Geometric Requirements for Modeling Polycrystalline Representative Volume Elements Using the Generalized Method of Cells

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To accurately predict the mechanical response of advanced metallic parts, the grain structure of the metal must be considered and coupled to the macroscale in a multiscale model. The size of the microscale representative volume element must be sufficiently large, and the grid used to discretize the microscale must be adequately refined, in order to ensure an accurate and converged solution. The generalized method of cells is used to predict the mechanical properties of polycrystalline representative volume elements of copper containing randomly oriented grains with the properties of a single face-centered-cubic crystal. Moreover, the results of a parametric study are used to conclude the geometric requirements for an objective microscale model, with respect to the elastic stiffness.

I. Introduction

The performance of high-temperature metallic alloy components is predicated upon the microstructure of the material. Multiscale modeling can be used to not only predict the performance of as manufactured materials, but it can also be used to design the material to meet specific performance requirements. To achieve this, robust models of the material polycrystalline microstructure, along with accurate, physics-based constitutive models must be linked to macroscale finite element method (FEM) models of the part. However, multiscale models can be computational cost prohibitive and there may be size effects. Thus, it is critical to understand the geometric requirements needed to construct an accurate and objective representative volume element (RVE) of the material.

The generalized method of cells (GMC) is a viable method for multiscale modeling of heterogenous materials and structures [1]. GMC coupled with FEM was used to model the deformation behavior of disk composed of a polycrystalline metal, and a two-phased, single crystal, Nickel-based super alloy, using a single crystal plasticity (SCP) model [2]-[3]. This work was later expanded to include a grain-size dependent SCP model [4][5]. More recently, GMC was used to model the evolution of porosity in an additively manufactured metal [6].

In this work parametric studies on the size of, as well as the number of subcells used to model, the RVE in GMC are conducted to determine the requirements for accurate and converged calculation of the effective elastic properties of a demonstrative metallic material composed of randomly oriented single crystal grains. The details on GMC simulations, and construction of the GMC RVEs are given in Section II, and the results are discussed in Section III.

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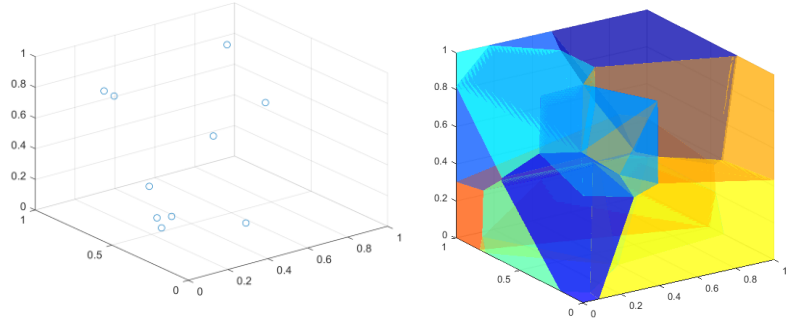
II. Details on Simulations and Construction of GMC Polycrystal RVE

Generation of the RVEs and MAC/GMC input files are scripted using MATLAB. The polycrystalline RVE is created in three main steps. First step is creating the Voronoi tessellation, where each polyhedron representing the Voronoi cell is used as a grain in the microstructure. In the second step, each of the subcells in the RVE are then assigned to the polyhedrons. This process is similar to voxel-based meshing in the conventional finite element method. Material properties for each grain are unique and depend on orientation of the crystals in the grain. The local properties and sub-volumes are homogenized assuming periodic boundary conditions to obtain the effective properties. Although the boundary conditions are strictly periodic, the arrangement of the grains does not necessarily require periodicity. RVEs with periodic grain structures are generated by creating a large point seed and constructing the RVE from a subset of that larger seed. In this study, several geometric modeling parameters are varied to understand their influence on the effective elastic properties of the material. These parameters include the number of grains in the RVE, the number subcells in the RVE, and periodic vs. non-periodic grain structure.

A. Voronoi Tessellation

The first step creates the tessellation by randomly placing points in the unit cube, which are the seeds to the Voronoi tessellation, see Figure 1a. Each of these seeds will become the center of the grain in the metal, as shown in Figure 1b. An open source 3rd party library VoronoiPolyhedrons is then used to produce the tessellation [7]. The call to the library returns the vertices of the polyhedron that defines the grain. An example of these polyhedrons in the unit cube is plotted in Figure 1. These vertices can be scaled in each direction to simulate elongated grains in a particular direction, if desired.



a) **b)**

Fig. 1 Voronoi polyhedron. a) Seeds for Voronoi tessellation. b) Final grain structure.

To enforce periodic grain structure, the method presented by Ref. [8] was followed. The seeds of the Voronoi tessellations are translated (copied) by one unit in each of the three dimensions. This increases the number of seeds by 27 times. The code assigns an identifying number to each seed before the copying to track the grains. Figure 2 shows the same set of seeds being translated by copying three times in each of the three dimensions. The planes shown represent the boundaries of each unit cell. The Voronoi tessellation is then found on the extended domain, which now extends from -1 to 2 in each direction. This ensures the periodic grain structure.

