Grain orientation stability and residual elastic energy induced by intergranular elastic interaction in rolled Al sheet

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Abstract. Plastic behaviors of grains in polycrystalline metals are induced by external loading and affected by intergranular elastic interactions during deformation. A proposed reaction stress (RS) model including the effects of external and intergranular interaction stresses can simulate the behaviors, whereas the necessary equilibria of intergranular stress and strain are reached reasonably. Rolling texture development in roughly elastic isotropic Al as an example is simulated based on the RS model, whereas main texture components can be predicted accurately. The level of intergranular interactions may fluctuate depending on many factors and become stable as texture forms at higher deformation degree, whereas all grains encounter similar deformation environment. Cube orientation indicates certain stability under the effect of RSs. A portion of elastic strain energy remains around the grains beside normal stored energy after deformation. The energy is orientation dependent and could not be predicted accurately by currently predominant crystallographic deformation theories and models based on Taylor strain principles. The elastic strain energy might affect the recrystallization process.

1. Introduction

Orientations of nuclei and recrystallization grains are related closely to the orientations of deformed grains. Therefore, the crystallographic deformation theories have attracted wide attention. It is known, for example, that cube oriented grains are not stable during rolling of FCC metals. However, cube texture appears very frequently in recrystallized FCC metal sheets. It is not yet entirely clear how those cube oriented nuclei could appear, although they may grow rapidly during recrystallization [1-3].
Recrystallization nuclei should somehow form in deformed matrix at early annealing stage. The deformed matrix offers not only an appropriate environment for rapid growth of grains, but also substructures with some special orientations for nucleation. Stress and strain equilibria are always maintained among the grains during deformation. However, distributions of stress and strain inside a rolling sheet are fluctuant in penetrating the polycrystalline body. It has been indicated that plastic deformation is conducted by combined activation of slips penetrating grains and some non-penetration slips around boundary areas [4]. Different combination of the slips in different grains helps to reach the fluctuant stress and strain equilibria in a nature way, and the fluctuation levels depend on grain orientations. After plastic deformation, some elastic stresses and strains will remain between grains in deformation matrix, which may provide extra recrystallization driving force in addition to ordinary stored energy. The extra driving forces may be grain orientation-dependent and affect the orientations of recrystallization grains.

Strain equilibrium in current theories and models including the viscoplastic self-consistent (VPSC) model [5], the advanced Lamel model [6], and the grain–interaction model [7], has been reached. However, the strains predicted by the models are not so fluctuant as they should be in penetrating the polycrystalline body, since the models are based on Taylor principles and prescribe in advance that strain tensor of grains or grain clusters is basically identical to the macroscopic strain tensor during plastic deformation. The strain prescription does not agree with the experimental observations very well [8]. On the other hand, for example for steel and Al alloy, the plastic deformation in VPSC model is accomplished mainly by penetrating slips. Therefore, the models can not predict the residual elastic stress and strain between grains after deformation accurately. In this work, we attempt to calculate the stability of different substructures of Al during rolling by means of a reaction stress (RS) model [4, 8], and to analyze the relationship between residual elastic energy and grain orientation after deformation.

2. Experimental observation
A 7.8 mm thick hot rolled and annealed band of industrial pure Al, as experimental material, was cold rolled for 10% reduction. Grains before and after the rolling are shown in Figure 1a and 1b. Many traces of active slip systems in different grains can be observed in Figure 1b. Figure 1c indicates the grain structure (full lines) determined by EBSD after rolling. The grain shapes should be similar to those indicated by dashed lines in Figure 1c, if they were deformed according to many current models based on Taylor principles [5-7], which are different from the experimental observations. Although the differences are not so drastic, the phenomenon implies that the multiple activation of slip systems does not agree with those predicted by many theoretical models above. Different slip systems may lead to different orientation evolutions and texture formation. The traces of slip systems indicate also, that many penetration slips occurred in the grains (Figure 1b) during deformation to achieve the necessary rolling strain. At the same time, there appear also many non-penetrating slips, including some slips closely localized around grain boundary (e.g. Figure 1d grain *) and some half penetrating slips (e.g. Figure 1d grain #). The non-penetrating slips help to reach the necessary intergranular strain and stress equilibria.
Figure 1. Grains of the 10% rolled Al sheet. (a) grains before rolling; (b) slip traces in the grains after rolling; (c) shape comparison of deformed grains (full lines) and those according to Taylor principles (dashed lines); (d) the penetrating slip (parallel full lines) and non-penetrating local slips (parallel dashed lines, including localized around boundary in grain * and half penetrating in grain #).

