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Finite element assessment of an affine self–consistent model for hexagonal polycrystals

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ABSTRACT

The present study aims at providing computations that can be used as reference solution to check mean-field nonlinear homogenization models for elastoviscoplastic constituents. These computations are based on finite element (FE) simulations of polycrystalline aggregates made of grains with hexagonal crystalline structure. A detailed statistical analysis has been performed for a specific grain located at the center of the aggregate by varying its neighboring grains. Comparisons are performed at the overall and local scales between simulations using the affine extension of the self-consistent scheme and the FE results for tensile and creep loading tests.

1. Introduction

Based on FE (Finite Element) simulations of microstructure, this study is devoted to develop a statistical approach in order to provide computations that can be used as reference solution to assess the accuracy of micro-mechanically based models. The full-field FE simulations on a Representative Volume Element (RVE) are used to calibrate micro-mechanically based constitutive models. The results are classically compared at two levels: the macroscopic level, using (i) the volume average over all Gauss points of the RVE (ii) and the phase scale, using the volume average over the Gauss points of the elements having the same orientation. This work focuses only on the assessement of the studied model on the phase level.

In the last decade, FE simulations of microstructure have been extensively used (i) to study the texture evolution during deformation processes, (ii) to predict stress/strain fields at local levels (intergranular and intragranular) (iii) and to calibrate micro-mechanically based constitutive models. Different techniques have been used in the literature to generate microstructure meshes. The first studies in this domain have used Voronoï tesselation algorithms in 2-D (Kumar and Kurtz, 1993; Watanabe et al., 2008; Weyer et al., 2002; Lebensohn et al., 2005; Saï et al., 2006) or 3-D (Kumar and Kurtz, 1994, 1995; Kumar et al., 1996; Barbe et al., 2001a, b; Kuprat et al., 2003; Diard et al., 2005) cases using a synthetic aggregate to provide a cubic domain. A non exhaustive list of studies devoted to real microstructure reconstruction coming from experimental data acquisition includes the works (Schmauder et al., 2003; Héripré et al., 2007; Bhandari et al., 2007; Musienko et al., 2007; Zhang et al., 2007; Zeghadi et al., 2007). A more realistic solution considering an RVE formed by non-truncated grains has been proposed by (Gérard et al., 2009; Hlilou et al., 2009; Abdeljaoued et al., 2009).

On the other hand, the classical self-consistent approach in which the concept of grain is replaced by the concept of crystallographic phase is adopted. Phases in the polycrystalline aggregate are defined according to the crystal orientation, that is all the grains with the same crystalline orientation belong to the same mechanical phase. For recrystallized alloys, the grains have equiaxed shapes and are randomly distributed. Consequently, the autocorrelation functions of the phases are spherical. The inclusion shape in the auxiliary Eshelby problem is related to these microstructural functions. The homogenization scheme assumes that each phase is

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embedded in a homogeneous effective medium (HEM), which is the rest of the aggregate. The overall behavior is then the average of the local behaviors over the crystallographic texture (Fig. 1). A particular attention is paid, here, to the grain located at the center of the aggregate. It will be referred to as CG (Central Grain). The CG is the furthest from the surface and then is less sensitive to the applied boundary conditions. The micro-mechanically based constitutive models will then be scrutinized against the full-field FE simulations for the CG. The approach can be summarized in the following steps:

1. The crystallographic orientation of the CG is assigned to a value between a set of selected Euler angles described in Section 3.2.
2. A random distribution of Euler angles is then assigned for the rest of the aggregate.
3. Boundary conditions are applied to the contour of the unitary cube as explained in Section 3.1. The mechanical response related to the CG is finally deduced.

To meet the assumptions of the self-consistent model, it is necessary to average the local fields of the CG. For this reason, the procedure described above is repeated as many times as necessary. The same steps, (1) to (3), are applied for a second crystallographic orientation of the CG. After N FE simulations are run, the average of strain and stress fields in the CG are calculated. The previous methodology is schematically summarized in Fig. 2. This procedure provides a realistic behavior of a given phase involving grains with the same orientation, different shapes and different neighborhoods in accordance with the self consistent formalism.