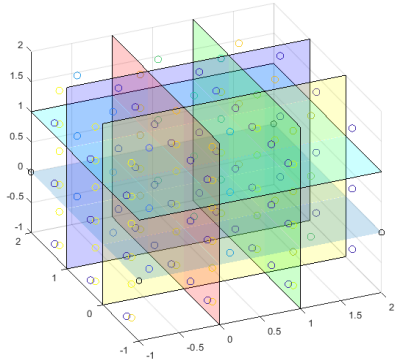


Fig. 2 Seeds for Voronoi tessellation with periodic microstructure.

B. Creating Subcell Grid

A utility of the library is then used to compute a set of linear inequalities. Each linear equation defines a plane that in turn define the boundaries of the polyhedron in either. A voxel gird is then created to represent the subcells of the RVE. Using the center coordinates of each subcell, the inequalities produced above are used to determine which grain each subcell belongs to. To avoid testing each subcell against each grain and increase the efficiency of the code, it is assumed first that the grain containing the adjacent cell will also contain the current subcell. If that is not the case, the membership within neighboring grains will be checked rather than arbitrarily checking other grains.

Parametric studies were conducted to study the sensitivity of the density of the subcell grid and number of grains in the RVE on the homogenized mechanical properties of the material, as well as the effect of the periodic grain structure. Examples of different, parameterized RVEs are plotted using the 3rd party open source library PLOTCUBE and shown in Figures 3 and 4 [9]. Figure 3 shows the RVEs with non-periodic grain structure. Figures 3a and 3b show RVEs with 10 grains with a 10 x 10 x 10 and 25 x 25 x 25 subcell grid, respectively. Meanwhile, Figures 3c and 3d show RVEs with 100 grains with a 10 x 10 x 10 and 25 x 25 x 25 subcell grid, respectively. Figures 4a-4d show RVEs generated using the same parameters except a periodic grain structure is enforced.

