Generalized self consistent polycrystalline model applied to heterogeneous materials exhibiting log normal grain size distribution

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ABSTRACT

A generalized self consistent approach, recently proposed by Jiang and Weng [1] for investigating the properties mechanical of nanocrystalline (NC) materials, is revisited and reformulated following an incremental scheme. The NC material is modeled as composed of spherical randomly distributed grains with a lognormal grain size distribution. Each oriented grain and its immediate grain boundary form a pair, which in turn is embedded an infinite effective medium with a property representing the average orientation of all these pairs. The plastic deformation of the grain phase takes into account the dislocation glide mechanism whereas the boundary phase is modeled as an amorphous material.

1. Introduction

NC and utrafine-crystalline materials (UFG) are research topic subjects that bridge several fields, from materials science to mechanical engineering since more than a decade [2]. This type of materials processes superior mechanical strength over their microcrystalline counterparts but limited plastic deformation. Both experimental and theoretical investigations show deformation mechanisms being dominated by the grain boundary phase activity. More generally, when the grain size decreases down to about tenth of nanometers, the yield strength increases linearly with the inverse square root of the grain size as described by the Hall-Petch law: $\sigma_y = \sigma_0 + kD^{-1/2}$, where σ_0 is the frictional stress, k the Hall-Pecth slope and D the mean grain size. Nevertheless, is should be noticed that the mechanical properties of a given material depend on the as-processed microstructure characteristics (such as the grain size distribution, the crystallographic texture, the grain boundary structure, the grain shape etc…) and not only on the mean grain size. Most of these microstructures characteristics are often out of reach experimentally. In the same time, numerical simulations are good means for predicting, optimizing, and controlling the processing of material. Jiang and Weng developed a generalized self consistent polycrystal model [1], based on Christensen and Lo's solution [3] and Lou and Weng's solution [4] to predict the influence of the as processed microstructure on the subsequent mechanical behavior.

In doing so, they considered solely the average grain size as structural parameter. However, experimental investigations do demonstrate that the grain size is dispersed in an interval within the lognormal distribution. Taking into account the lognormal distribution and the dispersion around the mean grain size allows to better simulating, with more accuracy, the behavior of the bulk NC or UFG materials and constitutes the goal of this study presented here.

2. The generalized self-consistent approach

In this paper, the generalized self-consistent model, recently proposed by Jiang and Weng [1], is rewritten following an incremental small strain scheme. The representative volume element (RVE) of this micromechanical model is an oriented grain identified by Eulerian angles (ϕ_1, θ, ϕ_2) and its immediate boundary forming a pair embedded in a homogeneous equivalent medium. Under the macroscopic Cauchy stress rate $\dot{\Sigma}_{ij}$, the plastic deformation of the grain is governed by its crystallographic slips systems. However the stress and strain of the surrounding grain boundary, modelled as an amorphous material, are closely related to the plastic strain of its enclosed grain. The nonlinear problem can be resoled by superposition of two linear auxiliary problems as schemes in Fig 1.

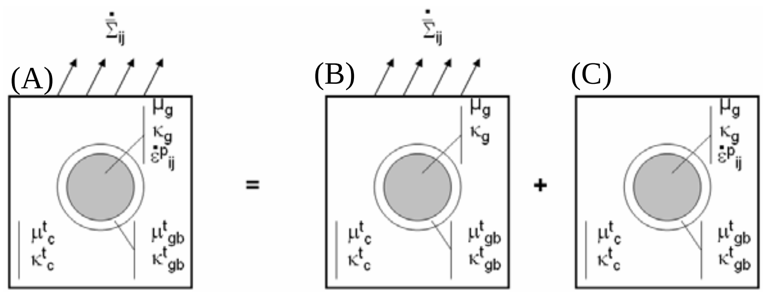

Figure 1. The decomposition scheme of the initial non-linear (A) problem into two linear auxiliary problems according to Christensen and Lo (B) and Lou and Weng (C).

