3-D Microstructural Modeling and Simulation of Microstress for Nickel Superalloys

VEXTEC Corporation, 5123 Virginia Way Suite C-21, Brentwood, TN 37027 USA

Abstract Statistical elastic micro-stress analysis of single-phase FCC polycrystalline metallic material has been conducted using 3-D microstructural cubic FEA model by Fortran-MSC Patran/Nastran software. In this paper, single-phase polycrystalline metallic material is modeled as an ensemble of grains, and all grains are assumed to have anisotropic mechanical properties with uniformly random orientations. The response of the polycrystal is the aggregate response of the constituent grains. Grain size, shape and orientation have been considered to study the micro-stress distribution in the model. Micro-stress analysis is performed using the statistical volume element (SVE) model with 200 grains. The results show that grain maximum stress and grain center stress have been found to be strongly correlated with the grain orientation and weak correlation with grain shape. The representative volume element (RVE) size for only one grain has been investigated. For illustrating, FCC materials, Nickel-based waspaloy, has been investigated. Finally, the micro-stress distribution difference for this SVE model under stress control and strain control has been investigated.

Keywords: anisotropy, grain size, orientation, random properties

1. Introduction

Macro-scale mechanical analysis usually lacks connection with the microstructure properties of the actual structure, and in most cases, the material is considered homogeneous in macro-level analysis. It is well known that, from a micro-scale prospective, the material is heterogeneous with spatial variations in the properties. A wide class of material microstructures display discontinuities in local properties, such as polycrystals and composite materials. One of the issues in solid mechanics analysis is the transition from a heterogeneous microstructure to an approximating continuum model. Random field models [1] have been established for the microstructural variations in the mechanical properties of heterogeneous materials which could be used in microstructure model [2] to predict micro-stress distribution within the polycrystalline metallic materials.

Voronoi tessellation has been widely used in mechanical engineering to generate 2-D or 3-D models to simulate microstructure of heterogeneous materials. Kumar [3] has developed a three dimensional method to establish a representative volume element (RVE) by Voronoi tessellation. The properties of the RVE model were investigated by Kumar, *et al.*[4] and found to be geometrically correct. The model has been used to investigate the micro-stress of different materials with anisotropic property in several studies [5, 6]. Limited number of three-dimensional cell model (only five grains in the cell) has been developed [7] which does not satisfy the need of statistical significance. Most simulations of material deformation and damage relied on the 2-D model [10-15] because they are much easier to build and solve. Ghosh and his coworkers [8, 9] have shown that 2-D Voronoi models are only effective for thin film structure, but for three-dimensional structures, the 2-D approximation is inaccurate and produced misleading micro-stress results. The micro-stress is particularly important in damage mechanisms that initiate on a very small scale such as fracture and fatigue [16].

In this paper, statistical elastic micro-stress analysis of single-phase FCC polycrystalline metallic material has been conducted using 3-D microstructural cubic FEA model which was presented in paper [2]. The single-phase polycrystalline metallic material is modeled as an ensemble of grains, and all grains are assumed to have anisotropic mechanical properties with uniformly random orientations. Using this method, a SVE is obtained, which is a polycrystalline aggregate of the individual grains. Each grain is considered a continuum material with anisotropic mechanical behavior. The properties are assumed to vary from grain to grain. The model is a random field model and includes uncertainties in grain size, shape, orientation. This paper presents the application of this automatic method to establish the mesodomain that considers the uncertainties mentioned above, and to study the macrostructural mechanical behavior from the view of micromechanics. Linear static stress analysis has been performed using the SVE model, and further, the von Mises stress of nucleation sites and the center of each grain, and maximum von Mises stress of each grain are presented. The results show that grain maximum stress and grain center stress have a strong correlation with the grain orientation and weak correlation with grain shape. The representative volume element (RVE) size for only one grain has been investigated. For illustrating, FCC material, Nickel-based Waspaloy, has been investigated, and its Ziner parameters is 2.54. The micro-stress distribution difference for this SVE model under stress control and strain control has been investigated.

