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MECHANICAL EFFECTS OF THE SELF-ORGANIZATION OF DISLOCATIONS AND RELATED CRITICAL CHARACTERISTICS*

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ABSTRACT: The effects of the dislocation pattern formed due to the self-organization of the dislocations in crystals on the macroscopic hardening and dynamic internal friction (DIF) during deformation are studied. The classic dislocation models for the hardening and DIF corresponding to the homogeneous dislocation configuration are extended to the case for the non-homogeneous one. In addition, using the result of dislocation patterning deduced from the non-linear dislocation dynamics model for single slip, the correlation between the dislocation pattern and hardening as well as DIF is obtained. It is shown that in the case of the tension with a constant strain rate, the bifurcation point of dislocation patterning corresponds to the turning point in the stress versus strain and DIF versus strain curves. This result along with the critical characteristics of the macroscopic behavior near the bifurcation point is microscopically and macroscopically in agreement with the experimental findings on mono-crystalline pure aluminum at temperatures around $0.5T_m$. The present study suggests that measuring the DIF would be a sensitive and useful mechanical means in order to study the critical phenomenon of materials during deformation.

KEY WORDS: dislocation patterns, work hardening, dynamic internal friction, critical phenomenon

1 INTRODUCTION

The plastic deformation of metal crystals involves intrinsically the multiplication/annihilation, reaction and movement of dislocations, consequently, leading to energy dissipation. This is a typical irreversible process far away from equilibrium state. As a result of dissipation structure formation, the ordered structures or patterns of dislocations can be formed through the self-organization process of dislocations[1]. This dynamical phenomenon shows the self-adjustability of materials to be compatible with the deformation and to resist failure, the same as bio-systems in adapting themselves to the environment. Meanwhile, there appear some distinct stages along the hardening curve, indicating the hardening behavior of crystals to vary with the self-organization process. Hence, for the purpose of resolving rationally the problem of the crystal hardening, it is essential to study the self-organization

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process of crystal dislocations and then to correlate dislocation patterns with the hardening behavior. This is an important tendency in the development of the modern hardening theory, in contrast to the classic one that addresses the dependence of the hardening only on the global dislocation density but not on the dislocation configuration.

Internal friction is considered as the macroscopic damping of kinetic energy during the vibration of substances caused by microstructural variation. Owing to its sensitivity to the evolution of the microstructure, measuring the internal friction has become an effective means used in materials science and condensed physics. By superposing a small vibrational stress upon the plastic deformation of materials, the internal friction measured in-situ is usually called the dynamic internal friction during deformation, or the DIF for brevity. With its relevancy to plastic deformation, the DIF provides us with important information about the movement, multiplication/annihilation and self-organization process of dislocations and, thus, is helpful to developing the correlation between the dislocation configuration and hardening. Some experimental and theoretical work has been done on the DIF, as reviewed critically by Zhou in his Ph.D. thesis[2]. It is worth noting that just like the classical hardening theory, the previous models for the DIF developed by researchers[3~6] are all based on the presumption that dislocations are arranged spatially in a statistically homogeneous manner. Therefore, the DIF is correlated to the mean values of the density, velocity and multiplication rate of dislocations and the contribution due to the dislocation patterning has not been taken into account in their models.

It includes both the positive and inverse problems of the transition from macro-scale to micro-scale and vice versa to determine the evolution of dislocation patterns based on the experimental findings on the DIF and then applying it to predicting the hardening behavior. The key issue related is to model the relation amongst the dislocation patterns, hardening and DIF. As the first step of the research, the single slip stage of crystal hardening will be focused in the present study of the relationship aforementioned. The present paper is divided into four sections. Firstly, a dislocation dynamics model for single slip proposed by the authors[7] will be outlined in Section 2, along with the characteristics of the self-organization of dislocations predicted based on it. Then, the macroscopic mechanical effect of the self-organization of dislocations on the hardening and DIF will be studied in Section 3. Next, in Section 4, we will give a comparison between the present theoretical result and experimental one available in the literature. Besides, the potential applications of the means of the DIF are discussed. Finally, a summary will be made on the present study in Section 5.

