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A FINITE DEFORMATION ANALYSIS OF POLYCRYSTAL BY CONSIDERING THE INFLUENCE OF GRAIN BOUNDARY*

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ABSTRACT By combining grain boundary (GB) and its influence zone, a micromechanic model for polycrystal is established for considering the influence of GB. By using the crystal plasticity theory and the finite element method for finite deformation, numerical simulation is carried out by the model. Calculated results display the microscopic characteristic of deformation fields of grains and are in qualitative agreement with experimental results.

KEY WORDS grain boundary, slip, slid, crystal plasticity, finite deformation

I. INTRODUCTION

Polycrystal is constituted of single grains with random orientation and GB. The width of GB of polycrystalline metal is small in general. Sometimes the influence of GB on the total characteristic of polycrystal is great. Much has been done on polycrystal. The pioneer work is Taylor's[1] rigid plastic model. T. H. Lin[2] extended Taylor's theory to include elastic deformation of grains. But they didn't consider the interaction between grains. Hershey[3] may be the first one who proposed the self-consistent idea and applied it to the calculation of polycrystal. By using famous Eshelby's[6] solution, Kroner[4], Budiansky et al. [5] developed the self-consistent method, and then Hill[7] made the method perfect. T. H. Lin[8], McHugh et al. [9], Harren et al. [10], Tokuda et al. [11] simplified the polycrystal as the assemble of some ideal grains and used Kelvin's solution or the finite element method to simulate the response of polycrystal. They considered the GB as geometrical boundary but didn't investigate the physical properties of GB. Zhong et al. [12] proposed the self-consistent-finite element method to simulate the sliding polycrystal. In this paper, GB and its influence zone are combined to form a boundary layer, and its mechanical property is different from that of a single grain. The deformation along GB and its normal direction can easily be considered because of the introduction of the grain boundary layer. By combining the model

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with the crystal plasticity theory, the finite element analysis for the plastic deformation of sliding polycrystal can be carried out.

I. THE GB MODEL AND DESCRIPTION OF DEFORMATION KINEMATICS

A two-dimensional model is considered in this paper for the convenience of calculation. The load is in-plane and GB is perpendicular to the plane. For FCC polycrystal, the normal direction of the plane is parallel to the crystal axis [0 1 1], while for BCC polycrystal, the normal direction of the plane is parallel to the crystal axis [1 0 0] if only the primary slip system is considered. The dislocation on GB can motivate GB to slip under an external load, and this will cause slip plastic deformation. The tangle and the pile up of dislocations on GB will result in high stress on GB, which can induce strain in the normal direction of GB. The general crystal plastic theory only deals with the slip deformation and can hardly deal with expansion strain produced by a normal deformation system (NDS). The meaning of NDS is that it can produce tensile or compression strain in the normal direction of GB. The material of GB considered here includes a slip system and an NDS. The slip plane of the slip system is GB and the slip direction is the tangential direction of GB. The expansion direction of NDS is the normal direction of GB. The mathematical description for the plastic deformation caused by the slip system is perfect. The kinematic description of NDS is given as follows. As shown in Fig. 1, xoy plane is a slip plane (GB) and z axis is the normal direction of GB. If expansion strain is ε, the plastic deformation gradient is:

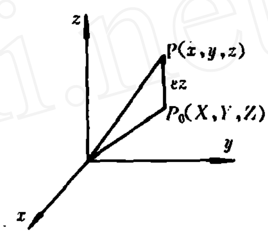


Fig. 1 Plastic deformation caused by NDS.

$$F^p = I + \varepsilon M \cdot M^T \tag{1}$$

$$\dot{F}^p = \dot{\varepsilon} M \cdot M^T \tag{2}$$

Using the Update-Lagrange method, there is:

$$\dot{F}^p \cdot (F^p)^{-1} = \dot{\varepsilon} M \cdot M^T \tag{3}$$

For simplicity, the resolved shear stress of the slip system is indicated by $\tau^{(\alpha)}, \alpha = 1, \cdots, N, N$ is the number of the slip system. The slip shear strain rate is $\dot{\gamma}^{(\alpha)}$, the normal stress of NDS is $\tau^{(N+1)}$, the expansion strain rate is $\dot{\gamma}^{(N+1)}$. Supposing the total deformation gradient is the superposition of the two kinds of deformation system, we have:

$$\dot{F}^p \cdot (F^p)^{-1} = \sum_{\alpha=1}^{N} \dot{\gamma}^{(\alpha)} S^{(\alpha)} \cdot M^{(\alpha)T} + \dot{\gamma}^{(N+1)} M^{(N+1)} \cdot M^{(N+1)T} \tag{4}$$