3. Reaction stress (RS) model

If a slip system in a grain is activated by external loading, the plastic strain tensor produced by the slip will induce stress and strain incompatibility. The slip must encounter resistance from the neighboring grains first in the form of elastic RSs. Plastic strain components produced will be partially reduced in an elastic manner, whereas the neighboring grains must also be strained elastically. Therefore, the incompatible plastic strains are relieved by the elastic strains of the concerned grain and its neighboring grains, between which stress and strain equilibria are reached elastically. The rolling stress tensor \([\sigma_y]\) bore by the concerned grain, according to \([4,8]\), becomes:

\[
[\sigma_y] = \sigma_y \begin{bmatrix}
\frac{1}{2} & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & -\frac{1}{2}
\end{bmatrix} - \sigma_y \begin{bmatrix}
-\mu e_{22} \frac{d}{b} & \mu e_{12} \frac{d}{b} & \mu e_{31} \frac{d}{b} \\
\mu e_{21} \frac{d}{b} & \mu e_{22} \frac{d}{b} & \mu e_{23} \frac{d}{b} \\
\mu e_{31} \frac{d}{b} & \mu e_{32} \frac{d}{b} & 0
\end{bmatrix}
\]  

(1)

where the first and second terms refer to the external rolling stress tensor and internal RS tensor, respectively; \(e_y\) denotes the plastic strain produced by the slip; 1, 2, and 3 represent the rolling direction (RD), transverse direction (TD), and normal direction (ND) of the rolling sheet, respectively; \(\sigma_y\) indicates the macroscopic flow yield stress during rolling; \(\mu\) specifies the generalized Schmid factor of the activated slip system; \(d\) corresponds to the effective distance between dislocations, and \(b\) is the length of the Burgers vector. The approximate relationship between \(\sigma_y\) and yield shear stress \(\tau_y\), and the \(d\) can be expressed according to Frank–Read theory as follows \([9]\):

\[
\tau_y = \frac{\sigma_y}{2} = \frac{Gb}{d} \quad \text{or} \quad d = \frac{2Gb}{\sigma_y}
\]

(2)
where $G$, in approximately elastically isotropic metals (such as Al), is shear modulus. The flow yield stress $\sigma_y$ of an annealed metal, i.e., $\sigma_{y0}$ denotes the yield strength, and its top limit in extremely hardened state, e.g., at $\varepsilon_{33}=-4.0$ (98% rolling reduction) can be the tensile strength $\sigma_b$. According to the conventional flow stress of most deformation metals, the flow yield stress $\sigma_y$ for the present simulation can be assumed to develop with rolling reduction $\varepsilon_{33}<0$ as follows:

$$\sigma_y = \sigma_{y0} + (\sigma_b - \sigma_{y0}) \cdot \frac{-\varepsilon_{33}}{4}$$

(3)

where $\sigma_{y0}=20$ MPa and $\sigma_b=50$ MPa are valid for Al, and $n=8$ is used in the present work. The RSs indicated in equation (1) accumulate during rolling until the Schmid factor of another slip system sufficiently increases and is instantaneously activated. The multiple slips can be alternatively followed step by step, and any requested combination of slip systems can be implemented.

However, the accumulated RSs should feature a limitation and a yield point that must not be exceeded. The limitations of deformation stresses should be $[\sigma_{ij}]_{\text{lim}}<a_{ij}\sigma_y/2$, where $a_{ij}$ represents the effective coefficient of maximal RSs at a range of 0 to 1 [8]. $a_{ij}=0$ means no RS, whereas $a_{ij}=1$ implies the highest level of RS. If any of the RSs acting on a grain reaches its up-limit, certain slip systems in the neighboring grains may be additionally activated locally in addition to the normal penetration slips.

In this case, the stress and strain equilibria are also maintained by the local plastic behavior around the boundary areas, as induced by several non-penetration slips, on which shear stress has reached the critical value for activation. The non-penetration characteristics of the slips imply that stress and plastic strain in equilibrium run from one grain over the boundary to another grain in a fluctuant way (Figure 1d) and cannot be similar to that predicted by Taylor principles. On the other hand, the non-penetration slips will induce also random orientation evolution, i.e. random texture.

It is necessary to prove whether the model can correctly predict deformation texture. An Al sample in commercial purity (99.9% Al) with 8.6 mm thickness and random initial texture was prepared. The sample was cold rolled to reductions of 70%, 90%, and 98% (true strain $\varepsilon_{33}$: $-1.2$, $-2.1$ and $-3.8$, respectively). Figure 2a shows the rolling textures in ODF sections, in which the copper and brass textures in $\phi_2=45^\circ$ section and S texture in $\phi_2=65^\circ$ section were observed [10].

Figure 2. Rolling texture of Al sheets. a. experimental observation; b. simulated based on the RS model including 20% random texture (936 initial random orientations; steps $\Delta\varepsilon_{33}=0.001$, $\alpha_{12}=0.7$, $\alpha_{23}=0.01$, $\alpha_{31}=0.001$, $\alpha_{22}=0.08$; ODF $\phi_2=45^\circ$ and $\phi_2=65^\circ$ sections, density levels: 1, 2, 4, 7, 11, 16, 22).

