Crystal Plastic Finite Element Simulation and Texture Analysis of Aluminum

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Abstract. The application of crystal plasticity in finite element codes is widely regarded as a valid way to represent the elasto-plastic behaviour of metal. Based on the rate-dependent crystal plastic constitutive model, the forming behaviour of the pure aluminium is studied in this paper. The stress distribution during the stretching, compressing, and shearing deformation is simulated, and it is concluded that the heterogeneity of the material deformation can be well reflected through the simulation with the crystal plasticity theory. At the same time, the pole figure and orientation distribution function (ODF) are obtained based on the numerical data, and the evolution of polycrystalline texture are analysed and predicted based on the simulation results obtained with the proposed crystal plasticity model.

1. Introduction

Accurate description of the anisotropic behavior of metal materials in the plastic forming process is always an attractive research issue in the calculation of plastic mechanics research and engineering applications. Therefore, a variety of plastic theories about metal materials have emerged. The crystal plasticity (CP) theory starts from the crystal structure of the material and explores the macroscopic deformation mechanism, so as to better understand the macroscopic plastic deformation of the material, reveal the law of material deformation, and optimize the forming behavior of the material [1].

In this paper, together with the crystal plastic finite element method (CPFEM), the single-crystalline and polycrystalline simulations of pure aluminum have been conducted with user material subroutine UMAT/ABAQUS. And through analyzing the pole figures and ODFs, the micro-texture of the material in the compressing, shearing deformation is compared. Therefore, it is of great significance to material forming, material strengthening, and plastic processing of materials.

2. Crystal plasticity theory

The CP theory has been widely used in the literature [2]. In this study, the single crystal constitutive equation is chosen.

$$\hat{\sigma} = L: D - \sum_{\alpha=1}^{n} (L: P_\alpha - \sigma \cdot Q_\alpha + Q_\alpha \cdot \sigma)\dot{\gamma}_\alpha \tag{1}$$

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Unlike the rate-independent crystal plasticity model, the value of slip shear rate is fixed. This paper uses the exponential function based rate-independent model proposed by Asaro and Rice et al [3].

$$\dot{\gamma}_\alpha = \dot{\gamma}_{\alpha 0}\left(\frac{\tau_\alpha}{g_\alpha}\right)^n sign(\tau_\alpha) \tag{2}$$

Where g_α denotes the strain hardening state of the crystal, and the strain hardening state of the actual crystal is very complicated. For this reason, it is considered only that it relates to the total amount of slip deformation γ, that is:

$$g_\alpha = g_\alpha(\gamma) \tag{3}$$

$$\gamma = \sum_{\alpha=1}^{n} |\gamma_\alpha| \tag{4}$$

In the cubic system, the hardening law of a single crystal slip system can be expressed as:

$$\dot{g}_\alpha = \sum_{\beta=1}^{n} h_{\alpha\beta}|\dot{\gamma}_\beta| \tag{5}$$

In the formula, $h_{\alpha\beta}$ is a function of γ, called the hardening modulus matrix, which contains the effects of self-hardening and latent hardening.

$$h_{\alpha\beta} = qh(\gamma) \tag{6}$$

The self-hardening function can generally be represented by a hyperbolic function:

$$h_{\alpha\alpha} = h(\gamma) = h_0 sech^2\left(\frac{h_0\gamma}{\tau_s - \tau_0}\right) \tag{7}$$

$$\gamma = \sum_{\alpha=1}^{n} \int_0^t |\dot{\gamma}_\alpha| dt \tag{8}$$

Among them, h_0 is the initial hardening rate, τ_0 is the yield shear stress, and τ_s is the flow stress saturation value. In addition, there are other hardening models that are not described here.

3. Simulation with single CP model

The above constitutive model is implemented with the user material subroutine UMAT in FE software ABAQUS. All the simulation of the metal forming processes will be conducted with the given CP model [4].

3.1. Discussion of RVE model

Usually, in order to verify the accuracy of the established model, a representative volume unit of material may be first established, abbreviated as RVE. The RVE is small in size, but it contains enough information about the microstructure. Therefore, the mechanical responses with RVE with defined loading can be used to verify the accuracy of the established crystal plasticity model.