The plastic deformation rate and spin rate are:

$$D^p = \sum_{a=1}^{N+1} P^{(a)} \dot{\gamma}^{(a)} \tag{5}$$

$$\Omega^p = \sum_{a=1}^{N+1} W^{(a)} \dot{\gamma}^{(a)} \tag{6}$$

where

$$\begin{cases} P^{(a)} = \frac{1}{2}(S^{*(a)} \cdot M^{*(a)T} + M^{*(a)} \cdot S^{*(a)T}) \\ W^{(a)} = \frac{1}{2}(S^{*(a)} \cdot M^{*(a)T} - M^{*(a)} \cdot S^{*(a)T}) \end{cases}, \quad a = 1,\cdots,N \tag{7}$$

$$\begin{cases} P^{(N+1)} = \frac{1}{2}(F^{*} \cdot M^{(N+1)} \cdot M^{*(N+1)T} + M^{*(N+1)} \cdot M^{(N+1)T} \cdot F^{*T}) \\ W^{(N+1)} = \frac{1}{2}(F^{*} \cdot M^{(N+1)} \cdot M^{*(N+1)T} - M^{*(N+1)} \cdot M^{(N+1)T} \cdot F^{*T}) \end{cases} \tag{8}$$

S^*, M^* are the slip direction and normal direction of the slip plane in deformed configuration respectively.

$$S^{*(a)} = F^{*} \cdot S^{(a)}, \quad M^{*(a)} = (F^{*})^{-1T} \cdot M^{(a)} \tag{9}$$

F^* is the elastic deformation gradient, the total deformation gradient F[14] is:

$$F = F^{*} \cdot F^{p} \tag{10}$$

The resolved shear stress of the slip system is:

$$\tau^{(a)} = \tau : P^{(a)}, \qquad a = 1,2,\cdots,N \tag{11}$$

The normal stress of NDS is:

$$\tau^{(N+1)} = \tau : (M^{*(N+1)} \cdot M^{*(N+1)T}) \tag{12}$$

The deformation rate and spin rate can be expressed as the sum of elastic and plastic part.

$$D = D^{*} + D^{p} \tag{13}$$

$$\Omega = \Omega^{*} + \Omega^{p} \tag{14}$$

Supposing the elastic property is not affected by deformation, we can get:

$$\overset{\nabla}{\tau} = L_c : D - \sum_{a=1}^{N+1} \lambda^{(a)} \dot{\gamma}^{(a)} \tag{15}$$

$$\lambda^{(\alpha)} = P^{(\alpha)} : L_c + \beta^{(\alpha)}, \qquad \alpha = 1,2,\cdots,N \tag{16a}$$

$$\lambda^{(N+1)} = P_s^{(N+1)} : L_c + \xi^{(N+1)} \tag{16b}$$

$$\beta^{(\alpha)} = W^{(\alpha)} \cdot \tau - \tau \cdot W^{(\alpha)}, \qquad \alpha = 1,2,\cdots,N \tag{17a}$$

$$\xi^{(N+1)} = -\left(\tau \cdot P_s^{(N+1)\mathrm{T}} + P_s^{(N+1)\mathrm{T}} \cdot \tau\right) \tag{17b}$$

$$P_s^{(N+1)} = (F^*)^{-1\mathrm{T}} \cdot M^{(N+1)} \cdot M^{(N+1)\mathrm{T}} \cdot (F^*)^{-1} \tag{18}$$

Assume that the relation between the shear strain rate and resolved shear stress is of a power law form including the relationship between the expansion strain rate and normal stress, as well,

$$\dot{\gamma}^{(\alpha)} = \dot{a}^{(\alpha)} \frac{\tau^{(\alpha)}}{g^{(\alpha)}} \left| \frac{\tau^{(\alpha)}}{g^{(\alpha)}} \right|^{1/m-1}, \qquad \alpha = 1,2,\cdots,N,N+1 \tag{19}$$

$g^{(\alpha)}$ is the α-th strain hardening value, the incremental form is generally assumed as:

$$\dot{g}^{(\alpha)} = \sum_{\beta=1}^{N+1} H_{\alpha\beta} \dot{\gamma}^{(\beta)} \tag{20}$$

To ensure high precision, the performed gradient method is used to calculate the shear strain rate and expansion strain rate.