All slip systems bear shear stress during deformation no matter they are active or not. The shear stress may reduce the necessary RS for additional activation of non-penetration slips, i.e., the effective
coefficients $a_{ij}$ are commonly lower than 1. The $a_{ij}$ must be determined for simulating the rolling texture and are influenced by grain orientations and those of the neighboring grains. The $a_{ij}$ of grains may be various because of different orientations of their neighboring grains, but will become stable during the rolling, since all grains fall into the same statistical environment with the formation of rolling texture. An appropriate values for the $a_{ij}$ are found to be $a_{12}=0.7$, $a_{23}=0.01$, $a_{31}=0.001$, and $a_{22}=0.08$. Figure 2b shows the simulation results, including 20% random texture resulting from the non-penetration slips. This outcome is closely similar to the experimental observations (Figure 2a) showing the central positions of copper, brass, and S textures and their peak densities. Therefore, the RS model can predict and reproduce the formation of rolling texture in Al correctly.

### 4. Stability of deformation substructure and residual elastic energy of grains based on RS model

The main texture components after heavy rolling of Al commonly include copper texture $\{90^\circ, 30^\circ, 45^\circ\}$, brass texture $\{35^\circ, 45^\circ, 0^\circ\}$ and S texture $\{55^\circ, 35^\circ, 65^\circ\}$ (Figure 2). Besides, the cube texture $\{45^\circ, 0^\circ, 45^\circ\}$ can be predicted in a relative wide range of higher $a_{ij}$ values (Figure 3).

![Figure 3](image_url)

**Figure 3.** Cube orientation after 95% rolling simulated based on the RS model under different $a_{ij}$ values ($a_{22}=0$), (ODF $\phi_2=45^\circ$ sections, steps $\Delta e=0.001$, density levels: 5, 10, 20, and 40).

It is obvious that cube orientation becomes stable locally in heavy rolling matrix if the RSs of grains reaches higher levels, which is unavoidable in an intricate rolling process. The corresponding stable cube substructure should be the source of cube nuclei of cube recrystallization texture.

The elastic stresses and strains induced by intergranular interactions will remain if external loading is removed. A part of the elastic energy of different grains remains in addition to normally stored energy. RSs $\sigma_{33}=0$ and $\sigma_{11}=-\sigma_{22}$ are valid, whereas deformation volume remains basically constant by the removal of external loading. The elastic energy $W$ around the boundary area can then be calculated according to the elastic theory and the remaining RS $\sigma_{ij}$ after deformation of differently oriented grains:

$$W = \frac{1}{2G} \left( \sigma_{12}^2 + \sigma_{23}^2 + \sigma_{31}^2 + \sigma_{22}^2 \right)$$

where $G=26$ GPa is valid for Al. The orientations based on RS simulation are classified into the main rolling texture components of copper, brass or S if their misorientations to the main components are less than 5°. The elastic energy of the orientations in the main texture components is calculated according to equation (4). Table 1 shows the average elastic energy of orientations in different textures in comparison with that of all orientations. The average elastic energy of cube orientation is also calculated in a similar manner under different $a_{ij}$ values. Notably, the orientations in different texture components indicate different levels of elastic energy under the same simulation conditions. Brass texture demonstrates much higher elastic energy in comparison with those of copper and S texture, and the elastic energy of cube texture could be very low or very high depending on $a_{ij}$ values (Table 1).
Table 1. Average elastic energy induced by intergranular mechanical interactions in different texture components during rolling simulation by the RS model

| Texture component | Effective coefficient $a_{ij}$ of maximal RSs | Rolling reduction |
|-------------------|---------------------------------------------|-------------------|
|                   | $a_{12}$ | $a_{23}$ | $a_{31}$ | $a_{22}$ | 70% | 90% | 98% |
| Brass             |         |         |         |         | 5009 Pa | 5499 Pa | 5922 Pa |
| S                 | 0.7     | 0.01    | 0.001   | 0.08    | 2749 Pa | 2865 Pa | 2642 Pa |
| Copper            |         |         |         |         | 2420 Pa | 2933 Pa | 2844 Pa |
| All orientations  |         |         |         |         | 2596 Pa | 3375 Pa | 3213 Pa |
| Cube              | 0.8     | 1.0     | 0.0     | 0.0     | 2526 Pa | 2066 Pa | 2311 Pa |
|                   | 0.3     | 1.0     | 1.0     | 0.0     | 8300 Pa | 9991 Pa | 7883 Pa |

Normally, the stored energy of deformed Al approximates 2MPa, and it reaches 0.3MPa in recovery state [9]. In comparison, the elastic stain energy (Table 1) is much lower. However, the level of elastic stain energy in differently oriented deformation grains can still exhibit certain effects during the following thermal treatment, including recrystallization nucleation and grain growth. The RS model indicates that the elastic strain energy retained around the cube structure may increases with increasing $a_{ij}$ levels (Table 1). The lower elastic energy may increase the stability of cube structure.

5. Summary
Real deformation behaviors of grains in Al do not agree with that predicted under Taylor principles. The RS model based on combination of external and intergranular interaction stresses can accurately predict textures in Al rolling sheets both in terms of orientation positions of the textures and their peak densities. Furthermore, according to the RS principles, cube orientation can achieve frequently certain stability in rolling process, which is of great significance for the formation of recrystallization cube texture. The residual elastic strain energy around the deformation grains is orientation-dependent, but is much lower than ordinary stored energy. The energy can lead to different orientation stabilities after deformation and may extend its influence to the subsequent recovery and recrystallization process.

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