they are sophisticated and based on large sets of parameters, are not able to reproduce all features of experimental ratchetting for a given set of material parameters (Bari and Hassan (2002)).

2 Modelling

2.1 Discretization of the volume of computation

As in Barbe et al. (2001a), the grains of the polycrystalline medium have the morphology of Voronoi polyhedra. They are obtained from a set of points randomly distributed in a three dimensional space—the nuclei; with the Voronoi tessellation, the medium is divided into convex polyhedra, each one being defined as the set of points closest to the nucleus of the polyhedron than to any other nucleus. The volume of study can be discretized regularly into $n \times n \times n$ brick elements so that, as in Nygards (2003), the grains are defined by sets of elements. It can also be discretized freely using tetrahedral elements which adopt the exact boundaries of polyhedra. Such a discretization is not an easy task, as noticed in Zhao et al. (2007). However it can be done using the free software Gmsh 1.60 (2005) but, as seen on fig. 1a, the number of nodes of the mesh becomes enormous as regards to the simple need to determine effective properties: to ensure the very complex geometrical constraints of the domain to be meshed, many very small elements are placed in the vicinity of polyhedra vertices. That is why a program has been developped, which is integrated in the software NePeR 1.5 (2006), and which allows to reduce considerably the number of required nodes as can be seen on fig. 1b. The processes by which such a reduction could be obtained are not detailed in the present work. They will be in the scope of a forthcoming communication.

2.2 Boundary conditions

The work of Kanit et al. (2003) has shown that the elastic effective properties of a random biphase material with strong contrast between properties are sensitive to the type of boundary conditions for a tensile test: homogeneous strain field on the contour, homogeneous stress field on the contour, periodic strain on the contour. In the present work, the purpose is not to study the effect of the boundary conditions. A mixed type of boundary conditions is used to model a simple axial loading for all the results presented hereafter: as a displacement is imposed in the direction of loading, the stresses in the perpendicular direction remain null.

2.3 Constitutive laws

Two types of anisotropic behavior have been attributed to the crystals:

- Isotropic transverse elasticity with coefficients corresponding to a zinc alloy.
Crystal plasticity assuming that plastic strain results from intragranular slip on slip systems, with parameters corresponding to INCO600 (Barbe et al. (2001a)); on every slip system, slip rate is deduced with a viscoplastic law from the resolved shear stress and the hardening contributions (isotropic and kinematic hardening); then stress and strain tensors are determined according to the crystallographic orientation through the Schmid tensor.

2.4 Computation

In the general case, the effective properties are the result of an ensemble average over the apparent (volume average) properties of a large set -hundreds of thousands of individuals- of random multicrystals. The following procedure is thus applied automatically for each multicrystal, controlled by a shell script:

- Voronoi tessellation and generation of the mesh according to the number of grains and to the discretization
- generation of the crystallographic orientations (isotropic)
- volume average over the multicrystal and storage of the result

Basic statistical treatments are then performed on the set of results obtained for \( N \) multicrystals:
- ensemble average \(< X >\) over the random variable \( X = \{x_i, i = 1, N\} : < X > = \sum_{i=1}^{N} x_i / N\)
- relative dispersion: \( D_{rel} = (\sum_{i=1}^{N} (x_i - < X >)^2)^{1/2} / < X >\)
3 Elasticity

The first investigation to make deals with the validity of the ergodicity hypothesis. To this concern, we have performed several thousands computations of multicroystals (called sub-domains hereafter) containing from 10 to 500 grains, and discretized with mapped meshes.

The dispersion and the mean value of lateral strain and axial stress is presented as a function of the number of grains per multicroystal (which corresponds in this text to the size of the sub-domain) on fig. 2. It is clear that ergodicity seems to be valid: (i) the number of grains per sub-domain has a neglectable effect on the apparent properties (ensemble average over sub-domains of a same size); (ii) as compared to the apparent properties obtained with 500 grains and \( 32^3 \) elements—a multicroystal which is considered large enough for providing effective properties of a polycrystal—, whatever the number of grains per multicroystal, the apparent properties are correct with an accuracy inferior to 1.5%. Furthermore, there is a very small effect of the sub-domain mesh size on the apparent properties and on the dispersion.

![Figure 2: Effect of the number of grains per sub-domain on the apparent properties in zinc and on its dispersion. The length of a vertical segment indicates the absolute dispersion](image)

4 Plasticity

The same kind of analysis as that made in elasticity is now under concern in elastoplasticity. Considering the axial stress obtained from mapped meshes, on fig. 3a, it is clear that there is a small effect of the number of grains per multicroystal as well as an effect of the size of sub-domains. These effects are not observed with free meshes respecting the morphology of Voronoi polyhedra (fig. 3b). That is why these effects could be related to the crude representation of convex polyhedra with ensemble of brick elements: such a discretization increases the total area occupied by the grain boundaries as compared to the original multicroystal defined by Voronoi tesselation; this way, it artificially increases the total volume of the regions where accommodation of plastic strains take place in the multicroystal and this increase is all the more important as the discretization is crude. This may explain why more plasticity is produced with \( 14^3 \) elements than with \( 18^3 \) elements for a same number of grains.

As a basic application to cyclic plasticity, we have performed cycles in simple tension-compression on several multicrystals of more than 200 grains: mapped meshes made of linear brick elements reported on fig. 4a and free meshes made of quadratic tetrahedral elements re-
Figure 3: Effect of the number of grains per sub-domain on the apparent axial stress in INCO600 and on its dispersion: (Left) mapped meshing, (Right) free meshing. The length of a vertical segment indicates the absolute dispersion.

Figure 4: Stress-strain curves of IN600 multicrystals submitted to a cyclic tension-compression test with imposed axial strain. (Left) mapped meshing, (Right) free meshing. Only points constitute results; lines are only meant to serve as guides to the eyes.

reported on fig. 4. In each case of mesh, all the curves merge into one, with a dispersion inferior to 2%. The quantitative discrepancy between the two cases of mesh is probably due to the difference in the degree of the elements.

5 Conclusions

The main conclusions pertaining to this analysis are the following:
(i) ergodicity hypothesis is valid in the case of elasticity, whatever the kind of meshing, mapped or free;
(ii) quadratic tetrahedral elements shall be used if one resorts to ensemble averaging for the determination of effective elastoplastic properties of polycrystals;
(iii) as concluded from several detailed analysis in previously cited works calling upon quadratic brick elements, the discretization does not need to be very fine as long as the number of grains in the multicrystal is large; typically of the order 10 elements per grain, tetrahedral of cubic;
(iv) the size of a representative volume element determined from a monotonic test remains the same for a cyclic test.

These results allow to define the possible configurations of FE computation to be retained for the study of cyclic multiaxial plasticity and more particularly ratchetting, two cases of loading for which the technique of FE crystalline plasticity could provide predictions in much better agreement with experiments than phenomenological modelling could ever do. Experimental and numerical tests are currently performed in LMR to address this question.

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References


