Influence of the elastic anisotropy on the initial yielding of polycrystals

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ABSTRACT

Based on the self-consistent estimate of the local stress field within an elastically anisotropic polycrystalline aggregate, an original definition of the initial yield surface of polycrystals is proposed. It makes use of the average and the standard deviation of the resolved shear stress on the different slip systems within a crystalline orientation. In the case of a copper polycrystal, our results show a strong influence of the stress heterogeneity with a decrease of the elastic limit estimate of about 20% compared to the customary estimates neglecting the intraphase field fluctuations. A good agreement with a full-field approach based on Fourier transforms is obtained.

1. Introduction

The experimental elastic limit of a polycrystalline metallic material is usually determined based on macroscopic stress-strain curves. A customary convention is to consider the macroscopic stress for an offset plastic strain of 0.2%. This definition gives necessarily an upper limit for the yield point of the polycrystal. On the other hand, the recent development of microdiffraction experiments allows to investigate the local plastic behaviour at the grain scale [1] and thus gives access to a local determination of the Yield Surface (YS) of a polycrystal. Such experimental results can be compared with predictions obtained with a micromechanical modelling which describes the heterogeneity of the mechanical fields resulting from the microstructural topology and the anisotropy of the elastoplastic constitutive behaviour. In the sequel, attention is focused on the role of the local elastic anisotropy since only *initial* yield surfaces will be considered.
Our study addresses the modelling of the YS of a polycrystal based on the local stress field. With this aim in view, we consider two types of micromechanical approaches: a full-field modelling based on Fourier transform and a mean-field modelling using the self-consistent scheme. Local definitions of the initial YS in the mean-field context are proposed and the results are compared with the full-field method.

2. Stress field within elastically anisotropic polycrystals

We consider isotropic polycrystals (i.e equiaxed grains and no preferred crystalline orientations) with anisotropic local elastic behaviour $\mathbf{C}(\mathbf{x})$. It is assumed that this random elasticity tensor field is Statistically Homogeneous and Ergodic (SHE). To be able to predict the initial yielding within a Representative Volume Element (RVE) of such polycristalline medium, it is necessary to describe the heterogeneity of the local stress field. This question is studied with different micromechanical approaches. In the sequel, all numerical applications have been performed with local elastic moduli of copper.

2.1 Full-field approach

The Fast-Fourier Transform (FFT) method has been proposed in [2] to determine the mechanical behaviour of a unit-cell representative of a heterogeneous material. It assumes periodic boundary conditions. This modelling makes use of a discrete spatial description of the microstructure and the local elastic behaviour. In the present case, the unit-cell adopted to represent an equiaxed polycrystalline microstructure is a 3D periodic Poisson-Voronoï tesselation (Fig. 1) made of 500 grains (i.e Voronoï seeds) with a one-to-one correspondence between the set of grains and the set of crystalline orientations. To use the FFT method, the Voronoï tesselation is discretized into a regular grid consisting of 128 x 128 x 128 voxels (6,300,000 degrees of freedom). Each grain thus comprises 4,200 voxels.

It is pointed out that the considered unit-cell is not a RVE of the polycrystal. To approximate the response of a RVE, a Monte-Carlo computation is performed by considering *N* different configurations of the unit-cell [3]. Different unit-cells are simulated by changing the Voronoï tesselation and keeping the same set of crystalline orientations. An estimate of the expectation of the stress and strain fields within a given crystalline orientation can thus be obtained. By using classical relations from the sampling theory, the relative error on the intracrystalline average fields can be obtained for a fixed number of configurations. In our case, 50 different unit-cells have been considered. With the local elastic moduli of copper, a relative error lesser than 2% is obtained. Note that each unit-cell is subjected to an uniaxial tensile loading along the z axis.

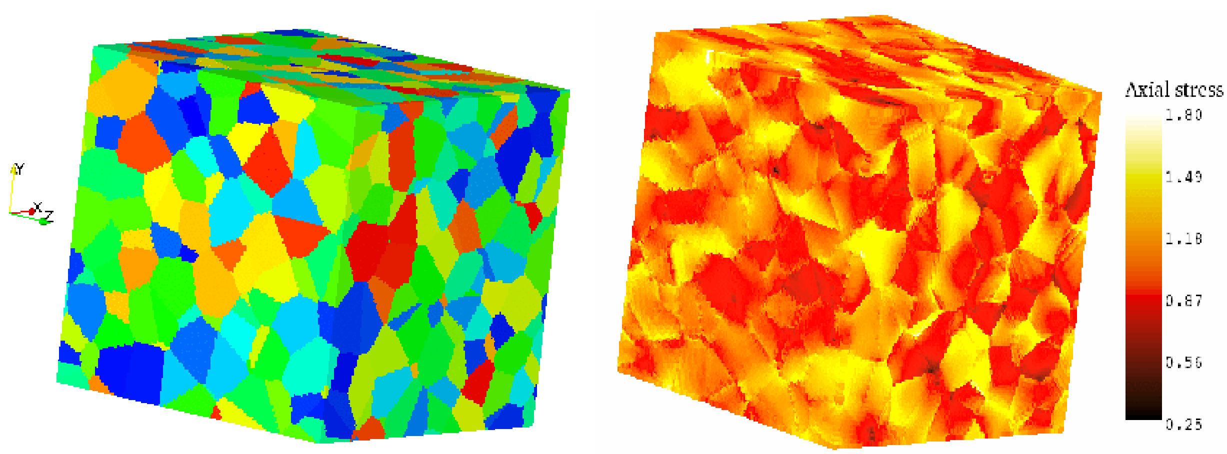

Figure 1. 3D periodic Poisson-Voronoï tesselation and field of the normalized axial stress s_{zz} for an uniaxial tensile test along the z axis.

