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Generation of 3D polycrystalline microstructures with a conditioned Laguerre-Voronoi tessellation technique

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ABSTRACT

Voronoi tessellation techniques are widely accepted methods for the generation of representative models of polycrystalline microstructures of metallurgic and ceramic materials. Contrary to most of the Voronoi-based tessellation methods developed, the Laguerre Voronoi technique provides control over the size and shape of the cells, therefore allowing to simulate accurately the grain structure of a wide range of materials. This paper presents a method for the generation of numerical models of 3D polycrystalline microstructures, based on the Laguerre-Voronoi tessellation technique. An innovative approach to define the additional parameters required by the Laguerre-Voronoi formulation for the generation of realistic 3D microstructures is presented, providing the algorithm with information on the given microstructure from a set of 2D micrographs easily obtainable experimentally. The method implemented efficiently avoids *degenerated* cells (affecting the quality of the final structure) and finds the most representative set of input values by comparing 2D sections of the numerical model against 2D imaging of real polished surfaces. In this paper, the capability of the method developed is verified by reproducing the microstructure of polycrystalline alumina with various ranges of grain sizes, deriving from different sintering procedures.

1. Introduction

The ability to accurately reproduce microstructural features is fundamental for the correct simulation of the micro-mechanical behaviour of polycrystalline materials. Therefore, numerical models which are not representative of the real microstructures will lead to incorrect prediction of both global and local phenomena. This is particularly important in brittle materials, whose failure is dominated by crack propagation mechanisms that are strongly dependent on the local geometric and physical phenomena, such as the location of grain boundaries, triple points, crystallographic misorientation and crack initiation.

Several techniques have been developed for the generation of 3D models of polycrystalline microstructures, based on both experimental measurements and numerical approaches. All algorithms for the generation of geometrically and physically representative 3D models of polycrystalline microstructures rely upon a variety of experimental techniques of *non-destructive* and *destructive* nature.

Within the first category, X-ray (micro-) diffraction microscopy provides 3D microstructural representations of a wide range of polycrystalline materials [19,26].

The destructive techniques are based on the interpolation of 2D images to reconstruct the 3D topology of the grain structure. A widely used technique is the "focused ion beam scanning electron microscope" (FIB-SEM), which consists of sectioning the material at given intervals taking SEM images of each surface [12].

The main disadvantage of the techniques based on the scanning of serial sectioned surfaces is the complex and time-consuming post processing required to analyse the amount of data produced. Moreover, the procedure might lead to non-unique topologies with apparent un-physical features (e.g. grain overlapping) in the reconstructed structure. However, in the recent years, the introduction of automated techniques (e.g. Robo-Met3D [24]) has reduced the computational cost and time of the procedure.

The algorithms for the generation of 3D models from the experimental data acquired can be divided in two main groups: the *specific* aiming to reconstruct the particular microstructure under consideration, and the *generic* aiming to construct statistically representative microstructures. The former methods normally require very large amount of data and, if relying upon the destructive data

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acquisition methods, cannot furbish simulations of the mechanical response that can be compared against experiments since the specific sample was destroyed during data acquisition on the microstructure itself. The latter approach is more versatile, as it allows for sensitivity studies of the behaviour of the material upon the variation in its microstructural properties, including the ability to compare the results of thus furbished simulations against corresponding experiments on samples which did not need to be assessed explicitly.

Several such generic numerical generation techniques developed over the years exhibit considerably different levels of accuracy in representing the materials under consideration.

The methods based on regular morphologies (e.g. cubes [21], dodecahedra [28], truncated octahedra [13]) have the advantage of a low computational cost for both the generation and the further spatial discretisation (i.e. meshing) of the grains. The simplicity of these methods is counterbalanced by their inability to reproduce the variability in shape and size of the grains, which makes them unable to simulate localised phenomena.

Voronoi tessellation, and its variants, provide an analytical formulation able to reproduce the non-regularity of polycrystalline morphologies. Additionally, the straight edges and the planar faces of the grains are advantageous for further spatial discretisation [1].

More complex methods, able to reproduce irregular morphologies by simulating the grain-growth kinetics, have also been developed (e.g. Montecarlo-Potts [29], Phase-Field [15], Surface Evolver [25]), but their complexity and high computational cost, restrict their use to simulate actual grain growth mechanisms.

Voronoi tessellations have dominated the modelling of metallurgic and ceramic microstructures in the recent decades because of the combination of the simplicity of formulation and the high representativeness of the results.

