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Micro–macro modelling of the effects of the grain size distribution on the plastic flow stress of heterogeneous materials

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Abstract

When the mean grain size of polycrystalline materials is larger than ~100 nm, it is commonly accepted for metals, intermetallics or ceramics that the plastic flow stress scales linearly with the inverse square root of the mean grain size (the so-called Hall–Petch behaviour). However, in this classic formalism, only the mean grain size is considered in a semi phenomenological way, and, the fact that the grains form a population of stochastic nature with different sizes and shapes is not stated. Here, a new self-consistent model making use of the "translated fields" technique for elastic–viscoplastic materials is developed as micro–macro scale transition scheme, and, the aggregate is composed of spherical randomly distributed grains with a grain size distribution following a log-normal statistical function. The constitutive behaviour of each grain is described by a partitioned strain rate into an elastic part and a viscoplastic part. The viscoplastic strain rate is described by an isotropic power law including the grain diameter through the reference stress. Numerical results firstly display that the plastic flow stress of the material depends on both the mean grain size and the grain size dispersion of the distribution. Besides, the role of the dispersion is more important when the mean grain size is on the order of the μm and the trend is a decrease of the flow stress with an increase of the dispersion. Secondly, predictions of second order internal stresses within the material indicate an increase in the internal stresses when grain size dispersion is increased, so that the plastic flow stress of the material depends on a competition between the respective distributions of internal stresses and individual flow stresses of the grains.

Keywords: Grain size distribution; Grain size effect; Plastic flow; Heterogeneous material; Micromechanical model

1. Introduction

The determination of the behaviour of heterogeneous materials with complex microstructures constitutes a challenge in the design of new materials and the modelling of their effective behaviour during their processing. The Hall–Petch relation [1,2] linking the yield strength to the mean grain size has been found to match quantitatively the grain size effect on the behaviour of polycrystalline aggregates. Originally, this relation which claims that the tensile yield stress of several polycrystalline steels scaled with the inverse square root of their mean grain size has been attributed by Hall and Petch to the development of intragranular dislocation pileups having a slip length proportional to the mean grain size. Indeed, to justify their experimental results, they used the theoretical model of an equilibrated pileup of straight dislocations developed by Eshelby et al. [3] to derive the aforementioned relation. Other authors [4,5] have also derived the Hall–Petch behaviour by measuring through TEM observations dislocation density within grains and by determining the increase of the plastic flow stress with the square root of dislocation density. It has been also found that grain boundaries are common sources of dislocations [6–8]. Anyway, the hypothesis of pileups to explain the Hall–Petch behaviour for the yield stress with a classical −0.5 exponent (inverse square root of mean grain size dependence) is still

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widely used by metallurgists [9–11] except for very large grained materials for which a -1 exponent (inverse mean grain size dependence) is rather found [12,13]. Furthermore, it has been shown that the Hall–Petch behaviour continues to be valid until a very fine grain regime (on the order of 100 nm) following Masumura et al. [14] who explored a lot of experimental data for many materials. A first micro–macro modelling considering grain size effect has been elaborated by Weng [15] who considered a Hall–Petch type equation with *a single valued grain size* at the scale of the slip systems and used the Berveiller–Zaoui's model [16] to derive the overall behaviour of copper polycrystals which leaded to a Hall–Petch type behaviour as well. More recently, non local dislocation mechanics models using the concept of geometrically necessary dislocations (GNDs) have been developed by Acharya and Beaudoin [17] and predict pretty well the strain-hardening rate dependence on grain size after the yield point making use of the evolution of GNDs (or equivalently the lattice incompatibility). In all these developments, only the *mean grain size* is considered.

Since the grain size distribution in heterogeneous materials provides heterogeneity, it appears fundamental to get an accurate description of the effect of grain size on the local interactions and behaviours, and also, a relevant mathematical description of the grain size statistics inherent to the processing route (prior working, annealing, etc.). Advanced homogenization techniques developed these last decades such that the self-consistent procedure did not focused on the effect of grain size distribution on the behaviour of heterogeneous materials and did not account for statistical description about grain diameters which are stochastic internal parameters of the microstructure. The objective of the present paper is to study in a systematic statistical way grain size effects on the macroscopic plastic flow stress of heterogeneous materials assuming a given grain size distribution *with higher moments than the mean grain size*. Especially, the role of the *grain size dispersion* is underscored. To achieve this objective, the present modelling includes three combined pillars depicted in Part 2: (i) a given statistical grain size distribution characterizing the heterogeneity of the aggregate associated with local grain size effect, (ii) some adequate constitutive relations at the scale of the grains including grain size as characteristic internal length scale parameter, (iii) a relevant scale transition scheme embodied here by a self-consistent model based on the "translated fields" technique developed for heterogeneous elastic–viscoplastic materials. Thus, intragranular plastic anisotropy and strain hardening are voluntary not taken into account since correlations between grain size and lattice orientation (crystallographic texture) need to be quantified for a complete description of couplings between texture and grain size. Furthermore, the case of nano-grained materials is not treated here (we only consider grain sizes larger than 0.1 μm) since grain boundaries may then occupy a non negligible volume fraction within the material and are willing to be regarded as a new phase [18]. Part 3 displays numerical results for heterogeneous materials with grain sizes log-normally distributed in terms of macroscopic plastic flow stress (or yield stress), local plastic strains and second order internal stresses.

In the whole paper, tensors are denoted by boldface symbols.

2. Model

In the present model, the RVE denoted V is constituted of N homogeneous grains (or crystallites) spherical in shape (i.e. approximately equiaxed after normal grain growth). The grain individual volumes (representing the heterogeneities) are supposed small compared with V. The grains are designated by the superscript "I" in the following ($I = 1, \ldots, N$). The present model first includes a representation of grain size distribution within the RVE using log-normal statistical functions (Section 2.1). The behaviour of the grains is regarded as elastic–viscoplastic without hardening because only the early stage of deformation (yield stress and transient regime) is considered. The spatial fluctuations of mechanical fields (assuming grain to grain compatibility) are due to grain size heterogeneities. These effects are captured assuming grain size dependent reference stresses within the viscoplastic constitutive formulation (Section 2.2). Then, a self-consistent scheme making use of the "translated fields" technique for elastic–viscoplastic materials is used as micro–macro scale transition to get the overall behaviour (Section 2.3).

2.1. Grain size distributions

On the topological point of view, the RVE is composed of spherical grains and we also assume that grain size is spatially non-correlated, which means that the spatial position of grains of a given diameter is truly random. Measured grain diameters follow approximately statistical log-normal density probability functions. These particular distributions have been often reported in the literature to fit real heterogeneous materials like polycrystalline metals or ceramics [19–21]. Recently, experimental observations for fine grained polycrystalline metals have also shown log-normal grain size distributions [22]. As reported in the literature [23], other types of grain size distribution may also occur in some cases but we limit ourselves to log-normal distributions.

A log-normal distribution function $\mathrm{Lgn}(M, S)$ of the variable D (with D positive, D being here the grain diameter) is defined so that the variable $x = \mathrm{Ln}(D)$ follows a normal distribution. M and S are respectively the mean value and standard deviation of the variable x. Thus, the probability density function for the log-normal distribution is (see e.g. the documentation of [24])

$$P(D|M,S) = \frac{1}{S\sqrt{2\pi}D} \exp -\frac{(\mathrm{Ln}(D) - M)^2}{2S^2}. \qquad (1)$$