2 DISLOCATION DYNAMICS MODEL

As suggested recently by Huang et al.[7], the dislocation population can be grouped into dipoles and mobile dislocations, with the former being slightly mobile, and their spatial density functions are denoted by ρ_d and ρ_m, respectively. In addition, the slip direction is denoted with x and the normal direction of the slip plane with y. Taken into account of the mechanisms of the drifting and conservative climbing of dipoles, and that of the slipping and cross-slipping of edge and screw dislocations, based on the long and short distance interactions between the two groups of dislocations as well as themselves, the governing equations for dislocation dynamics are obtained as follows

$$\left.\begin{aligned}\partial_t\rho_d &= D^d_{xx}\partial_{xx}\rho_d + D^d_{yy}\partial_{yy}\rho_d + f(\rho_d) - d/\rho_d + g\rho_m\rho_d \\ \partial_t\rho_m &= D^m_{xx}\partial_{xx}\rho_m + D^m_{yy}\partial_{yy}\rho_m + D^m_{zz}\partial_{zz}\rho_m + \\ &\quad 2D^m_{xz}\partial_{xz}\rho_m + d/\rho_d - g\rho_m\rho_d\end{aligned}\right\} \tag{1}$$

where D^d_{xx}, D^d_{yy}, D^m_{xx}, D^m_{yy}, D^m_{zz}, D^m_{xz} are diffusion coefficients. The term of $g\rho_m\rho_d$ means that mobile dislocations are captured by dipoles at rate of g and so becomes the sink of mobile dislocations and the source of dipoles. The term of d/ρ_d represents the mobilization of the dislocations captured, where d is the main controlling parameter (bifurcation parameter) related to the external force. The function $f(\rho_d)$ expresses the generation rate of dipoles resulting from the other mechanisms. The governing equations are non-linear reaction-diffusion equations that determine the dynamical mechanism of the self-organization process of dislocation populations. As compared with those suggested by Walgraef et al.[8], the three-dimensional rather than two-dimensional movement of mobile dislocations has been considered and more physically reasonable reaction terms have been included in the present equations. The initial spatial distribution of dislocation populations is assumed to be homogeneous, with periodic boundary conditions.

Linear stability analysis has shown that when the bifurcation parameter d reaches a critical value

$$d_c = \frac{1}{2}g\rho_d^{0^3}\left(\sqrt{\frac{a}{g\rho_d^0}} + \sqrt{\frac{D^d_{yy}}{D^m_{yy}}}\right)^2 \tag{2}$$

where $a = -f'(\rho_d^0) > 0$, the homogeneous state of dislocation populations, ρ_d^0 and ρ_m^0 satisfying

$$f(\rho_d^0) = 0 \qquad \rho_m^0 = \frac{d_c}{g\rho_d^{0^2}} \tag{3}$$

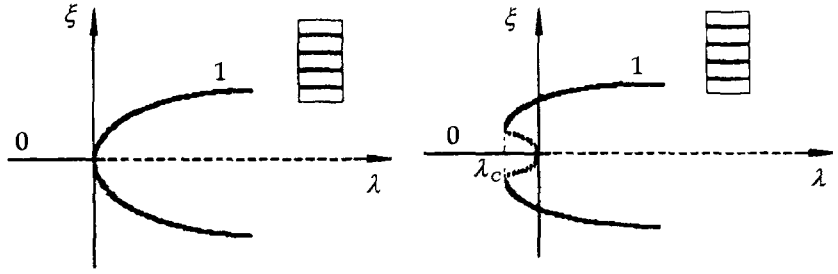
may loss its stability and the following embryo of dislocation pattern appears

$$\rho_d = \rho_d^0 + \hat{\rho}_d \qquad \rho_m = \rho_m^0 + \hat{\rho}_m \tag{4}$$

with

$$\left\{\begin{array}{c}\hat{\rho}_d \\ \hat{\rho}_m\end{array}\right\} = \xi(\lambda)\sin(q_{cy}y + \varphi)\left\{\begin{array}{c}1 \\ -\dfrac{D^d_{yy}}{D^m_{yy}}\left(1 + \sqrt{\dfrac{a}{g\rho_d^0}\dfrac{D^m_{yy}}{D^d_{yy}}}\right)\end{array}\right\} + O(\xi^2) \tag{5}$$

