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Generation of statistically representative synthetic three-dimensional microstructures

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ABSTRACT

This study provides a general framework for the creation of three-dimensional microstructures for anisotropic two-phase materials with complex morphologies. The ability to create synthetic microstructures that are statistically representative of real materials is dependent on the ability of the generation algorithm to meet the assigned statistics. Hence, the fidelity of the synthetic microstructure depends on the efficiency of the generation process. The generated microstructures were statistically evaluated with respect to the target distribution for grain size, shape, orientation and phase volume fraction. This serves a dual purpose of validation of the packing algorithm and quantification of the 3D microstructures.

According to a 2008 National Research Council study, the Integrated Computational Materials Engineering (ICME) approach aims to link "*computational tools with product performance analysis*" with the intention of reducing the time and cost of developing new materials [1]. One of the key tenets of ICME is the quantification of the structure-property relationships [2]. Conventionally, these relationships have been studied empirically using approximate measures of microstructure and qualitative deductions. These microstructure models aim to replicate the mean values of microstructural descriptors and assume highly idealized grain morphologies. However, many material failure mechanisms, like crack nucleation and growth, depend critically on the local distribution and tail behavior of microstructural descriptors [3,4]. These factors limit the practicality of these models in structure-property predictions and highlight the need for more accurate representations of microstructure.

The advent of advanced 3D characterization techniques and robust image analysis tools makes the complete 3D representation of real materials viable. Direct 3D measurements using high-energy X-ray diffraction microscopy [5,6] and serial sectioning combined with electron microscopy [7–9] are two possible routes. However, direct measurements can be very expensive, tedious and prone to aleatoric variability due to local effects. An alternative approach is to create digital 3D microstructures that are statistically representative of real microstructures and can be used in predictive studies. Rather than creating an exact spatial replica of real microstructure, this method aims to capture the statistical distribution of features within a microstructure [10,11]. The ease and versatility of this approach facilitates generation of multiple instantiations of the same microstructure thereby helping in isolating the effects of local variations.

Most of the prior efforts in synthetic microstructure generation focused on single-phase materials with regular grain shapes. However, most aerospace alloys have multiple phases and complex grain structures and texture [12,13]. These microstructures present unique challenges in the packing of grains and hence require different considerations compared to single phase equiaxed microstructures. The current study provides a general framework for the generation of representative two-phase synthetic 3D microstructures which comprises of HCP particles in larger BCC grains. This is especially aimed towards two-phase titanium alloys like Ti-6Al-4V, Ti-5Al-5Mo-5V-3Cr and Ti-10V-2Fe-3Al [14–16]. An open source software package developed by the Air Force Research Laboratory and BlueQuartz Software for microstructural analysis called *DREAM.3D* has been used in this study [17]. A preliminary step in the generation of synthetic microstructures is quantitative characterization of experimentally measured microstructures, however that is outside the scope of the current work and has been described

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by other researchers [18–20]. The focus of the current work is to examine if 3D microstructures representative of real two-phase alloys can be created, given a set of statistical goals. The accuracy and precision of synthetic microstructure generation have been evaluated by comparing statistical distributions for grain size, grain shape, texture and volume fractions of the phases. This serves a dual purpose of validation of the packing algorithm and quantification of the actual distributions in the microstructure, which will impact its behavior when used for its intended application such as deformation simulations.

The development of DREAM.3D follows previous efforts to generate voxel-based polycrystalline microstructures [21–23]. Initialization of the synthetic volume is done by creating a cuboidal box on a regular grid with specified dimensions and grid resolution. If the use case requires the use of a representative volume element (RVE), then the parameters of the synthetic initialization must be based on sensitivity studies that have determined the domain size necessary to achieve convergence for the property of interest [24]. DREAM.3D fills space by packing shape primitives into the synthetic volume [17]. The most common primitive is an ellipsoid, but other shapes may also be used. The packing of ellipsoids is an optimization problem subject to multiple constraints corresponding to the assigned parameters for the distribution in grain size, shape, neighbors, and orientation. The grains are then swapped until the maximum possible volume is filled while ensuring that the target morphological statistics are matched. After the initial placement, the grains are allowed to grow with different rates in different directions until the grains impinge and fill the synthetic volume completely.

