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Quantitative comparison between simulated and experimental FCC rolling textures

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Abstract. The degree of similarity between simulated and experimental fcc rolling textures is characterized by a single scalar parameter. The textures are simulated with a relatively simple and efficient 1-point model which allows us to vary the strength of the interaction between the grains and the surrounding matrix and the scheme for the calculation of the lattice rotation. For the copper-type texture the best agreement between simulation and experiment is obtained by {111}<110> slip combined with relaxed constraints according to a procedure different from the traditional scheme for relaxed constraints. A Sachs-type model without any volume effect of deformation twins provides a very high degree of similarity between simulated and experimental brass texture. Addition of volume fractions of deformation twins corresponding to those observed experimentally has practically no effect on the simulated textures.

1. Introduction

The existence of two different types of fcc rolling texture, the copper-type texture and the brass-type texture, is the classical problem within the field of deformation texture. The history of the investigations of the two types of fcc rolling texture has been reviewed by Leffers and Ray [1]. The development of the copper-type texture is favoured by high stacking fault energy, high rolling temperature and low strain rate while the development of the brasstype texture is favoured by the opposite set of conditions. As also reviewed by Leffers and Ray there is by now general agreement that the development of the copper-type texture can be simulated by models with {111}<110> slip. There is not a corresponding general agreement about the simulation of the development of the brass-type texture. According to the predominant ideas it may be simulated by a combination of {111}<110> slip and a volume effect of deformation twinning as originally suggested by Wassermann [2] or by {111}<110> slip only with a special pattern of deformation and lattice rotation, e.g. [1,3,4]. In the present work we do strictly quantitative comparisons between the simulated and experimental textures via a single scalar correlation factor obtained from the procedure developed by Tarasiuk and Wierzbanowski [5]. This correlation factor involves all components/aspects of the textures considered. We also show the simulated and experimental ODFs [6].

Our present simulations refer to {111}<110> slip without and with deformation twinning. Our model is a rather simple 1-point model which includes the possibility to vary the strength of the interaction between the grains – from very weak to very strong – and to make a choice between two procedures for the calculation of the lattice rotations. The simulated and experimental textures correspond to the reduction of 60%.

2. Computational procedure

2.1. The polycrystal deformation model

The model for plastic deformation of polycrystals proposed by Leffers [7,8] and further developed by Wierzbanowski et al. [9,10] is used to simulate the texture formation during rolling deformation. The elastic-plastic isotropic interaction between a grain and its environment is expressed as:

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where σ_{ij} and ε_{ij}^{p} are the stress and plastic strain tensors of a grain, Σ_{ij} is the stress applied to the material, E_{ij}^{p} is the plastic deformation of the sample and L is a scalar interaction parameter. Equation (1) was used by Berveiller and Zaoui [11] with $L = \alpha \mu$ where μ is the shear modulus and α is an elastic-plastic accommodation factor suggested to be in the range 0.01-0.1. This equation was successfully appliedd for the interpretation of residual stress measurements [12, 13]. For the materials we are going to simulate, copper and brass, this corresponds to an approximate L range of 500-5000 MPa. We examined a continuous transition from Sachs to Taylor type models by doing the simulations with a range of Lvalues: 10, 30, 100, 300, 1000, 3000 and 5000 MPa. Other equations define the deformation model (cf. [7-11]), e.g., active of slip systems are selected on the basis of the Schmid law, the linear hardening law is used and the plastic strain increment of a grain is:

$$\delta \varepsilon_{ij}^{p} = \frac{1}{2} (m_{i}n_{j} + m_{j}n_{i}) \delta \gamma$$
⁽²⁾

where **m** and **n** are unit vectors along the *[uvw]* slip direction and the *(hkl)* slip plane normal and $\delta\gamma$ is a slip shear increment. The sample strain is the average of grain strains.

