; 9. Variation of brass orientation {110}⟨112⟩ of fcc at 99.9% rolling reduction with change of NT shear ratio under complex relaxed constraints model with constant NR shear ratio of 0.6 according to the present several models when the specified plane is plane "2".

.t two shears occur on each of two veral combinations of shears system ed on the minimum shear magnitude ulation under relaxation with shear ng direction) shows that copper ori- ng only in Taylor's five shears model report under full constraints. The ormal strain) of NR. The maximum Taylor's five shears model to such as r hand, brass orientation decreased del. Secondly the simulation under nents between normal direction and sed with NT and disappeared more while brass orientation {110}⟨112⟩ f NT in Taylor's five shears model to selection of *none* shear plane to se of brass orientation is shown also nes) or eight (i.e. four 'two shear'

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Processing Path Model to Describe Texture Evolution During Mechanical Processing

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tract. Using a processing path model based on the conservation principle in the orientation space explicit solutions be formed linking any final (desired) microstructure to a given initial state for polycrystalline materials. The model texture coefficients in spherical harmonics expansion to as materials descriptors to represent the texture state of rystalline materials. In this work, the effect of increasing the maximum number of texture coefficients used in the s expansion (represented by L_{max}) on the prediction of texture and its accuracy is fully studied.

roduction

e has been much progress in the development of a framework for microstructure sensitive design of polycrystalline erials in recent years [1-4]. The new methodologies concentrate on the development of inverse techniques viding mechanical designer the modeling tools for design path along the direction of performance → properties & irement → microstructure → processing path rather than the more traditional direction flowing from microstructure property. The present work is focused on the linkage between processing and microstructure (specifically texture) that there is a direct analytical form linking the final microstructure to the initial with a limited number of process meters. Many efforts were invested to arrive at a mathematical representation of microstructure including chemical ponents, phases, grain shape, grain boundary orientation, crystal orientation distribution (texture) and so on. Some perties such as embrittlement and fracture are more related to the grain boundary distribution and character than ure. Some global properties, such as elastic modulus and yield strength, are primarily dependant on texture. In this y we concentrated on texture evolution.

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

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

ϕ_1, ϕ and ϕ_2 are Euler angles for the orientation g. ODF can be presented as a weighted sum of hornormal basis function (spherical harmonics) [3]:

$$f(g) = \sum_{l=0}^{\infty} \sum_{m=0}^{M(l)} \sum_{n=0}^{N(l)} F_l^{mn} \dot{T}_l^{mn}(g) \tag{2}$$

The set of texture coefficients $\{F_l^{mn}\}$, is used to represent texture and predict macroscopic perties. The advantage of using texture coefficients to represent the texture state of polycrstalline terials is that the macroscopic properties can be characterized by these coefficients linearly. The es representation can used to calculate macroscopic property $\overline{P}$, as in the following:

$$\overline{P} = \sum_{l=0}^{\infty} \sum_{m=0}^{M(l)} \sum_{n=0}^{N(l)} F_l^{mn} p_l^{mn} \tag{3}$$

Here p_l^{mn}'s are property coefficients.

In our previous work [3,4,5], a processing path model was proposed to simulate texture evolution during deformation in cubic and hexagonal material. Kalidindi et. al. used this relationship to derive the elastic properties of polycrystalline cubic copper from the set of texture coefficients:

$$\overline{C}_{1111} = 209.92 - 20.386F_4^{11} + 30.390F_4^{12} - 40.202F_4^{13} \tag{4}$$

In this relationship, effective stiffness C_{1111} is represented as a function of a set of limited number of texture coefficients $\{F_4^{11}, F_4^{12}, F_4^{13}\}$.

This model was also used to give optimal processing path through a streamline family of processing paths. In teh following this model is examined further to simulate texture evolution.

Processing Path Model

There are many models proposed to simulate and predict texture evolution of polycrystalline materials during mechanical deformation based on crystal plasticity and phenomenological modeling. These models can predict microstructure evolution, given the initial microstructure, deformation mode and other parameters representating other details of the microstructure. However it is difficult to use these models to arrive at an analytical tool to predict microstructure at any time during deformation.

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 proposed by Clement and Bunge [7-11] et. al. The orientation space is constructed by theree Euler angles $\{\phi_1,\phi,\phi_2\}$, (Fig.1) with a density parameter defined as $\rho = f(g)$. The flux rate in the orientation space is $R(g)$. According to the conservation principle:

$$\frac{\partial\rho(g,\eta)}{\partial\eta} + div[\rho(g,\eta)R(g)] = 0 \tag{5}$$

Here η is the deformation parameter which is a function of time t. Substituting Eq. (5) with the relationship of the density and the spectral expansion of texture, we get:

$$\sum_{lmn}\frac{dF_l^{mn}(\eta)}{d\eta}\dot{T}_l^{mn}(g) + \sum_{\lambda\sigma\rho}F_\lambda^{\sigma\rho}(\eta)div\left(\dot{\overline{T}}_\lambda^{\sigma\rho}(g)R(g)\right) = 0 \tag{6}$$

