Investigations on the Reliability of FEA Calculations on the Microscopic Scale

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ABSTRACT

Local stress fluctuations and effective material behavior of polycrystalline materials are studied using a representative volume element. The microstructure is modeled by a Voronoi-tessellation with random orientations of the crystallographic axes of each grain. Finite-element-analyses are carried out for different grain geometries and materials. High stress localizations are observed. The scatter of the effective properties is reduced with increasing number of grains.

In order to analyze the influence of the anisotropic material on a real micro component, a tooth profile of a planetary gear was mapped upon characteristic Voronoi-tessellations. A high influence of the grains on the stress distribution is observed. The maximum stresses occur at both tooth roots depending mainly on the crystallographic grain orientations in the critical area. An enormous scatter of the stress maxima is observed. This has to be taken into account for the reliable dimensioning of micro components.

Keywords: anisotropy, FEA, grain, microstructure and Voronoi-tessellation

1 INTRODUCTION

The Finite-element-analysis is more and more used in the calculation of micro components. In general, consciously or not, it is assumed that the component contains a sufficient large number of grains over a characteristic profile. Only for this case the assumption of isotropic and homogeneous materials holds.

If the number of grains within the micro component falls below a certain value dependent on its structure and its single crystal parameters, then the microstructure has to be included in the dimensioning process. The local stress distribution can be heavily influenced by the grains.

This work is therefore a first important step to achieve reference values for the engineer about the validity of classical design concepts on a microscopic scale.

2 MICROMECHANICS

For micromechanical investigations we consider a volume element with an inhomogeneous linear elastic material behavior. To describe the overall behavior the local fields at the microscale are replaced by their spatial mean values:

$$\langle \sigma \rangle = \frac{1}{|V|}\int_V \sigma(x)\,dV, \qquad \langle \varepsilon \rangle = \frac{1}{|V|}\int_V \varepsilon(x)\,dV.$$

With the help of these macroscopic values the overall elasticity tensor can be defined as

$$\langle \sigma \rangle = C^* : \langle \varepsilon \rangle.$$

The definition of transversal isotropic overall parameters such as Young's moduli E_1^*, E_2^* and E_3^* is straightforward. To solve the boundary value problem in the volume element either linear displacements or constant tractions are imposed

$$u(x)\big|_{\partial V} = \varepsilon^0 \cdot x, \qquad t(x)\big|_{\partial V} = \sigma^0 \cdot n(x).$$

This is the typical framework in micromechanics to calculate overall properties of heterogeneous materials [1], [2]. In this work it is used to study the scatter of the effective behavior and the local fluctuations of inhomogeneous microstructure.

2.1 Model of the grain structure

We use a Voronoi-tessellation to simulate a realistic grain geometry of a polycrystalline material [3], [4]. A Voronoi-tessellation represents a cell structure constructed from a point process by introducing cell walls perpendicular to lines connecting neighboring points. The point process can be chosen in a way, which describes the real grain structure the best. The most simple and common choice is a Poisson-Point-Process with uniformly distributed independent points, see figure 1.

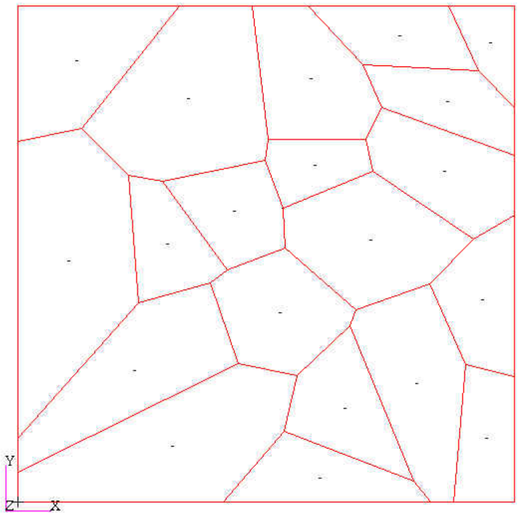

Figure 1: Voronoi-tessellation with 20 cells.

To describe a more irregular grain structure, a Cluster-Point-Process can be used. If on the other hand the grain structure is more regular, than a so called Hardcore-Point-Process is suitable with lower boundary for the distance between neighboring points.

2.2 Mesh generation

The mesh generation is performed automatically with the macrolanguage PCL within the pre-postprocessor MSC.Patran. For details of meshing see [5].