where $\hat{\rho}_m/\rho_m^0 \ll 1$, $\hat{\rho}_d/\rho_d^0 \ll 1$, $q^2_{cy} = \sqrt{(ag\rho_d^0)/(D^d_{yy}D^m_{yy})}$ and φ is the phase and ξ the coefficient dependent on the bifurcation parameter $\lambda = d - d_c$. Furthermore, the non-linear bifurcation analysis has also indicated that the bifurcation is in the form of fork as shown in Fig.1, in which Fig.1(a) is referred to as super-critical bifurcation and Fig.1(b) as sub-critical one. It is noted that $\xi(\lambda) = 0$ is the trivial solution corresponding to the homogeneous state and $\xi(\lambda) \neq 0$ the non-trivial one corresponding to the dislocation structure periodic along y direction. That is to say, the spatial distribution of dislocations has the symmetry broken along the normal direction of the slip plane. This structure stands for a layer-structure with the layers mainly comprised of the dipoles parallel to the slip plane, and in the gap between any two neighboring layers, the density of mobile dislocation is higher while that of dipoles is lower. That is just a typical dislocation structure often observed experimentally in the stage of single slip, termed carpets[9]. It is different from another typical dislocation structure,



(a) (b)

Fig.1 Bifurcation figure of the dislocation pattern formation
0 — homogeneous state, 1 — carpets

termed walls, which is also a layer-structure but whose layer planes are perpendicular to the slip plane.

3 HARDENING AND THE DYNAMIC INTERNAL FRICTION DURING DEFORMATION

3.1 Hardening

The plastic slip strain rate in a single crystal is given by Orowan's formula

$$\dot{\gamma} = \rho_m v_m b \tag{6}$$

where b is the norm of Burger's vector and v_m represents the collective velocity of mobile dislocations which, based on the classic relation of dislocation dynamics, is related to effective resolved shear stress τ_e through

$$v_m = M\tau_e^n \tag{7}$$

in which M stands for the mobility coefficient, n is the reciprocal of the velocity sensitivity exponent and

$$\tau_e = \tau - \alpha G b \rho_d^{1/2} \tag{8}$$

where G is the elastic shear modulus, α the non-dimensional constant and τ the applied resolved shear stress assumed to be uniform within the crystal.

Near the critical point, expanding ρ_m, v_m in (6) into series and ignoring the high-order terms give

$$\dot{\gamma} = \left(\rho_m^0 + \hat{\rho}_m\right)\left(v_m^0 + \frac{\partial v_m}{\partial \tau}\Delta\tau + \frac{\partial v_m}{\partial \rho_d}\hat{\rho}_d\right)b \tag{9}$$

Defining the mean of $\dot{\gamma}$ around the crystal volume V as the macroscopical plastic strain, then, by using (5~8), we have

$$\bar{\dot{\gamma}} = \frac{1}{V}\int_V \dot{\gamma}\mathrm{d}V = \bar{\dot{\gamma}}^0 + nMb\rho_m^0\tau_e^{n-1}\Delta\tau + \frac{1}{4}\alpha nMGb^2(\rho_d^0)^{-1/2}\tau_e^{n-1}\frac{D_{yy}^d}{D_{yy}^m}\left(1+\sqrt{\frac{a}{g\rho_d^0}\frac{D_{yy}^m}{D_{yy}^d}}\right)\xi^2 \tag{10}$$

For the case of constant strain rate, $\bar{\dot{\gamma}} = \bar{\dot{\gamma}}^0 = \rho_m^0 v_m^0 b$, it is readily shown that

$$\Delta\tau = -\frac{1}{4}\frac{\alpha G b}{\rho_m^0(\rho_d^0)^{1/2}}\frac{D_{yy}^d}{D_{yy}^m}\left(1+\sqrt{\frac{a}{g\rho_d^0}\frac{D_{yy}^m}{D_{yy}^d}}\right)\xi^2 \tag{11}$$

As ξ is small, there would appear in this case a phenomenon that the stress decreases slightly or remains unchanged approximately near the critical point as a result of the dislocation pattern formation.