Further utilizing the spectral expansion, we define:

$$div\left(\dot{\overline{T}}_\lambda^{\sigma\rho}(g)R(g)\right) = -\sum_{lmn}A_{\lambda l}^{mn\sigma\rho}\dot{T}_l^{mn}(g) \tag{7}$$

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

$$\frac{dF_l^{mn}(\eta)}{d\eta} = \sum_{\lambda\sigma\rho}A_{\lambda l}^{mn\sigma\rho}F_\lambda^{\sigma\rho}(\eta) \tag{8}$$

After integrating Eq. (8), the processing path function is presented below:

$$F(\eta) = e^{A(\eta-\eta_0)}F(\eta_0) \tag{9}$$

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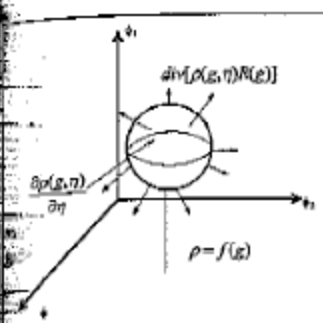

Fig. 1. Illustration of conservation principle in orientation space.

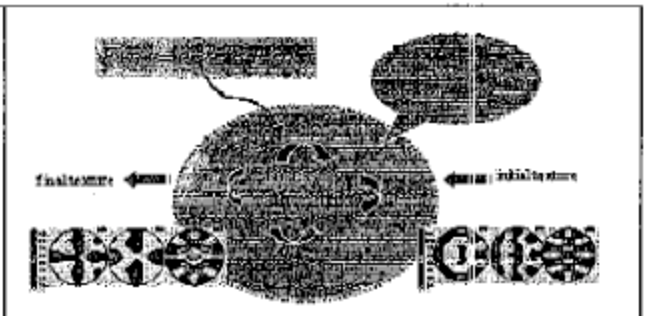

Fig. 2. Application of texture evolution matrix in inverse materials design. The goal is to find an optimized solution of processing path

Texture evolution matrix A is an intrinsic property of materials. The model as illustrated in Fig. 2, can be used as a processing recipe 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

Based on the previous study [4-6], we now focus on the effect of increasing the order L on improving the precision of texture evolution during mechanical deformation. Expansion of texture function in Eq. (2) implies that $f(g)$ will be described more precisely when the order l is increased to larger values. If the crystal system is cubic and the sample system is orthortropic, then $L_{min}=4$, and Eq. (3) becomes:

$$\begin{aligned} f(g) &= \sum_{l=0}^{L_{max}} \sum_{m=0}^{M(l)} \sum_{n=0}^{N(l)} F_l^{mn} \hat{T}_l^{mn}(g) \\ &= F_0^{11}\hat{T}_0^{11}(g) + F_4^{11}\hat{T}_4^{11}(g) + F_4^{12}\hat{T}_4^{12}(g) + F_4^{13}\hat{T}_4^{13}(g) \\ &= \hat{T}_0^{11}(g) + F_4^{11}\hat{T}_4^{11}(g) + F_4^{12}\hat{T}_4^{12}(g) + F_4^{13}\hat{T}_4^{13}(g) \end{aligned} \tag{10}$$

Increasing L_{max}, the error in the calculation of ODF or the deviation of $f(g)$ from the real value will be smaller. Fig. 3 presents (111) pole figure of the initial state, a pseudo random distribution. After a uniaxial extention to a strain of 0.2, the numerical experimental pole figure is given in Fig. 4a. Using a modified Taylor Model [12-13],the first order prediction of texture evolution in cubic materials can be calculated. For the processing path model with $L_{max}=4$, the texture evolution parameter A can be described by a 4×4 matrix. The calculated pole figure from this 4×4 A according to processing path function, Eq. (13), is shown in Fig. 4b. It gives a rough representation of (111) fiber texture. When L_{max} is increased to 12, there are 30 nonzero texture coefficients. (111) pole figures from 30 ×30 A is shown in Fig. 4c. The (111) fiber texture is much clearer than that in Fig. 4b. Fig. 4d is recalculated (111) pole figure from A in the case of $L_{max}=22$. It is very close to the experimental result shown in Fig. 4a.

Fig. 3. (111) pole figure of the initial state.

Fig. 4. (111) pole figures at a strain of 0.20 during tension. (a)numerical experiment result from Taylor model; (b)recalculated from processing path model using L_{max}=4; (c) recalculated using L_{max}=12; (d) recalculated using L_{max}=22.

Increasing the dimension of texture evolution matrix will improve the prediction of texture evolution at the expense of computation time.