It has to be noted, that not every realization of the point process leads to a “meshable” tessellation due to the requirements on the geometry of the finite element method. For a reliable linear elastic analysis all angles within the polygons should exceed 30° and the aspect ratio of the shortest and longest line should be lower than 1:500.

A meshable tessellation is simply obtained with the trial-and-error-method. For a large number of grains (>1000) this can be difficult. To achieve an aspect ratio of 1:500, about 500 trials are needed to get a meshable Voronoi-tessellation with 1000 grains.

Numerical simulations have shown that the subset of meshable tessellations has similar statistical properties as the set of all tessellations, e.g. the standard deviation of the surface of a cell is nearly the same. So the restriction to meshable tessellations is not severe.

2.3 Model of the crystallographic orientation

The grains are considered as single crystals with anisotropic elastic behavior. The orientation of the crystallographic axes is described with the three random Euler angles

$$\varphi \in [\,0,2\pi\,[\,,\quad \theta \in [\,0,\pi\,[\,,\ \text{and}\quad \Psi \in [\,0,2\pi\,[.$$

To model an isotropic macroscopic material behavior, an isotropic orientation distribution of the random variables φ, θ and Ψ is used.

3 APPLICATION

In order to analyze the influence of the materials microstructure (grain size, number of grains, grain orientation) and the material parameters (single crystal parameters) on the stresses of a real component, the studies of Weyer and Fröhlich are applied to the geometry of a tooth of a planetary gear [1], [2].

The Institute of machine design of the University of Karlsruhe is dealing within the scope of the DFG founded collaborative research center (Sonderforschungsbereich) “Development, production and quality assurance of primary shaped micro components from metallic and ceramic materials” with the development, design and dimensioning of a micro planetary gear train.

The tooth profile of a planet wheel was mapped upon characteristic Voronoi-tessellations with 20 and 50 grains, see figure 2. Unnecessary finite elements outside the tooth profile and even whole grains have been removed. After that the mesh has been adapted to the geometry of the planet wheel. The tooth has been fixed and a load according to the operating conditions was imposed on the tooth flank.

For the anisotropic calculations the grains are modeled as anisotropic single crystals with random crystallographic orientations. To compare these with results of isotropic calculations, analyses which are neglecting the microstructure are carried out, too. This approach is commonly used in FE-analysis of micro components. The Hill’s average of the elastic single crystal values is chosen as the isotropic material parameters [6].

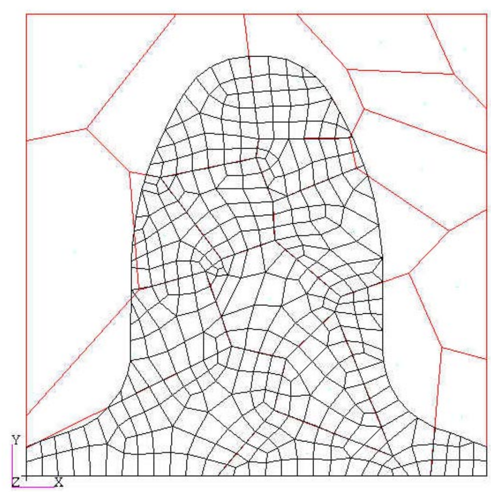

Figure 2: Tooth profile with mesh.

4 RESULTS

First, the local fluctuations inside the volume element are examined. Figure 3 shows the probability density of the stress component σ_{11} for 500 grains and 18.000 finite elements, averaged over 50 realizations of the orientation distributions.

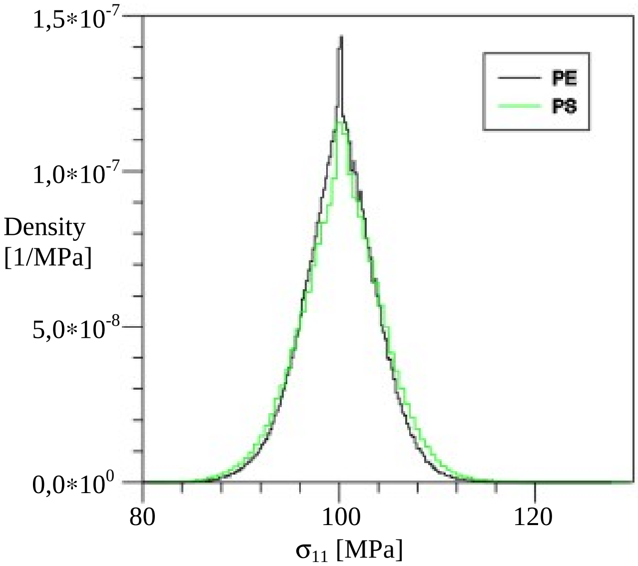

Figure 3: Probability density for σ_{11}. (PS: Plane stress, PE: Plane strain)

A linear traction in x_1-direction with σ_{11}^0=100MPa is applied. The single crystal data for alumina has been used [7]. The scatter for plane stress is slightly higher than for plane strain.
In Table 1, the mean values and the standard deviation of the stress components are given for a model with 1000 grains.

