3D DIGITAL MICROSTRUCTURES FOR MODELING POLYCRYSTALLINE SOLIDS

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A set of tools is described for creating digital three-dimensional microstructures and transforming them into finite element meshes for computational solid mechanics. The approach is based on statistical information from experimental measurements using automated electron back-scatter diffraction on orthogonal cross-sections. The microstructures currently allow grain shape, texture and grain boundary character to be matched to the measurements in a single-phase material. Grain shapes are abstracted in terms of distributions of either ellipsoids in 3D or ellipses in 2D sections. Grain orientation and grain boundary misorientation textures are quantified with distributions in a homochoric space. Simulated annealing is used to match the digital microstructures to the experimental information. The discretization of the microstructure can be realized by either a Voronoi tessellation or on a regular grid (voxels on a simple cubic lattice). Extensions of the method are described that generate finite element meshes based on either the tessellations or the regular grid. The resulting 3D digital microstructures are useful for a wide variety of applications. Examples are given for generating models of commercial aluminum alloys and two-phase materials. Applications of the approach range from fatigue crack initiation to the mechanical properties of foams.

Key words: digital microstructures, statistical reconstruction, crystallographic texture