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Evolution of dislocation cells during plastic deformation①

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Abstract: In recent years, materials with ultrafine grain size(UFG) have attracted much attention. By using severe plastic deformation(SPD) techniques, materials with fine grain size as small as 200－250 nm have been obtained. However, the nature of the grain boundaries has not been theoretically understood. It is still an unsolved question whether or not finer grain sizes down to 100 nm could be reached. A semi-quantitative model for the evolution of dislocation cells in plastic deformation was proposed. The linear stability analysis of this model leads to some interesting results, which facilitate the understanding of the formation of cell structures and of the factors determining the lower limit of the cell size of SPD materials.

Key words: evolution of dislocation cells; ultrafine grain; severe plastic deformation
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1 INTRODUCTION

It is expected that materials with fine grain size have good performances during service. With the development of new materials processing techniques, such as equal channel angular extrusion (ECAE), bulk materials with ultrafine grain size (UFG) can be produced. However, further clarification on the nature of grain or cell boundaries is needed. Thus, it is still under study whether the severely plastically deformed(SPD) material is truly polycrystalline down to grain sizes of 100 nm[1]. The deformation mechanisms and their simulation need further research.

In recent years, the evolution of dislocation patterns has attracted much attention to achieve deep understanding of the deformation mechanisms. It is found that dislocation patterns appearing in deformed metals belong to the combination of the four basic patterns found in copper under cyclic deformation at room temperature[2]. Rolling and torsion lead to a cell structure belonging to the basic patterns[3-6]. Dislocation cell or subgrain is readily formed in the process of creep and drawing[7-9]. With the development of computer technology, many researchers have studied dislocation patterning by computer simulation. For example, Abraham et al[10] simulated the plasticity of FCC crystals by using molecular dynamics in approaching micron scale using up to one billion atoms. The evolution of dislocation patterns could be visual on the computer. Their work has important significance in the establishment of continuum theories for plastic deformation in small structures. In theoretical studies of the formation of dislocation patterns, Holt[11] investigated the rearrangement of screw dislocations under the drive of applied stress without considering the generation and annihilation of dislocations. In 1985, Walgraef and Aifantis[12] indicated that plasticity should be viewed as a nonlinear irreversible process driven to a far from dynamic equilibrium point. The evolution of dislocation patterns is a typical nonlinear phenomenon that should be described by the principle of dissipative structure and synergetics. This method has been widely used in plasticity, especially in strain hardening[13, 14].

In the process of severe plastic deformation, dislocations are generated, which move and interact mutually. By the self-organization of dislocations, cell structures are formed and then shrink down to a steady dimension[15-19]. With this consideration, we can assume that the lower limit grain size of SPD materials should be equal to the possibly formed minimum cell size. In this paper, an attempt is made to establish a semi-quantitative model of the evolution of dislocation distributions. By the theoretical analysis of this model, we obtain

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two generally noteworthy formulae and a criterion for the limiting cell size. These results will promote the understanding of the mechanism of the cell forming process.

2 MODEL

For the sake of simplicity, we consider here only a hierarchy of mobile and immobile dislocations. It is assumed that the dislocations are straight lines, with the Burgers vector parallel to the x direction, unlike dislocations moving with the same rate in opposite directions, and all of the slip systems are active simultaneously where the changes of dislocation density are the same.

In the light of the theory of dissipative structures and the principle of synergetics, any kind of dislocation should obey the following transport-reaction equation[12, 20-22]:

$$\frac{\partial \rho_k}{\partial t} + \mathrm{div}\boldsymbol{J}_k = g_k \tag{1}$$

where the subscript k denotes the dislocation type, which is denoted by $k=$ m and $k=$ i for mobile and immobile dislocations, respectively; $\boldsymbol{J}$ denotes the flux of dislocation, and g the generation and reaction term. These terms can be readily expressed in terms of dislocation theory[15, 16]. Hence, we obtain the semi-quantitative dislocation model as follows:

$$\frac{\partial \rho}{\partial t} = -\frac{\partial(\rho_m v)}{\partial x} - B\frac{\partial}{\partial x}\left[\psi\left(12\frac{\partial \rho}{\partial x} + \frac{n^2}{\rho}\frac{\partial^3 \rho}{\partial x^3}\right)\right] + D - E\rho_m - F(1+\varphi^2)\rho^3 \tag{2}$$

where n indicates the number of dislocation spacing, v the gliding rate of dislocations, ρ the total dislocation density, ρ_g the difference between the densities of the positive and negative dislocations, which is expressed as[17, 18]:

$$\frac{\partial \rho_g}{\partial t} = \frac{\partial(\rho_m v)}{\partial x} \tag{3}$$

The factors ψ and φ are as follows:

$$\psi = \frac{\rho_0}{\rho} \tag{4}$$

$$\varphi = \frac{|\bar{\rho}_g|}{\rho_{\max}} \tag{5}$$

B, D, E and F are coefficients.

In the process of plastic deformation, the compatibility condition should be satisfied, as follows[16]:

$$\dot{\gamma} = \frac{\dot{\tau}_e}{G} + b\rho_m v \tag{6}$$

where $\dot{\tau}_e$ is the derivative of effective shear stress τ_e with respect to time, G the shear modulus, v the gliding rate of dislocations. That is to say, at any given local place, the total strain rate is the sum of elastic and plastic strain rate. Based on Eqns. (2-6), a qualitative study of the evolution of cell structure can be made, and some interesting results can be obtained.

3 MECHANISM OF EVOLUTION OF DISLOCATION ARRANGEMENT AND LOWER LIMIT SIZE OF CELL STRUCTURE

The established model is a nonlinear partial differential equation, which contains some unknown coefficients. Therefore, it is difficult to obtain a theoretical solution by using this model. However, we can make a linear stability analysis to achieve some interesting results and to obtain a good understanding of the evolution process. It is known that dislocations tend to form ordered structures of alternative appearing of high and low dislocation density zones. Therefore, we can express the function of spatio-temporal distribution of dislocation by using Fourier expansion. Assuming the investigated system length to be $2l$, the solution of the model can be considered as the superposition of an initial dislocation density ρ_0 and a number of dislocation density waves[15-17]:

$$\rho = \rho_0 + \sum_{i=1}^{\infty} C_i \cos\frac{i\pi x}{l} \tag{7}$$

where C_i is the amplitude of the waves. Substituting Eqn. (7) into Eqn. (2), and taking into account the orthogonality relations of the trigonometric function, we can obtain a set of equations as follows:

$$\dot{C}_j = \omega_j C_j + \xi \tag{8}$$

where ξ is a trivial term that does not affect the evolution of the system.

$$\omega_j = \left[\frac{12B\psi\pi^2}{l^2} + \frac{s\pi^2}{2l^2\rho_0^3}\left(\frac{\dot{\gamma}\sqrt{\rho_0}}{b} - \frac{\dot{\rho}_0}{2}\right)\right] j^2 - \frac{B\psi n^2\pi^2}{l^4\rho_0} j^4 - 2F\rho_0 \tag{9}$$

The characters of the system are mainly determined by the value and variation of ω_j[17]. When ω_j is negative, the system remains stable. Otherwise, the system will lose its stability. Since different j corresponds to different ω_j, it is significant to know the change of ω_j with j as well as which j is the dominant wave number. Let

$$\frac{\partial \omega_j}{\partial j^2} = 0 \tag{10}$$

Then

$$j_d^2 = \left[12B\psi\rho_0 + \frac{s}{2\rho_0^3}\left(\frac{\dot{\gamma}\sqrt{\rho_0}}{b} - \frac{\dot{\rho}_0}{2}\right)\right]\frac{l^2}{2B\psi n^2\pi^2} \tag{11}$$

where j_d denotes the dominant wave number, s the ratio of the effective and the threshold stresses.