2. Statistical volume element cubic model generation

Most metallic materials used in engineering design are polycrystalline. The mechanical behavior of these materials is determined by grain sizes, strengths, shapes and orientations. To study the property of polycrystalline structures at the micro scale, simulation of grain microstructure is necessary. Voronoi tessellation is a method that has been used in several studies of grain morphology. The majority of these studies have been two-dimensional simulations. However, three-dimensional analysis is needed to truly understand grain orientation effects on microstructural behavior because grain orientation varies in three dimensions.

The proposed microstructure simulation method relies on the physical process of forming granular pure metal with no defects (such as voids, cracks, etc.) under uniform cooling rates The results are observed to agree well with the experimentally observed statistics of the material microstructure. The following assumptions on grain growth are made:

1. The grain growth is isotropic; that is, the grain will grow at the same velocity in all directions. Constant velocity occurs when each grain cools at the same rate. Therefore, this assumption is valid for single-phase materials with spatially consistent cooling rates.
2. The grain growth will stop to form a grain boundary in one direction when it meets another growing grain boundary, but the grain will continue to grow along other directions. The grain growth process will end when its growth stops in all directions.
3. There is no grain growth in the area of an already existing grain i.e., the grains are not allowed to overlap.
4. The volume is fully populated with grains i.e., there are no voids.

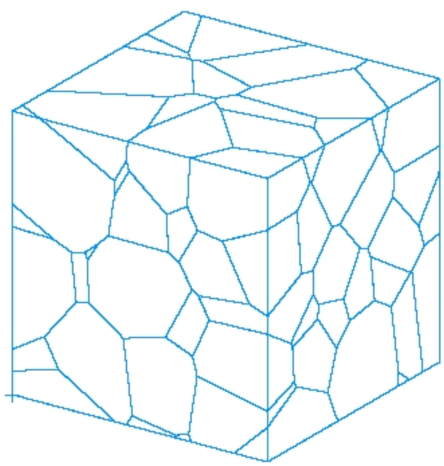
Figure 1: Cubic solid model

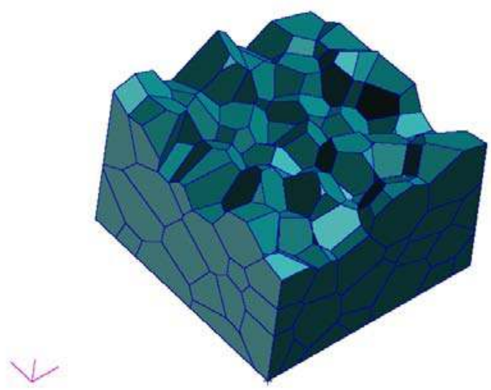
Figure 2: Part of simulated model

The statistical volume element cubic model is shown in Figure 1, which is generated by the method presented in [2], and part of the simulated model is shown in Figure 2. The mechanical behavior of these materials is determined by grain sizes, shapes and orientations. The SVE cubic model is a polycrystalline aggregate of the individual grains. Each grain is considered a continuum material with anisotropic mechanical behavior.

