ANALYSIS ON CYCLIC PLASTICITY AND STRESS DISTRIBUTION OF POLYCRYSTAL AT GRAIN LEVEL

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ABSTRACT

To investigate the macroscopic and microscopic mechanical behavior of polycrystalline materials under the conditions of cyclic loading, a Voronoi polycrystalline aggregation model was employed to study the statistical distribution of stress and strain, and macroscopic cyclic plasticity, for a copper polycrystalline material. The algorithm for solving the visco-plastic constitutive relations that describing the slipping plasticity for single crystal grain of the polycrystalline material applied in the present paper was suggested by Zhang et al. (2004a, 2004b), in which the Cauchy stress tensor is taken as the basic variable to be solved by Newton-Raphson iterations. On the basis of calculation of single crystal constitutive equations, the simulation for a FCC copper polycrystal were carried out under the cyclic loading of symmetrical tensile and compression. According to the results, the distribution of microscopic stress, strain and effective plastic strain, and coefficient of variation (the ratio of the standard deviation to the mean) were analyzed, which shows the heterogeneities of microscopic stress and strain in the Voronoi polycrystal tessellation caused by the randomness of the grain crystals in the polycrystal aggregate. Meanwhile, the curve of mean stress and strain for the Voronoi polycrystalline tessellation were also calculated, the results can reasonably describe the Bauschinger effect and cyclic hardening characteristic of polycrystalline materials.

It is necessary to point out that, in the present paper, the cyclic characteristic of polycrystalline material is not set prior. The cyclic plasticity of the Voronoi tessellation is completely obtained from the results modeled by the tessellation associated with the known mechanical behavior of a single crystal, under the cyclic load condition.

1 INTRODUCTION

From the microscopic of view, the mechanical behavior of polycrystalline materials and the microscopic stress and plastic slip deformation can be calculated by using crystal plastic theory and numerical simulation. On the basis of crystal plastic theory, Taylor model, which assumes the volume and deformation of grains are identical, can be used to study the cyclic plasticity of polycrystalline materials (Turkmen et al., 2002；Peng and Fan，2003）. However, the main aim of these researches is to obtain the macroscopic mean behaviors, by which the heterogeneous characteristic between the grains is ignored.

Representative volume element (RVE) is a general model to study the micro-mechanical behavior in the microscopic level. The RVE for polycrystal consists of a number of grains, so its statistic mechanical behavior is very similar with the macroscopic mechanical characteristic. In principle, such a RVE can describe the heterogeneous characteristic and statistic characteristic, because by which the information of randomness of the polycrystalline micro-structure can be preserved. By using Voronoi polycrystalline aggregation model, Barbe et al. (2001), Zhang et al. (2004a) and Zhang et al. (2004b) carried the analyses of the difference of stress between the grains under the monotonic loading. Under the cyclic loading conditions, such a research for the heterogeneous stress and strain by polycrystal tessellation so far is absent.

2 RVE OF A POLYCRYSTALLINE MATERIAL

To consider the randomness of size, shape and orientation of grains, the Voronoi polycrystalline aggregation model was chosen as the RVE in the present paper. The grains in Voronoi tessellation are polyhedron generated by random arrangement of grain nuclei, and their orientations are also arranged randomly. For every grain, the elastic and inelastic mechanical characteristic is anisotropic. Due to there are enough grains in the RVE, the global response and macroscopic average mechanical behavior is approximately isotropic. Then the volume statistical stress and strain are defined as:

$$\Sigma_{ij} = \frac{1}{V}\int_V \sigma_{ij} dV, \quad E_{ij} = \frac{1}{V}\int_V \varepsilon_{ij} dV \cdot \tag{1}$$

