On Improving Predictions of Texture Evolution Using Processing Path Model

Über die verbesserte Vorhersage der Gefügeentwicklung mittels des Processing-Path-Modells

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The processing path model based on the conservation principle in the orientation space allows us to optimize processing path from a given initial state to a desired final microstructure for polycrystalline materials. This model uses texture coefficients in spherical harmonics expansion as descriptors to represent the texture state of polycrystalline materials. In this work, the effect of increasing the number of texture coefficients used in the series expansion (decided by l_{max}) on the prediction accuracy of texture evolution is investigated.

Key words: Processing path, materials design, texture evolution, microstructure, property

Das Processing-Path-Modell zur Gefügeentwicklung, das in dieser Studie entwickelt wurde, basiert auf dem Erhaltungsprinzip im Orientierungsraum und ermöglicht die endgültige Mikrostruktur - aus den ursprünglichen Mikrostrukturdaten eines polykristallinen Materials - vorauszusagen. Um den Gefügestatus eines polykristallinen Materials zu beschreiben, verwendet dieses Modell zur Materialbeschreibung Gefügekoeffizienten in sphärisch-harmonischer Reihenentwicklung. In dieser Arbeit wurde die Auswirkung einer Erhöhung der Gefügekoeffizienten in der Reihenentwicklung (dargestellt durch l_{max}) auf die Voraussage des End-gefüges untersucht.

Schlüsselworte: Bearbeitungsweise, Materialdesign, Gefügentwicklung, Mikrostruktur, Materialeigenschaften

Introduction

The development of microstructure sensitive design (MSD) framework for polycrystalline materials has evolved a great deal in recent years [1-3]. This methodology exploits the fact that all aspects of materials properties can be efficiently represented in a common Fourier space. The evolution of texture during mechanical deformation can be represented as a path line (processing path) in the microstructure hull. Each point in this Fourier space stands for a unique texture, associated with corresponding properties. The present work concentrates on the relationship between the process and the microstructure (specifically texture) such that there is a direct analytical solution linking the final microstructure to the initial one with a limited number of process parameters. Many efforts were invested to arrive at a mathematical representation of microstructure including chemical components, phases, grain shape, grain boundary orientation, crystal orientation distribution (texture) and so on. Although some local properties are more related to the other characters than texture, most global properties, such as elastic modulus and yield strength, are primarily dependant on texture. In this study we concentrated on texture evolution.

Basic properties can be linearly represented by the quantitative descriptors of microstructure using statistical homogenization relations [1,2]. For the purpose of the present work, we limit the microstructure representation to texture represented by orientation distribution function (ODF) *f(g)*:

$$f(g)dg = \frac{dV(g)}{V} = f(\phi_1, \phi, \phi_2) \tag{1}$$

Here, V is the total volume and $dV(g)$ is the volume with orientation g represendted by the Euler angles ϕ_1, ϕ and ϕ_2. The ODF can be presented as a weighted sum of orthornormal basis functions T^{i} (spherical harmonics)[4]:

$$f(g) = \sum_{l=0}^{\infty} \sum_{m=0}^{M(l)} \sum_{n=0}^{N(l)} F_t^{mn} T^{\ddot{i}^{mn}}(g) \tag{2}$$

The weight parameters F in the above equation represent the texture coeffecients. In our previous work [3,5,6], a processing path model was proposed to simulate texture evolution during deformation in cubic and hexagonal materials. This model was also used to give optimal processing path through a streamline family of processing paths. In the following, this model is examined further to simulate texture evolution.

Processing Path Model

The details of the processing path model were presented elsewhere [4-6]. Here the basic features are summarized below. This model is based on the conservation principle in the orientation space [7-11]. The orientation space is constructed by three Euler angles $\{\phi_1,\phi,\phi_2\}$, with a density parameter defined as $\rho=f(g)$. The flux rate in the orientation space is $R(g)$. According to the conservation principle:

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$$\frac{\partial \rho(g,\eta)}{\partial \eta} + div[\rho(g,\eta)R(g)] = 0 \qquad (3)$$

