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Evaluation of mobile dislocation density based on distribution function of dislocation segments①

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Abstract: A function is offered to represent the distribution of reduced length of dislocation segments. The segment distribution of materials, e. g., MgO and Cu, can be well described by taking appropriate values of parameters m and n. Based on this function, a model for evaluating the mobile dislocation density is developed. Provided the total dislocation density and applied stress are known, the mobile dislocation density could be readily assessed by using this model. For pure copper the mobile dislocation density and strain rates at deferent strains are evaluated. The calculated results are consistent with the known experimental data.

Key words: mobile dislocation; dislocation segment; distribution function
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1 INTRODUCTION

Mobile dislocation density is an important parameter in the study of plasticity, especially in the study of dislocation patterning[1-4]. Many researchers have done their best to this subject, and developed models to assess the mobile dislocation density[5-11]. Since both the mobile dislocation density and its velocity are dependent on the applied stress and total dislocation density, it is difficult to determine their exact magnitudes. In the past years, there have been some publications concerning the direct measurement of mobile dislocations and its velocity[12-14]. However, these studies are only limited to some special materials, e. g., ionic crystals or metals deformed in the superconducting state (at much low temperature). As for the common metals deformed at room and high temperatures, the mobile dislocation density is still hard to be directly measured, and generally studied by indirect method. Therefore, this subject is so far still opening for research[15, 16].

In this paper, a simple function is offered to describe the distribution of dislocation segments. Based on this function, a model for evaluating the mobile dislocation density is derived. And the theoretical calculation for MgO and pure copper are compared with the known experimental.

2 MODEL

As described by former researchers, dislocations in metals can be assumed to be links or segments. When the effective shear stress acting on a segment exceeds a critical value, it will become mobile. Thus

$$l_c \geqslant \alpha G b / \tau_e \tag{1}$$

where l_c is the critical length of dislocation segments, α is a coefficient close to unity, G is the shear modulus, b is the Burgers vector, τ_e is the effective stress that is the sum of applied stress τ_a and the long internal stress τ_i:

$$\tau_e = \tau_a + \tau_i \tag{2}$$

For simplicity, we only consider the reduced length of dislocation segments which is defined as

$$x = l / L_{avg} \tag{3}$$

where l is the length of the dislocation segment and L_{avg} is the average length of dislocation segments. We expect to use a function, $\Phi(x)$, to describe the distribution of dislocation segments, and $\Phi(x)\,dx$ to express the probability that segments have the reduced length between x and $x + dx$. It is obviously that $\Phi(x)$ should satisfy the following conditions:

$$\left.\begin{array}{l} \Phi(0) = 0 \\ \Phi(+\infty) = 0 \\ \int_0^{+\infty} \Phi(x)\,dx = 1 \\ 0 \leqslant \Phi(x) \leqslant 1 \end{array}\right\} \tag{4}$$

As we know, a complex function can be approximately expressed by using Taylor expansion. Therefore, $\Phi(x)$ could take the form of the power function. A simple integrable function satisfying the above conditions is

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$$\Phi(x)=(m+1)(n-1)x^{m}(1+x^{m+1})^{-n} \quad (5)$$

where m and n are positive constants for specific metals. Function $\Phi(x)$ has the maximum extreme value at point x_p in $(0, +\infty)$:

$$\left.\begin{aligned} x_p &= \left[\frac{n}{m}+n-1\right]^{-\frac{1}{m+1}} \\ \Phi_{max} &= \frac{(m+1)(n-1)}{\left[\frac{n}{m}+n-1\right]^{\frac{m}{m+1}}\left[1+\left[\frac{n}{m}+n-1\right]^{-1}\right]^{n}} \end{aligned}\right\} \quad (6)$$

According to the definition of $\Phi(x)$, we have

$$\left.\begin{aligned} \rho'_m &= \int_{x_c}^{+\infty} x\,\Phi(x)\,dx \\ \rho'_i &= \int_0^{x_c} x\,\Phi(x)\,dx \\ \rho' &= \int_0^{+\infty} x\,\Phi(x)\,dx \end{aligned}\right\} \quad (7)$$

where $\rho'_m=\rho_m/L_{avg}$, $\rho'_i=\rho_i/L_{avg}$, $\rho'=\rho/L_{avg}$ and $x_c=l_c/L_{avg}$. Therefore, the ratio of mobile dislocation density to total dislocation density is

$$\frac{\rho_m}{\rho}=1-\frac{\rho'_i}{\rho'} \quad (8)$$

and the average dislocation segment length is

$$L_{avg}=\frac{\rho}{(m+1)(n-1)\int_0^{+\infty} x^{m+1}(1+x^{m+1})^{-n}dx} \quad (9)$$

Substituting Eqns. (5) and (7) into Eqn. (8) yields

$$\frac{\rho_m}{\rho}=1-\frac{\int_0^{x_c} x^{m+1}(1+x^{m+1})^{-n}dx}{\int_0^{+\infty} x^{m+1}(1+x^{m+1})^{-n}dx} \quad (10)$$

Provided m and n are integers, we can explicitly write the expression of the integral in Eqn. (10). If n is a rational number, it can be expressed as the form:

$$n=n_1/n_2 \quad (11)$$

where n_1 and n_2 are mutually prime numbers.