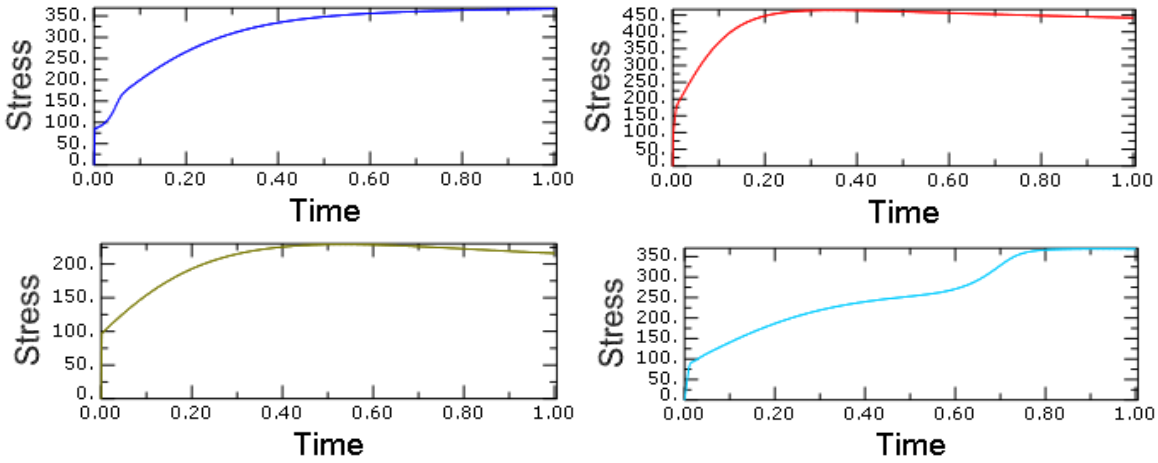

Figure 1. Stress - time curves of RVE model.

As can be seen from Figure 1, with the different loading directions, the yield points obtained with different defined RVE model are different from each other. This shows that the material constitutive model established in this paper can well represent the anisotropic behaviour. Moreover, the numerical value of the yield point is close to the actual yield point of pure aluminum, so the crystal plasticity model adopted this time has certain feasibility. In addition, the actual yield stress range for pure aluminum is from 90 to 120 MPa.

3.2. Simulation of the stretching, compression and bending of the cantilever beam

After completing the analysis of the stress response of the RVE model, a cantilever beam geometry model was established to simulate the stretching, compressing, and bending deformation of the cantilever beam.

Figure 2 shows the stress distribution of the material after stretching, compression and shearing deformation, respectively. In each process, obvious stress concentration appears on the side of the material, and only the middle part of the fixed end has a small stress value. In addition, during the bending deformation of the simulated cantilever beam, the stress concentration of the cantilever beam is present.

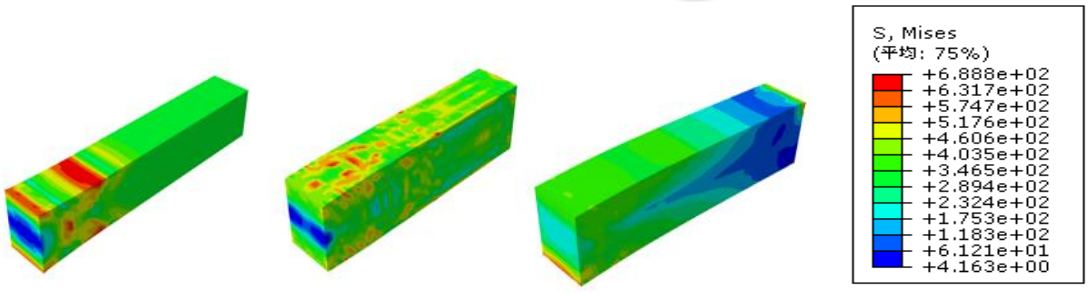

Figure 2. Simulation of different processes with CP model.

It can be seen that the simulation results with the single CP material model clearly show the phenomenon of the non-uniform stress, and which is difficult to obtain the same result through the macroscopic material model. It also reflects the validity of crystal plasticity theory from the perspective of dislocations. To describe the plastic deformation behavior of the material, it is a good

reflection of the non-uniformity of the stress change in the plastic deformation of the crystal material, so as to more truly reflect the deformation of the material.

4. Polycrystalline simulation and texture analysis

Based on Taylor's homogenized model, a polycrystalline model is built and applied to simulation. At the same time, by plotting pole figures and ODFs, the density distributions of orientation are analyzed, and the corresponding textures and evolution rules can be studied.

4.1. Simulate based on the Taylor model

With reference to the work by Marin [5], a polycrystalline model is established to simulate the compressing and shearing deformation in this paper. The model is shown in Figure 3. It contains a sufficient number of single crystal grains with different orientations, but its deformation is uniform. So that it fits well with the requirements of Taylor's homogenization theory.

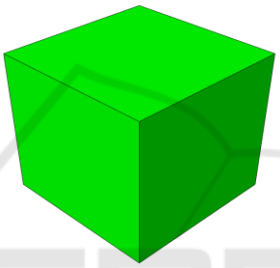

Figure 3. Polycrystalline model with 500 grains' orientations.