For the homogeneous state before dislocation patterning, it is shown through (3) and (6~8) that

$$\dot{\gamma} = \frac{dMb}{g(\rho_d^0)^2}\left(\tau - \alpha Gb(\rho_d^0)^{1/2}\right)^n \tag{12}$$

In general, d increases monotonously with τ and so does the dislocation density with strain during the earlier stage of deformation. Therefore, it is easy to know from (12) that τ increases also with strain to keep the constant strain rate, i. e., the crystal hardens during the earlier stage. Meanwhile, averaging (4) and (5) over the volume leads to

$$\bar{\rho}_d = \rho_d^0 \qquad \bar{\rho}_m = \rho_m^0 \tag{13}$$

It means that near the bifurcation point, although the mean dislocation densities remain constant, significant changes occur in the behavior of the hardening. Hence, the dislocation pattern is more important to the hardening than the dislocation density itself.

3.2 The dynamic internal friction

If a mechanical vibration is superposed to the plastic deformation of crystals, the DIF is defined as

$$Q^{-1} = \frac{1}{2\pi}\frac{\Delta W}{W} \tag{14}$$

where W is the total free vibration energy and ΔW the damping of the energy per cycle induced by the microstructural modification. According to Ke and Zhang[3], the vibrational resolved shear stress, $\tau' = \tau_0' \sin\omega t$, takes part in the plastic deformation and then results in the DIF, where τ_0' is the amplitude and ω the circular frequency of the vibration. Expanding $v_m = v_m(\tau_e)$ into series and neglecting the terms of high order in view of $\tau_0' \ll \tau$, we get

$$v_m = v_m(\tau_e + \tau') = v_{m0} + \frac{\mathrm{d}v_m}{\mathrm{d}\tau_e}\tau' \tag{15}$$

where v_{m0} is the velocity of mobile dislocations without vibrational stress action. When the dislocation density is homogeneous, we have

$$\Delta W = \int_0^{2\pi/\omega} \rho_m v_m b\tau' \mathrm{d}t \tag{16}$$

Substituting (15) into (16) and then carrying out integration, by means of (6,7), yield that

$$\Delta W = \frac{n\pi\tau_0'^2}{\omega\tau_e}\dot{\gamma} = \frac{n\pi\tau_0'^2}{\omega\tau_e n_p}\dot{\varepsilon} \tag{17}$$

where $\dot{\varepsilon}$ is the tensile strain rate (neglecting elastic strain) and n_p the orientation factor of the tension axis. The total free vibration energy is

$$W = \sigma_t^{0^2}/2G = \tau_0'^2/2Gn_t^2 \tag{18}$$

where σ_t^0 is the amplitude of the vibrational stress and n_t its orientation factor. Combining (17) and (18) gives

$$Q^{-1} = \frac{n_t^2}{n_p}\frac{nG\dot{\varepsilon}}{\tau_e\omega} \tag{19}$$

For the tension with constant strain rate, $\dot{\gamma} = \rho_m v_m b = \text{const}$, in view of (7), we get

$$\frac{\mathrm{d}\tau_e}{\mathrm{d}\varepsilon} = -\frac{\tau_e \mathrm{d}\rho_m/\mathrm{d}\varepsilon}{n\rho_m} \tag{20}$$

As $\mathrm{d}\rho_m/\mathrm{d}\varepsilon > 0$ during the earlier stage of deformation, it follows directly that $\mathrm{d}\tau_e/\mathrm{d}\varepsilon < 0$ and thus, from (19)

$$\frac{\mathrm{d}Q^{-1}}{\mathrm{d}\varepsilon} = -\frac{n_i^2}{n_p}\frac{\mathrm{d}\tau_e}{\mathrm{d}\varepsilon}\frac{nG\dot{\varepsilon}}{\tau_e^2\omega} = \frac{n_i^2}{n_p}\frac{\mathrm{d}\rho_m}{\mathrm{d}\varepsilon}\frac{G\dot{\varepsilon}}{\tau_e\rho_m\omega} > 0 \tag{21}$$

That is to say that the DIF increases also with strain in the earlier stage of deformation where dislocations are distributed uniformly in a statistical sense.