The increment of the shear strain from time t to $t+\Delta t$ is

$$\Delta\gamma^{(\alpha)} = \gamma^{(\alpha)}(t + \Delta t) - \gamma^{(\alpha)}(t) \tag{21}$$

If a linear interpolation is employed within the time interval, we have:

$$\Delta\gamma^{(\alpha)} = \left[(1-\theta)\dot{\gamma}^{(\alpha)}(t) + \theta\dot{\gamma}^{(\alpha)}(t+\Delta t)\right]\Delta t \tag{22}$$

where $0 \leqslant \theta \leqslant 1$. To expand (19) in Taylor's series, we have

$$\begin{aligned} \dot{\gamma}^{(\alpha)}(t+\Delta t) &= \dot{\gamma}^{(\alpha)}(t) + \left.\frac{\partial\dot{\gamma}^{(\alpha)}}{\partial\tau^{(\alpha)}}\right|_t \Delta\tau^{(\alpha)} + \left.\frac{\partial\dot{\gamma}^{(\alpha)}}{\partial g^{(\alpha)}}\right|_t \Delta g^{(\alpha)} \\ &= \mathrm{Sgn}(\tau^{(\alpha)})\dot{a}^{(\alpha)}\left[\frac{\tau^{(\alpha)}}{g^{(\alpha)}}\right]^{1/m}\left[1 + \frac{1}{m}\left(\frac{\Delta\tau^{(\alpha)}}{\tau^{(\alpha)}} - \frac{\Delta g^{(\alpha)}}{g^{(\alpha)}}\right)\right] \end{aligned} \tag{23}$$

$$\Delta\tau^{(\alpha)} = \dot{\tau}^{(\alpha)}\Delta t \tag{24a}$$

$$\Delta g^{(\alpha)} = \dot{g}^{(\alpha)}\Delta t \tag{24b}$$

Using the formulae of $\dot{\tau}^{(\alpha)}$ and $\dot{g}^{(\alpha)}$, we can obtain

$$\sum_{\beta=1}^{N+1} M_{\alpha\beta}\Delta\gamma^{(\beta)} = F^{(\alpha)} \tag{25}$$

where

$$M_{\alpha\beta} = \delta_{\alpha\beta} + \left(\frac{\theta\Delta t\dot{\gamma}_i^{(\alpha)}}{m}\right)\left[\frac{\lambda^{(\alpha)} : P^{(\alpha)}}{\tau^{(\alpha)}} + \mathrm{Sgn}(\tau^{(\alpha)})\frac{H_{\alpha\beta}}{g^{(\alpha)}}\right] \tag{26a}$$

$$F^{(\alpha)} = \left[\dot{\gamma}_i^{(\alpha)} + \left(\frac{\theta\Delta t\dot{\gamma}_i^{(\alpha)}}{m\tau^{(\alpha)}}\right)\lambda^{(\alpha)} : D\right]\Delta t \tag{26b}$$

By choosing appropriate $\Delta t, M_{\alpha\beta}$ will be positive, then the shear strain rate and expansion strain rate increments can be obtained from (25).

Ⅱ. CALCULATION RESULTS

The finite element method for finite deformation is used in the calculation in this paper. The Update-Lagrange method is used and variational formulation is based on the following equation:

$$\int_v\left[L_{ijkl}D_{kl}\tilde{D}_{ij} - 2\sigma_{ik}D_{kj}\tilde{D}_{ij} + \sigma_{kl}\frac{\partial V_m}{\partial x_k}\frac{\partial V_m}{\partial x_l}\right]\mathrm{d}v = \int_s\dot{T}_i\tilde{V}_i\mathrm{d}s \tag{27}$$

where L_{ijkl} is an elastic tensor because of the use of the rate-dependent constitutive relation (19) and the performed gradient method for calculating $\Delta\gamma$. The body force is neglected, $\dot{T}_i$ is the load rate, V_i and D_{ij} are velocity and velocity rate respectively, $\tilde{V}_i$ and $\tilde{D}_{ij}$ are virtual velocity and virtual velocity rate respectively.

The calculating model is shown in Fig. 2. There are 23 single grains in the polycrystal, and the grains' orientation is of approximately random distribution. The boundary conditions are:

$$\begin{cases} X = 0, & \dot{u} = 0, & \dot{\tau}_{xy} = 0 \\ X = L, & \dot{u} = \dot{U}, & \dot{\tau}_{xy} = 0 \\ Y = 0, & \dot{\tau}_{xy} = 0, & \dot{\tau}_{yy} = 0 \\ Y = H, & \dot{\tau}_{xy} = 0, & \dot{\tau}_{yy} = 0 \end{cases} \tag{28}$$

