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Mechanic-Stochastic Model for the Simulation of Polycrystals

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Mechanic-Stochastic Model for the Simulation of Polycrystals

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Abstract

A mechanic-stochastic model for the mechanics of polycrystal material based on the single crystal orientations is presented. With this method, the distributions of strain and stress tensor components can be obtained in practice. Specific examples of computed distributions are shown, together with the distributions of the FEM-calulated mechanical responses of a polycrystal.

1. Introduction

During the production of metallic microcomponents, the local anisotropies of the materials become large enough to cause a strong influence in the resulting mechanical responses. For this reason, a model for the mechanical simulation of such pieces has to drop all isotropic assumptions and include the stochastic distribution of the microstructure.

In this work, we present a stochastic model of the microstructure in a polycristal (Section 2), together with some simulated distributions of the elastic tensor components and the corresponding elastic responses calculated using a Finite Element Method in a three-dimensional material piece (Section 3).

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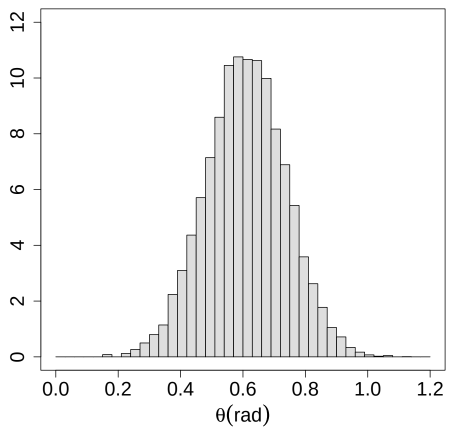

Figure 1: Histogram for the distribution of the projected nutation angle.

2. Stochastic model

The stochastic model bases on the orientations of a crystalite in the RTN system. The orientation of a crystalite in a polycrystal is described by a rotation g, which maps the RTN system on the crystal physical system. These rotations constitute the rotation group SO(3). All distributions on this group are described by the formula $d\mu = f(g)dg$, $g \in$SO(3), with the invariant measure $dg = \frac{\sin\theta d\theta}{2}\frac{d\varphi_1}{2\pi}\frac{d\varphi_2}{2\pi}$, and density of distribution $f(g) = \sum\limits_{l=0}^{\infty}\sum\limits_{m,n=-l}^{l} C^l_{mn}T^l_{mn}(g)$.

The way to derive the canonical normal distributions (CND) [1] lies in the application of Parthasarathy's [2] central limit theorem (CLT) for the rotation group. The concept of small rotations [3] is used for this purpose. The set of small rotations corresponds to a certain set of Euler angles:

$$\begin{cases} 1-(e'_z,e_z) = 1-\cos\theta \leq a \\ 1-(e'_x,e_x) = 1-\cos\varphi_1\cos\varphi_2+\sin\varphi_1\sin\varphi_2\cos\theta \leq b \\ 1-(e'_y,e_y) = 1+\sin\varphi_1\sin\varphi_2-\cos\varphi_1\cos\varphi_2\cos\theta \leq b \\ 0 \leq a,b \ll 1 \end{cases} \tag{1}$$

Here, (e_x,e_y,e_z) form a basis before a small rotation is applied and (e'_x,e'_y,e'_z) thereafter. The set of small rotations is now represented by the

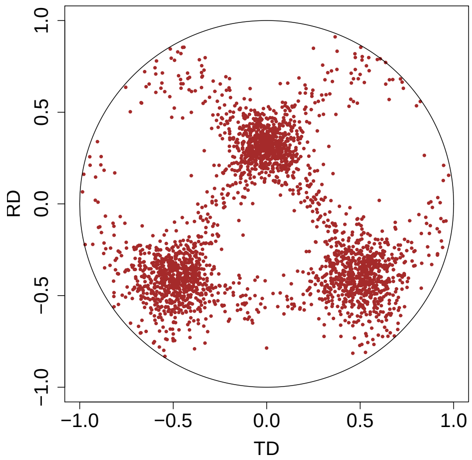

Figure 2: $< 100 >$ pole figure given a RTN texture.

region $\Pi(a,b) = \left\{(\varphi_1, \theta, \varphi_2) : \ \theta \le \sqrt{2a} = \bar{a} \ , \ |\varphi_1 + \varphi_2| \le \sqrt{2b} = \bar{b}\right\}$.