In general $\rho_0 \geqslant 10^7\ \mathrm{m}^{-2}$, the magnitude of b is in the order of 10^{-10} m, s in the order of 1, $\psi \approx 1$. If the strain rate is in the range of $1-10^{-4}\ \mathrm{s}^{-1}$, the second term in the brackets of Eqn. (11) can be

neglected. Thus

$$j_b = \frac{l\sqrt{6\rho_0}}{n\pi} \tag{12}$$

The critical dislocation density corresponding to the dominant wave number j_d is as follows:

$$\rho_c = \frac{2}{3}\left[\frac{n\pi j_d}{2l}\right]^2 \tag{13}$$

Eqns. (12) and(13) are helpful to understanding the evolution of the cell structure, which will be discussed later. It is reasonable to consider the cell size to be the dominant wavelength. Then the subsequent cells will have the size

$$d_{sub} = \frac{2l}{j_d} = \frac{2n\pi}{\sqrt{6\rho_0}} \tag{14}$$

Since the elastic interactions between dislocations will be screened beyond a critical distance(assumed here n times the average dislocation distance)[17, 19], n might be as small as one with regard to a high dislocation density. Therefore, the minimum size of cells or subgrains is

$$d_{min} = \frac{2\pi}{\sqrt{6\rho_{cmax}}} \tag{15}$$

where ρ_{cmax} denotes the maximum dislocation density in cell interiors. For cold-deformed metals, the dislocation density in cell walls can reach the order of 10^{16} m^{-2}, and in cell interiors the order of 10^{14} m^{-2}. Then the minimum size reached by SPD is 115 nm(corresponding to $\rho_{cmax} = 5 \times 10^{14}$ m^{-2}).

4 DISCUSSION

When we ignore the interaction existing in the system, i. e. the term in the right-hand side of Eqn. (1) or the last three terms of Eqn. (2), we can also obtain the above results, i. e. Eqns. (12 – 15). This facilitates the whole derivation process. This result is consistent with that of Holt[11].

It is shown from Eqn. (12) that the dominant wave number j_d is only dependent on the system length and the dislocation density. The larger the system length is, the larger the dominant wave number will be, i. e. the more the cells will be. For a given deformation, as the dislocation density increases, the smaller dominant wave number j_d will appear at first. Hence, the cell number increases with strain up to a steady value. If we consider $2l$ as the diameter of the initial grain size, the cell forming condition can readily be satisfied in large grains. When the grain sizes are smaller than a critical value, cells will not be formed further. Therefore, we can say that in any plastic deformation there exists a lower limit size for cells. It is obvious that the grain sizes obtained by SPD techniques cannot break through this limit too.

With regard to SPD-copper with the grain size of 200 – 250 nm undergoing fatigue deformation, the stress applied must be smaller than that in the SPD process. Taking into account the features of deformation, the dislocation density during fatigue cannot exceed that in SPD. In terms of Eqn. (14), the cells cannot be formed in the existing grains. This is in consistence with Ref. [1]. Another similar example is superplastic deformation[16]. Because of its high straining temperature and its low strain rate, the produced dislocations disappear readily. Thus, the dislocation density is very low in the interiors of the grains, and cells cannot be formed.

In terms of Eqns. (12 – 15) as well as the discussion above, it is obvious that the generation of cells(or subgrains) does not depend on the physical parameters of the materials, only on a structural parameter, i. e. the dislocation density. This reflects a general character of materials. Therefore, we can study the microstructural properties based on the combination of dislocation theory with synergetics. This is the fundamental approach to predict the microstructural behavior.

5 CONCLUSIONS

1) The formulae for dominant wave number j_d, critical dislocation density ρ_c and lower limit size d_{min} are generally applicable to materials.

2) It is hard to achieve a grain size smaller than 100 nm for materials deformed by severe plastic deformation.

3) When a SPD material undergoes fatigue deformation, cells are hardly formed in the interior of grains or preexisting cells or subgrains.

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