The hardening law used in this paper is Asaro's hardening law:

$$H(\gamma) = H_s + (H_0 - H_s)\mathrm{sech}^2\left(\frac{H_0 - H_s}{\tau_s - \tau_0}\gamma\right) \tag{29a}$$

$$H_{\alpha\beta} = H(\gamma)[q + (1 - q)\delta_{\alpha\beta}] \tag{29b}$$

There are three slip systems in the single grain and one slip system in GB, and only the elastic deformation is considered in the normal direction of GB. The elastic properties of single grains and those of GB are equal. The elastic constants are $E = 1000\tau_0$. $\nu = 0.3$, the initial resolved critical shear stress of single grains is the same as that of GB, and the value is τ_0, the parameters in the hardening law are chosen as follows. $H_0 = 8.9\tau_0, H_s = 0.0, \tau_0 = 60.84$ MPa, $q = 1.2$, reference

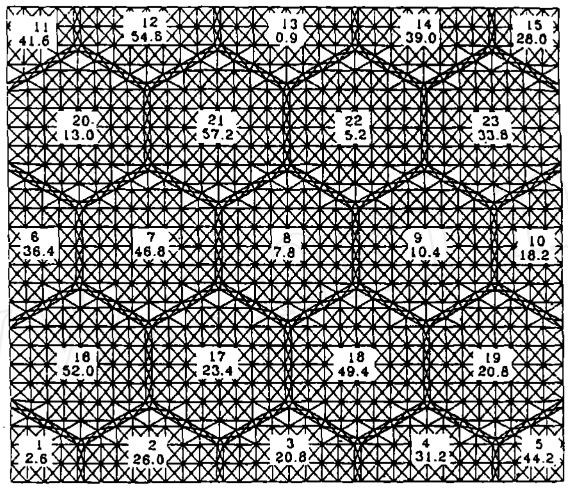


Fig. 2　Initial finite element mesh of polycrystal and orientation of single crystal (real digit represents orientation angle, integer digit represents single crystal).

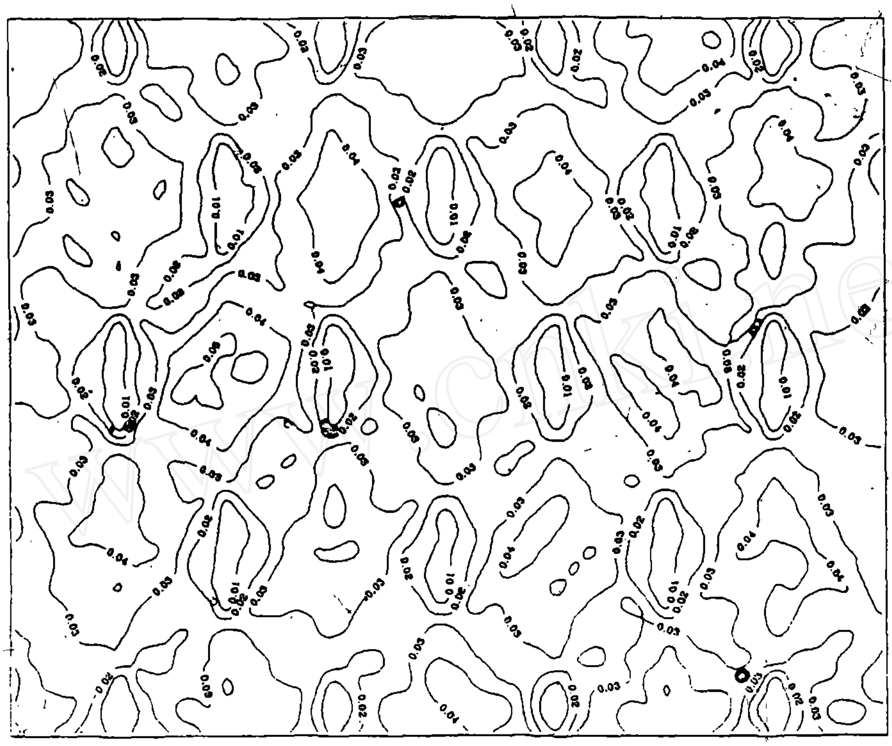
strain rate $\dot{a}=0.001$, rate sensitivity $m=0.005$.

The triangle element is used in calculation. The total number of elements is 3708, that of nodes is 1919.