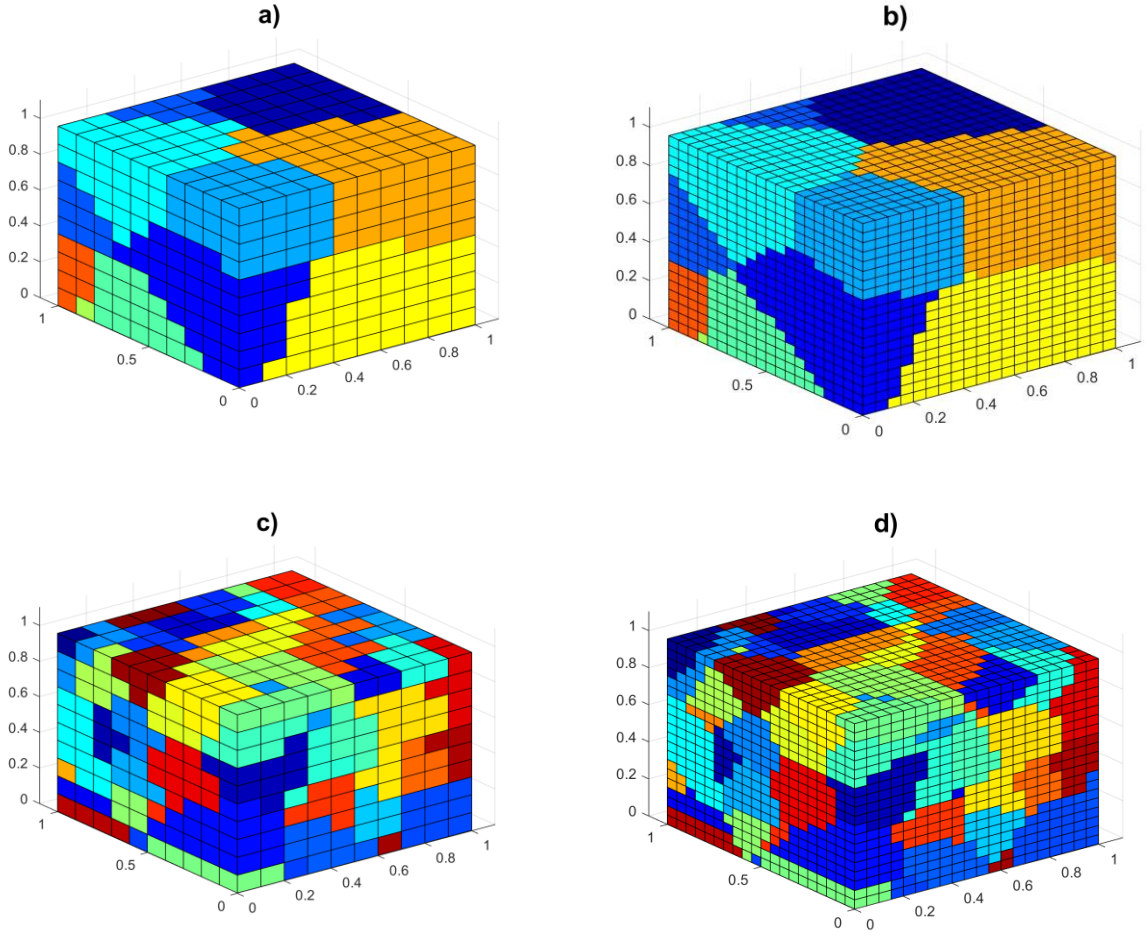


Fig. 3 Parameterized polycrystalline RVEs with non-periodic grain structure. a) 10 grains, 10 subcells per direction. b) 10 grains, 20 subcells per direction. c) 100 grains, 10 subcells per direction. d) 100 grains, 20 subcells per direction.

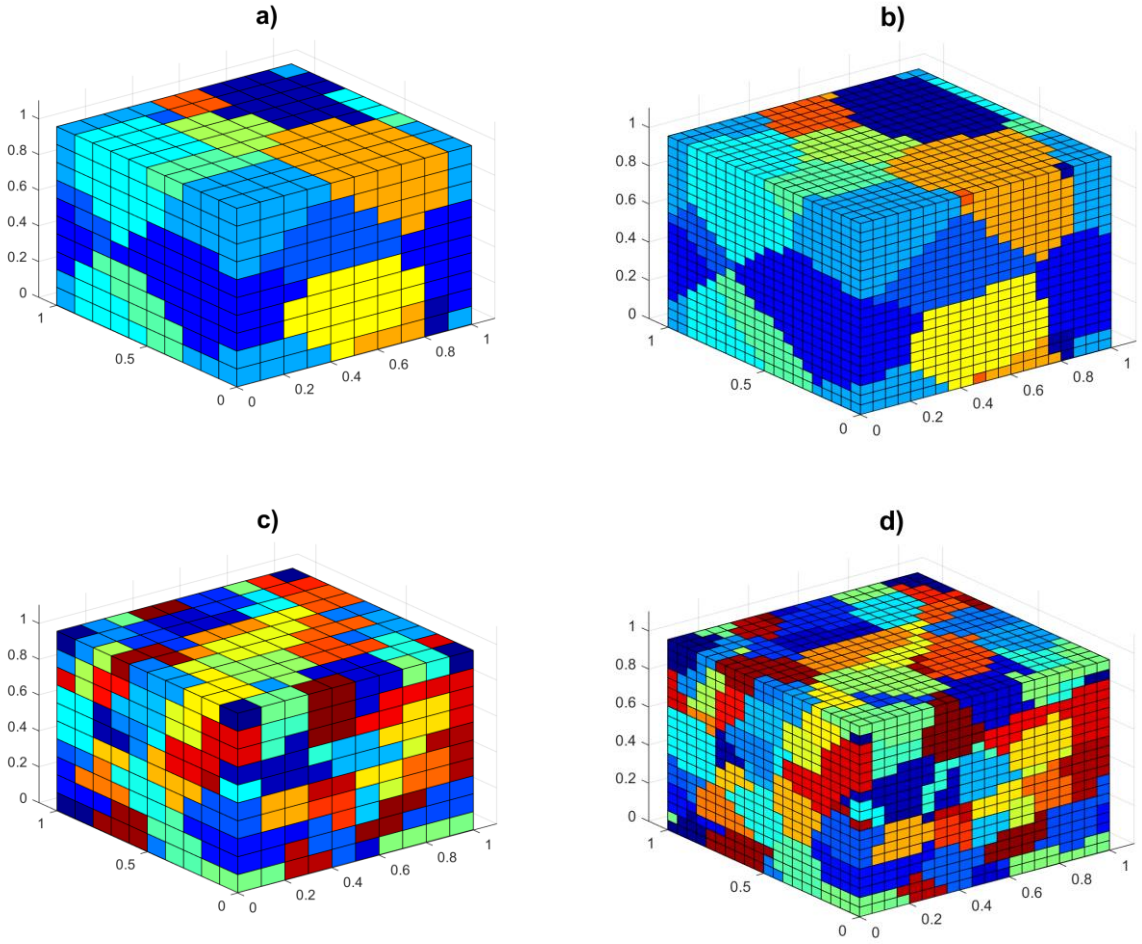


Fig. 4 Parameterized polycrystalline RVEs with non-periodic grain structure. a) 10 grains, 10 subcells per direction. b) 10 grains, 20 subcells per direction. c) 100 grains, 10 subcells per direction. d) 100 grains, 20 subcells per direction.

C. Assigning Local Properties and Calculating Effective Properties

Each grain contains single crystals all oriented in the same direction. The elastic cubic stiffness properties for face-centered-cubic (FCC) copper are assumed ($c_{11} = 168400\ MPa, c_{12} = 121400\ MPa,\ c_{44} = 75400\ MPa$) [2]. However, the crystalline orientation among the grains is varied. These material properties are simply assigned by randomly rotating the elastic tensor of the single crystal material randomly selected coordinate frame of the grain. Homogenization of the RVE to calculate the effective properties is conducted using triply-periodic GMC (GMC3D) [1]. Since the orientation of the grains are random, the effective properties are generally anisotropic.