2.2. Lattice rotations

As first pointed out by Hosford [14] and recently recapitulated by the present authors [1,3,4] there is an ambiguity in the calculation of the lattice rotation resulting from a given slip event. For plane strain/rolling as described with 1-point models there are two possible lattice-rotation schemes which we here, in accordance with the designations used in [3,4], refer to as "Classical Condition", *CL*, and "Preservation Condition", *PR* (the same quantities were designed as: *MA* and *PSA* in [15]). Let us take the total sample rotation and the rotations of the individual grains to be zero. Then, according to *CL*, the grain lattice rotation $d\omega_{ii}^{latt(CL)}$ must be added in order to compensate for the plastic rigid body rotation:

$$\delta \omega_{ij}^{latt(CL)} = -\delta \omega_{ij}^{p} = -\frac{1}{2} (m_{i}n_{j} - m_{j}n_{i}) \,\delta\gamma \tag{3}$$

CL is the classical lattice-rotation scheme used in solid mechanics.

On the other hand, during the *rolling process* initially equiaxed grains get flattened parallel to the rolling plane and elongated parallel to the rolling direction. In this situation it is logical to assume that a plate of material initially parallel to the rolling plane ($x_1 x_2$) preserves this orientation after deformation and that a string of material initially parallel to the rolling direction (x_1) preserves this orientation. This leads to the following lattice rotation (*PR*):

$$\delta \omega_{21}^{latt(PR)} = -\delta e_{21}^{p} = -m_{2}n_{1}\delta\gamma$$

$$\delta \omega_{31}^{latt(PR)} = -\delta e_{31}^{p} = -m_{3}n_{1}\delta\gamma$$
with: $\delta \omega_{ij}^{latt(PR)} = -\delta \omega_{ji}^{latt(PR)}$. (4)
$$\delta \omega_{32}^{latt(PR)} = -\delta e_{32}^{p} = -m_{3}n_{2}\delta\gamma$$

2.3. The correlation factor

For the comparison of the simulated textures with experimental ones we use a correlation factor R which expresses the degree of similarity between two textures. R = 1 means that the two textures are identical, and decreasing R values reflect a decreasing degree of similarity. R is calculated - from pole figures or orientation distribution functions, ODFs – with a linear-regression procedure developed by Tarasiuk and Wierzbanowski [5]. The resulting R values are particularly sensitive to the positions in pole figure/Euler space. It is considered that for $R \ge 0.8$ there is a reasonable agreement between simulated and experimental textures.

3. Results

In this section we present our results for the various combinations of lattice-rotation scheme and interaction strength (L values). We refer to the reduction of 60%.

3.1. Simple <110>{111} slip

The correlation factor between the textures simulated for $<110>\{111\}$ slip and the copper-type experimental texture, R_C , and the correlation factor between the textures simulated with $<110>\{111\}$ slip and the brass-type experimental texture, R_B , as functions of L are shown in Fig. 1 for *CL* and *PR* lattice rotation definitions. For the highest L value one notices that the R values (both R_C and R_B) are (practically) identical for *CL* and *PR* in accordance with the statement from [3] that *CL* and *PR* lead to the same lattice rotations for high L values.



Fig. 1. Correlation factors R_c and R_B versus L for CL and PR lattice rotation with <110>{111} slip mode.

For the higher values of *L* there is agreement between the textures simulated with both lattice-rotation schemes and the experimental copper-type texture ($R_c > 0.8$). The agreement is the best for L = 1000 MPa combined with *CL*: $R_c = 0.86$, approaching "really good agreement". For the lower values of *L* the textures simulated with *PR* agree reasonably well with the experimental brass-type texture: $R_B = 0.83$.



Fig. 2. ODFs simulated with CL lattice rotation and $<110>{111}$ slip mode for and L=1000 MPa together with the experimental copper ODF. The copper component C (•) and the brass component B (ϕ) are marked.

Fig. 2 shows the ODFs simulated with *CL* lattice rotation for an *L* value of 1000 MPa together with the experimental copper ODF. The figure confirms the above statement that *CL* lattice rotation leads to a copper-type simulated texture for L = 1000 MPa. Fig. 3 shows the ODFs simulated with *PR* lattice rotation for an *L* value of 10 MPa together with the experimental brass ODF. The figure confirms the statement that *PR* lattice rotation leads to a brass-type simulated texture for low L values. In both cases the intensities of simulated textures are higher than those of experimental ones but their shapes and characters agrees very well.

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Fig. 3. ODFs simulated with PR lattice rotation and $<110>\{111\}$ slip mode for L=10 MPa together with the experimental brass ODF. The brass component B (ϕ) is marked.