The sequence of measures $d\mu_n = f_n(g)dg$, with f_n denoting the rectangular distribution in $\Pi(a_n, b_n)$, $a_n = \bar{a}/\sqrt{n}$, $b_n = \bar{b}/\sqrt{n}$ corresponds to the sequence of convolutions $d\mu_n^{*n}$, which converges for $n \to \infty$ to the canonical normal distribution on SO(3) with parameters $\bar{a}^2/8$ and $\bar{b}^2/6$ [3].

The realisation of the random variable $g \in$SO(3) with distribution $d\mu_n^{*n}$ is now the product of the small random rotations $g = g_1 g_2 ... g_n$, where $g_i = g(\varphi_1^i, \theta^i, \varphi_2^i) \in$SO(3) with rectangular distribution in $\Pi(a_n, b_n)$.

The distribution of crystalite orientations may be modelled by Monte Carlo simulation and the material parameters of interest can be derived from them. Figure 1 shows the distribution of the projection of the nutation angle θ on the sphere for selected values of $\bar{a} = 0.25$, $\bar{b} = 0.65$ and $n = 50$ for the texture (1,1,2)[$\bar{1}$,$\bar{1}$,1]. This distribution results from 10000 realizations. Figure 2 shows the pole figure for the same texture.

The tensor representation of the rotation group $C_{ijkl} = g_{ip} g_{jq} g_{km} g_{ln} c_{pqmn}$ leads now to the equations $C_{ij} = c_{ij} + \mu^c \Lambda_{ij}(\varphi_1, \theta, \varphi_2)$, where $\mu^c = c_{11} - c_{12} - 2c_{44}$ is the measure of anisotrophy. The resulting distributions of the stiffness matrix components under $\bar{a} = 0.2$, $\bar{b} = 0.4$ are shown in the Figures 3.