III. Results and Discussion

A parametric study was conducted to determine how many subcells were needed to achieve a converged effective stiffness as a function of the number of grains in the RVE. I.e., at what point is the change in the effective stiffness of the RVE, calculated using GMC3D, negligible as the discretization of the RVE is refined? In addition, a statistical study was performed to identify if the mean and standard deviation of randomly generated RVEs would converge as more grains are included in the RVE. The results of this study yield guidelines for discretization and size requirement for a statistical RVE (SRVE) [10].

A. Grid Density Requirements for Converged Properties

10 RVEs were created with the total number of grains N_{grains} ranging from 10 grains to 100 grains in increments of 10, using the procedure descried in Section II.A. The RVEs were assigned an N x N x N grid via the method in Section III.B. The baseline grid was N = 10. The size of the grid N was increased by one, and the effective properties for each RVE were calculated until N=30. Note for a given number of grains in the RVE, only the grid was changed, not the Voronoi tessellation seeding. For brevity, only select results from 10, 30, 60 and 100 grains are presented in this subsection.

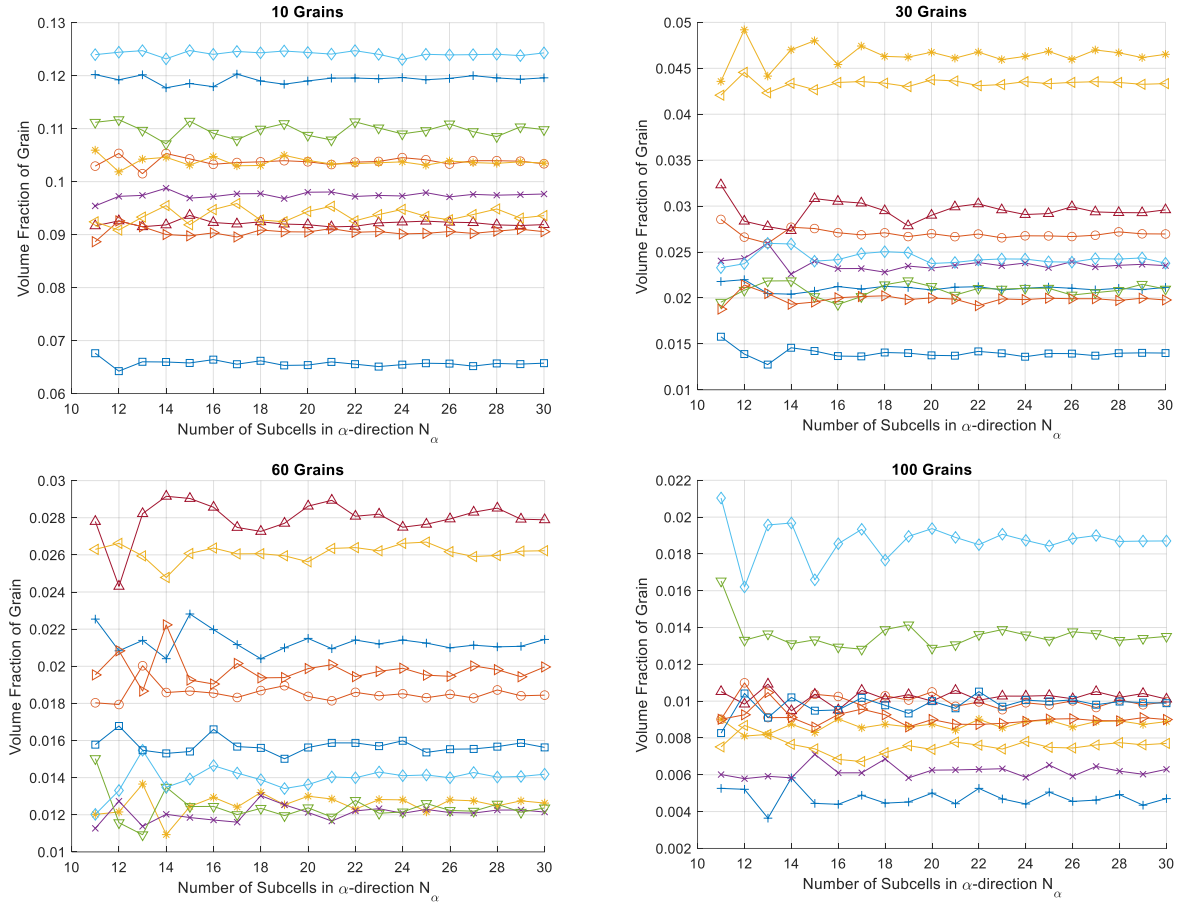


Fig. 5 Local volume fraction of grains as a function of number of subcells in RVE for RVEs with 10, 30, 60, and 100 grains.

