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Effects of grain size distribution and stress heterogeneity on yield stress of polycrystals: A numerical approach

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ABSTRACT

This paper addresses the relation between the grain size distribution, the elastic stress field fluctuations and the description of incipient plasticity in polycrystals with local elastic anisotropy. We propose a numerical approach based on full-field computations on polycrystalline microstructures. The generation of microstructures with prescribed grain size distribution and grain shape is made by combining dense-sphere packing with Power diagrams. By using a local plastic criterion based on the stress field statistics, it is shown that the macroscopic Hall–Petch relation significantly depends on the grain size distribution and the stress heterogeneity. Previous results of the literature obtained with mean-field approaches are confirmed by our study.

1. Introduction

A polycrystalline material is a heterogeneous material with a random microstructure whose heterogeneity originates from the spatial variation of the crystalline orientation field together with the anisotropy of the single crystal. When the characteristic size of the grains is of the order of hundreds of μm or more, the statistical information on the morphological and crystallographic textures, based on *n*-point correlation functions, allows to derive bounds and estimates for effective linear (elasticity, conductivity, etc.) and nonlinear (plastic yield stress, electric hysteresis, etc.) properties [1,2]. These estimates depend on the shape of the correlation functions but not on their characteristic lengths. However, for polycrystals with smaller grain size, the effective properties may exhibit a dependence with the characteristic size of the heterogeneities. Consequently, the sole information on the shape of the *n*th order probability density functions is inadequate. In plasticity, a well-known relation exists between the grain size and the yield stress: the Hall–Petch effect [3,4]. It predicts a linear increase of the yield stress with respect to the inverse of the square root of the grain size. The modeling of this dependence can be addressed by using strain gradient plasticity models with higher order stresses [5–7] or by introducing geometrically necessary dislocations [8], whose density is related to the gradient of the plastic slip [9,10]. An alternative (phenomenological) approach is to consider a classical framework with a grain size dependence of parameters of the constitutive behavior (namely, the critical resolved shear stresses). This approach has been initially proposed in the context of the self-consistent scheme with a Hall–Petch type relation for the critical resolved shear stress on each slip system [11] for polycrystals with uniform grain size. The influence of a grain size distribution on the yield stress has been later investigated with the Taylor model [12] and the self-consistent scheme [13]. These models consider the average stress field within the grains to describe the initial yield stress. This assumption is known to deliver irrealistic self-consistent estimates, in the case of a uniform grain size, for cubic polycrystals exhibiting elastic anisotropy [14]. It has been recently shown that this shortcoming only arises if the intragranular stress heterogeneity is not accounted for in the criterion describing the inception of plasticity. The early plastic yielding, which occurs well below the conventional macroscopic yield stress can be indeed described by the self-consistent model which in turn coincides with reference full-field results on polycrystalline aggregates [15]. Following these results, the present study aims at investigating the effect of elastic anisotropy on the initial yield surface of polycrystals by considering their grain size distribution. For this goal, we adopt a numerical full-field approach allowing to perform computations on 3D polycrystalline unit-cells with prescribed morphological parameters. More specifically, the Fast-Fourier Transform (FFT) method [16,17] is used since it permits efficient calculations (for periodic boundary-value problems) based on digital images of the microstructure. This feature is particularly attractive in the case of complex microstructures presenting a large number of grains with varying sizes.

The experimental characterization of three-dimensional polycrystalline microstructures has been recently made possible with the development of X-ray diffraction contrast tomography [18].

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Consequently, the description of the effective response and local fields of real polycrystalline samples is now conceivable [19,20]. However, such experimental data remain relatively scarce. An alternative procedure consists in reconstructing three-dimensional microstructures from EBSD orientation maps obtained by consecutive polishing. Albeit possible (see, for instance, [21]), this procedure is particularly tedious and implies the destruction of the investigated sample. Following these remarks, it appears that a workable full-field analysis on polycrystalline microstructures with various grain size distributions must rely in practice on artificial microstructures which match given morphological characteristics. Besides, this approach is relevant in view of the design of microstructures.

The paper is organized as follows. Firstly, we present the numerical scheme used for the generation of polycrystalline microstructures. It combines a dense-sphere packing algorithm [22] with Power diagrams [23]. Illustrative examples encompass unimodal, bimodal as well as lognormal grain size distributions. The ability of the method to build polycrystalline aggregates with anisotropic grain shape is also emphasized. Secondly, the initial yield surface of copper polycrystals with varying grain size distribution is studied based on a statistical description of the stress field. Previous mean-field results concerning the effective Hall–Petch relation [3,4] are confirmed and the importance of the intragranular stress heterogeneity is further highlighted.