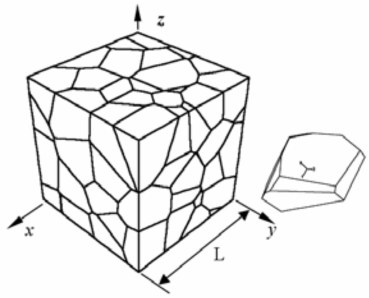


Fig. 1 Voronoi model with 100 grains

To save machine time, in this paper, only 100 grains are arranged in the aggregate. And its finite element mesh consists of 28558 tetrahedron elements with 5793 nodes (see Fig.1). For the primary analysis, the anisotropic behavior for every grain is set identical. And the microvoids and microcracks in the RVE are not considered. The corresponding single-crystal constants are obtained from Asaro and Needleman (1985). The crystal lattice is cubic and the elastic constants are $C_{11} = 51.227\,\text{GPa}$, $C_{12} = 36.93\,\text{GPa}$ and $C_{44} = 22.937\,\text{GPa}$. The parameters for the crystal viscoplastic model are $\tau_0 = 60.84\,\text{MPa}$, $\tau_s = 109.51\,\text{MPa}$, $h_0 = 541.5\,\text{MPa}$, $\dot{\gamma}_0 = 1\times10^{-3}/\text{s}$, $q = 1$ and $k = 200$. And the copper single crystal has a FCC octahedron slip system.

3 CONSTITUTIVE MODEL AND CALCULATION ALGORITHM

The stress calculations can be performed according to the formulation in the ABAQUS theory manual for the current configuration:

$$^{t+\Delta t}\boldsymbol{\sigma} = \Delta\boldsymbol{R} \cdot {}^{t}\boldsymbol{\sigma} \cdot \Delta\boldsymbol{R}^T + \Delta\boldsymbol{\sigma}(\Delta\boldsymbol{D}), \tag{2}$$

where $\boldsymbol{\sigma}$ is the Cauchy stress tensor which is work-conjugate to the rate of deformation $\boldsymbol{D}$ (the reference configuration is the current configuration), $\Delta\boldsymbol{\sigma}$ the incremental stress tensor caused by the constitutive behavior, and $\Delta\boldsymbol{R}$ the incremental rotation matrix describing the rigid body rotation for the corresponding material point. Here, t and $t+\Delta t$ denote the initial and end times of the incremental period, respectively. In the above equation, the first term on the right describes the stress change caused by a pure rigid body rotation during the time increment, while the second term denotes the incremental stress determined by the material constitutive behavior. The incremental Cauchy stress tensor under the current configuration can be calculated according to Hooke's law:

$$\Delta\boldsymbol{\sigma} = \overset{<4>}{\boldsymbol{C}}_G : \Delta\boldsymbol{\varepsilon}^e, \tag{3}$$

where $\overset{<4>}{\boldsymbol{C}}_G$ is the fourth-order tensor of anisotropic elasticity of the material with respect to the global axes, which is obtained from rotational transformation with respect to the crystal axes, and $\Delta\boldsymbol{\varepsilon}^e$ is the incremental elastic logarithm strain tensor. Then, Eq.(2) can be rewritten as:

$$^{t+\Delta t}\boldsymbol{\sigma} = \Delta\boldsymbol{R} \cdot {}^{t}\boldsymbol{\sigma} \cdot \Delta\boldsymbol{R}^T + \overset{<4>}{\boldsymbol{C}}_G : \Delta\boldsymbol{\varepsilon}^e. \tag{4}$$

Due to the addition decomposed of velocity gradient tensor, the Eq. (3) can be written as:

$$\Delta\boldsymbol{\sigma} = \overset{<4>}{\boldsymbol{C}}_G : (\Delta\boldsymbol{\varepsilon} - \Delta\boldsymbol{\varepsilon}^p), \tag{5}$$

where, $\Delta\boldsymbol{\varepsilon}^p$ is plastic strain increment, $\Delta\boldsymbol{\varepsilon}$ is the incremental logarithm strain tensor. By using the evolvement law of plastic deformation gradient,

$$\dot{\boldsymbol{F}}^p = \left[\sum_{\alpha=1}^{n} (\boldsymbol{m}^{(\alpha)} \otimes \boldsymbol{n}^{(\alpha)})\dot{\gamma}^{(\alpha)}\right] \cdot \boldsymbol{F}^p, \tag{6}$$

Therefore, the formulation of increment plastic strain can be defined and calculated. And the incremental resolved shear strain can be calculated by linear superposition during an incremental time period:

$$\Delta\gamma^{(\alpha)} = [(1-\eta)\,{}^{t}\dot{\gamma}^{(\alpha)} + \eta\,{}^{t+\Delta t}\dot{\gamma}^{(\alpha)}]\Delta t\,, \tag{7}$$

where $0 < \eta \le 1$ is a constant, and ${}^{t}\dot{\gamma}^{(\alpha)}$ and ${}^{t+\Delta t}\dot{\gamma}^{(\alpha)}$ are respectively the initial and end values of the rate of resolved shear strain for the α -slip system, which can be described by viscoplastic power law (Hutchinson, 1976).