	Alumina		Barium Titanate	
Model	Plane strain	Plane stress	Plane strain	Plane stress
σ_{11}	100 ± 2,9	100 ± 3,2	100 ± 10,4	100 ± 11,9
σ_{22}	0 ± 2,7	0 ± 2,8	0 ± 8,0	0 ± 8,1
σ_{12}	0 ± 1,5	0 ± 1,7	0 ± 4,8	0 ± 5,5

Table 1: Mean value and standard deviation of the local stress fields in MPa for a model with 1000 grains.

It can be seen that the highest scatter is obtained for σ_{11} (approx. 10%) and the lowest for the shear component σ_{12}. These results can be used as a measure of localization in a real heterogeneous microstructure compared with the homogenized medium. It has to be mentioned that the variance of stress is influenced by the chosen boundary condition, at least for a small number of grains.

The overall Young's modulus E_1^* has been calculated for Poisson-Voronoi-tessellations with 5 to 1000 grains. Figure 4 shows E_1^* for 50 realizations of the orientation distribution using linear displacement boundary conditions.

It can be seen that the mean value is approximately constant and the scatter decreases with increasing number of grains. In Table 2 the mean value and the standard deri-

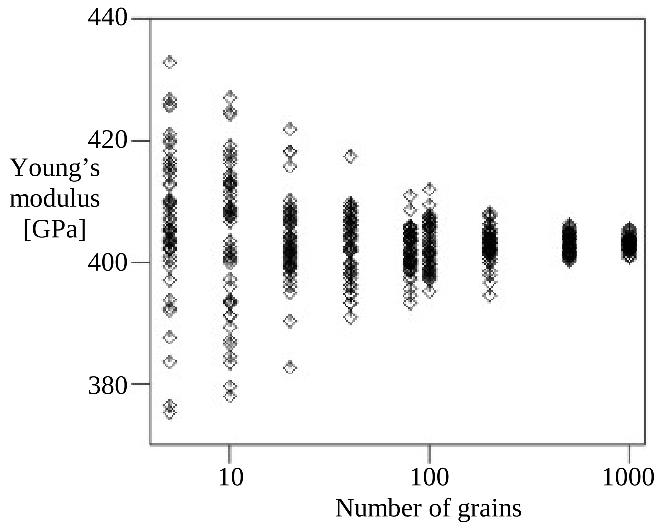

Figure 4: Overall Young's modulus E_1^* depending on the number of grains

vation of E_1^* for 100 grains is listed for different single crystal values. Of course, the single crystals with a higher degree of anisotropy (e.g. zirconia) lead to a higher scatter.

Material [7]	E_1^*	**Scatter**
Al_2O_3	402,7 ± 4,0	1,0 %
$BaTiO_3$	152,3 ± 8,9	4,7 %
Steel 316	207,1 ± 6,5	2,9 %
ZrO_2-3mol Y_2O_3	209,2 ± 6,0	4,3 %
ZrO_2-8mol Y_2O_3	225,6 ± 7,2	2,9 %

Table 2: Mean value, standard deviation, and scatter of E_1^* for different single crystal values in GPa.

Different realizations of the Poisson-point-process show a similar behavior. The scatter for Cluster-point-processes is significantly higher as for a Poisson- or Hardcore-point-process with the same number of cells.

Due to the anisotropic material behavior on the microscale and the limited number of grains, C^* will be anisotropic even for an isotropic orientation distribution. The degree of anisotropy is reduced for increasing number of grains.

As a second part, the influence of the grains on the stresses of the tooth profile has been analyzed. The tooth profile has been calculated with different materials (alumina, zirconia and steel 316) for isotropic and anisotropic microscopic material behavior.

