Virtual 3D microstructures with specified characteristics of state variable distributions

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Abstract. For a wide variety of model calculations a hypothetical 3D microstructure is required as input. Although experimental data are frequently used to this purpose, 3D microstructures are difficult to measure experimentally. In order to circumvent these difficulties, a virtual microstructure generator to simulate a specific 3D material microstructure is proposed. Such a virtual microstructure could serve as input for different types of models, would allow a faster model prototyping, would help to explore the boundary conditions of models and reduces the number of unnecessary experimental measurements. In the current paper, the method to generate and to control the grain size distribution as well as texture are discussed.

Introduction

Polycrystalline metallic solids are composed of a contiguous set of crystal grains. Such a set and its properties constitute the microstructure and can be partially described using statistical parameters like grain size, crystallographic orientation and misorientation distributions. To a large extent the microstructure of a polycrystal determines its engineering behavior by controlling *e.g.* mechanical, corrosion and magnetic properties. In the last decades a large number of models has been developed claiming to account for a variety of material responses and some of these may benefit from calculations employing 3D (three dimensional) microstructures as an input.

During the development of a microstructurally based material model a set of different input parameters are required for validation and optimization. In order to avoid time-consuming and sophisticated 3D measurements of microstructures a framework for virtual microstructure generation is proposed here. A virtual microstructure is a model itself, capable of generating a numerical representation of numerous microstructural features that are able to substitute for experimental data when used as input to microstructural models. Virtual microstructures are very handy to produce test case samples, which can be used for fast modeling prototyping and microstructural design since they may cover a very large spectrum of microstructural state variables even outside the range of practical implementation. Such capacity helps one to find the boundary conditions and the crucial state variables in a model. It is important to state that the aim is not to completely replace experiments but reduce their number and improve their efficiency by predefining which samples are better suited for experimental validation. Once validated and with the boundary conditions checked, it is also useful to look for optimum microstructures when one wants to design a material.

In the past decades metallurgists and scientists have been looking at the microstructure and defined a broad range of parameters to characterize them. However to create a virtual microstructure the opposite exercise has to be done, *i.e.* starting from a set of microstructural state variables, conveniently expressed as statistical distribution functions, a 3D set of contiguous

grains needs to be created which represents the virtual microstructure. Because microstructures are very complex objects some assumptions are required to simplify the framework. Therefore, it is assumed here that the microstructure is fully characterized by a set of crystal orientations of a single phase that are assembled in a contiguous volume, ignoring in-grain heterogeneities. The input parameters of the microstructure generator can be specified as a set of distribution functions and their relations like grain morphology, orientation and grain boundary character. Additional features such as number of neighbors, triple junction angles or clustering of some properties might be considered as well, but are ignored for the time being. The current paper will report the results when the grain size and texture distribution functions are given as input.

Method

In the proposed framework, surfaces are the main representative objects. Each grain is represented by a set of surfaces forming a closed volume rather than a set of subvolumes in a grid as *e.g.* voxels in a cubic grid space. This choice allows for a more precise description of grain boundaries and associated properties (such as *e.g.* local GB curvature), and on the practical side it also allows for a compact data description and thus a faster calculation. In the first version of the model the boundaries are composed of flat surfaces, but in future these flat surfaces will be converted to polynomial piecewise surfaces. If necessary, further post-processing conversion to voxels or meshes can be carried out for the sake of compatibility with others model formats such as *e.g.* finite elements and phase field modeling.

The grains are first created using the concept of Voronoi cells, which consist of a mathematical concept where a space $\mathbb{R}^n$ is partitioned starting from a set of points $p \in \mathbb{R}^n$. Each cell is defined by a region in the space where all distances are closer to its central point p than the central points from any other cell. Voronoi structures bear a one-to-one relation with Delaunay triangulation [1]. Both concepts provide equivalent information but stored in different ways, the so called duality property, that allows a straightforward bijective conversion between them. Even though there are algorithms to directly calculate Voronoi cells, an indirect method that calculates the Delaunay triangulation first and then converts it to Voronoi cells is used here.