The stress-strain relation of each oriented grain is given by

$$\dot{\sigma}_{ij}^{(g)} = C_{ijkl}^{(g)} \left(\dot{\varepsilon}_{kl}^{(g)} - \sum_s \nu_{kl}^{(s)} \dot{\gamma}^{(s)} \right) \tag{1}$$

where $C_{ijkl}^{(g)}$ is the crystal elasticity tensor, $\dot{\gamma}^{(s)}$ is the shear rate, $\nu_{kl}^{(s)}$ is the Schmid factor tensor of the slip system s, defined as the tensor product of the unit slip direction tensor and the slip plane normal tensor of the considered slip system.

The plasticity of the grain-boundary phase is isotropic and incompressible (p=0). The yield function described by [5]: $\sigma_e^{(gb)} = \sigma_y^{(gb)} + h_{gb} (\varepsilon_e^{p(gb)})^{n_{gb}}$ where $\sigma_e^{(gb)}$, $\varepsilon_e^{p(gb)}$ and $\sigma_y^{(gb)}$ are the Mises' effective stress, effective plastic strain and the yield strength initial of grain boundary respectively. The parameters h_{gb} and n_{gb} are the material constant related to the grain boundary. The grain boundary thinness was given a value of δ=1 nm [1].

3. Results and discussions

The application of the present model for the copper processed by inert gas condensation method [6] was presented in this section. Fig. 2a compares the true stress-true strain curve obtained from experimental tensile test at room temperature at the strain rate of $10^{-4}s^{-1}$ and the one of the current model prediction. Three types of material, corresponding to three different mean grain sizes of 49 nm, 110 nm and 20 μm, were studied. It is clear that the flow stress depends on the grain size and the simulation compares fairly well with the experimental results.

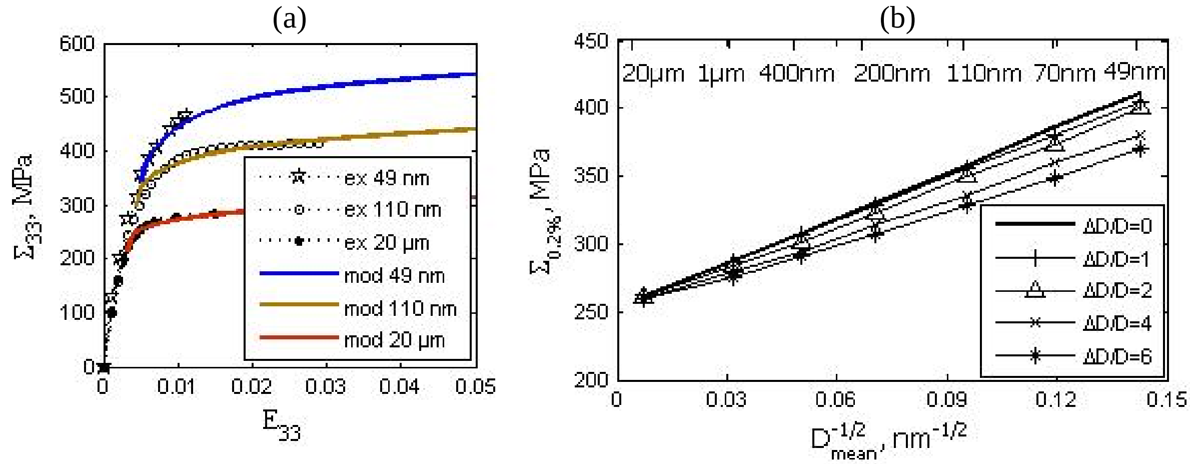

Figure 2. (a) Calculated (mod) and experimental (ex) stress-strain relations of copper with different grain sizes. (b) Predicted flow stress at 0.2% plastic strain as a function of mean grain size for different relative dispersion ΔD/D.