We also studied the influence of L_{max} on the evolution of individual texture coefficients such as F_4^{11}, F_4^{12} and F_4^{12}. These three texture coefficients are are sufficient for the representation of elastic properties. Bunge [3] pointed that when the crystal system is cubic and the sample system is orthortropic, a limited number of texture coefficients are needed to relate the texture coefficients and elastic properties, as shown in Eq. (4). That is to say, $l \le 4$. In this case, three texture coefficients $\left\{F_4^{11}, F_4^{12}, F_4^{13}\right\}$ are enough for the calculation of the elastic properties. From the texture evolution matrix $A_{tension}$, $A_{compression}$ and $A_{rolling}$ in the processing path model and Eq. (5), we can obtain the evolution of elastic property C_{1111} during mechanical deformation, as shown in Fig. 5.

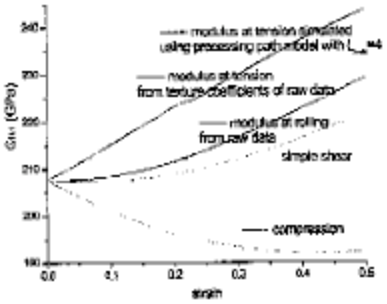

Fig. 5 Evolution of stiffness matrix C1111 during different processing methods calculated from the texture coefficients set, $\left\{F_4^{11}, F_4^{12}, F_4^{13}\right\}$, representing the state of polycrystalline materials.

It is shown that with the increase of strain, C_{1111} increases very fast in tension, decreases in compression and increases slightly in rolling and simple shear. Texture evolution matrix can then be used as a guide to achieve a particularly desired elasticity modulus. Fig. 5 also shows C_{1111} from the simulated data using the processing path model with L_{max}=4. The simulated modulus is very close to the numerical experimental result. It is clear that L_{max}=4 provides a first order simulation on the evolution of property. It is important to predict the evolution of texture coefficients F_4^{11}, F_4^{12} and F_4^{13} precisely. To examine the precision, we define an error parameter as shown below:

$$error_l^{ave} = \frac{1}{N}\sum_{i=1}^{N}\left({}^{i}F_l^{ave}{}_{recalculated} - {}^{i}F_l^{ave}{}_{experimental}\right) \qquad (11)$$

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model using L_{max}=4; (c) recalculated using

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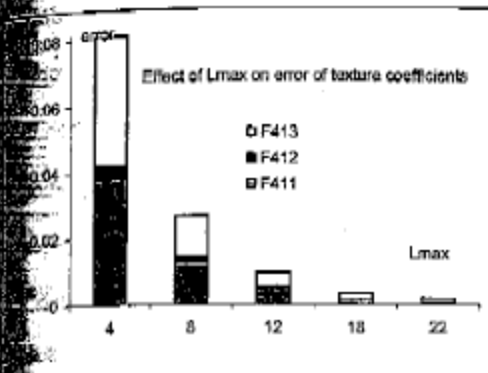

6. Effect of L_{max} on the error of texture coefficients, $error_4^{11}$, $error_4^{12}$ and $error_4^{13}$, recalculated from processing path model during tension.

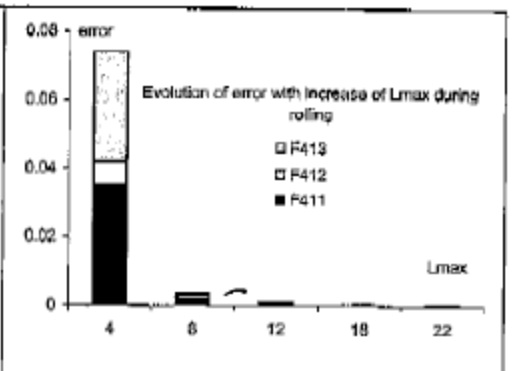

Fig. 7. Effect of L_{max} on the error of texture coefficients, $error_4^{11}$, $error_4^{12}$ and $error_4^{13}$, during rolling.

Fig. 6 shows the evolution of error during tension from 0% to 40%. Two features are obvious. First, the error is very small even when L_{max} is as small as 4. Second, the error of three texture coefficients continue to decrease further with the increase of L_{max}. $error_4^{11}$ decreases from 0.038 when $L_{max}=4$ to 0.00086 when $L_{max}=22$, while $error_4^{12}$ decreases from 0.004 to 0.0001 and $error_4^{13}$ from 0.039 to 0.00086. These two features also presented in other cases. Fig. 7 shows the evolution of error during rolling from 0% to 40%. With the increase of L_{max}, the dimension of texture evolution matrix **A** used in Eq. (10) increases from 4×4 to 172×172. Processing path function using larger **A** will predict the evolution of texture coefficients better with the sacrifice of computation time. Comparing with Bunge's works [7-9], processing path model gives a good simulation in the evolution of texture. This is attributed to the processing path function which is a continous integral function while Bunge's method loses the required presicion by using a stepwise integral method.

Conclusion

To predict the evolution of texture coefficients, a processing path model based on the conservation principle in the orientation space was proposed. 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.

Acknowledgement

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