It is worth noting that the consistency of the adopted approach was already checked for linear elastic behavior (Priser, 2008) by comparison with analytical solution obtained with the help of self consistency theory. An examination of local and global stress fields in a spherical inclusion obeying a cubic elastic behavior and embedded in an infinite medium subjected to homogeneous strain at infinity have demonstrated that the convergence of the FE results to the analytic solution is achieved (Bornert et al., 2001) after 1000 realizations. A similar study was performed in the work of Castro Moreno et al. (2012) in which the FE aggregate was subjected to isotropic loading and to a shear loading in order to estimate the elasticity constants (i.e. bulk modulus and shear modulus of the HEM). Two microstructures of 343 ($7 \times 7 \times 7$) and 512 ($8 \times 8 \times 8$) grains are used respectively. In the following, OD342 will refer to the microstructure of 343 grains and OD511 will refer to the microstructure of 512 grains. A crystal plasticity material model, taking into account the hexagonal lattice and the crystallographic orientation, was assigned to each grain. It was shown that the FE computations correctly predict the elasticity constants and the stress-strain fields in the CG for two materials. The results were assessed by comparison to analytical results given in (Berveiller, 1978).

In the present work, FE computations using a crystal plasticity model are performed to simulate a polycrystalline aggregate submitted to tensile, relaxation and creep loadings. The results are compared with the predictions of a micromechanical model based on the self-consistent affine scheme (Masson and Zaoui, 1999; Brenner et al., 2002).

Comparable investigations can also be found in (Lebensohn et al., 2004a, b; 2011). The paper is organized in the following manner: The main lines of constitutive equations for the single crystal model are recalled briefly in Section 2. In Section 3, the FE mesh, the boundary conditions and the statistical analysis of the FE results are presented. The constitutive equations of the affine type formulation are recalled in Section 4. Comparisons between the affine type model and FE simulations are shown in Section 5 for the central grain as well as the for overall behavior. In addition to the tensile test, which is fundamental in characterizing the mechanical properties, focus is set on the elastoviscoplastic behavior of HCP materials through creep and relaxation tests.

2. Constitutive equations for the single crystal

A simplified elastoviscoplastic single crystal model is used to describe single crystal behavior. It assumes, in the framework of small perturbation, an additive decomposition of the elastic and the viscoplastic strain rates; the elastic part is obtained by the Hooke's law:

$$\underset{\sim}{\dot{\varepsilon}} = \underset{\sim}{\dot{\varepsilon}}^{p} + \underset{\sim}{\dot{\varepsilon}}^{e} \qquad \underset{\sim}{\dot{\sigma}} = \underset{\approx}{\mathbf{C}}\, \underset{\sim}{\dot{\varepsilon}}^{e} \tag{1}$$

where $\underset{\approx}{\mathbf{C}}$ is the fourth-rank tensor of elastic moduli. The so—called resolved shear stress τ^s acting on a particular slip system (s) is given by the relation:

$$\tau^s = \underset{\sim}{\sigma} : \underset{\sim}{\mathbf{m}}^s \tag{2}$$

where $\underset{\sim}{\sigma}$ is the stress tensor in the grain and $\underset{\sim}{\mathbf{m}}^s$ is the orientation tensor attributed to the slip system (s):

$$\underset{\sim}{\mathbf{m}}^s = \frac{1}{2}\left(\underset{\sim}{\mathbf{l}}^s \otimes \underset{\sim}{\mathbf{n}}^s + \underset{\sim}{\mathbf{n}}^s \otimes \underset{\sim}{\mathbf{l}}^s\right) \tag{3}$$

$\underset{\sim}{\mathbf{n}}^s$ and $\underset{\sim}{\mathbf{l}}^s$ are the “slip plane” normal vector and the “slip direction” vector in this plane, respectively. The resolved shear stress τ^s can be related to the corresponding shear rate $\dot{\gamma}^s$ via a power law expression:

$$\dot{\gamma}^s = \dot{\gamma}_0 \left(\frac{|\tau^s|}{\tau_0}\right)^n sign(\tau^s) \tag{4}$$

A specific material parameter τ_0 is considered for each slip system family: basal (3 systems), prismatic (3 systems) and second-

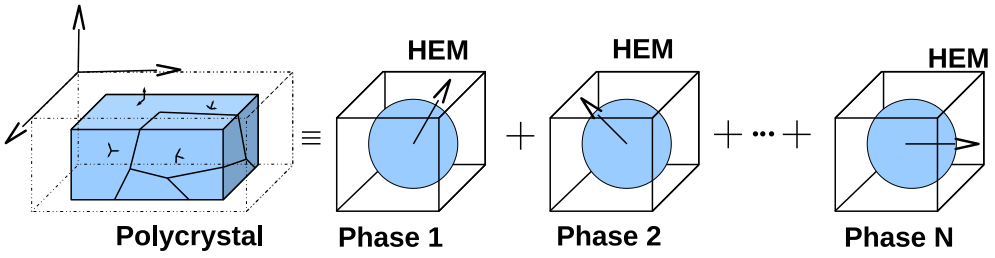

Fig. 1. Eshelby's problems for equiaxed polycrystals.