In the above formulae, ${}^{t+\Delta t}\dot{\gamma}^{(\alpha)}$, ${}^{t+\Delta t}\boldsymbol{\sigma}$ and $\Delta\boldsymbol{\varepsilon}^{p}$ are unknown, whereas they are not independent of each other. To solve the unknown variable, an algorithm using mixed implicit Newton-Raphson iteration suggested by Zhang et al. (2004a, 2004b）was applied in this paper.

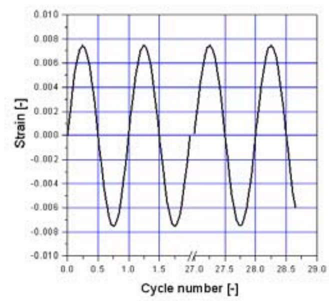


Fig. 2 Macro strain loading cycle（±0.075）

4 NUMERICAL ANALYSIS

Assuming the material undergoes a uniaxial macroscopic uniformed deformation in z direction, and then the boundary condition of polycrystal tessellation shown as Fig. 1 can be written as:

$$\left.\begin{array}{llllll} x=0, & u=0; & y=0, & v=0; & z=0, & w=0 \\ x=L, & u=U; & y=L, & v=V; & z=L, & w=W \end{array}\right\}, \tag{8}$$

where, u, v and w are the displacements respectively in x, y and z direction, $L=1$, U and V are respectively the displacements on the boundary plane, which were determined by finite element constraint equation, W the boundary displacement is given to simulate the uniaxial stretch, and $W = W_0 \sin(0.05t)$ with $W_0 = 0.75$. The relation between the macroscopic uniaxial strain for the RVE and cycle number was shown as Fig. 2. The amplitude is identical for tensile and compression.

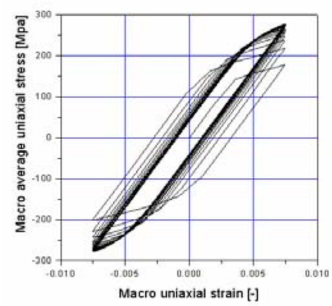
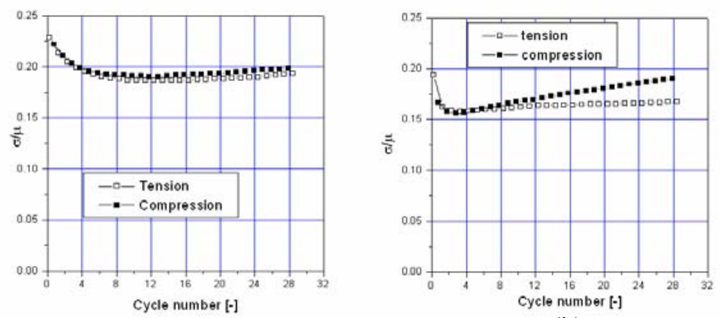


Fig. 3 Cyclic stress strain curve

<u>Cyclic hardening and hysteresis loop of polycrystal</u>

Under the given cyclic strain load condition, macroscopic uniaxial mean stress and mean strain curve for the RVE is shown in Fig. 3. At the early stage of cyclic loading, the flow stress increases with the cyclic number, which implies the material undergoes plastic hardening. But the hardening is weakening with the cycle number increasing and the stress and strain curve gradually goes stable to form a stable hysteresis loop when the cyclic number exceeds 10, (see Fig. 3). At the same time, the stress strain curve in Fig.



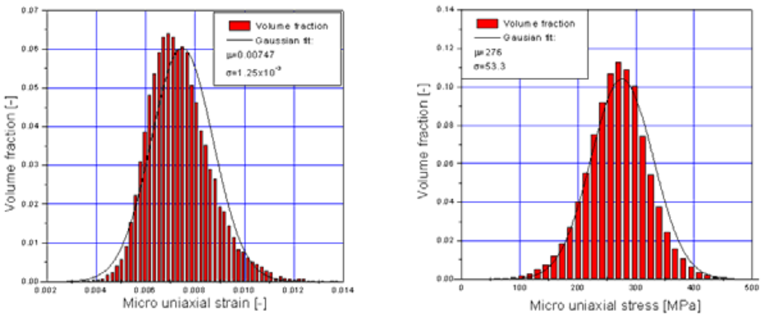
(a) (b)

Fig. 4 COV at tension/compression peak with cyclic number: (a) for micro longitudinal stress; (b) for micro longitudinal strain

3 also observably displays the Bauschinger effect by the polycrystal tessellation under cyclic loading. These results imply that the cyclic characteristic strongly depends on the residual stresses caused by heterogeneities of the polycrystal.