The effective elastic properties heterogeneous materials are primarily driven by the volume fraction of its constituents. Figure 5 shows the volume fraction of the grains in the RVEs as a function of the number of subcells used to discretize the RVE. To minimize clutter, results for only 10 grains per RVE are presented. These simulations were conducted to understand how the discretization affects the accuracy of the desired volume fraction for each grain and to determine how many subcells are required to minimize this error. Because of the voxel grid used in GMC3D, the convergence in the local volume fractions is not monotonic and the numerical volume fraction will oscillate around the desired volume fraction. The total change in the local volume fractions Δv was calculated as the grid is refined,

$$\Delta v = \frac{\sqrt{\sum_{g=1}^{N_{grains}} \left(v_g^{N-1} - v_g^{N}\right)^2}}{N_{grains}} \tag{1}$$

where v_g^N is the local volume fraction for grain g and a N x N x N grid. Figure 6 shows number of subcells in the grid when Δv < 0.01. Note, it was not feasible to achieve Δv < 0.001 and still maintain a computationally tractable RVE,

so a threshold of 0.01 was chosen which corresponds to an average change of less than 1% in the local volume fractions of the grains as compared to the previous grid. Figure 6 shows the results for all 10 RVEs and, for most RVEs, N=16 is sufficient to produce less than a 1% average change in the local volume fraction of the grains. When compared to Figure 5, it does appear that the local volume fractions begin to settle. However, to ensure convergence in the effective properties of the RVE, a larger value for N, N=20, was chosen for the statistical study in Section III.B. Please refer to Figures 3b, 3d, 4b, and 4d for images of demonstrative RVEs with this level of refinement.

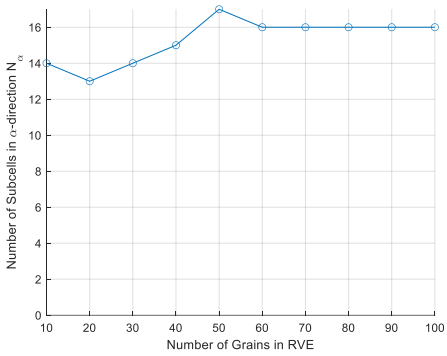


Fig. 6 Number of subcells as a function of number of grains in RVE when the total change in local volume fraction Δv is less than 0.01.