Here η is the deformation parameter. Substituting Eq. (2) with the relationship of the density and the spectral expansion of texture, we get:

$$\sum_{lmn} \frac{dF_l^{mn}(\eta)}{d\eta} \dot{T}_l^{mn}(g) + \sum_{\lambda\sigma\rho} F_\lambda^{\sigma\rho}(\eta) div\left(\dot{\dot{T}}_\lambda^{\sigma\rho}(g)R(g)\right) = 0 \qquad (4)$$

Further utilizing the spectral expansion, we define:

$$div\left(\dot{\dot{T}}_\lambda^{\sigma\rho}(g)R(g)\right) = -\sum_{lmn} A_{l\lambda}^{mn\sigma\rho} \dot{\dot{T}}_l^{mn}(g) \qquad (5)$$

The rate of change of the texture coefficients F_l^{mn} are now derived as:

$$\frac{dF_l^{mn}(\eta)}{d\eta} = \sum_{\lambda\sigma\rho} A_l^{mn\sigma\rho} F_\lambda^{\sigma\rho}(\eta) \qquad (6)$$

After integrating Eq. (6), the processing path function is presented below:

$$F(\eta) = e^{A(\eta-\eta_0)} F(\eta_0) \qquad (7)$$

Texture evolution matrix A is an intrinsic property of the material. The model can be used to find a processing schedule to achieve a desired texture from the initial by calculating the corresponding texture evolution matrix. The present work focuses on the improvement of the predictive capability of the model.

Results and Discussion

For this work we start with a numerically constructed FCC polycrystal which exhibits a nearly random texture (*Fig. 1*). The use of Taylor model, with 400 random orientations, allows us to generate the evolution of the microstructure for tension, compression and rolling. The first part of this work used three constant strain increments (2 %, 1 % and 0.2 %) to generate data from 0 % to 50 % strain and varied the value of l_{max} to the values 4, 8, 12, 18, and 22. For each of these values, the matrix evolution has been calculated using Eq. (6). The use of repeated Richardson extrapolation permitted us to find a better approximation of the matrix evolution. It is important to note that the size of the texture evolution matrix A increases with the increase of l rank. Its size is 4x4, 13x13, 36x36, 100x100 and 172x172 for $l_{max} = 4$, $l_{max} = 8$, $l_{max} = 12$, $l_{max} = 18$ and $l_{max} = 22$ respectively. The use of Eq. (7) allows us to compute texture coefficients from 0 % to 50 % using our initial texture. Bunge [3] pointed out that when the crystal system is cubic and the sample system is orthortropic, a limited number of texture coefficients with $l \leq 4$ are needed to relate the texture coefficients and elastic properties. In this case, three texture coefficients $\{F_4^{11}, F_4^{12}, F_4^{13}\}$ are enough for the calculation of the elastic properties. Here we compared these principle texture coefficients, obtained by Taylor and those obtained by the processing path model using the least mean square error.

$$error_l^{mn} = \frac{1}{N}\sqrt{\sum_{i=1}^{N} ({}^{i}F_l^{mn} recalculated - {}^{i}F_l^{mn} Taylor)^2} \qquad (8)$$

The calculated errors obtained in tension, rolling and compression for each of the three texture coefficients F_4^{11}, F_4^{12} and F_4^{13} are shown in *Figure 2*. It is evident that the increase of l rank generates a major decrease in error.

Each of the data obtained by the processing path model at $l_{max} = 4$, 12 and 22 for several strains have been used to generate pole figures for tension, compression and rolling. These pole figures have then been compared to those numerically generated using Taylor model. Since the simulation results for all the strains follow the same pattern of deformation we depict only the results for 20 % in *Figure 3*.

After deformation to a strain of 20 %, the Taylor-based pole figure is given in the first column. Using the processing path

Fig. 1. (111) pole figure of the initial state.
Abb. 1. (111)-Polfigur des ursprünglichen Gefüges.