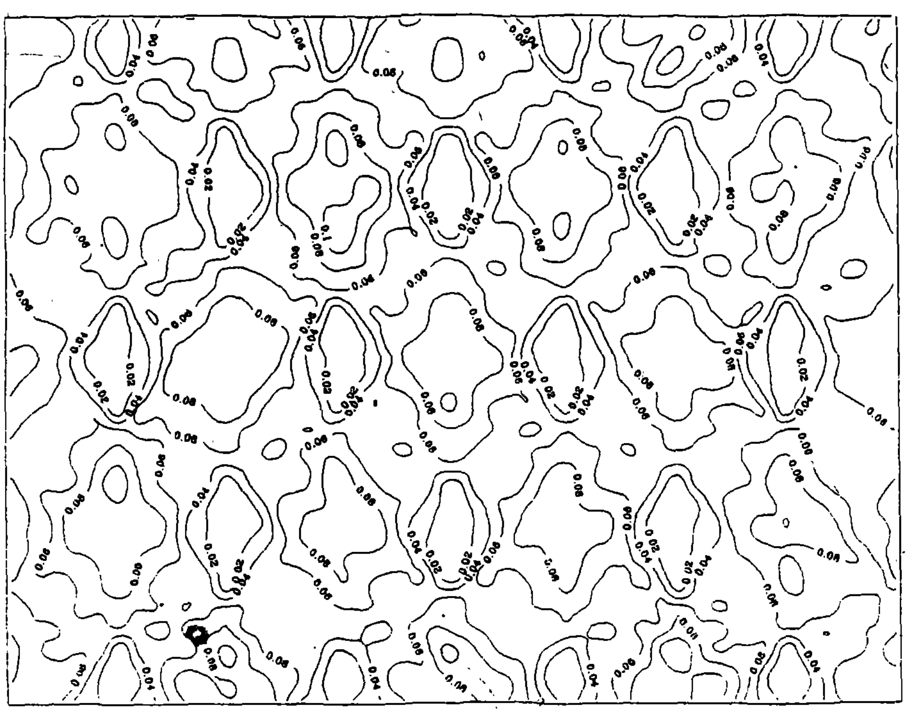
Figures 3a,b,c,d represent the contours of ε_x of polycrystal under engineering strain $e=0.03$, 0.06, 0.10, 0.15. From Fig. 3a, it can obviously be seen that the larger the Schmidt factor, the larger the deformation is in grain. For example, the orientation angle of number 7 is $46.8°$, its Schmidt factor is large, the maximum deformation in it is also the maximum value in polycrystal. The orientation angle of grain numbered 5 is $44.2°$, of which the Schmidt factor is also large, but the largest deformation value in it is not the maximum value in polycrystal because of the constraint of boundary. Figures 3b,c,d, show that the phenomenon is not obvious, when the deformation increases.

Figures 4a,b,c,d indicate the distribution of ε_x along y axis on the cross section of $x/L=0.184$, perpendicular to x axis under engineering strain $e=0.03$, 0.06, 0.10, 0.15 respectively. The meaning of Figs. 4e,f,g,h is the same as that of Figs. 4a,b,c,d. But the cross section is at $x/L=0.559$.

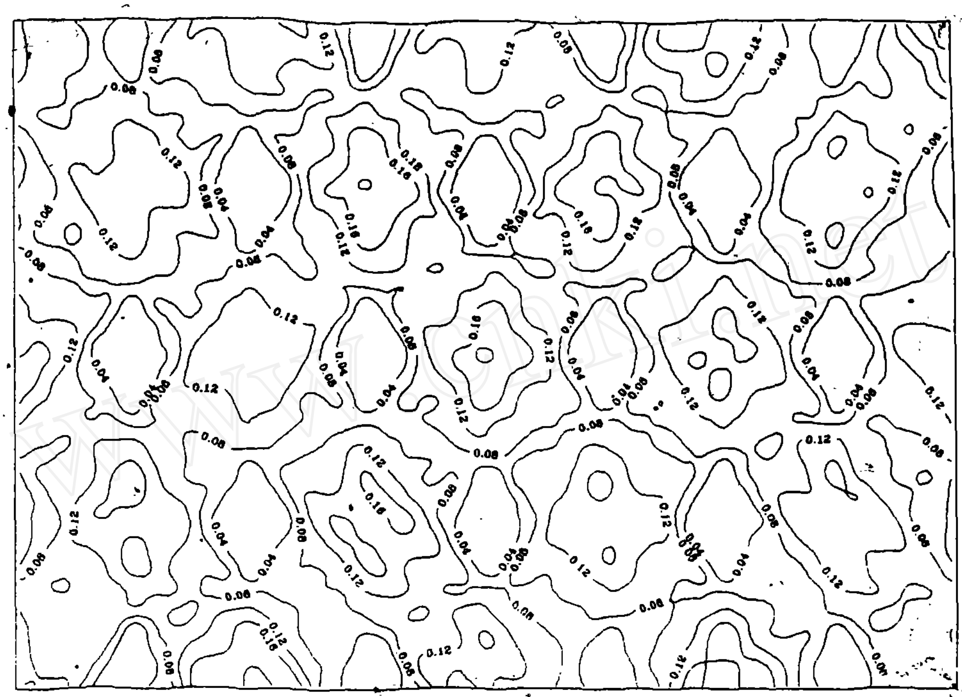
Figures 5a,b,c,d represent the distribution of ε_x on cross section at $y/H=0.25$ along x-axis under engineering strain $e=0.03$, 0.06, 0.10, 0.15. The strain on GB is smaller than that on grains. The meaning of Figs. 5e,f,g,h is similar to that of Figs. 5a,b,c,d. But the cross section is at $y/H=0.5$. The same conclusion can be obtained and the results are in qualitative agreement with the experimental results shown in Fig. 6.