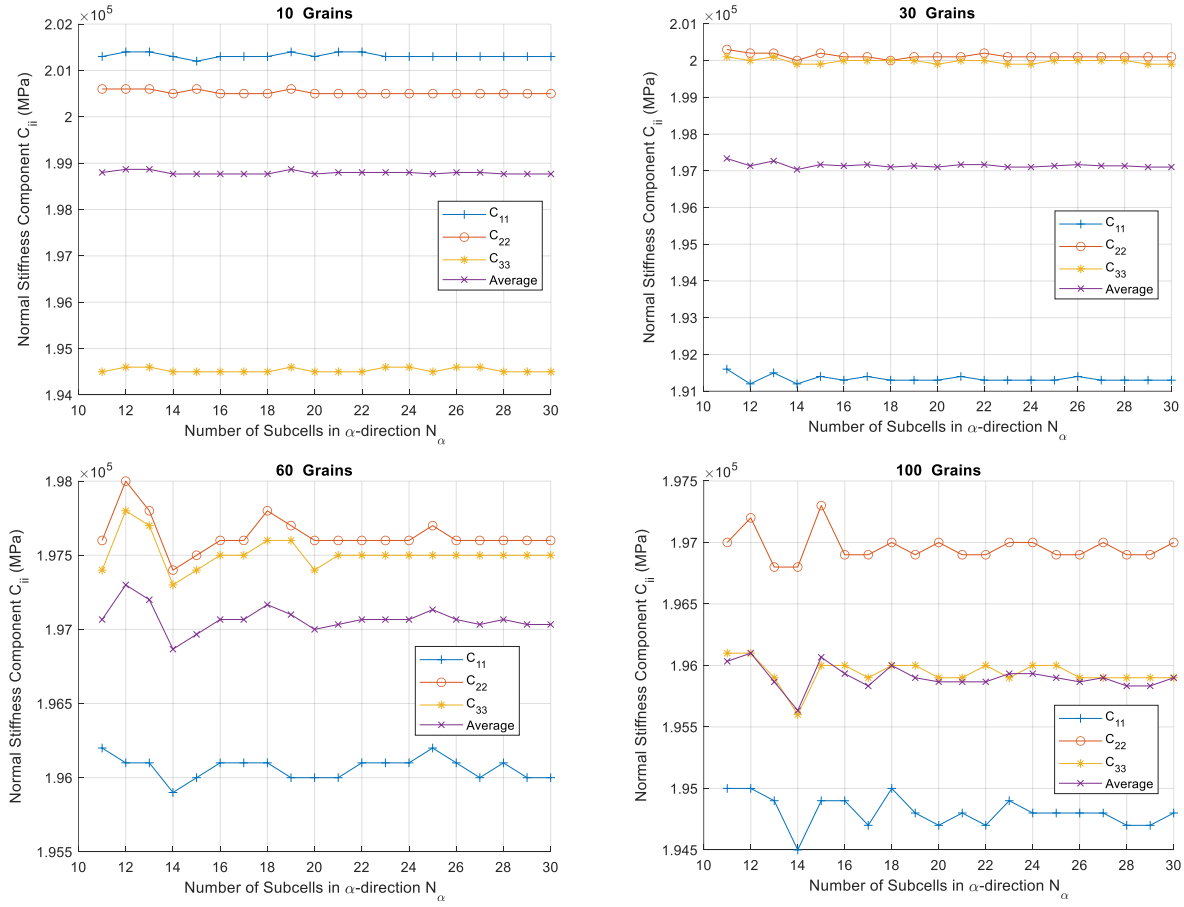


Fig. 7 Normal components of the effective RVE stiffness matrix C_{11}, C_{22}, C_{33}, and their average as a function of number of subcells in RVE for RVEs with 10, 30, 60, and 100 grains.

Figure 7 shows the normal components of the effective stiffness matrix C_{11}, C_{22}, C_{33} and their average as a function of the number of subcells in the RVE for 10, 30, 60, and 100 grains. It can be observed that, more subcells are needed to achieve convergence in these properties as the number of grains is increased. As such, only the results for the RVEs with 100 grains are shown for the other components of the stiffness matrix in Figure 8. Figure 8a and 8b show the normal coupling and shear terms in the stiffness matrix and the convergence of these terms are aligned with what is seen in Figure 7 for 100 grains. Since the grains are randomly oriented and are themselves anisotropic, the effective properties of the RVE will be generally anisotropic. The statistical average of the properties of the RVE will result in isotropic properties, representing the bulk material at the macroscale. The normal-shear and shear coupling terms are plotted as a function of the number of subcells for RVEs with 100 grains in Figures 8c and 8d. It can be seen, there is appreciable of scatter amongst these terms. Overall, the results shown in Figures 7 and 8 support the choice of N=20 to obtain converged properties. The statistical study, presented in the next subsection, on the size of the RVE ranging from 10 to 100 grains.