3.2. <110>{111} slip with random stresses added

Leffers [16] suggested a "modified Sachs model" for the simulation of the brass-type texture. In our terminology the modified Sachs model corresponds to a combination of <110>{111} slip, *PR* lattice rotation and low *L* values with random stresses added [7,8]. We add six components of random stress each with a random value between \pm a maximum value which is 35% of the deterministic applied stress Σ_{11} (Eq. 1). A given random-stress component is allowed to operate in a number of steps randomly selected between zero and 30 % of the average number of steps needed to reach 60% reduction. The random stresses were originally introduced with the specific purpose of mimicking the interaction with individual neighbouring grains which, in 1-point models, is a random effect. Their magnitude was established by trial-and-error. Fig. 4 shows R_C and R_B as functions of L for PR lattice rotation calculated for <110>{111} slip with random stresses added. The overall picture is similar to that in Fig.1, but some of the actual values of R_c and R_b have changed. The best agreement with the experimental copper texture (for moderately high L values combined with CL) is unchanged as compared with Fig.1 (highest R_c value is 0.86 in both figures). The best agreement with the experimental brass texture (for low L combined with PR) has improved very significantly as compared with Fig. 1 (highest R_B value increased from 0.83 to 0.92). This is nearly a perfect agreement.



Fig. 4. Correlation factors R_B and R_C versus L for CL and PR lattice rotation calculated for <110>{111} slip with random stresses added.

Fig. 5 shows the ODF simulated with *L* value of 10 MPa, *PR* lattice rotation and <110>{111} slip with random stresses added together with the experimental brass ODF. As compared with Fig. 3 there are certain changes. For instance the simulated ODF in Fig.5 is less sharp than this in Fig. 3. As already reflected in Fig. 4 there is a very good agreement between simulated and experimental textures.



Fig. 5. ODF simulated with L = 10 MPa combined with PR lattice rotation for $<110>{111}$ slip with random stresses added together with the experimental brass ODF. The brass component B (\blacklozenge) is marked.

3.3. <110>{111} slip with <112>{111} twinning added

It is obvious that a possible volume effect of deformation twins on the formation of the brasstype texture must be seen together with the experimentally observed volume fraction of deformation twins in materials developing a brass-type texture. According to [1] there are only two reliable series of observations: In brass with 15% zinc rolled to reductions of about 40% the volume fraction of deformation twins is only few percent, and in brass with 30% zinc rolled to 76% reduction the volume fraction of deformation twins is less than 25%. By interpolation we derive a volume fraction of deformation twins of ~15% for our reduction of 60%, and this is basically the volume fraction that we use in our simulations.



Fig. 6. Correlation factors versus *L* for *CL* and *PR* lattice rotation with 15% volume fraction of deformation twins.

We only consider twinning in the matrix material. We do not consider detwinning in the twins. Deformation twinning is introduced in our simulations with the procedure suggested by Tomé et al. [17]. Fig. 6 shows the correlation factors versus *L* for *CL* and *PR* with a 15% volume fraction of deformation twins. Comparison with Fig. 1 shows that the addition of 15% twins has a negligible effect on the correlation factors (and hence on the textures) in the case of *PR* lattice rotation. In the case of *CL* rotation twinning slightly increases values of R_B – but not enough to obtain a satisfactory agreement with experimental brass texture, particularly so for the higher values of *L* (R_B smaller than 0.6). This lacking effect of the 15% twins goes beyond earlier observations by Kalidindi [18]. He found that the addition of a 22% twin volume fraction had a "very minor" effect on the Taylor-simulated texture.

It should be mentioned here that the 'modified Sachs model, which gives a nearly perfect prediction of the brass type texture, can be explained by a formation of thin twin lamellae (not volume twins !) parallel to primary slip systems planes [1]. This favors a long action of primary slip systems by blocking a passage of dislocations to secondary slip systems, hence the 'Sachs type' behavior is realized.

4. Conclusions

Our results lead to the following conclusions:

- Use of correlation factor, based on linear regression, permits to compare precisely the predicted and experimental textures,

- There is no problem with explaining the copper type texture formation: strong interactions (*L* of the order of 1000 MPa) and preferably *CL* lattice rotation,

- The best agreement with brass type texture is obtained for weak interactions (L of the order of 10 MPa) and PR lattice rotation,

- Adding of *volume* twinning in realistic amount does not explain the brass texture formation when using strong interaction and *CL* rotation definition.

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