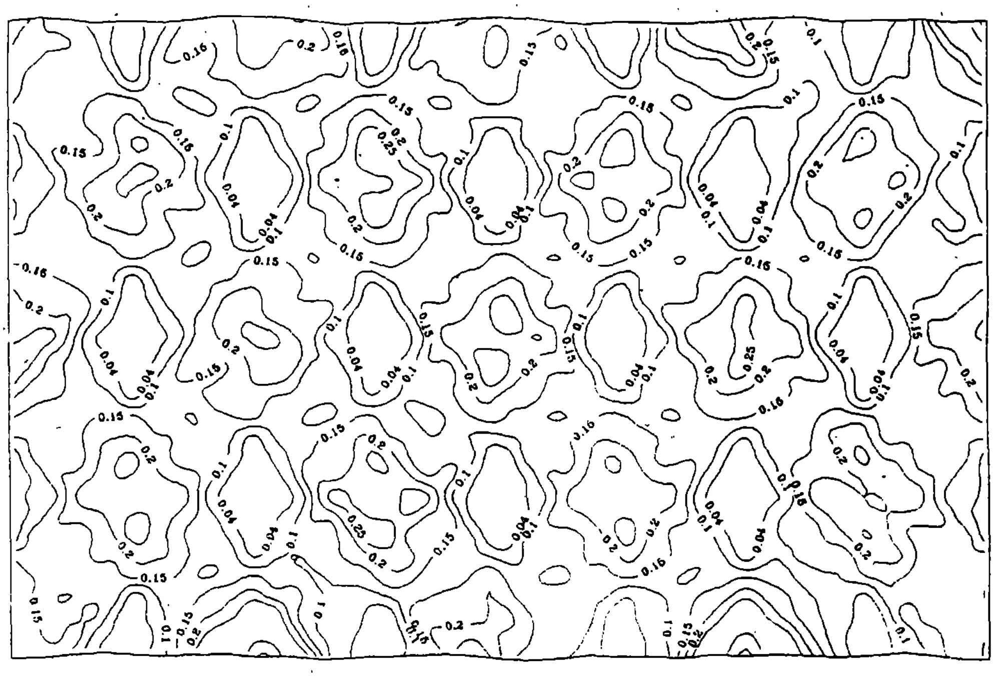
(a)　$e=0.03$



(b)　$e=0.06$



(c) $e=0.10$



(d) $e=0.15$

Fig. 3 Contours of e_s of polycrystal under different engineering strains.