3. Statistical volume element cubic model and linear statistical analysis

It was shown that SVE cubic models with 100, 150 and 200 grains have congruence results considering different SVE cubic model grain sizes effect [2]. In this paper, a SVE cubic model with 200 grains has been chosen to investigate elastic analysis of a single-phase polycrystalline metallic material through micro-level response and all stresses are relative (local stress/applied stress). Only the tension loading case has been applied to the model. An elastic analysis of a single phase polycrystalline metallic material is considered for illustration. A cubic SVE with dimensions of $10 \times 10 \times 10$ (Figure 3) is automatically created using the tessellation-PATRAN program (TPP). The boundary and loading conditions are shown in Figure 3 which represents SVE of 200 grains with mesh of 11333 nodes and 60134 four-node tetrahedral elements. Nodes *A(0,0,10)*, *B(0,0,0)*, *C(10,0,0)*, *D(0,10,10)*, *E(10,10,10)*, and *F(10,10,0)* are the corner nodes of the SVE model. Nodes *A*, *B*, and *C* are on bottom surface of the SVE model, while nodes *D*, *E*, and *F* are on top surface of the SVE model. The SVE model is subjected to an external pressure *P* of 10 psi in the negative y direction on top surface of the SVE model. On bottom surface of the SVE model, node *A(0,0,10)* is fixed with constrain of x=0, y=0, z=0; node *B(0,0,0)* is constrained with y=0, z=0; and all other nodes on the bottom surface are constrained with y=0 as described in the follow equation:

$$\begin{cases} x=0,\ y=0,\ z=0 & \textit{Node A} \\ y=0,\ z=0 & \textit{Node B} \\ y=0 & \textit{All nodes on the bottom except node A and B} \\ P=-10\ psi & \textit{Top surface} \end{cases}$$

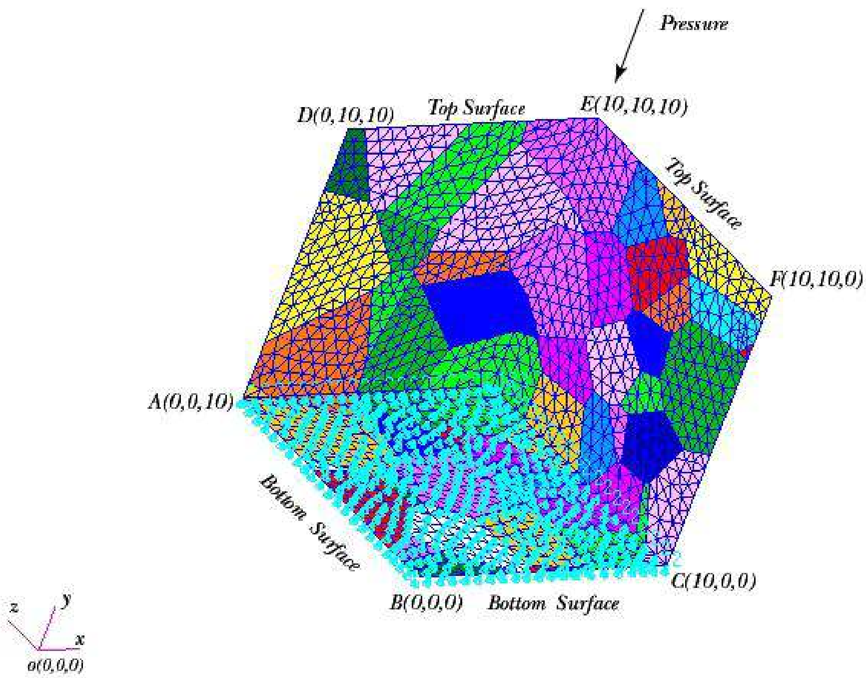

Figure 3: Boundary and loading conditions, Material properties of cubic model

4. SVE cubic model statistcal micro-stress distribution investigation

Statistcal micro-stress distribution has been investigated using the SVE cubic model created by the method presented in paper [2]. In all SVE cases, von Mises stress at the center of each grain is studied when considering boundary effect, geometry effect, orientation and grain shape effect to the micro-stress distribution of the SVE cubic model. It is necessary to mention that the definition of grain center location in the SVE cubic model is different from the definition of the grain 'seed' location mentioned in paper [5]. The grain center location is at the volumn center of each grain, while the grain 'seed' location is the location where grain is assumed to start to grow.