Figure 5 shows the distribution of the Mises-stress for a calculation carried out with anisotropic grains. It can be seen that the stress obviates a specific grain inside the tooth profile due to the dependence of the stiffness from the grain orientation.

For the isotropic calculation the maximum stress is at the left tooth root. In the anisotropic case two possible locations for the global stress maximum can occur: Preferably the left but also the right tooth root. The location of the maximum is mainly depending on the specific crystallographic orientation of the grains situated at the tooth root.

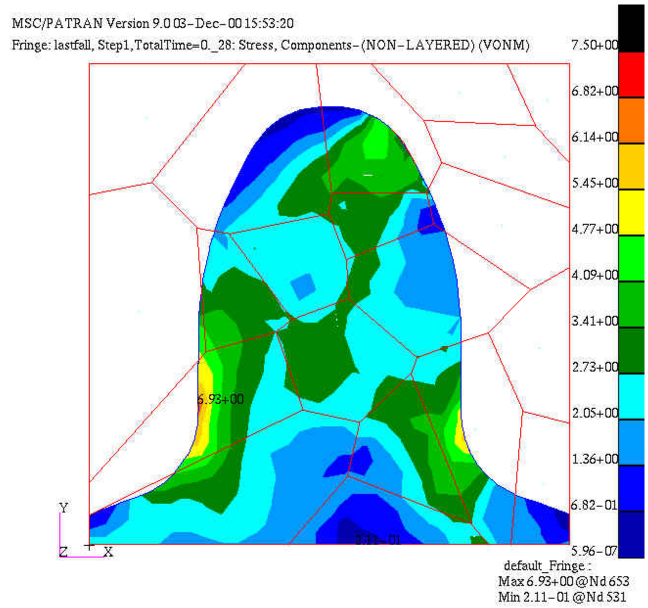

Figure 5: Mises-stress in the tooth for anisotropic zirconia grains.

Figure 6 shows the scatter of the local stresses at the left tooth root for different materials. Because of the different anisotropy of the single crystal values the lowest scatter occurs for alumina, the highest scatter for zirconia. The model with 20 grains leads to a scatter of about 5% and 21%, respectively. The reduction of scatter with an increasing number of grains, as noticed in figure 4, can not be observed, here. The scatter of the mean value remains for 50 grains. The right tooth root shows a similar behavior with a lower mean value.

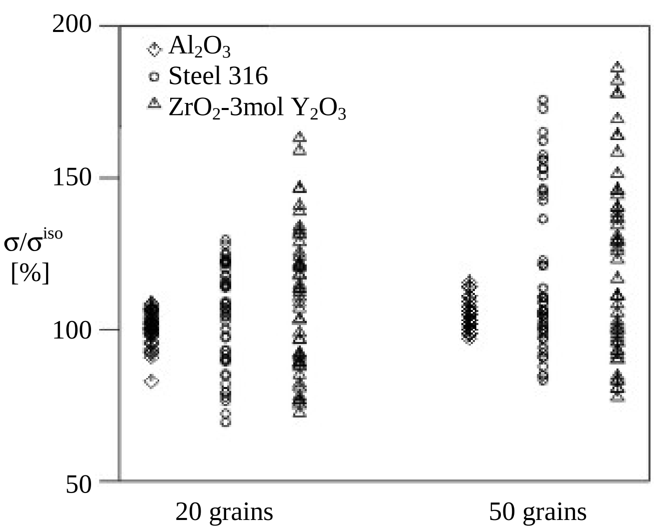

Figure 6: Results of the stress on the left tooth root in relation to the result for the isotropic calculation.

The scattering is mainly caused by the grain orientation in the considered location. Obviously, this effect is hardly influenced by the number of grains in the tooth, as there is no averaging involved. In comparison to the results of the isotropic calculations stress maxima for anisotropic calculations can be up to 100% higher.

For a high reliability of a micro component a suitable crystallographic orientation of the grains in the critical areas is necessary. If a selection of the crystallographic orientation is not possible the resulting higher stress maxima have to be taken into account for dimensioning.

5 CONCLUSION

Local stresses and overall material parameters of polycrystals have been calculated. High stress fluctuations inside the microstructure and a reduced scatter of the effective properties with increasing number of grains were observed.

FE-analysis of the tooth profile of a planetary gear has been carried out. The grains show a heavy influence on the stress distribution. It has been noticed that the stress maxima occur at one of the tooth roots depending mainly on the crystallographic orientation of the grains in these critical areas.

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