Automated Meshing of Evolving Microstructures From High-Throughput Grain Growth Simulations

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Abstract

Microstructure evolution simulations using the kinetic Monte Carlo algorithm and the phase field method are routinely used to model and simulate sintering and densification of ceramic and metallic materials. Understanding evolution of microstructural features is important as these are known to influence different materials properties, e.g., strength through the Hall-Petch effect. After modeling microstructural evolution, finite element analysis is often desired to determine the properties or the response of the resulting microstructure. In addition, certain properties such as the electrical conductivity might be desired at each time-step of the microstructure evolution simulation. Therefore, the process of obtaining the microstructure output at a given simulation time-step, meshing that structure, and solving for its properties through FEA software needs to be automated. The COMSOL Multiphysics® software has powerful solvers to determine these properties and can be automated through the LiveLink™ for MATLAB® interface. However, adequately meshing these structures is challenging as there can be a multitude of voids, phases, material properties, and interfaces that must be accounted for reliably. We detail a method that uses LiveLink™ for MATLAB® to automate the handling of the output microstructures from the SPPARKS framework, through a robust meshing routine using functions from the ISO2MESH toolbox, to solving for the electrical conductivity of the microstructure in the COMSOL® software. Specifically, we will address the meshing routine which can be used to provide compatible meshes from voxelized 3D matrices that could be generated for all sorts of geometries and applications. We detail how we are able to automatically determine and maintain the domain information so that the appropriate material properties can be assigned to specific regions of the geometry. In addition, this method will efficiently mesh the geometry by using a finer mesh at the interfaces and a coarser mesh towards the grain centers. To illustrate some of the utility to this method, we simulate the relationship between the microstructure and its electrical conductivity over the course of the densification process using the AC/DC module. Electrical properties for alumina are used. The simulation shows that the microstructure increases in conductivity as the pore volume is removed and is validated by similar, experimental observations.