4.1 Grain orientation and von Mises relationship in the SVE cubic model

This section investigates the relationship between grain orientation and micro-stress distribution within SVE cubic model. In this paper, five sets of grain orientation have been studied using the SVE cubic model. Grain orientation has been defined by three Euler angles, θ_1, ϕ and θ_2, which can be obtained by rotating θ_1 about original Z-axial first, then rotating ϕ about primary Y-axial, and finally, rotating θ_2 about double primary Z-axial. In this paper, orientation factor is defined as $\sin\theta_1 \cos\phi$. The micro-stress distribution is related with orientation factor using this SVE cubic model. There are five orientation cases for each of the single-phase polycrystalline metallic material. The relationship between the maximum von Mises stress of each grain and its orientation factor are shown in Figure 4 and Figure 5, which show that grain orientation is a strong influence on maximum von Mises stress of each grain. When orientation factor value

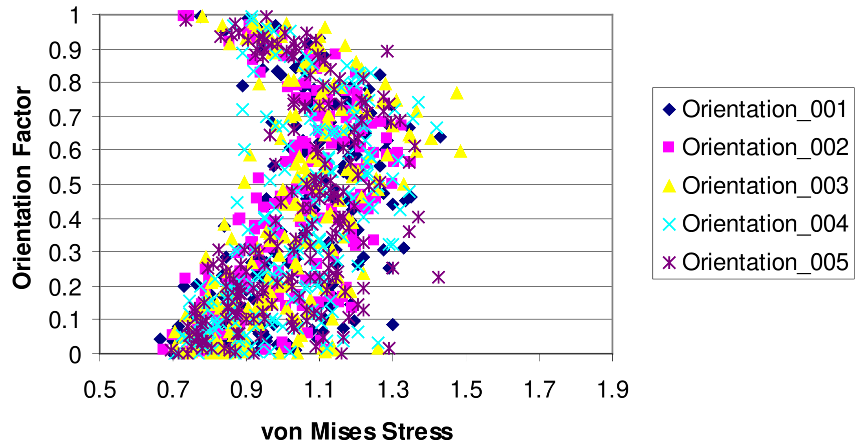

Figure 4: Grain orientation relationship with von Mises stress at the center of each grain for nickel-based Waspaloy material

ranges form 0.5 to 0.9, the corresponding grain would be in the range of maximum von Mises stress is high. As to the von Mises stress at the center of each grain in the SVE cubic model, the same trend occurs as shown in Figure 4 and Figure 5. The von Mises stress at center of each grain has a strong relation with its corresponding orientation factor within the SVE cubic model.

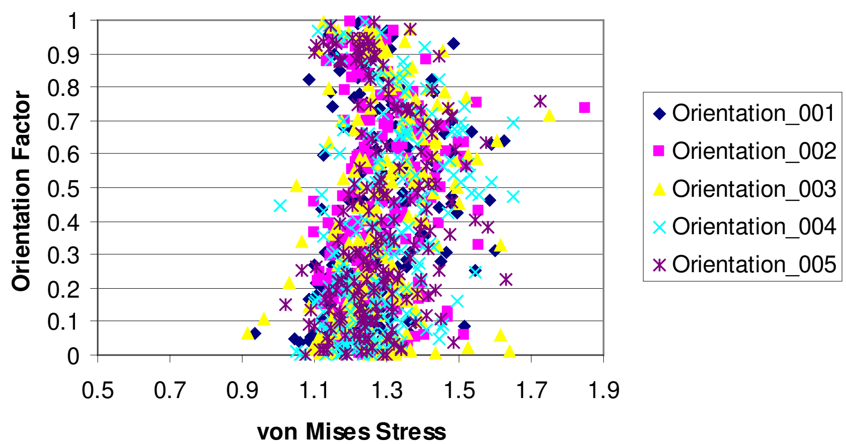

Figure 5: Grain orientation relationship with maximum von Mises stress of each grain for nickel-based Waspaloy material

