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An automated procedure for geometry creation and finite element mesh generation: Application to explicit grain structure models and machining distortion

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ABSTRACT

Explicit grain structure models within finite element (FE) computational tools are essential for conducting crystal plasticity simulations to elucidate the three-dimensional (3D) topological effects of microstructural evolution on micromechanical fields during plastic deformation. Such full-field framework can predict not only texture evolution but also the development of intra- and inter-granular misorientation, grain shape, and grain boundary character distribution in polycrystalline metals. This paper develops an automated procedure for the geometry creation and FE mesh generation of explicit grain structures to facilitate full-field crystal plasticity modeling of complex shapes other than cuboids. The procedure consists of: (1) generation of a synthetic voxel-based microstructure of cuboidal shapes using the software called digital representation environment for the analysis of microstructure in 3D (DREAM.3D), (2) cutting of the model into a final shape by Boolean operations in Abaqus software, and (3) generation of volume FE mesh for the shaped polycrystalline aggregate using a custom-built toolset involving Patran software. Explicit grain structure FE models for micropillar compression and for micro-tube forming are created as examples. To further demonstrate the utility and robustness of the automated procedure for making multiple cuts while attaining the state of stress equilibrium after each cut, machining distortion of an Inconel 718 aircraft engine disk is modeled. The starting material for machining had a distribution of bulk residual stresses resulting from prior thermo-mechanical processing. Specifically, turning and broaching operations are carried out using the procedure. During machining, the disk distorts as material is removed, while bulk residual stress fields evolve to reach a new equilibrium. The disk distortion during the material removal is predicted using the developed automated procedure in Abaqus.

1. Introduction

Computational mechanics of polycrystalline materials often employs full-field calculations of mechanical fields. The term 'full-field' indicates that constituent grains explicitly interact with each other, while the micromechanical fields, defined in term of stress and strain, are equilibrated under the strain compatibility conditions in a discretized spatio-temporal domain. Since critical aspects of extreme material behavior such as void nucleation are governed primarily by local strain concentrations, knowledge of plasticity processes at grain scale is necessary for understanding and predicting material behavior. Starting from the work reported in [1], the finite element (FE) numerical method has been extensively used to solve for such fields, often with a sub-grain FE mesh resolution [2–13]. Under uniform macroscopic loading, these models reveal heterogeneous deformation because they account for the spatial distribution of grain size and shape of constituent grains and their inherent anisotropy and inter-granular interactions. A Green function method provides an alternative to FE when solving the field equations over a spatial domain [14]. The methodology was initially developed to calculate the effective and local mechanical response of composites [15] and later advanced to calculate the visco-plastic deformation of polycrystalline metals [16]. It relies on the efficient fast Fourier transform-based algorithms to solve the convolution integral representing stress equilibrium under the strain compatibility over a voxel-based microstructural cell, which is periodic and initially cubic or a rectangular parallelepiped (cuboidal). Such microstructure cells are primarily aimed at understanding behavior of a material. While computationally

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efficient [17–19], this methodology is at a disadvantage relative to the crystal plasticity FE (CPFE) methods because many applications of polycrystal plasticity are in the form of more complicated shapes, and requiring boundary conditions that are not periodic. Moreover, the grain boundaries are not present as continuous surfaces in these voxel-based microstructural cells. In contrast to full-field models, mean-field models calculate homogenized material response without accounting for any grain-to-grain interactions [20–32].

In early works, CPFE studies have ignored the morphology of grains [33–39]. In subsequent developments, simple geometries such as cuboids, rhombic dodecahedrons, and truncated octahedrons were used to represent grains in CPFE primarily because these constructs can be readily generated over a spatial domain representing a microstructure [40–42]. Because of their uniform and highly simplified grain morphology, compared to a real microstructure, these CPFE models were unable to accurately capture the inter-granular and intra-granular mechanical fields [43]. These early models were also unable to effectively represent the structure of grain boundaries. More recently, individual grains have been modeled using many finite elements [5,6,44–47]. These studies confirmed that the grain morphology plays a significant role in determining stress-strain heterogeneities.