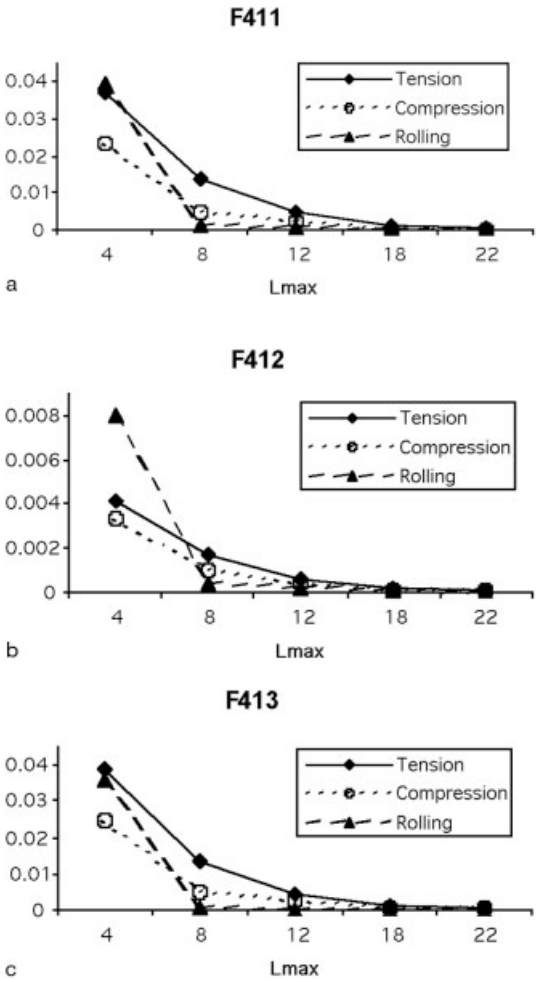

Fig. 2. Mean square error between experimental and recalculated texture coefficients, a) F_4^{11}, b) F_4^{12} and c) F_4^{13}.
Abb. 2. Effektiver Fehler zwischen experimentellen und berechneten Gefügekoeffizienten, a) F_4^{11}, b) F_4^{12} and c) F_4^{13}.

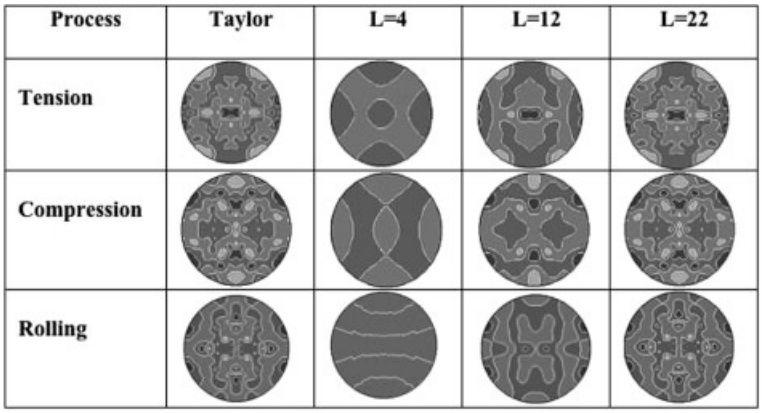

Fig. 3. (111) pole figures for tension, compression and rolling obtained for strain of 20 %.

Abb. 3. (111)-Polfiguren für Zug, Druck und Walzen bei einer Dehung von 20 %..

model with $l_{max} = 4$, the calculated pole figures according to processing path function, Eq. (7), are shown in the second column. It gives a rough representation of a fiber-like texture for all tests. When l_{max} is increased to 12, the (111) pole figures are shown in the third column. The results are much closer to the Taylor model prediction than those obtained for $l_{max} = 4$. The last column contains the recalculated (111) pole figures in the case of $l_{max} = 22$. These results are in agreement with the Taylor model result shown in first column. For all cases it is evident that the increase of l rank produces the same effect on the evolution of the pole figure for all tests. When increasing l_{max}, the deviation of the orientation distribution function $f(g)$ from the real value will be smaller.

Conclusion

A processing path model based on the conservation principle in the orientation space was proposed to predict the evolution of texture coefficients. A texture evolution matrix A is defined and used in the processing path function to describe the evolution of texture coefficients. With the increase of l_{max}, the dimension of A increases, the processing path model predicts the evolution of texture and individual texture coefficients more precisely. From our results, l_{max} should be expanded to 22 for a complete representation of texture although $l_{max} = 4$ seems to be enough when only F_4^{11}, F_4^{12} and F_4^{13} are of interest.

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