4.2 Representative volume element (RVE) size study for one grain

The question arises as to how big the SVE need to be to predict statistically significant variation in stress for one grain? The SVE cubic model as shown in Figure 6 was used to investigate this question. Assuming a randomly chosen grain (Figure 7) on the surface of the SVE cubic model (Figure 6), the maximum von Mises stress of this grain and von Mises stress at the center of this grain are shown in Figure 10 and Figure 11 after analyzing finite element results and considering six sets of grain orientation in the SVE cubic mode. The geometry of first layer of grains of this specific grain is shown in Figure 8 with 11 grains, and the geometry of second layer grains is shown in Figure 9 with 37grains. For this particular exterior grain, its RVE size has been studied the following way:

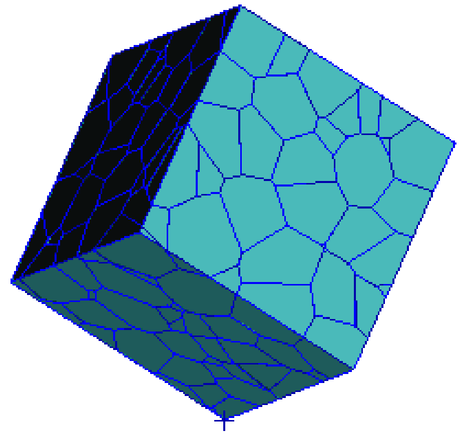

Figure 6: SVE model of microstructure

1. Consider six sets of grain orientation to study the C.O.V. of center stress for the particular grain.
2. Fix the orientation of the particular grain in six cases, and study the stress distribution within the grain and C.O.V. of center stress of the grain.
3. Fix the orientation of the particular grain and all its first layer neighbor grains in six cases, and study the stress distribution within the grain and C.O.V. of center stress of the grain.
4. Fix the orientation of the particular grain and all its first layer neighbor grains and second layer neighbor grains, and study the stress distribution within the grain and C.O.V. of center stress of the grain.

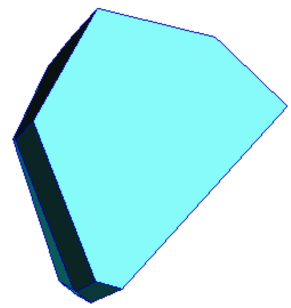

Figure 7: The grain need to be considered.

From the results listed in Table 1, it is found that the difference of maximum von Mises stress for the specific grain on the surface of SVE cubic model is convergent from 0.419 to 0.070, and coefficient of variance (C.O.V.) is convergent from 0.118 to 0.023 during Case 0 to Case 3 finite element analysis, which can also be found in Figure 10. At the same time from the results listed in Table 2, it is found that the difference of grain center von Mises stress for the specific grain on the surface of SVE cubic model is also convergent from 0.468 to 0.065, and C.O.V. is convergent from 0.175 to 0.027 during Case 0 to Case 3 finite element analysis, which can also be found in Figure 11. It means that the RVE size of one grain needs at least two layers of neighbor grains, and there is less effect on micro-stress of the specific grain if just changing grain orientation beyond the second layer within the SVE cubic model. Here, due to the specific grain is an exterior grain, its first layer has 11 grains, and its second layer has 37 grains only.

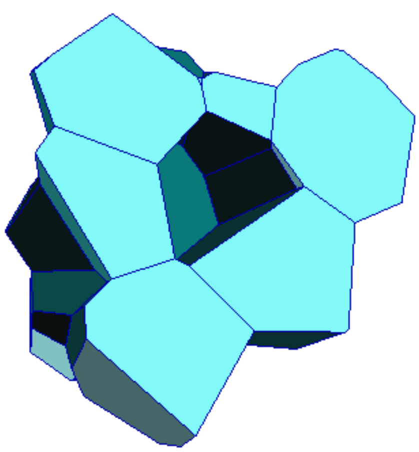

Figure 8: First layer grains of the grain

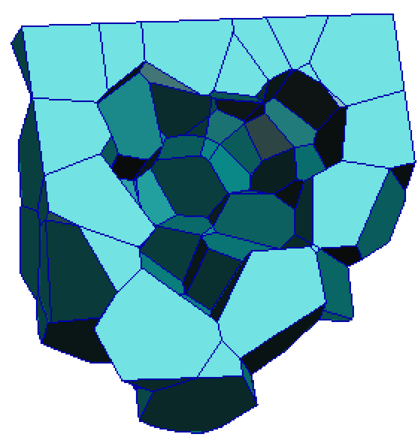

Figure 9: Second layer grains of the grain

Table 1: Maximum von Mises stress difference and its C.O.V. of the specific grain