Modeling the evolution of grain structure along with grain boundaries with plastic deformation is necessary for a more complete understanding of local and overall material response. To this end, FE models allow for grain boundary representation as discretized surfaces. A widely use methodology for voxel-based explicit grain structure generation is the Voronoi tessellation method along with various extensions [45,46,48–51]. However, polyhedral-shaped non-uniform grain shapes created by the Voronoi tessellation methods are often unrealistic because rules for the organization and geometrical constraints of the grains produced are not unique. In addition, the grain boundaries appear as coarse disordered polygons. To relax these limitations, DREAM.3D (the digital microstructure analysis environment in 3D) software has recently been developed by U.S. Air Force Research Laboratory and Blue Quartz [52,53]. The software is a result of the work conceived in [54]. While well suited for generating voxel-based grain structures in cuboidal shapes with surface mesh over grain boundaries, meshing of grain structures in 3D is yet to become a capability of the software. In recent work, we have developed and integrated a set of tools relying on the grain boundary surface mesh from DREAM.3D to create volume mesh of high quality over grains, ensuring the conformal conditions between constituent grains [55,56]. The conformal conditions between constituent grains means that neighboring grains share triangular elements at grain boundaries.

Experimental techniques have also been developed to acquire voxel-based grain structure data in 3D, which can be used as a direct input into CPFE simulations. An automated robotic serial sectioning device has been developed to capture 2D images for every slice at a high rate [57,58]. The 2D images are stacked and post-processed to form a 3D microstructure. The crystallographic information can be supplied from EBSD, which can be periodically performed by interrupting the automated robotic serial sectioning procedure. Another technique, known as focused ion beam electron backscattered diffraction (FIB-EBSD), uses the FIB to perform the serial sectioning and EBSD to create the crystallographic map for each section [59–64]. Finally, the most advanced technique for acquiring such data is *in-situ,* non-destructive near-field high-energy X-ray diffraction microscopy (nf HEDM) [65–69]. Data defining the state of grain structure, crystal lattice orientations, lattice strains and associated residual stresses, various defects such as voids, and even dislocation density acquired using these experiments can be used to initialize and critically verify full-field models.

Voxel-based microstructural data can also be obtained by numerical models such as phase field models [70], Potts (Monte-Carlo) grain growth models [71,72], and cellular automata recrystallization models [73,74].

While such measured and simulated voxel-based grain structures can directly represent the finite element mesh (e.g. every voxel is a brick element) utilized in a CPFE simulation [75,76], typically the data is further processed by smoothing the voxel description of grain boundaries using various interpolation methods. Such interpolation methods are conveniently available within DREAM.3D, which can produce triangular grain boundary surface mesh of appropriate size. Most importantly, the data is post-processed to reduce the number of discrete elements to a computationally manageable resolution.

As mentioned above, the grain size, shape, and crystallographic orientation strongly influence the local mechanical behavior of a material [77–79]. To capture heterogeneous deformation behavior of polycrystals, grain structures can be explicitly modeled using CPFE methods. This is particularly true in simulations of micro-forming processes such as forming of micro-tubes [80,81] and various micromechanical tests such as micro-pillar compression [49]. As a result, there is a demand for creating grain structures for various specimen geometries to facilitate accurate simulations.

This work develops an automated procedure for the geometry creation and subsequent mesh generation of complex shapes in 3D. An explicit grain structure FE model of a micro-pillar for compression and a micro-tube for microforming are created to demonstrate the utility of the procedure for subsequent CPFE modeling. To further demonstrate the robustness and utility of the procedure, machining distortion of an Inconel 718 aircraft engine disk is modeled [82,83]. Multiple cuts intrinsic to the machining process are performed in an automated manner while attaining the state of stress equilibrium after each cut under a clamped condition and in the unclamped i.e. free state of the disk after machining. Aircraft engine disks are typically forged followed by heat treatment and machining [82,83]. Thus, the starting material for machining had a distribution of bulk residual stresses resulting from prior thermo-mechanical processing. In general, local residual stresses can be induced during machining, but the bulk residual stresses remain primarily from prior processes [84–87]. The extent of cutting induced stresses depends on machining parameters such as feed rate, depth of cut, and cutting speed, which have major influence on the surface integrity of a machined part. The model developed here considers the residual stresses from prior thermo-mechanical processes, but not the cutting induced stresses. During machining, the workpiece distorts as material is removed, while bulk residual stress fields evolve to reach a new equilibrium. The comparisons between the measured distortion trends and the numerical predictions are presented and discussed. Good predictions demonstrate that the model is well suited for evaluating distortions during and after machining.

2. Automated procedure

Predictive capabilities of models such as CPFE are greatly improved by explicitly meshing grain structure and grain boundary surfaces. Creation of realistic grain structure models has been significantly advanced with the introduction of DREAM.3D [53]. This software, among other features, can generate 3D synthetic voxel-based microstructures and triangular surface mesh representing grain boundaries. The output of DREAM.3D in terms of the grain boundary surface mesh is a starting point for volume mesh generation. In recent work, we have developed an integrated toolset for volume meshing of grain structure models starting from the surface mesh [55]. However, the 3D grain structure models