The key point to generate a proper grain size distribution using Voronoi cells is to find a proper set of central points that reproduces the user specified grain size distribution. The user provides the grain size distribution function $f(gs)$ as well as the lower and upper limits $gs \in [a, b]$, thus defining the *target* distribution. If n points are randomly placed in a box of which the size depends on the number of grains n and the average grain size of the target distribution, the resultant distribution is the so-called Poisson-Voronoi which exhibits a lognormal distribution with a variance of 0.424 [2]. Even though this distribution might be useful in some specific cases, in more general cases the target distribution will deviate from the lognormal one and may exhibit a different variance or even a bimodal structure. In order to transform the initial set of points in a valid one where the Voronoi cells follow the target distribution a Reverse Monte Carlo (RMC) algorithm is used [3]. Both target and current distributions are discretized into histograms with volume fractions p_i in each bin and the error function described in Eq. 1 is employed for convergence.

The orientation assignment starts once a suitable grain size distribution is found. The target distribution is obtained from a discretized Orientation Distribution Function (ODF) in Euler space. To the purpose of discretization the inverse of the Cumulative Distribution Function (CDF) is sampled by a uniform distribution, very much similar to the method proposed by Toth and Van Houtte [4]. The CDF is constructed by numerical integration of the ODF along its three angles, as describe in Eq. 3 where $v_{i,j,k}$ is the volume fraction in a discrete position of the Euler space.

$$\text{error}_{GS} = \sum_{i=1}^{N} (p_i - p_i^{target})^2. \tag{1}$$

$$\text{error}_{ODF} = \sum_{i=1}^{N} \sum_{j=1}^{M} \sum_{k=1}^{L} (v_{i,j,k} - v_{i,j,k}^{target})^2. \tag{2}$$

$$\text{CDF}(N, M, L) = \sum_{i=1}^{N} \sum_{j=1}^{M} \sum_{k=1}^{L} v_{i,j,k} \sin \Phi \Delta\phi_1 \Delta\Phi \Delta\phi_2. \tag{3}$$

Even though the method described above allows a fair ODF sampling , each sampled orientation has implicitly the same weight or volume fraction. It means that when the orientations are associated to the grains and the grain set has a non-uniform volume fraction distribution, the resultant ODF is very much likely to be distorted. On the other hand there are an infinite set of orientations that when associated with a certain set of grains will result in equivalent ODFs. This shows how ill-posed the problem might be *i.e.* in its present form it is not guaranteed that a unique solution can be found. In order to specify a unique solution the missing state variables like misorientation or grain boundary character distributions should be included. For the moment the model does not include any of those parameters, therefore RMC will be applied to enforce a *possible* association between orientations and volume fractions using the error function described in Eq. 2.

Example

One example displaying the current capabilities of the virtual microstructure generator will be given. A set of 1000 grains was generated and fitted into a bimodal spectrum composed by overlapping two normal distributions. The first distribution, that was obtained by placing points randomly, is shown in Fig. 1(a). As expected, it resembles a lognormal distribution with a variance of approximately 0.43 that is typical for Poisson-Voronoi statistics. Finally, after the RMC iterations, the desired distribution is obtained as one can observe in Fig. 1(b).

Once the grain set is defined, the following step is to create the texture by assigning orientations to each grain. Given a target ODF, orientations were sampled and assigned randomly to the grains, see Fig. 2(b). As expected, the distribution does not match with the target distribution, Fig. 2(a), because of the non-uniform grain size. After the RMC iterations a valid configuration was achieved as shown on Fig. 2(c).