2. Generation of microstructures

2.1. Coupling Laguerre diagrams with dense sphere packing: background

2.1.1. Voronoi and Laguerre diagrams

Voronoi diagrams are widely used to construct artificial polycrystalline microstructures since they mimic the homogeneous crystal growth process [24]. A Voronoi diagram (Fig. 1) is a partition of space D which relies on N initial points $g_i \in D$, $i \in [0,N]$ called *germs*. Each grain $G_i \subset D$ is defined as the subset containing all the points closer to one germ than any other germ. Let $p \in D$ a point in space D.

$$p \in G_i \iff \forall j \neq i; \quad \|p - g_i\| < \|p - g_j\| \tag{1}$$

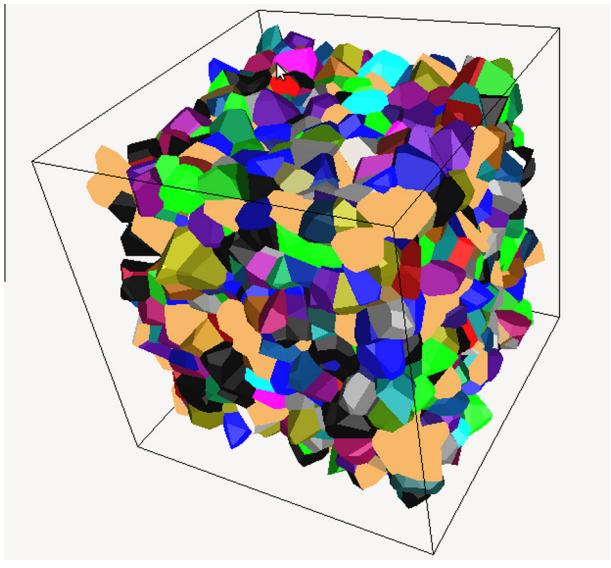

Fig. 1. A Poisson–Voronoi diagram with 2000 germs.

By construction, the interfaces between grains are planar and grains are convex polyhedra. Their faces can be obtained by using the Delaunay triangulation which is the dual graph of the Voronoi tessellation. Additional periodicity constraints have to be imposed on the tessellation to avoid artificial boundary effects.

The control of the grain volume distribution is obviously related to the spatial distribution of the germs. To represent equiaxed polycrystalline microstructures, a natural choice is to adopt a Poisson process to generate the germs. It leads to an isotropic microstructure with an almost uniform grain size. Dating from the work of Kumar et al. [25,26], this microstructural model is widely used to study the physical properties of equiaxed polycrystalline microstructures since it mimics the homogeneous crystal growth process[see, for instance, [27,28]]. By definition, this process provides no control on the microstructural features (i.e. grain size distribution and shape). To gain control on the grain repartition, a possibility is to adopt a Neyman-Scott or Gibbs process which helps obtaining aggregates of grains with different sizes [29]. However, the shape of the grains remains uncontrolled. An alternative approach to gain control on the grain size is to make use of Laguerre diagrams (also known as Power diagram) [23,30]. Each grain $G_i^L \subset D$ is now defined as the subset containing all the points for which the power distance relative to the sphere with center c_i and radius w_i is smaller than the power distance with any other spheres. The grain $G_i^L \subset D$ is defined as:

$$p \in G_i^L \iff \forall j \neq i; \quad \|p - c_i\|^2 - w_i^2 < \|p - c_j\|^2 - w_j^2 \tag{2}$$

A Voronoi diagram is a Laguerre diagram for which all weights are equal. Interfaces between adjacent grains are planar and grains are convex polyhedra.

Laguerre diagrams and regular triangulations are dual. The vertices of the regular triangulation are the germs of the corresponding Power diagram, edges correspond to faces and the vertices of the Power diagram are the orthogonal centers of the triangulation [31]. Weight is similar to a distance and it enables some control of the size of grains. The larger the weight, the bigger the grain. If the germs c_i are randomly distributed, the Laguerre diagram can present the following shortcomings:

(i) The point c_i may not be within the grain G_i^L.
(ii) A germ may result in an empty grain.

Such problems are overcome when points c_i are taken as centers of non-overlapping spheres of radius $r_i \geqslant w_i$. In this particular case, each grain contains the sphere it comes from. If the volume fraction of the sphere packing is large enough, grains are expected to have low aspect ratios and the grain size distribution is expected to be similar to the diameter distribution of the spheres. Being able to pack efficiently dense sets of non-overlapping spheres can thus provide control on resulting grain size distribution and grain shape.

2.1.2. The Lubachevsky–Stillinger algorithm

To represent realistic polycrystalline microstructures, a Power diagram seeded by a random packing of spheres has been considered for this study. Many algorithms have been designed to study random dense packing of hard spheres. Among the most successful, the Lubachevsky–Stillinger (LS) algorithm [22] is able to fastly pack a large number of polydisperse spheres. It is possible to pack ellipsoids [32] and it has been used to generate random microstructures in the range of fiber-reinforced materials [33].

The LS algorithm is an event-driven molecular dynamic algorithm. At $t = 0$, spheres (Fig. 2) are reduced to points. Each radius increases proportionally to time t and each center moves with a constant velocity. As spheres collide, the algorithm changes their