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PII: S0045-7825(17)30702-8
DOI: https://doi.org/10.1016/j.cma.2017.10.029
Reference: CMA 11657

To appear in: *Comput. Methods Appl. Mech. Engrg.*

Received date : 11 September 2017
Revised date : 26 October 2017
Accepted date : 30 October 2017

Please cite this article as: R. Quey, L. Renversade, Optimal polyhedral description of 3D polycrystals: Method and application to statistical and synchrotron X-ray diffraction data, *Comput. Methods Appl. Mech. Engrg.* (2017), https://doi.org/10.1016/j.cma.2017.10.029

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Optimal polyhedral description of 3D polycrystals: method and application to statistical and synchrotron X-ray diffraction data

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Abstract

A methodology is presented for optimal polyhedral description of 3D polycrystals from experimental properties. This is achieved by determining, by optimization, appropriate attributes of the seeds of Laguerre tessellations. The resulting tessellations are optimal in the sense that no further improvements are possible using convex geometries. The optimization of Laguerre tessellation combines a new, computationally-efficient algorithm for updating tessellations between iterations to a generic optimization algorithm. The method is applied to different types of experimental data, either statistical, such as grain size distributions, or grain-based, as provided by synchrotron X-ray diffraction experiments. It is then shown how the tessellations can be meshed for finite-element simulations. The new method opens the way to more systematic and quantitative analyses of microstructural effects on properties. The presented algorithms are implemented and distributed in the free (open-source) software package Neper.

Keywords: Microstructure, Laguerre tessellation, optimization, micromechanics

1 Introduction

The influence of the microstructure on the mechanical and physical properties of polycrystalline materials has been known for a long time. The average grain size, for example, is responsible for the so-called "Hall-Petch strengthening" [1, 2] and is important for fatigue resistance [3, 4]. The grain size distribution has similar effects, albeit generally less pronounced [5, 6]. Of course, these phenomena are directly related to the stress and strain heterogeneities developing at the microstructure scale [7]. In the past 15 years, large efforts have been conducted to analyse experimentally the local deformation of polycrystalline materials in 3D using synchrotron X-ray diffraction. These methods provide both the grain structure of polycrystalline materials [8, 9] and the local stresses and lattice rotations [10–13] that develop as they are deformed. Numerical methods are available to simulate these phenomena [14–22], e.g. the widely-used finite element method [14–20]. Simulations can then be compared to experiments [19, 20] or used alone to analyse systematically the influence of microstructural attributes, on condition that appropriate polycrystal models are available.

As the (morphological) properties of polycrystalline microstructures result from material's chemistry and elaboration, they can be simulated using physical models, e.g. the phase field model [23, 24]. Geometrical models, in comparison, are conceptually simpler and computationally cheaper. A polycrystal can for example be represented by a packing of ellipsoids combined with simple growth [25]. These approaches generally provide microstructures of high fidelity but do not offer full control on them. Moreover, the microstructures are in general complex, as they can include general (non-convex) grain shapes which can only be described on grids of voxels, which is not adapted to standard, conformal meshing [26]. Such is also the case for polycrystal images provided by synchrotron X-ray diffraction [8, 9], which motivated the development of dedicated meshing procedures [27, 28]. In contrast, geometrical models such as Voronoi or Laguerre tessellations can be described in a compact, scalar fashion, using sets of points, lines, surfaces and volumes. A major advantage is that they can be meshed with relatively standard approaches [26], while their cells being necessarily convex is often a minor limitation for representing polycrystals [29]. Voronoi tessellations, in particular, have been widely used in numerical simulations in the past few years [7, 19, 20, 30–35] but only partially reproduce elementary polycrystal properties such as their grain size distribution [26].

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