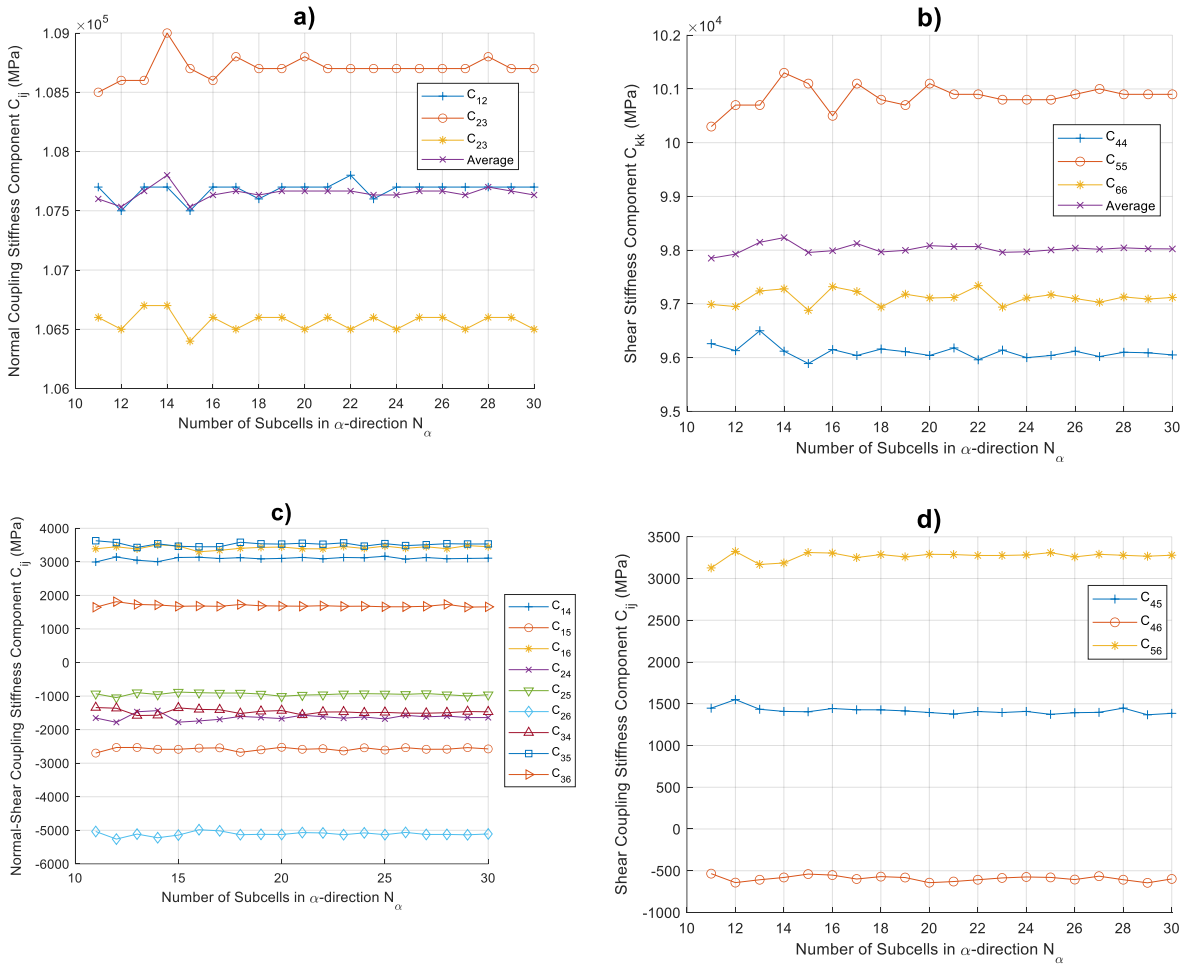


Fig. 8 Components of the effective RVE stiffness matrix C_{ij} as a function of number of subcells in RVE for RVEs with 100 grains. a) Normal-shear coupling terms. b) Shear terms. c) Normal-shear coupling terms. d) Shear coupling terms.

B. Number of Grains Required for a Statistically Representative Volume Element

The previous section studied the requirements in the grid needed to model the RVE to achieve converged elastic properties with GMC3D for an RVE size up to 100 grains. However, for each RVE size, i.e., number of grains in the RVE, only on instance of the microstructure was considered. To insure the RVE is truly representative of the bulk material, it must be large enough to capture the statistical variability observed in the bulk material [1]. In this subsection the results form a statistical analysis are presented to determine the size of the RVE for this material. For

each RVE size, ranging from 10 to 100 grains in increments of 10, 100 instances were analyzed using GMC3D with a 20 x 20 x 20 grid.

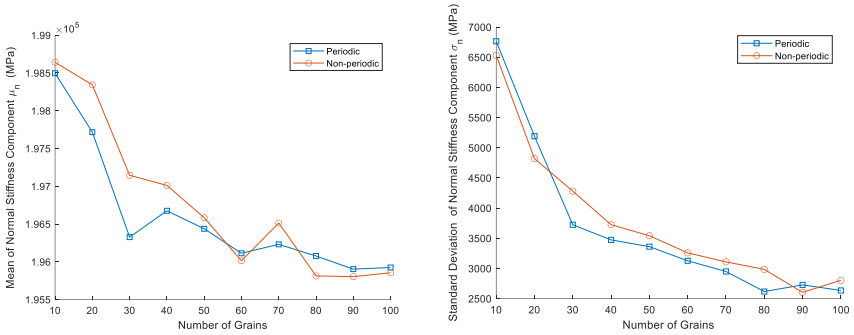


Fig. 9 Mean and standard deviation of normal components of stiffness matrix for RVEs with increasing number of grains with and without periodic microstructure.

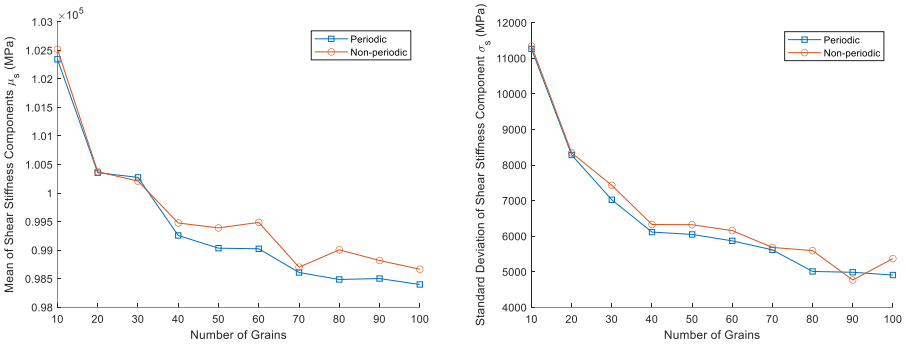


Fig. 10 Mean and standard deviation of shear components of stiffness matrix for RVEs with increasing number of grains with and without periodic microstructure.

Figures 9 and 10 show the mean and standard deviation of the normal components of the effective stiffness matrix as a function of the number of grains. Based on these charts it appears that the mean and standard deviation have of these properties are converged when the number of grains in the RVE is between 80 and 90. A similar response is observed in the terms that couple the normal strains due to Poisson effect, shown in Figure 11. Since the single crystal grains are anisotropic, the effective properties of the RVE may contain normal-shear coupling terms. However as shown in Figure 12, these terms average out to be nearly zero. Finally, the mean of the shear coupling terms do not seem to be converging, even though the standard deviation is (Figure 13). The enforcement of a periodic microstructure did not have a significant impact on these results.