Case	Case 0	Case 1	Case 2	Case 3
Maximum - Minimum	0.419	0.172	0.100	0.070
C.O.V.	0.118	0.051	0.027	0.023

Table 2: Grain center von Mises stress difference and its C. O.V. for the specific grain

Case	Case 0	Case 1	Case 2	Case 3
Maximum - Minimum	0.468	0.177	0.146	0.065
C.O.V.	0.175	0.087	0.059	0.027

* Case 0 --- Original six sets of grain orientation within the SVE cubic model.
Case 1 --- The specific grain with fixed orientation.
Case 2 --- The specific grain and its first layer with fixed orientation.
Case 3 --- The specific grain, its first and second layer with fixed orientation.

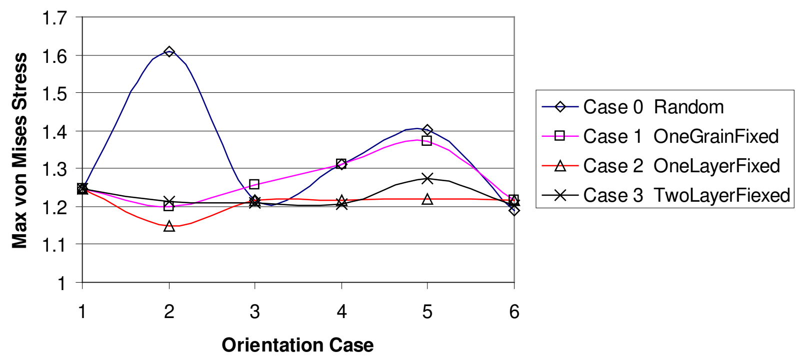

Figure 10: Maximum von Mises stress of grain

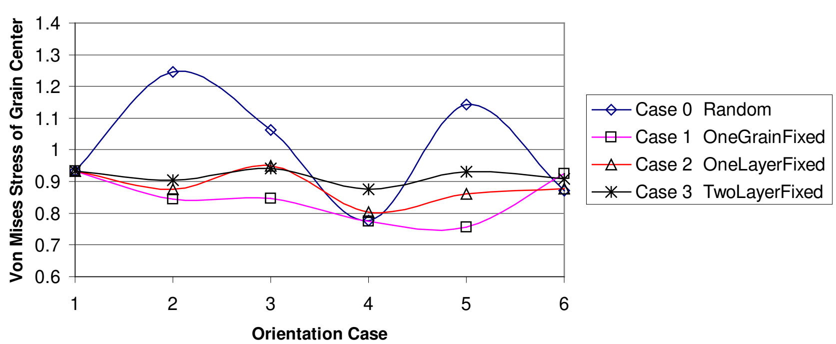

Figure 11: von Mises stress at grain center

4.3 Micro-stress differenece for stress control and strain control boundary condition

The question arises as to the difference between stress controlled and strain controlled boundary conditions. For the stress control boundary condition micro-stress analysis, 10 psi pressure is applied on the top surface of the SVE cubic model as shown in Figure 3. In order to compare the micro-stress distribution under strain control boundary condition, strain is applied on the top surface of the SVE cubic model which is equivalent average displacement under the stress control boundary condition. There are two sets of orientation investigated for both the stress control and strain control boundary condition. The grain maximum von Mises stress and grain center von Mises stress distribution of the SVE cubic model have been obtained as shown in Figure 12 and Figure 13, respectively. The maximum von Mises stress of each