The statistical character of uniaxial stress and strain

At the strain peak of tensile and compression, the relations between the coefficient of variation (COV, the ratio of the standard deviation to the mean) of the microscopic uniaxial stress σ_{33} and strain ε_{33} with cyclic number are shown as Fig.4. Here, σ and μ are standard deviation and mean for stress and strain respectively. At the early stage of cycle load beginning, the COV squints towards decreasing, and in the successive loading cycle, the COV for both stress and strain tends towards increasing gradually. At the same time, the COV for strain under the compression loading is higher than that under the tensile cyclic loading. It is probably reason caused by the few number of grains in the polycrystal aggregate that the response of the RVE under tensile and compression is not very symmetric. On the other hand, the COV for stress under the tensile and compression load condition are approximatively identical. The reason is maybe that the stress is not very sensitive to the change of strain during plastic deformation. According to the results, the configuration of statistical distribution of stress σ_{33} and strain ε_{33} has weak relation with the cyclic number. Fig. 5 shows the statistic distribution of stress σ_{33} and strain ε_{33} under the tensile displacement peak of the 28th cycle, and the distributions are basically Gaussian.



(a) (b)

Fig. 5 The statistical distributions at the tension peak of 28th cycle: (a) for micro tension strain; (b) for micro tension stress.

Statistical character of effective plastic strain

The development of COV of microscopic effective plastic strain for polycrystal aggregate under the cyclic loading is shown as Fig.6. Here, the microscopic effective plastic strain ε_{eq}^{p} ($\varepsilon_{eq}^{p}=\int_{0}^{t}\sqrt{\frac{2}{3}\dot{\varepsilon}_{ij}^{p}\dot{\varepsilon}_{ij}^{p}}\,dt$) represents the microscopic plastic deformation accumulation of a material point in crystal grain of the RVE. From the Fig.6, the COV is globally to increase although the decreasing can be found during early stage of cycle, due to only a very few grains have plastic slipping and the distribution on effective plastic strain is very non-uniformed, the COV is higher. However, with the cycle number increasing, plastic slipping takes place in more and more grains, which causes the COV starts to decreases. But with cyclic number increasing further, the plastic strain in some grains apt

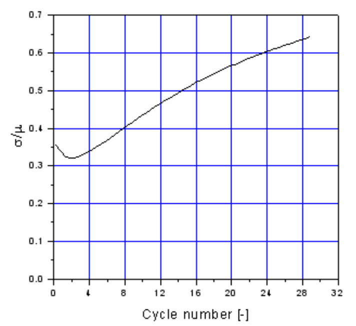


Fig. 6 The COV for micro effective plastic strain at strain cycle peak with cycle number.

to slipping will increase much faster than the others because the orientations; this will make micro plastic strain going to heterogeneous, then the COV will increase gradually.

The distributions of effective plastic strain of the RVE during the deformation process were shown in Fig. 7. At the early stage of cyclic loading, only a few crystals have plastic deformation, and