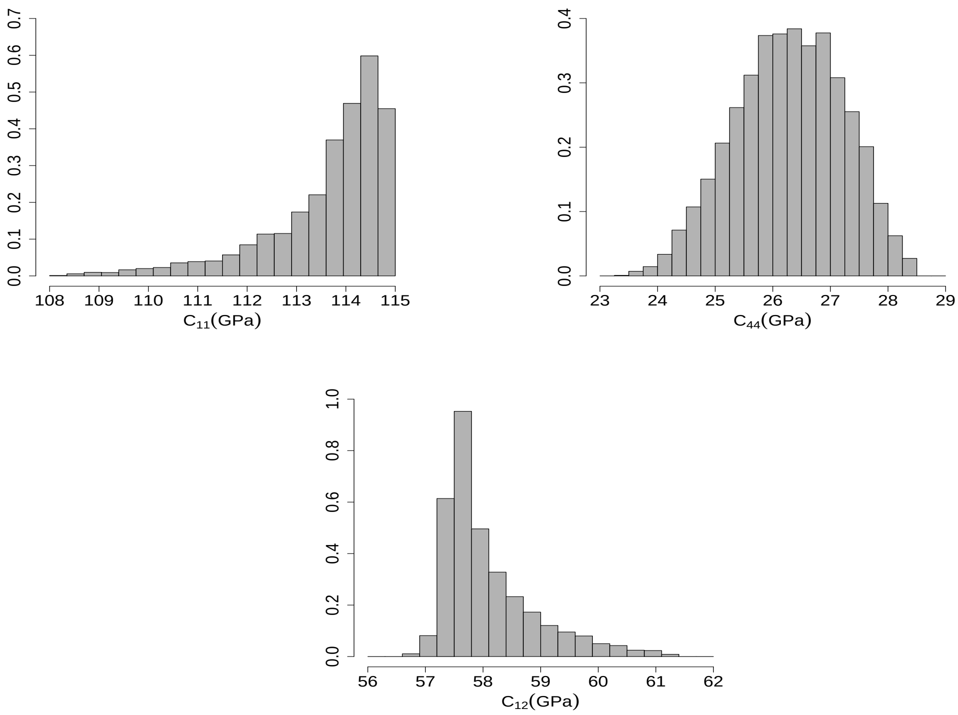

Figure 3: Aluminium; $c_{11} = 108.2$, $c_{44} = 28.5$ and $c_{12} = 61,3$ GPa.

3. Finite Element Simulations

In order to show the effects of the texture-imposed material properties, thousand pieces of size $0.45 \times 0.45 \times 0.45$ were simulated usnig a domain decomposition in 20 grains and applying an artificial strain in x-direction of 1%. For each grain, the location of the center was selected randomly and the components of the elastic moduli were taken from the stochastically calculated tensors (cf. Section 2).

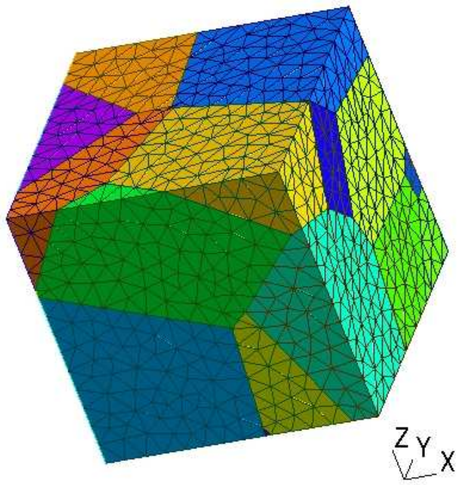

Figure 4: One of the simulated cells.

Figure 4 shows an example of the domain decomposition for one of the thousand simulated pieces. The different colors correspond to different grains. The simulations are performed using the Aluminium distributions shown in Figure 3.

Figure 5 shows the obtained distributions for the different components the volume averaged stress tensor[1]. The values of this stresses were obtained after a FEM simulation for an applied srain in x-direction of 1%.

[1]The volume averaged components of the stress tensor are $\bar{\sigma}_{ij} = \frac{1}{V}\int_\Omega \sigma_{ij}$, with V the volume and Ω the domain of the piece.

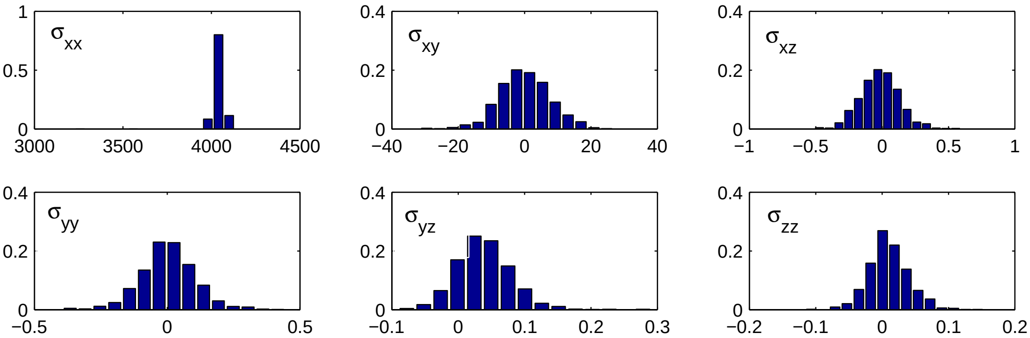

Figure 5: Distributions of obtained stresses under an applied strain of $\varepsilon_{xx} = 0.01$.

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