Figure 4 shows the stress curves of polycrystalline model during compressing and shearing deformation, respectively. It can be seen from Figure 4 that the stress curves of polycrystalline model in different deformation processes are approximately the same. This is because, the grains have different orientations and they are randomly distributed at the mesoscale scale. However, when turn to the macroscopic scale, the mechanical behavior of the materials will show a feature of isotropic based on the statistical principle.

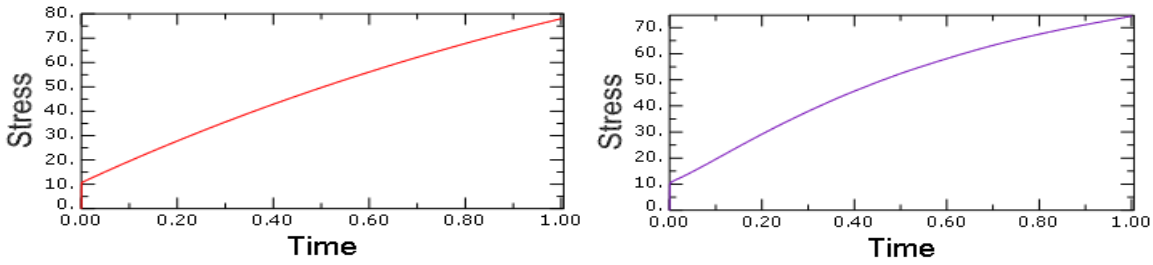

Figure 4. Stress - time curves of polycrystalline model.

4.2. Simulation of texture evolution

The pole figure describes the three-dimensional spatial distribution of the crystal with two-dimensional images. If no texture appears, the density distribution of the pole figure should be uniform, as shown in the Figure 5.

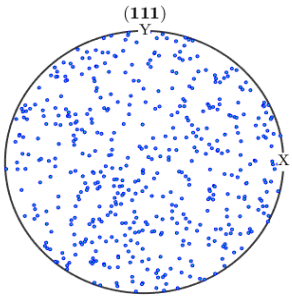

Figure 5. Pole figure without texture.

As shown in Figure 6, the pole figure after compressing and shearing deformation are obtained. Due to the different ways of deformation, there are differences in the evolution of the pole figure. For the pole figure of compressing deformation, the density of the poles in the middle is low, and then the orientation tends to concentrate in a local range. The pole figure of shearing deformation differs greatly from the compressing. Its distribution of orientation is concentrated in the center, but new textures are also generated at the edge of the pole figure.

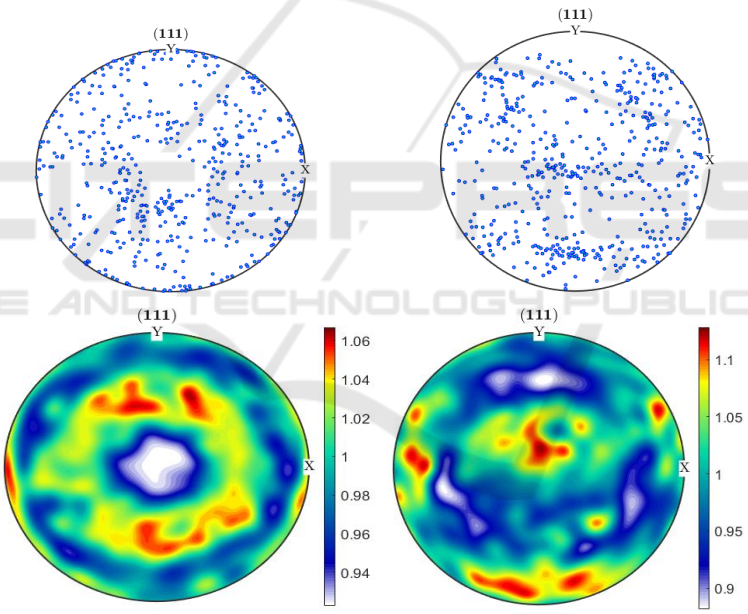

Figure 6. Pole figures in different process.

However, the pole figure shows a two-dimensional space that has certain limitations of describing the three-dimensional spatial distribution of the crystalline orientation. Therefore, with three spatial Euler angles as the variables, the orientation distribution function (ODF) is established to express the spatial distribution of the crystalline orientation, and the resulting figure is called an ODF figure. It can show the density and distribution of the texture in the form of iso-density lines.

Figure 7 shows the ODFs of compression deformation. By using the increment step as a variable, it is possible to show the evolution of texture during the deformation. It can be seen that the distribution of orientation on the same crystalline surface has a certain rule, and new texture will emerge during deformation.