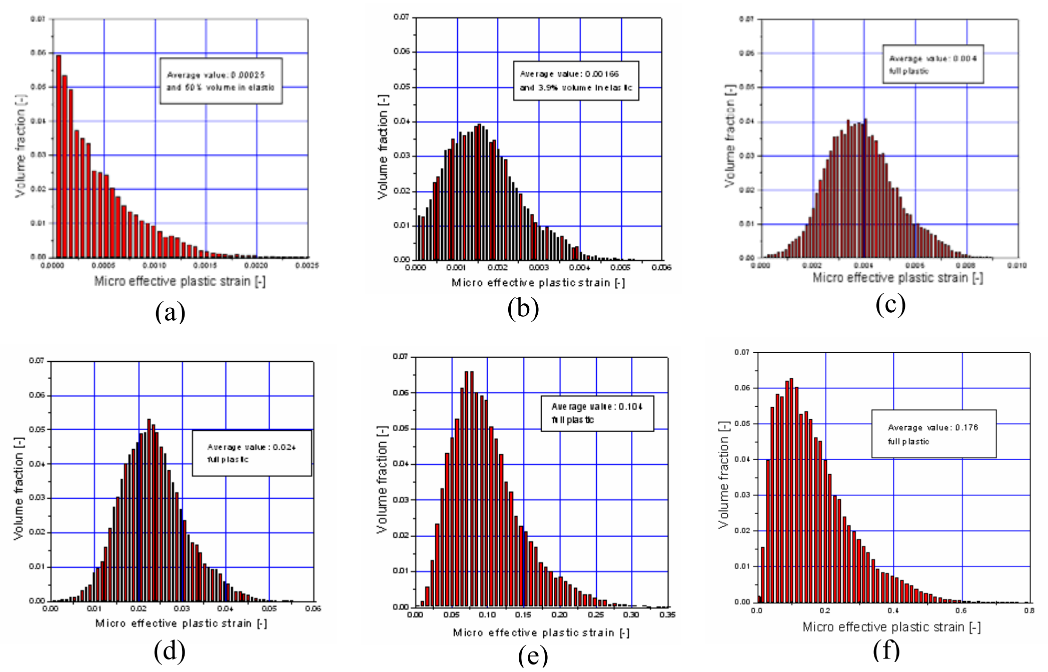


Fig. 7 Evolution of the distribution of micro effective plastic strain with cycle number increasing.

other grains are still in elastic (Fig. 7(a)). In the successive loading cycle, more and more grains turn to plastic, the distribution of microscopic effective plastic strain in the polycrystal aggregate become Gaussian gradually((Fig. 7(b,c,d)). With the increasing of cycle number, due to the influence of orientation of grains is getting stronger, the microscopic effective plastic strain of a minority of grains increase faster and faster, which makes the deviation distribution of the strain((Fig. 7(e,f)). In this process, the heterogeneities of the microscopic effective plastic strain become fairly strong and the plastic deformation will develop on a minority of grains with the successive loading cycle.

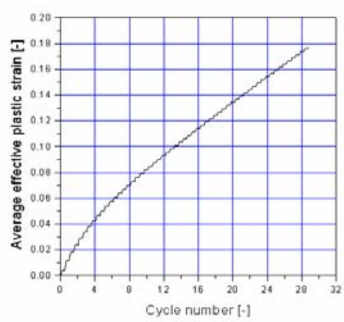


Fig. 8 Statistical average effective plastic strain with cycle number.

Mean effective plastic strain

The statistical mean value of microscopic effective plastic strain in the polycrystal material $\bar{\varepsilon}^p_{eq}$ ($\bar{\varepsilon}^p_{eq} = \frac{1}{V}\int_V \varepsilon^p_{eq} dV$) can represent the average plastic deformation of the RVE. Here, Fig.8 gives this mean values variable curve with the number of loading cycle. From this figure, it can be shown that the mean plastic strain tends to linear increasing with the cyclic number.

5 CONCLUSIONSS

According to the main results of this paper conclusions can be obtained as below:

1. Under the uniaxial symmetry tensile and compression cyclic load condition, the statistical stress and strain curve of the Voronoi polycrystal RVE, in which the slip system for grain crystal has isotropic hardening feature, presents cyclic hardening phenomenon and Bauschinger effect. And the curve will gradually become a fairly stable hysteresis loop after a few loading cycles.
2. The distributions of microscopic uniaxial stress and strain of the RVE are Gaussian. At the initial stage of deformation, the COV (reflect heterogeneous degree) may decrease, and then increase gradually with the plastic strain under given cycle loading.
3. The statistic distribution of accumulation of microscopic effective plastic strain is approximately Gaussian in the initial stage of plastic deformation, but it will change to non-Gaossian with the loading cycle increasing. Its COV has an obvious increase with cycle loading increasing.
4. Under the uniaxial symmetrical tensile and compression load conditions, the growth for the accumulation of microscopic effective plastic strain is nonlinear in the beginning of cyclic load, but curve's tendency will turn linear with the cycle increasing.

It is necessary to point out that in the present paper the cyclic characteristic of polycrystalline RVE is not prior set. The cyclic plasticity of the RVE is completely obtained from the results calculated by the Voronoi tessellation associated with the mechanical behavior of single crystal, under the cyclic load condition. And the results seem as reasonable.

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