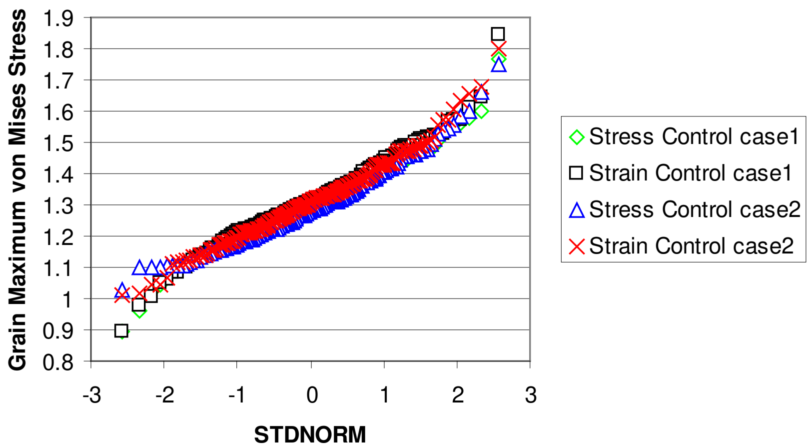

Figure 12 Grain maximum von Mises stress under stress control and strain control boundary condition

grain under strain control boundary condition is slightly higher than that of under stress control boundary condition in each orientation sets for the SVE cubic model. The same phenomenon is seen with the grain center von Mises stress. The overall micro-stress distribution is very similar under both loading conditions, and the only difference between them is that the top two layers of grains have slightly different micro-stress distribution, but other part of the model have exactly the same micro-stress distribution. This indicates that stress control and strain control only affect top two layer micro-

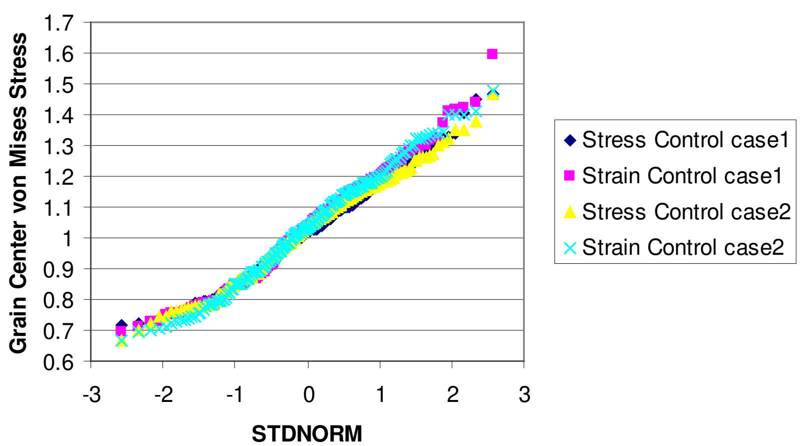

Figure 13 Grain center von Mises stress under stress control and strain control boundary condition

stress distribution using this SVE cubic model i.e., the boundary condition only effects local to the boundary and the random nature of the microstructure tends to eliminate the effect of the boundary condition.

5. Conclusions

Statistical elastic micro-stress analysis of single-phase FCC polycrystalline metallic material has been conducted using 3-D SVE cubic model by Fortran-MSC Patran/Nastran software. In this paper, single-phase polycrystalline metallic material is modeled as an ensemble of grains, and all grains are assumed to have anisotropic mechanical properties with uniform random orientations. The response of the polycrystal is the aggregate response of the constituent grains. Grain size, shape and orientation have been considered to study the micro-stress distribution in the model. Micro-stress analysis is performed using the statistical volume element (SVE) model with 200 grains. The representative volume element

(RVE) size for only one grain has been found that at least it needs two layers of grains surrounding the specific grain. The micro-stress distribution difference for this SVE model under stress control and strain control has been investigated, and find that only top two layers of grain with different stress distribution, other part of the model have almost the same stress distribution.

Acknowledgments

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