Define the DIF after dislocation pattering as the average over the volume of Q^{-1}. Then from (19) and (6~8), we obtain

$$\begin{aligned}\overline{Q^{-1}} &= \frac{1}{V}\int_V Q^{-1}\mathrm{d}V = \frac{n_i^2 nMGb}{V\omega}\int_V \tau_e^{n-1}\rho_m \mathrm{d}V = \\ &\frac{n_i^2 nMGb}{V\omega}\int_V \left[(\tau_e^0)^{n-1} + (n-1)(\tau_e^0)^{n-2}\left(\Delta\tau - \frac{1}{2}\alpha Gb(\rho_d^0)^{-1/2}\hat{\rho}_d\right)\left(\rho_m^0 + \hat{\rho}_m\right)\right]\mathrm{d}V = \\ &Q_0^{-1} + \frac{n_i^2 n(n-1)MGb}{\omega}(\tau_e^0)^{n-2}\rho_m^0\left[\Delta\tau + \frac{1}{4}\frac{\alpha Gb}{\rho_m^0(\rho_d^0)^{1/2}}\frac{D_{yy}^d}{D_{yy}^m}\left(1 + \sqrt{\frac{a}{g\rho_d^0}\frac{D_{yy}^m}{D_{yy}^d}}\right)\xi^2\right]\end{aligned} \tag{22}$$

in which

$$Q_0^{-1} = \frac{n_i^2 nMGb\rho_m^0(\tau_e^0)^{n-1}}{\omega} = \frac{n_i^2}{n_p}\frac{nG\dot{\varepsilon}^0}{\tau_e\omega}$$

corresponds to the DIF when dislocations are distributed uniformly. For the deformation with constant strain rate, applying (11) it follows readily that

$$\overline{Q^{-1}} = Q_0^{-1} \tag{23}$$

It shows us an interesting result that just after dislocation pattern is formed the DIF remains unchanged. Consequently, there occurs a flat stage in the DIF versus strain curve near the bifurcation point. In other words, we may say that the bifurcation point is a turning point of the DIF versus strain curve. This result, to the author's knowledge, has not been obtained before.

4 DISCUSSION

Figure 2 depicts the experimental curves of the DIF (Q^{-1}-ε) and hardening (σ-ε), respectively, for the constant velocity of tension at different strain rates[2,10]. The circular frequency, ω, used for measuring the DIF is 1.0 Hz and the tested material is the crystal of pure aluminum (99.999%), whose tension orientation is [331]. The test temperature is 190°C ($0.5T_m$). As shown in Fig.2, in the earlier stage of tensile deformation, both the DIF and flow stress enhance acutely until their maximum is reached near $\varepsilon = 1\%$. Next, the flow stress reduces slightly or remains unchanged, and so does the DIF, except for Fig.2(a). If our attention is restricted to the experimental findings within the range of small deformation, it is easy to know that the tension with constant velocity is equivalent

approximately to that of constant strain rate. Moreover, despite the fact that [331] is the orientation corresponding to double-slip, the interaction between the two slip systems is weak because they share a common slip plane. Therefore the macro-mechanical behavior is similar to that corresponding to the orientation of single-slip (which stands for the superposition of two single-slips). Comparing the experimental findings on the macro-mechanical behavior as well as the related critical phenomenon with theoretical results obtained in the last section, it is suggested strongly that the point of $\varepsilon = 1\%$ might be the bifurcation point for the onset of the dislocation patterning.