The size of a grain can be represented by its equivalent spherical diameter (ESD), which is the diameter of a sphere with the same volume as the grain. It is generally assumed that the ESD of the grains follows a log-normal distribution [25]. The parameters that define the log-normal size distribution are the mean (μ) and standard deviation (σ) of $log(ESD)$ values. Deviations from log-normal behavior at extreme values can be controlled by specifying lower and upper cutoff values (m, M) in terms of multiples of σ away from μ. The actual bounds of the ESD values are therefore $exp(\mu - m * \sigma)$ and $exp(\mu + M * \sigma)$. The morphology of the grains in the microstructure can be controlled by varying aspect ratios through modification of the axis lengths (A:B:C in decreasing order). In order to fully characterize the 3D shape of the grains, two aspect ratios (B/A and C/A) are required. The aspect ratios are assumed to follow a beta distribution and are defined by the shape parameters α and β. Similarly, other microstructural metrics like neighbors distribution and Ω_3 distribution can also be specified [26]. In addition to the morphological descriptors, the crystallography of the grains can be defined by specifying a list of orientations with different relative weights to form an orientation distribution function (ODF) for each constituent phase [27]. For microstructures with more than one phase, the overall space is divided amongst the phases according to their relative volume fractions. The morphological and crystallographic statistics are defined for each phase separately. An additional consideration for multi-phase microstructures is the orientation relationship (OR) between the phases. During phase transformations, there typically exists a relationship between specific planes and directions of the parent and product phases based on the minimization of interface energy [28]. Most titanium alloys predominantly follow the Burgers OR $\left((0001)_{hcp}//\{011\}_{bcc}, \left[11\bar{2}0\right]_{hcp}//\langle 1\bar{1}1\rangle_{bcc}\right)$ [29]. This transformation has 12 distinct variants as there are two possible $\langle 1\bar{1}1\rangle$ directions on each of the six $\{110\}$ planes [30].

Although DREAM.3D provides a convenient user interface to build synthetic microstructures, this process can be automated using a command line application called PipelineRunner. Python scripts were written to perform systematic parameter sensitivity studies.

Three-dimensional synthetic microstructures representative of two-phase titanium alloys were generated for different combinations of morphological and crystallographic parameters. The generated microstructures comprise of a single large BCC grain containing many platelet-shaped HCP grains (an example shown in Fig. 1a). Since the BCC grain size in titanium alloys is typically 2 to 3 orders of magnitude higher than the HCP grain size, only the statistics of HCP grains are of interest in the current study.

Microstructures were created with different values of the mean size μ while other size parameters were not altered. Other aspects of the microstructure like grain shape (10:10:1 ratio), crystallographic texture (no selection), phase fractions (30% HCP), domain size (128^3) and resolution (1) were kept fixed (at baseline values) for the size sensitivity analysis. The efficiency of the microstructure generation process is evaluated by monitoring the ability to reproduce the size distribution for different values of assigned μ. 20 instantiations were generated for each μ in order to determine the repeatability of the process. Fig. 1b plots the σ against μ for the observed grain size distribution in the generated microstructures such that each point in the plot corresponds to one of the instantiations. At lower values of μ, the points are concentrated but relatively far away from the target values of μ and σ. On the other hand, the points are much more spread out at higher values of μ.

In statistical terms, the microstructure building is not accurate at low μ and not precise at high μ. The low precision at high μ is due to the lack of statistically significant number of grains as the domain size and volume fraction are held constant. The trend in accuracy is less obvious and the relatively low accuracy at the smallest μ can be because the grains at the lower tail of the distribution have too few voxels and cannot match the target statistics correctly. Microstructures generated at $\mu = 1$ with better resolution ($\Delta r = 0.5$) but the same total volume show an improvement in accuracy. Also, microstructures at $\mu = 4$ with larger domain size ($N = 256^3$) but the same resolution show a better precision. The trends in accuracy and precision have been shown in Fig. 1c.

Matching the average size quantities is necessary but does not completely capture the size distribution. Fig. 1d shows the calculated grain size distribution based on the assigned parameters along with the observed probability density from one of the instantiations. The tail behavior is better visualized in probability plots of the cumulative distribution function. Fig. 1e shows the probability plots for assigned and observed distributions for different μ values.

Microstructures were generated with $\mu = 2$ and $\sigma = 0.2$ for different HCP volume fractions (f_α). The spread in the observed values of μ and σ is shown in Fig. 2a. A clear trend is observed in the accuracy of observed μ values with changing f_α. It was observed that precision is not a concern while analyzing the volume fractions and 20 instantiations of the same volume fraction showed negligible spread. Hence, single instantiations were carried out different f_α values (shown by the blue line in Fig. 2b) to elucidate the interrelationships between different parameters. An important observation is that a volume fraction higher than 60% could not be achieved. Packing of second phase particles is done one-at-a-time unlike the all at once approach used for packing of primary phase grains. The current packing algorithm for particles does not allow the ellipsoids to grow into each other. However, high volume fractions are achievable in the existing framework by allowing for multiple attempts to insert second phase grains iteratively into the microstructure. HCP grains were inserted into the parent phase microstructure to form an intermediate microstructure. In the next step, grains were inserted into the intermediate microstructure and this process is repeated till the desired fraction is achieved. Fig. 2b shows the resulting volume fractions for different number of insertion steps during the microstructure generation. For example, $f_\alpha = 0.75$ can not be achieved using one step, but two steps with an assigned fraction of 0.75 meets the target, as shown in Fig. 2c. The need to track the