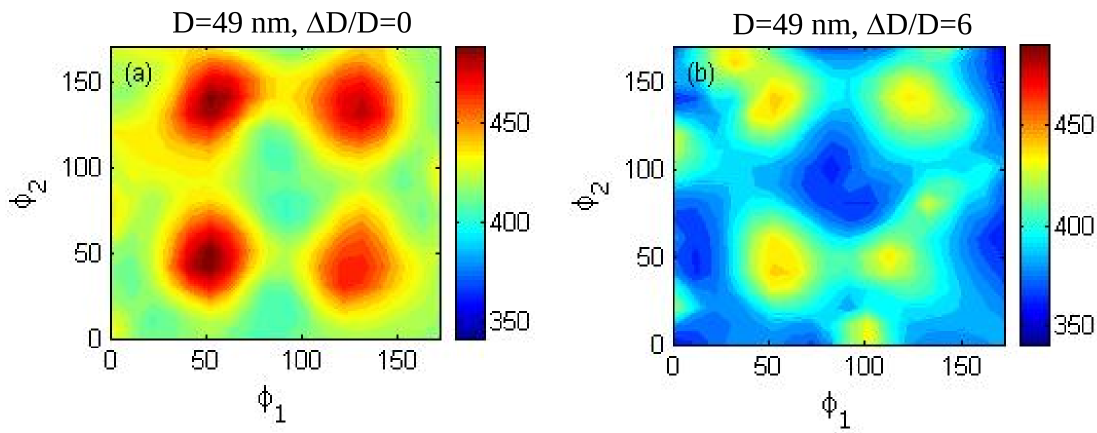

Figure 3. Map for the effective stress of the grain phase (at the overall axial plastic strain level E^p=1%) in terms of the orientation of the grain (random orientations) at mean grain size D_{mean}=49 nm and different relative dispersion.

A procedure is used to generate different discrete lognormal distribution with given means and dispersions [7]. The flow stresses at 0.2% plastic strain are plotted in Fig. 2b as a function of $D_{mean}^{-1/2}$. The relative dispersion ΔD/D takes the values 0, 1, 2, 4, 6 and all the curves appear to be quite linear. Our results, like those presented by Berbenni et al [7], display a unique effect of the grain size dispersion which becomes more significant at the NC regime (49 nm).

Fig. 3 illustrates the evolution of effective stress of the grain phase (which is defined as $\sigma_e^{(g)} = \left(\frac{3}{2} \sigma_{ij}^{'(g)} \sigma_{ij}^{'(g)} \right)^{1/2}$) at the overall axial plastic strain level E^p=1% taking into account the initial grain orientation, different mean grain sizes and associated relative dispersions. It can be seen that in the all cases, the effective stress of the grain phase is heterogeneous and the high effective stresses are located at (ϕ_1, ϕ_2) = (50°,50°), (50°,125°), (125°,50°) and (125°,125°). In the case of (D_{mean}=49nm, ΔD/D=6), the effective stress exhibits more heterogeneity than the other cases with the presence of additional high effective stress located at (ϕ_1, ϕ_2) = (0°,110°), (40°,160°), (100°,0°), and (130°,80°) (see Fig. 3b). Comparing the effective stress in the case of the coarsest mean grain size D_{mean}=20µm with no dispersion (ΔD/D=0) to the case of a broader dispersions like ΔD/D=6, the resulting stress fields are very close (in position and levels) (not show here). As for the NC sample (D_{mean}=49nm), a loss of the effective stress fields is found when the two extreme dispersions ΔD/D=0 and ΔD/D=6 (Fig. 3a and 3b) are compared. These results confirm that the effect of the grain size dispersion on the effective stress fields at E^p=1% becomes more significant at finest mean grain sizes.

As in previous work [7], we have numerically investigated the hypothesis that broad dispersions tend to reduce the grain size dependence whereas the individual grain behaviour is grain size dependent.

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