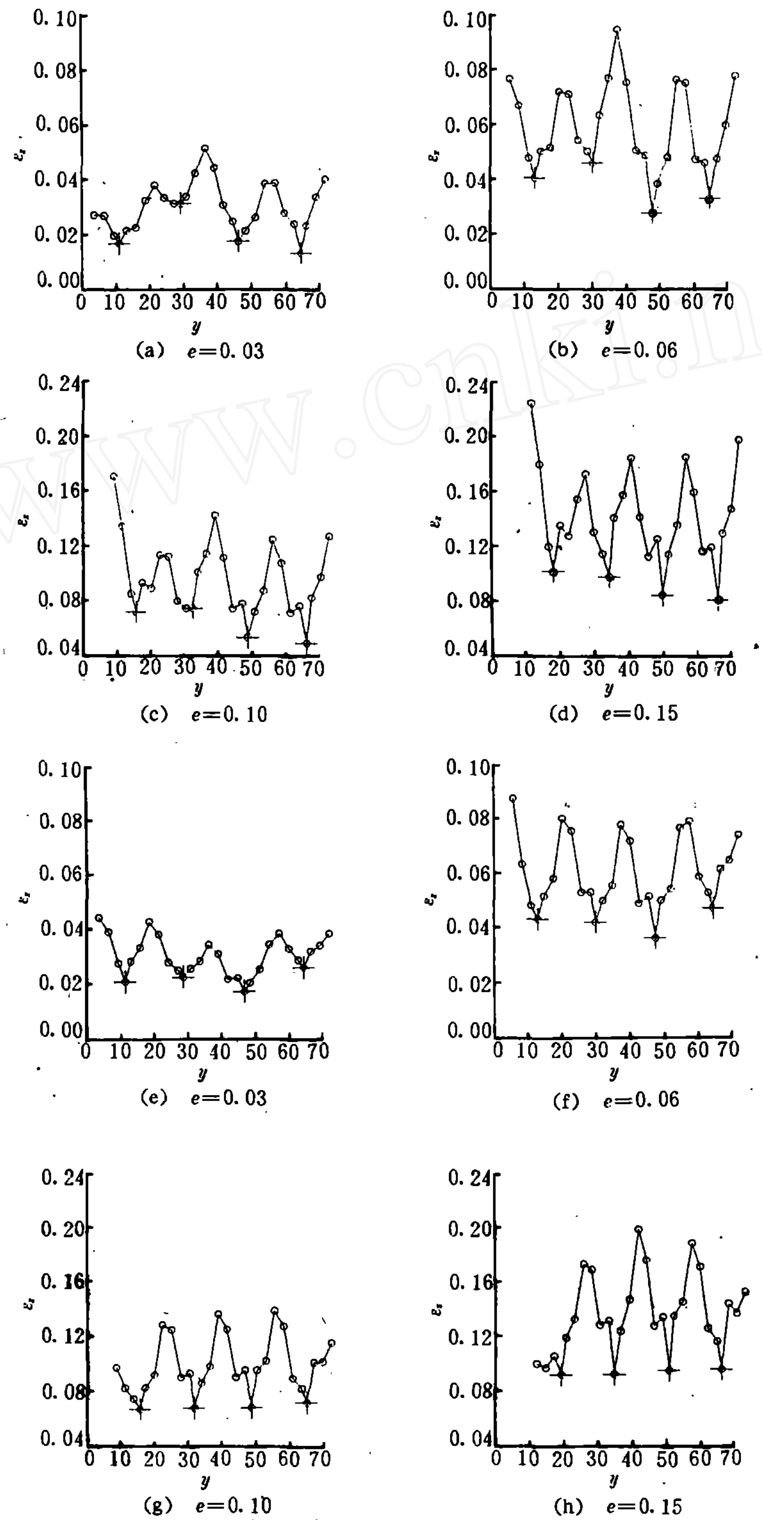


Fig. 4 Distribution of ε_x of cross section perpendicular to x axis

The cross section is at $x/L=0.184$ for above and $x/L=0.559$ for below.