Among the several variation of the Voronoi tessellation algorithm available in the open literature, Poisson-Voronoi, Hardcore-Voronoi, and Laguerre-Voronoi formulations are widely accepted to generate tessellations statistically representative of real polycrystalline microstructures. Whilst the first two variants offer only a limited control over the shape and size of the cells, the Laguerre-Voronoi method modifies more deeply the formulation of the tessellation by imposing constraints on the initial state [20], thus allowing to model a wider range of grain structures (e.g. metals [9], foams [14], granular matter [4]).

The increased modelling capability offered by the Laguerre-Voronoi tessellation, however, comes at the cost of a non-bijective relation between the nuclei and the cells, for which a conditioning method is needed.

In this paper, the improvement offered by the implementation of the Laguerre-Voronoi tessellation, expressed in terms of representativeness of the microstructurals models generated, is illustrated. A novel methodology for the conditioning of the nuclei seeding procedure, to prevent the occurrence of *degenerated cells* within the structure, is implemented. The presence of many more degrees of freedom (i.e. weights) requires a technique for the extrapolation of the input parameters from experimental measurements. In particular, to illustrate the effectiveness of the proposed method, the approach presented in this paper relies solely upon the data collected from 2D SEM images of polycrystalline microstructures. The models generated using that data are then analysed using virtual serial-sectioning in order to generate 2D data for direct comparison against the SEM micrographs of the materials under consideration. Finally, a method to optimise the input of the Laguerre-Voronoi tessellation (i.e. weights) is described, showing the excellent agreement reached between numerical and experimental results.

2. Voronoi-based tessellation algorithms

Among the numerical techniques developed to generate representative models of polycrystalline microstructures, the Voronoi tessellation techniques are generally considered to offer an excellent compromise between representativeness and simplicity of formulation.

In this section, first the classic formulation is illustrated, highlighting its limits in representing real polycrystalline microstructures, then the methodology developed to reproduce experimental measurements, based on the Laguerre-Voronoi modification, is presented.

2.1. Formulation of the Voronoi tessellation

Given a finite set of *N nuclei* arbitrarily positioned in the space $\Re^3$, the Voronoi tessellation decomposes the three-dimensional space into one *cell* per each nucleus, consisting of all the points closer to the generating nucleus than to any other nucleus. Mathematically it can be expressed as:

$$\{R_{P_i}\} = \{x \in \Re^3 : ||\mathbf{P_i} - \mathbf{x}|| \leqslant ||\mathbf{P_j} - \mathbf{x}||\} \quad j = 1, 2, \ldots, N : j \neq i \tag{1}$$

where $\mathbf{P_j}$ is the position of the j-th nucleus, R_{P_i} is the cell associated to the nucleus $\mathbf{P_i}$, and $\mathbf{x}$ is the position of a generic point in $\Re^3$.

From this formulation, it is clear that the only control over the cell size and shape is given by imposing constraints on the nuclei seeding procedure. The *Poisson* [16] and *Hardcore* [11] constraints are arguably the most common additions to the Voronoi tessellation.

The Hardcore-Voronoi tessellation, in particular, has often being used to generate statistically representative models of metallurgic [11] and ceramic [8] polycrystalline microstructures, as well as of granular matter [7]. It offers the possibility to control the sphericity of the grains through the definition of a single scalar value: the *Hardcore radius* ρ, that represents the minimum distance between the nuclei during the seeding process. In 3D this operation can be expressed as:

$$||\mathbf{P_i} - \mathbf{P_j}|| = \sqrt{\sum_{k=1}^{3} (P_{i_k} - P_{j_k})^2} > \rho \quad \forall (i,j) = 1, 2, \ldots, N : j \neq i \tag{2}$$

The introduction of three more parameters allows for a certain degree of control over the shape of the grains, by defining a privileged growing direction of the cells (i.e. Extended Hardcore [8]).

However, the distribution of grain size of all the Voronoi assemblies based on constraints of the nuclei seeding exhibits a typical bell-shaped curve, as reported by [20], which is not necessarily representative of real granular materials.

In particular, they are not able to represent the wide range of real grain sizes and the presence of large grains within the microstructure, as illustrated in Section 3.

2.2. Laguerre-Voronoi tessellation

In place of the *Eulerian* distance used in the classic Voronoi formulation, the Laguerre-Voronoi tessellation introduces the so-called *power-distance*, defined as:

$$pow(\mathbf{x}, (\mathbf{P_i}, w_i)) = ||\mathbf{P_i} - \mathbf{x}||^2 - w_i \tag{3}$$

where $\mathbf{x}$ is the position of a generic point in $\Re^3$, $\mathbf{P_i}$ the position of the generic i-th nucleus, and w_i the weight associated to it. Note that, if all the weights are equal, the power distance reduces to the Euclidean.