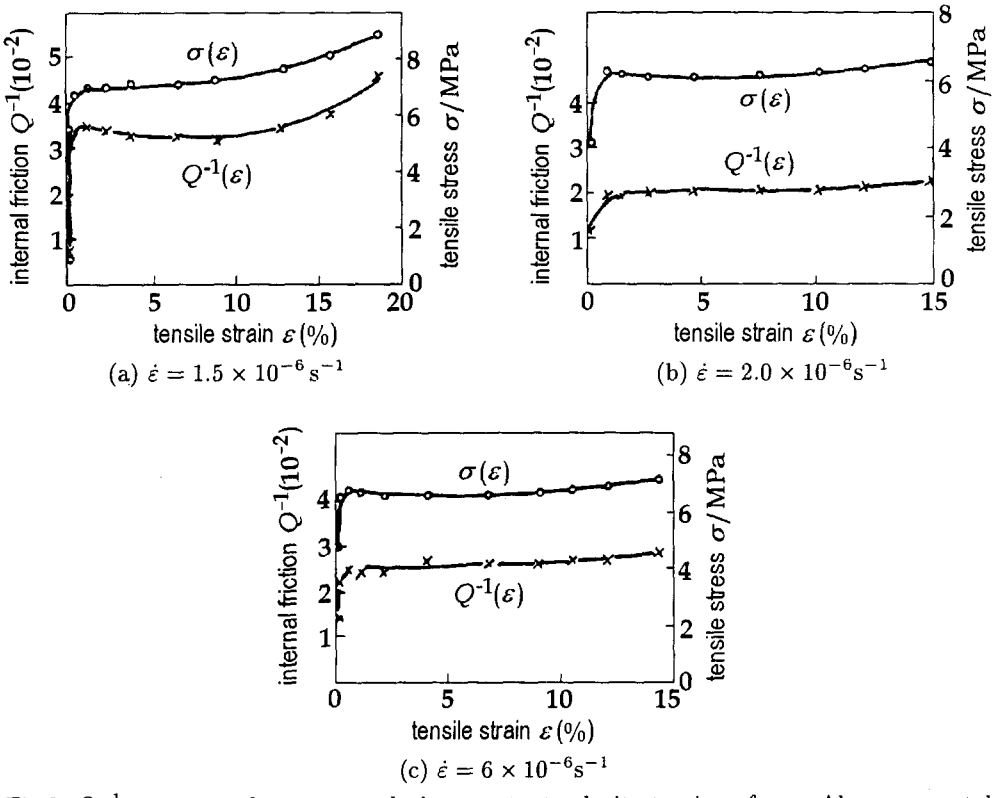
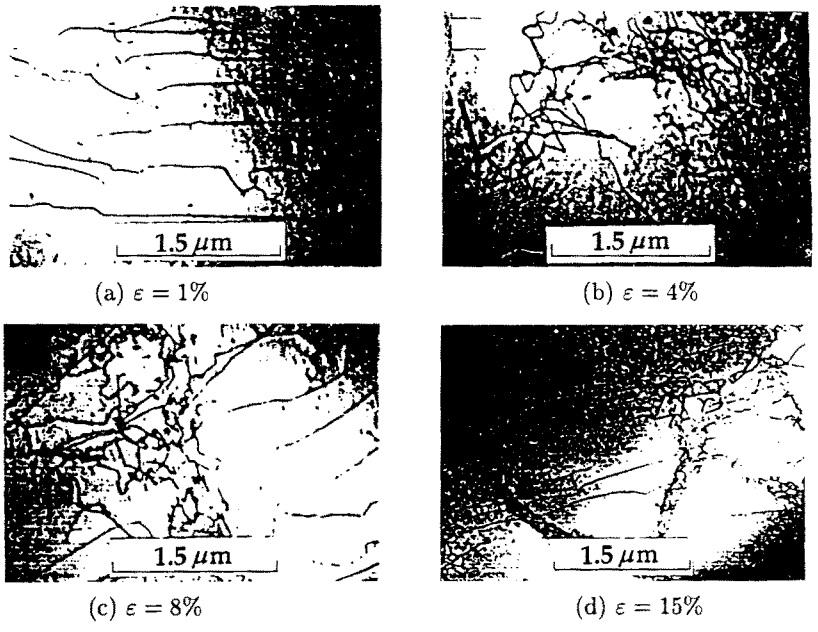


Fig.2 Q^{-1}-ε curve and σ-ε curves during constant velocity tension of pure Al mono-crystals
Tension orientation: [331]; Temperature: 190°C; Frequency: 1.0 Hz