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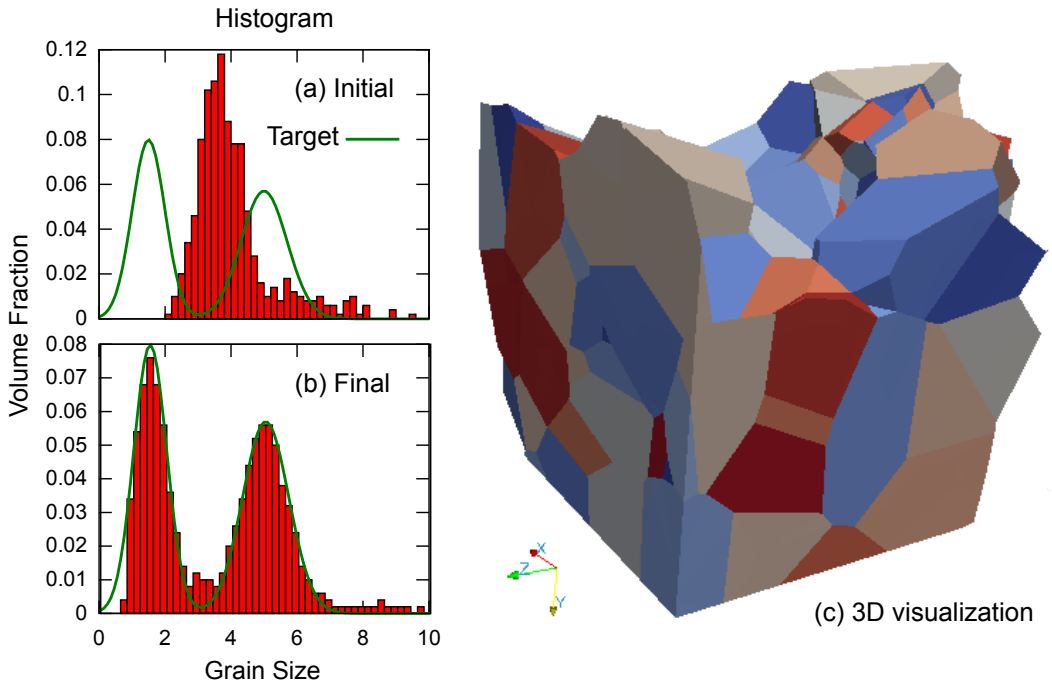

Fig. 1: Generation of 1000 grains that correspond to the target distribution composed by two overlapping normal distributions ($\mu_1 = 1$, $\sigma_1 = 0.5$, $\mu_2 = 5$, $\sigma_2 = 0.7$). (a) The initial distribution after random positioning of points. (b) Final distribution after RMC iterations. (c) 3D section of the resultant grain set.

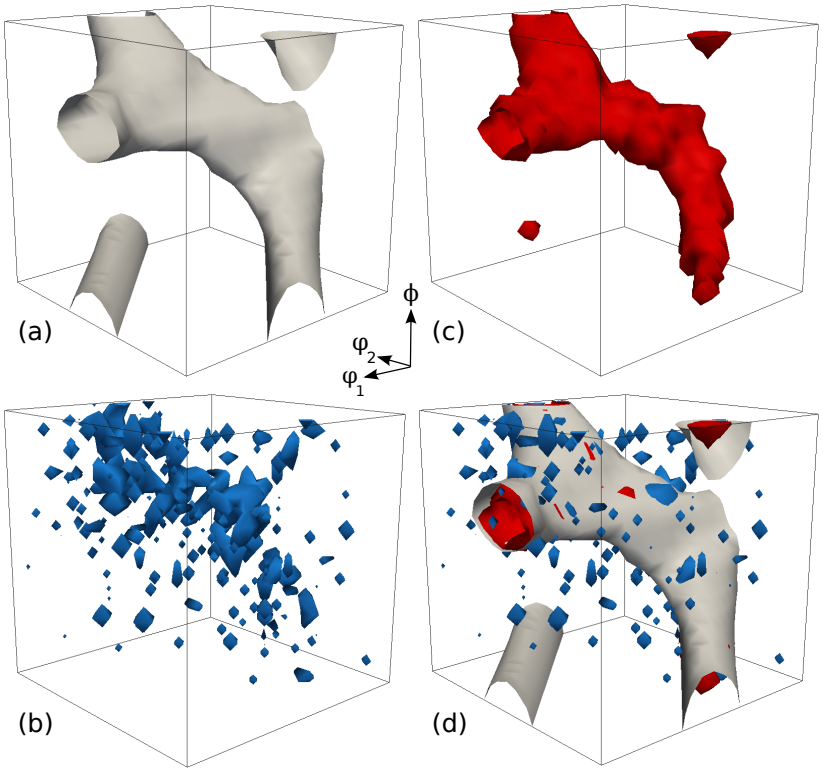

Fig. 2: Texture reconstruction. (a) Target ODF with typical $\alpha - \gamma$ fibers obtained experimentally. (b) Initial ODF after random assignment of sampled orientations to grains. (c) Final ODF after RMC iterations. (d) Overlay of the previous three states.