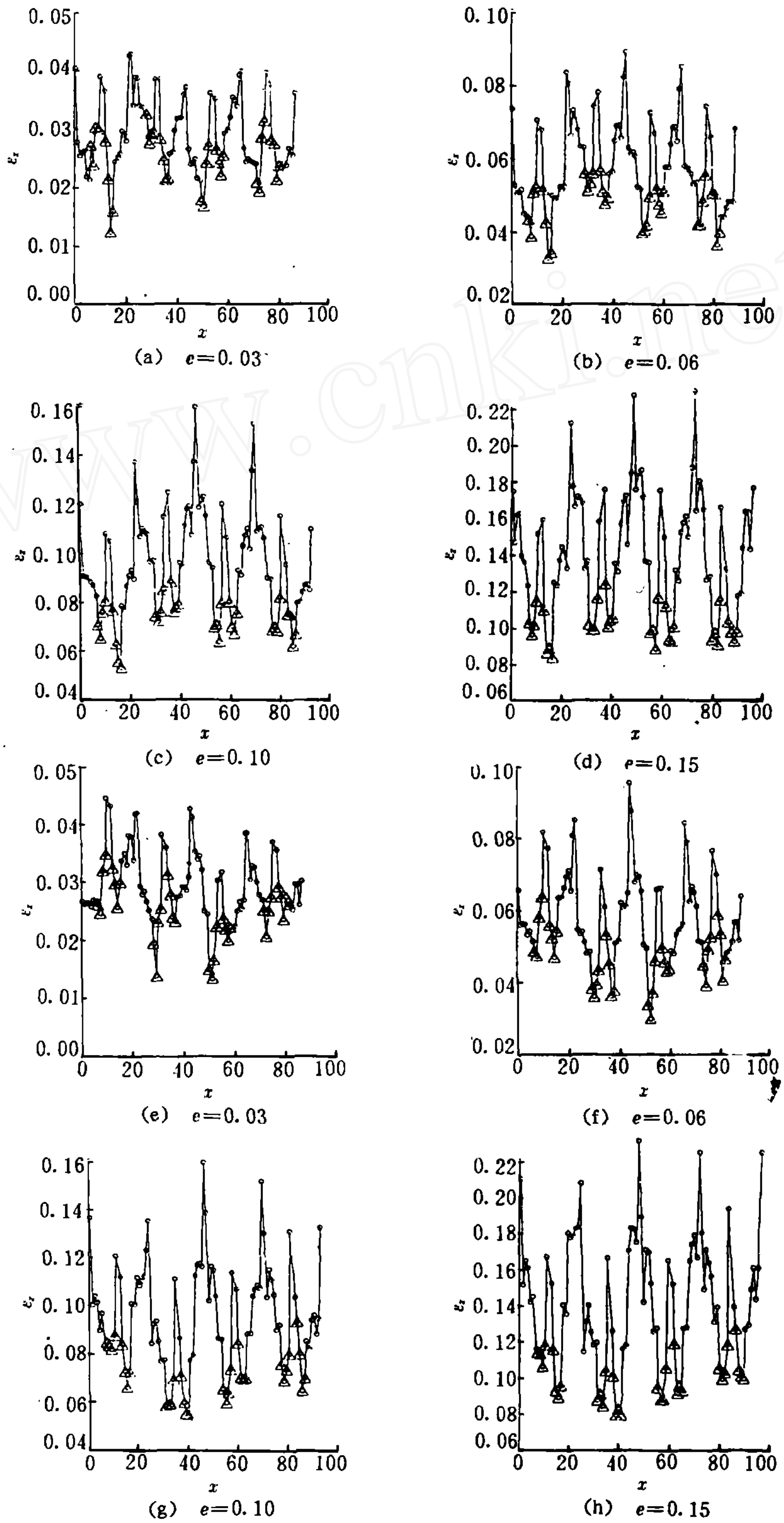


Fig. 5 Distribution of ε_x of cross section perpendicular to y axis. The cross section is at $y/H=0.25$ for above and $y/H=0.5$ for below. "Δ"represents GB, "∘" represents single crystal.

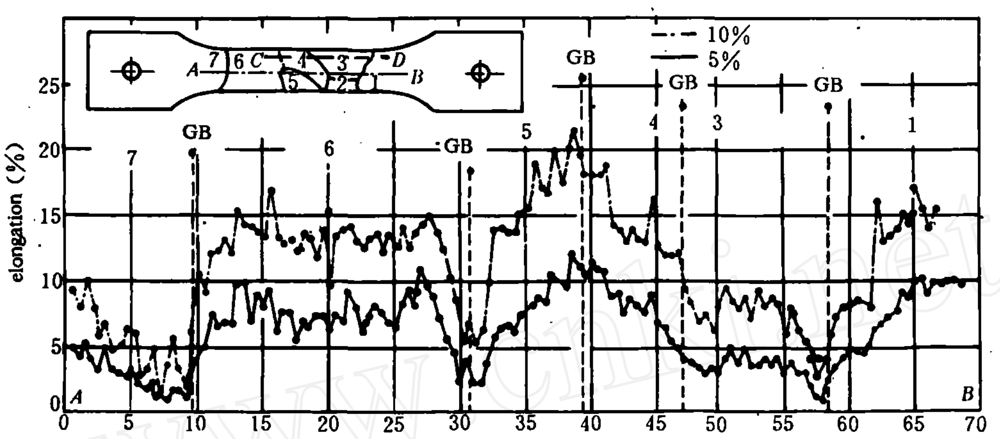


Fig. 6 The variation of local elongation of aluminium polycrystal.

Ⅳ. CONCLUSION AND DISCUSSION

The conclusions are as follows:

(1) By combining GB and its influence zone as a grain boundary layer, a sliding polycrystal plastic theory model is established to deal with sliding and expansion on GB.

(2) The larger the Schmidt factor is, the larger the deformation in the grain when the engineering strain of polycrystal is small. This phenomenon is not obvious when the engineering strain increased because of the influence of GB and the interaction between grains and grain's orientation.

(3) The deformation on GB is smaller than that in grains only when the sliding can take place at GB, while the expansion can hardly take place along the normal direction of GB.

(4) The plastic deformation of a polycrystal is not homogeneous as is the deformation inside grains.

(5) The simulated results by the finite element method for finite deformation are in qualitative agreement with those of experiment for polycrystal.

The model in this paper is a two-dimensional one. There are only three slip systems in grains and one slip system plus one NDS in GB. In an actual polycrystal, the interaction between slip systems and geometrical form and physical characterizations are very complex. In further research, we can measure some parameters in the model by high-tech experiment. Another way is to combine some parameters measured with the mathematical programming method to obtain the other parameters, and then we can calculate the response of the polycrystal quantitatively.

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