Figure 3 is the results of TEM observation on dislocations by Zhou et al.[2,10]. The experimental condition is the same as indicated in Fig.2(a). From the TEM experimental observation, there are a few dislocations in the samples of the raw material. When $\varepsilon = 1\%$ is reached, the dislocation density becomes higher but distributes in a statistically homogeneous fashion. Lately, when the strain increases to 8%, dislocation clustering appears. Furthermore, when the strain reaches 15%, a distinct dislocation pattern forms. In general, it is hard to determine by TEM observation the exact position of the bifurcation point where dislocation patterns start to be formed, since the dislocation pattern just formed is merely the small embryo. Therefore, only a disorder state of dislocation populations with the high density could be observed in this stage. Until the embryo grows up to some extent, the clustering of dislocations becomes visible. However, the system has been far away from the bifurcation point. On the other hand, as known from the theoretical analysis presented in

Section 2, the macro-hardening and the DIF curves are sensitive to the bifurcation point and so exhibit the critical phenomenon. Combining the macro-mechanical phenomenon and the findings of microstructural observation, it could be expected that there has been the embryo of dislocation pattern in the configuration displayed in Fig. 3 (a), that is to say that the point of $\varepsilon = 1\%$ is just the critical point of the bifurcation.



(a) $\varepsilon = 1\%$ (b) $\varepsilon = 4\%$

(c) $\varepsilon = 8\%$ (d) $\varepsilon = 15\%$

Fig.3 TEM photographs corresponding to the different positions in the curve of Q^{-1}-ε indicated in Fig.2(a)

The experimental results as shown in Fig.2 and Fig.3 support both macroscopically and microscopically the theoretical correlation, as given in Section 3, between the dislocation pattern and strain hardening as well as the DIF. Hence, it has been illustrated experimentally and theoretically how dislocation patterns affect significantly the macro-mechanical properties. More meaningfully, it provides us with a potential means to study the DIF using the dislocation pattern or vice versa. There are many critical phenomena in the dissipative process of the nonlinear and non-equilibrium complex systems, which have been attracting academic concerns. From the critical phenomenon of complex systems, many important information on the internal dynamical mechanisms can be captured such as the omen of phase transformation or catastrophe induced by the self-organization process of the system. With the sensitivity of the DIF to the self-organization of dislocations, it is suggested that the measuring of the DIF is a useful mechanical means to study experimentally the critical phenomenon of the plastic deformation of metals and could be manipulated in a simple way. In addition, if the lithosphere is viewed as a nonlinear dynamical system, it is easily understood that the means of the DIF is closely similar to the loading-unloading method used effectively to predict earthquake. In fact, measuring the DIF stands for superposing a loading-unloading process to the dynamical system and then examining the dissipation of the energy in order to uncover the internal evolution of the lithosphere. Therefore, the research of the DIF can be extended to the cases involving not only the plastic deformation but also the other mechanisms of dissipation such as damage for studying the strength and

durability of materials.

5 CONCLUSION

In the present paper, the classic models for the hardening and the DIF corresponding to homogeneous dislocation configurations have been modified to be applicable to more general cases that take into account of dislocation patterns. Besides, by combining the evolution of dislocation pattern determined by nonlinear dislocation dynamics, the correlation between the dislocation pattern and hardening as well as the DIF has been obtained. Some conclusions could be made as follows for the tension with constant strain rate.

(1) In the early stage of deformation, the flow stress and the DIF increase with the density of dislocations. Near the critical point, the homogeneous dislocation configuration becomes unstable and the density of dislocations reaches the maximum. Consequently, dislocation patterning begins. However, in the neighborhood of critical point, the global density of dislocations and the DIF remain unchanged, and the flow stress either starts to decrease or keeps approximately constant. It means that the turning points in the curves of hardening and the DIF are consistent with the point of bifurcation of dislocation pattering.

(2) As compared with the experimental results of Al mono-crystals, the theoretical results achieved in the present paper are supported experimentally by both the macro-mechanical response and microstructural dislocation configuration observation.

(3) In the earlier stage of deformation, the hardening and the DIF are mainly governed by dislocation density, while in the middle and later stages, dislocation patterns become more important.

(4) Measuring the DIF is an effective mechanical means for studying the critical phenomenon.

The present study has been restricted to the phenomenon near the bifurcation point of dislocation patterning in the stage of single slip. Those corresponding to double-slip or multi-slip and far from the bifurcation point are worth exploring further with the help of computer simulation.

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