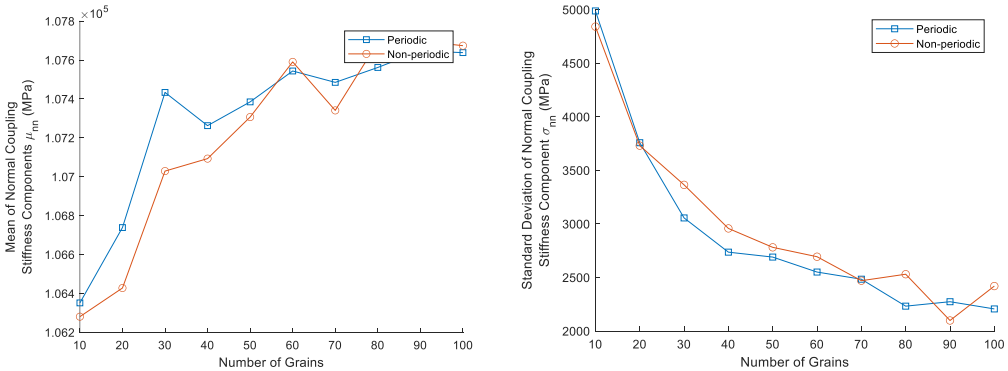


Fig. 11 Mean and standard deviation of normal coupling components of stiffness matrix for RVEs with increasing number of grains with and without periodic microstructure.

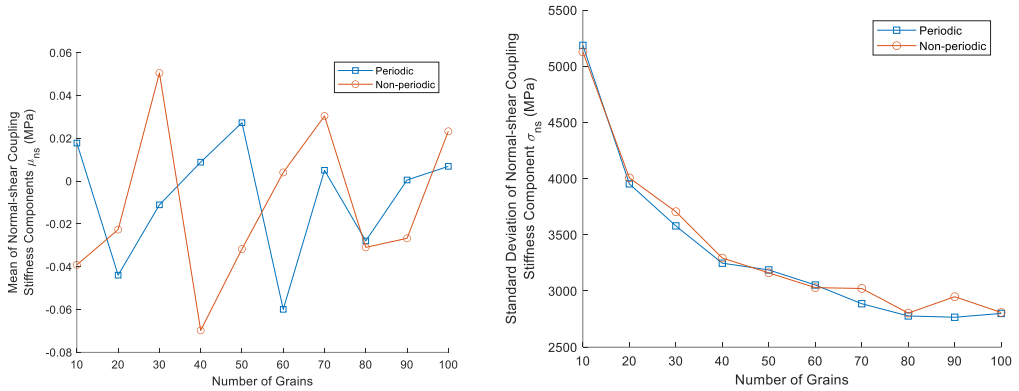


Fig. 12 Mean and standard deviation of normal-shear coupling components of stiffness matrix for RVEs with increasing number of grains with and without periodic microstructure.

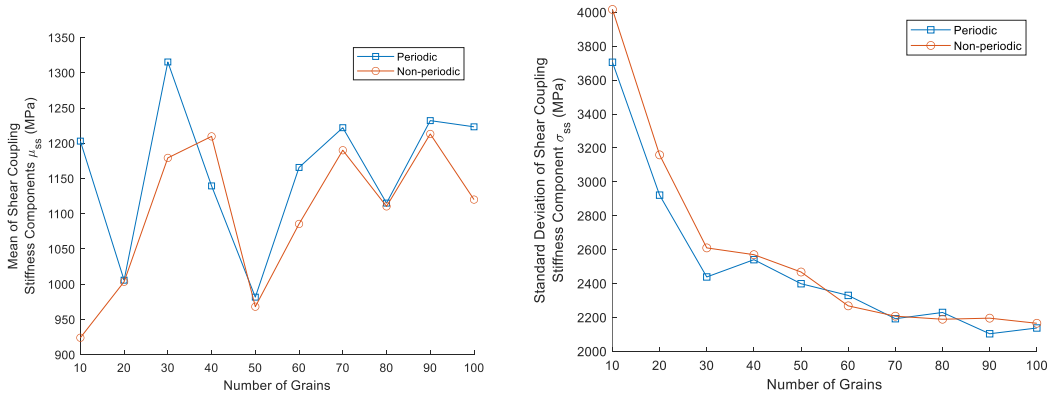


Fig. 13 Mean and standard deviation of shear coupling components of stiffness matrix for RVEs with increasing number of grains with and without periodic microstructure.

IV. Conclusion

The focus of this manuscript is to determine geometric requirements for modeling polycrystalline RVEs with GMC3D. The first study was focused on determining the number of subcells required to get a converged solution for a range of number of grains. It can be concluded that a grid of 20 x 20 x 20 subcells is sufficient to obtain converged properties for an RVE containing up to 100 grains. Next a statistical study was conducted and determined that the size of the SRVE should contain between 80 and 90 grains. Only 100 instances per RVE size were analyzed, so a more thorough statistical analysis may yield different results. Furthermore, the conclusions drawn here only hold for similar linear elastic materials. The results will change if the degree of anisotropy of the phases change. Moreover, a similar study should be conducted if the local deformation is nonlinear.

Acknowledgments

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