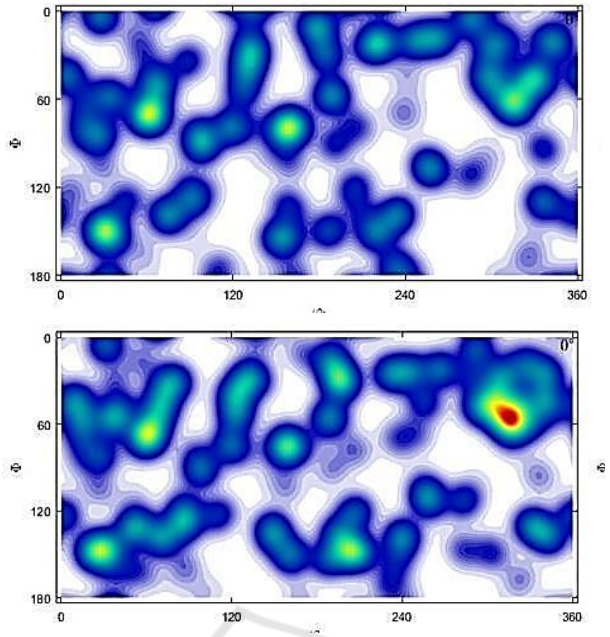

Figure 7. ODFs at different increments.

Figure 8 shows the ODFs of shearing deformation at different Euler angles. As it can be seen from the figure, there is large difference in density distribution on different crystalline faces. This is mainly determined by the initial orientation and the loading path of grains.

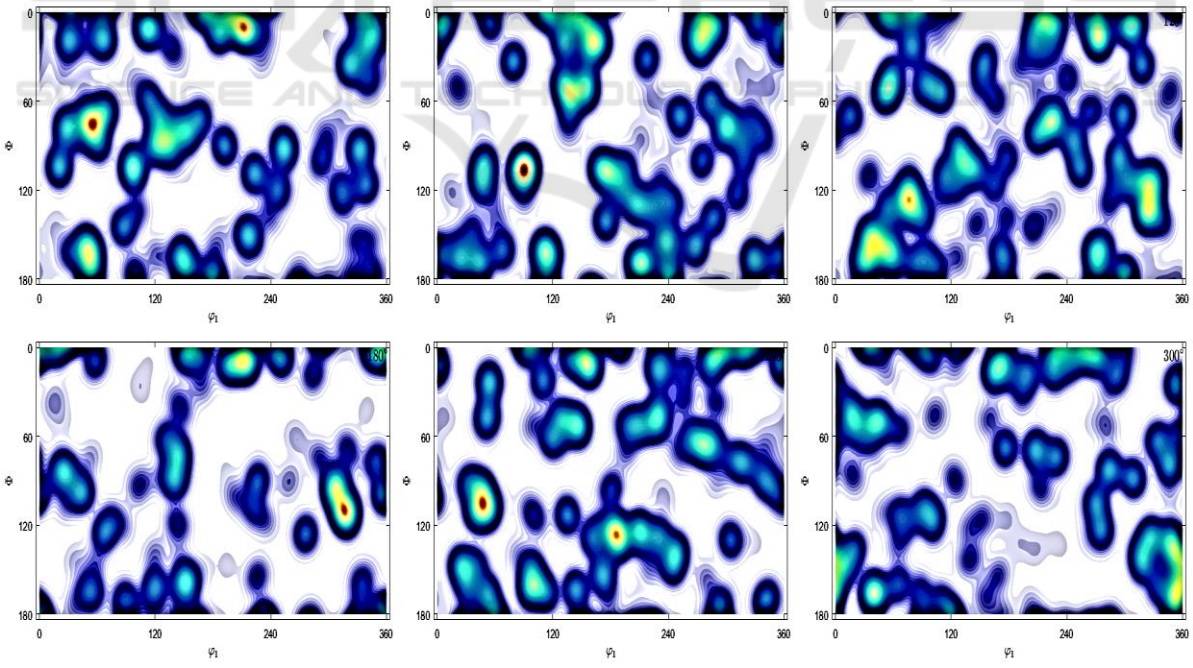

Figure 8. ODFs at different Euler angles.

5. Conclusions

Based on the theory of crystal plasticity, the model of pure aluminium single crystal and polycrystal is completed in combination with the user material subroutine, and the plastic deformation behaviors are simulated. In the single crystal simulation process, a RVE model which contains enough information about the microstructure is established. The anisotropy of the established crystal plasticity model is verified by comparing the different yield points in each stretching direction.

By simulating the stretching, compressing and bending deformation of the cantilever beam, there are obvious non-uniform stress distributions in the model. It is also reflected that the crystal plasticity theory which considers the plastic deformation behavior is closer to the true deformation of the material. Based on Taylor homogenized model, the polycrystalline model is established and its mechanical response is predicted. At the same time, pole figures and ODFs are plotted, which can predict the evolution of textures well.

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