For each configuration, a highly heterogeneous stress field is obtained. Indeed, the local axial stress component can reach almost twice the macroscopic value (Fig. 1.). Obviously, this stress fluctuation will give rise to an early plastic yielding within the polycrystal as compared to the isotropic elastic case.

Concerning the intracrystalline strees field, it is interesting to note that it does not follow a Gaussian distribution for each single configuration but it tends to such a distribution when it is averaged over the 50 different configurations (Fig. 2). This observation is consistent with previous results obtained on a RVE for a model 2D polycrystal with Voronoï microstructure [4].

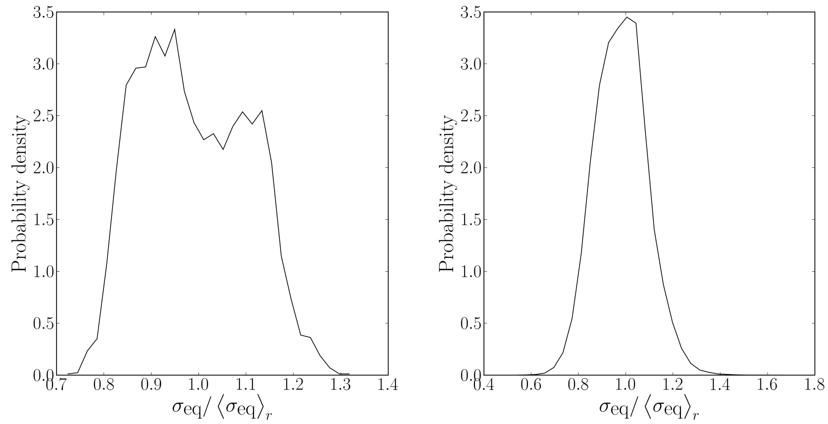

Figure 2. Probability densities of the normalized equivalent local stress for a given crystalline orientation. Left: single unit-cell configuration. Right: 50 unit-cell configurations.

2.2 Mean-field approach

The mechanical field fluctuations within a SHE polycrystalline aggregate can alternatively be quantified by using a mean-field approach making use of the elementary Eshelby's localisation relation. Such procedure rely on astatistical description of the microstructure via the *n*-points correlation functions. In this framework, it has been established that the self-consistent scheme (SC) is attained for "perfectly disordered" polycrystalline microstructures [5]. In the linear elasticity context, the mean-field approaches give an estimate of the first and second moments of the intraphase mechanical fields within the heterogeneous medium. For the considered polycrystalline microstructure, the average and the variance of the stress and strain fields for each crystalline orientation within a RVE can thus be obtained using the self-consistent scheme. In general, they have to be evaluated numerically. A good agreement between the FFT computation and the SC estimate has been previously reported for the intraphase first and second moments of the fields within polycrystalline microstructures [4,6]. In the present case, since the full-field approach shows that the fields follow a normal distribution, it is pointed out that the self-consistent scheme then leads to a particularly relevant estimate of the intraphase stress field distribution.

3. Yield surface estimate and stress heterogeneity

Based on the statistical description of the intraphase stress field available with the self-consistent scheme, it is proposed to define a *probability yield surface* related to the level of intraphase heterogeneity which is accounted for. By using the classical Schmid criterion, it is assumed that the yielding occurs in the polycrystal when some *reference* resolved shear stress (RRSS) reaches a critical value. In the context of self-consistent estimates, the RRSS usually corresponds to the maximal value of the average per crystalline orientation of the resolved shear stress on the different slip systems. Such definition leads to an upper bound for the initial YS. More realistic estimates can be obtained by using both *average* and *standard deviation* per crystalline orientation to define the RRSS. More precisely, it is proposed to define the RRSS as the upper value of a given confidence interval on the resolved shear stress distribution. SC estimates of the YS for tensile-torsion tests are reported on Fig. 3. with different definitions: average, 68%, 95% and 99% confidence intervals.

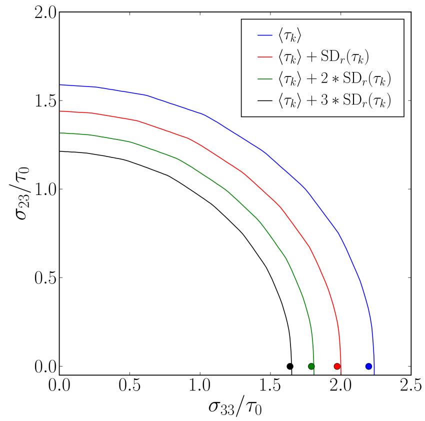

Figure 3. Prediction of the initial YS of an isotropic copper polycrystal using the SC scheme (lines) with different definitions of the RRSS. The points are FFT results for uniaxial tension.

4. Concluding remarks

(i) In the particular case for which the local fields within a 'composite' follow a normal distribution, the mean-field approaches deliver an accurate description of this distribution.
(ii) SC estimates of the YS is strongly influenced by the stress field heterogeneity which results from the local elastic anisotropy. If we adopt the 95% CI defintion, the estimate of the elastic limit in uniaxial tension is decreased by ~20% compared to the customary average definition.
(iii) A very good agreement is obtained between the FFT and the SC estimates for the initial tensile elastic limit. The discrepancy is consistent with the error of the ensemble averaging.

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