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Modeling the effect of voxel resolution on the accuracy of phantom grain ensemble statistics

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ABSTRACT

The spatial resolution of experimental three dimensional (3D) mesoscale microstructural data has typically been prescribed using simple rules. For example, serial section experiments often attempt to collect at least ten sections through the average feature, however, this rudimentary guidance likely results in data under- or oversampling depending on the measurement(s)-of-interest. This study investigates one approach for determining a minimally sufficient resolution for 3D microstructural data using computer-generated phantoms of polycrystalline grain microstructures. These phantom microstructures were generated on a voxel grid with high resolution and used as reference volumes, which were then progressively down-sampled to coarser resolutions. Discrete probability density functions (PDFs) of morphological descriptors were constructed from both the reference and down-sampled volumes, and the similarity between the PDFs was quantified using a modified version of the Bhattacharyya Coefficient. Analysis of the data revealed that the grain size and the number of nearest neighbor grains have distributions relatively insensitive to changes in resolution, whereas shape parameters including ellipsoid aspect ratios (b/a and c/a) and the moment invariant Ω_3, have higher sensitivities.

1. Introduction

The importance of characterizing microstructure in three dimensions (3D) to accurately quantify the true size, true shape, local neighborhood, and connectivity of microstructural features has been well documented [1,2]. Recent technological advances have contributed to the development of automated and semi-automated microstructure characterization systems that can collect large 3D data sets of material microstructure [3–5]. Furthermore, the wide availability of advanced computing power has led to the development of software that is capable of creating virtual (phantom) 3D microstructure data that closely mimics the real microstructure [6]. The maturation of both experimental and computational 3D microstructure data generation methods has provided the material community with an

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unprecedented ability to digitally represent the morphology of microstructural ensembles with high fidelity. These digital representations are likely to play a key role in the success of recently instituted Integrated Computational Materials Engineering (ICME) initiatives [7–9].

In 2D quantitative microstructural analysis, it is well-known that low resolution images (corresponding to large pixels relative to the size of the feature-of-interest) can result in a loss of microstructural information. Conversely, excessively high resolution images result in a needlessly large memory size and may not provide any significant improvement in the accuracy of the desired analysis [10]. Naturally, the same problem exists for 3D microstructural data, and thus it is necessary and prudent for efficient quantitative microstructural analysis to determine the optimal resolution for data sampling, including both in- and out-of-plane sampling resolutions. This issue is especially important for data collection methods like serial sectioning, as simply collecting data at higher and higher resolutions may not be practical, due to the potential cubic growth in both collection time and computational resources for data post-processing and analysis. Note also that the estimation of the uncertainty associated with digital representations of microstructure has been underdeveloped [11].

The use of phantoms, i.e., simulated objects that mimic the expected characteristics of experimental data, has recently been employed to study the effect of image resolution on the accuracy of measurements derived from image data. For example, the accuracy of selected size and shape parameters relative to the spatial resolution of tomographic X-ray data was examined using cylindrical-shaped phantoms [12]. Re-sampling of the cylinder data to lower resolutions in this study resulted in approximately 100 and 1000 voxels per cylinder being required to keep the cylinder surface area and 3D Feret shape, respectively, below ~10% error. Another recent work investigated the effect of spatial resolution on very small (<50 grains) phantom grain ensembles, for selected regional and topological grain properties [14]. Error analysis was performed for the volume, surface area, and mean width of each grain, as well as the length of each triple line and the location of each quad point. The accuracy of quantitative measurements from digital 2D images was also investigated by Tiwari and Tewari, although this study only considered the effect of sampling resolution using simple objects such as lines and circles [13].

In contrast to these prior efforts that examine the effect of spatial resolution on the measurements of individual features, this study examines the effect of spatial resolution on discrete PDFs derived from analysis of 3D phantom grain ensemble microstructures consisting of thousands of grains. Phantom voxel-based microstructures have been generated with very high spatial resolution relative to the typical microstructural feature (e.g., grain), providing a common reference from which to quantitatively assess the effect of sampling resolution. The minimum voxel resolution required to accurately represent the statistics of the phantom reference volumes has been determined by down-sampling the volumes, both isotropically and anisotropically. The isotropic scheme re-samples the reference volume using a progressively coarser isotropic voxel array, whereas the anisotropic scheme allows an “out-of-plane” voxel dimension to vary at multiples of the “in-plane” resolution, simulating a potential issue encountered in experimental data collection. We have quantified the relationship of the down-sampled volume to the reference volume by comparing mean values as well as the geometric similarity of full PDFs via a modified version of the Bhattacharyya Coefficient, for distributions of grain size, shape, and the number of nearest neighbors.

2. Phantom Voxel-based Microstructure Creation and Down-sampling

The creation of the reference volumes and subsequent down-sampling was performed using the 3D material analysis software DREAM.3D, which stands for Digital Representation Environment for Analyzing Microstructure in 3D (dream3d.bluequartz.net). The procedure used to create and resample these volumes is described in the following subsections.

2.1. Phantom Generation Procedure

A lognormal grain size distribution was used to instantiate phantom grain ensembles for this study, with a mean and standard deviation of $\mu = 0.85$ and $\sigma = 0.705$. The mean of the distribution corresponds to an equivalent sphere diameter of 3.0, and the standard deviation selected results in a heavy tail for the lognormal distribution, providing a variety of large and small grains for all of the reference volumes; note that we have selected a hard limit for the lognormal size distribution, where the maximum equivalent sphere diameter is equal to 14.0. The shapes of the grains were constrained to be nearly equiaxed with no preferential spatial orientation. The reference volumes all contained over 3000 grains, including approximately 1500 grains that did not contact the surface of the reference volumes. Surface grains are considered to have biased microstructural statistics and therefore were not considered in this analysis. The spatial resolution for each reference volume was selected to have 30 voxels spanning the diameter of a grain that corresponds to the mean of the lognormal grain size distribution. Hereafter, we refer to spatial resolution of both the reference and down-sampled volumes relative to the mean grain diameter, and have termed this value VRAD (Voxels Relative to the Average feature Diameter).

Five reference volumes were generated using the lognormal grain size distribution parameters listed above. For the interested reader, a more detailed review of synthetic microstructure generation methods has been reported previously [6], and a basic outline of the microstructure generation procedure is as follows. First, the dimensions of the phantom microstructural volume were defined based on the desired number of grains and their associated size distribution. Next, a geometric packing algorithm was used to fill the space with sampled grains, where the grain sizes were randomly selected from the prescribed lognormal distribution. During grain placement, the grains were allowed to be inserted, removed, or translated within the volume, and final grain placement was based on matching a