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Abstract

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Reconstruction and stochastic 3D modeling of grain boundaries in polycrystalline materials from incomplete data, using tessellations with flat and curved facets

Joint with Lukas Petrich, Jakub Staněk, Mingyan Wang, Carl E. Krill III and Volker Schmidt

Polycrystalline materials are composed of a space-filling system of so-called grains. The microstructure of polycrystalline materials, i.e., morphological properties of the grains, plays a key role for physical phenomena such as grain growth. Full information about the shape of the grains can be acquired, e.g., by three-dimensional electron backscatter diffraction (3D-EBSD), whereas by far-field three-dimensional X-ray diffraction (3D-XRD) microscopy the only geometrical information that can be obtained are the centers of mass and volumes of each grain. The advantage of the latter measurement technique is that it allows to quickly investigate large numbers of grains without destroying the specimen in the process, rendering it a good solution for in situ experiments.

In this talk, a method to predict the full 3D information of the grain system, based on a 3D-XRD measurement is presented. We assume that the system of grains can be represented as a *Laguerre tessellation*, which is a space-filling system of convex polytopes. Laguerre tessellations can be generated by points with real-valued marks. From the information about centers of mass and volumes of grains, we construct such a system of marked points, which acts as a generator for a Laguerre tessellation. The system of marked points is iterativeley refined such that the centers of mass and volumes of the polytopes in the Laguerre tessellation approximately correspond to the values obtained from the 3D-XRD measurement.

So far, we have assumed that the grain boundaries are flat, such that we can model the grains as convex polytopes. However, for some materials, the boundaries may be curved. In this case, the concept of a Laguerre tessellation can be adapted to generate a space-filling system of non-convex grains. This can, e.g., be done using the *spherical growth tessellation*, which can also be generated from a system of marked points. We present a stochastic 3D model for polycrystalline

AlCu samples based on a spherical growth tessellation. By the aid of this model, virtual polycrystalline microstructures can be generated, the statistical properties of which approximately match the ones extracted from 3D image data of real microstructures. In addition, by a systematic variation of model parameters, virtual polycrystalline materials with different morphological properties can be generated. These structures can, e.g., be used as input for simulations of grain growth in polycrystalline materials.