Thus Eqn. (10) can be expressed as the following form:

$$\frac{\rho_m}{\rho}=1-\frac{\int_{(1+1/x_c)^{1/n_2}}^{+\infty} t^{n_2-n_1-1}(t^{n_2}-1)^{-p}dt}{\int_0^{+\infty} t^{n_2-n_1-1}(t^{n_2}-1)^{-p}dt} \quad (12)$$

where $p=\frac{1}{m+1}-n+2$, $t=\left[1+\frac{1}{x}\right]^{\frac{1}{n_2}}$. If p is integer, integral in Eqn. (12) can be explicitly expressed. It is easy to verify that only p takes 0 or 1 will the following conditions be satisfied:

$$\left.\begin{aligned} & n+n/m-1>0 \\ & n>1 \\ & m+n/m-3<0 \\ & \Phi_{max}<1 \end{aligned}\right\} \quad (13)$$

Hence, Eqn. (12) can be expressed as follows:

$$\frac{\rho_m}{\rho}=\begin{cases} 1-\left[1+\frac{1}{x_c}\right]^{1-n} & (p=0) \\ 1-\frac{\int_{(1+1/x_c)^{1/n_2}}^{+\infty} t^{n_2-n_1-1}(t^{n_2}-1)^{-p}dt}{\int_0^{+\infty} t^{n_2-n_1-1}(t^{n_2}-1)^{-p}dt} & (p=1) \end{cases} \quad (14)$$

Eqn. (5) is the basic distribution function and Eqn. (10) is the model for predicting the mobile dislocation density.

3 APPLICATIONS

3.1 Distribution of dislocation segments

Function $\Phi(x)$ expresses the distribution of dislocation segments. It will not vary with strain and temperature for a specific metal. Figs. 1 and 2 show the theoretical curves of $\Phi(x)$ for $p=0$ and 1, respectively. It is shown that the larger the magnitude of m, the further the peak of the curve approaches to the right-hand side. If m is fixed and the value of n increases, the peak value of $\Phi(x)$ also increases and the distribution of x tends to less spread. Figs. 3 and 4 show the comparison of present modeling with the theoretical distribution in Ref. [7]:

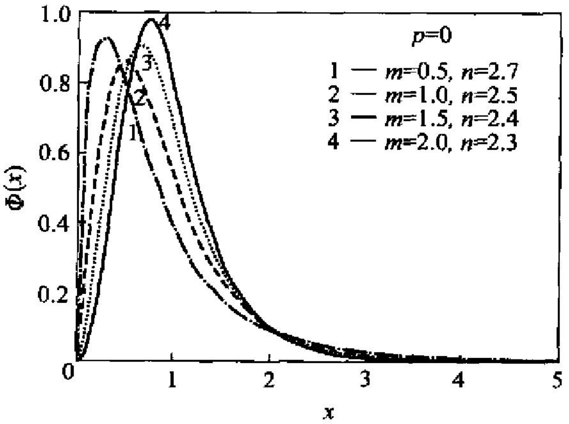

Fig. 1 Theoretical curves of dislocation segment distributions for $p=0$

$$L_{avg}\Phi(L)=\frac{k^{k+1}}{k!}\left[\frac{L}{L_{avg}}\right]^{k-1}\exp\left[-k\frac{L}{L_{avg}}\right] \quad (15)$$

and the experimental results for MgO and pure copper[15], respectively. It is shown that the present function gives a better description of the distribution of dislocation segments. The peak reduced length of dislocation segments corresponding to the maximum value of $\Phi(x)$ predicted by the model of Ref. [7] seems to be larger than the experimental result for MgO (Fig. 3). While the curve predicted by present model is closer to the experimental points.

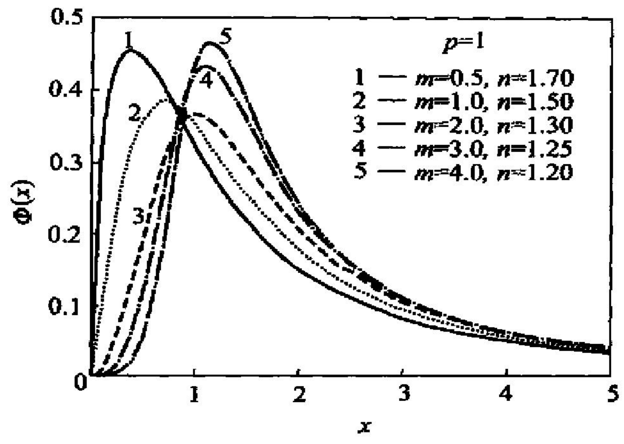

Fig. 2 Theoretical curves of dislocation segment distributions for $p = 1$

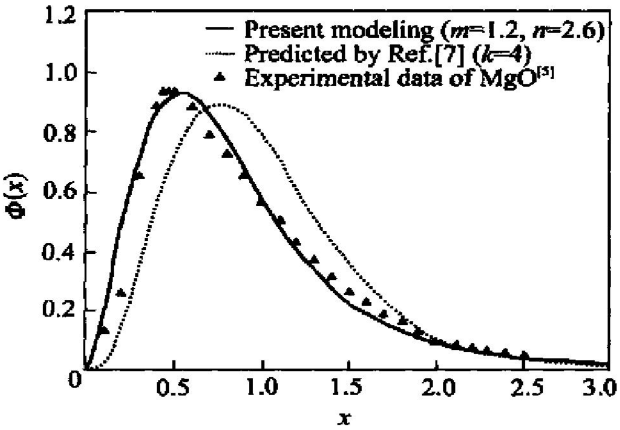

Fig. 3 Comparison of present modeling for MgO with experimental results and modeling by Ref. [7]

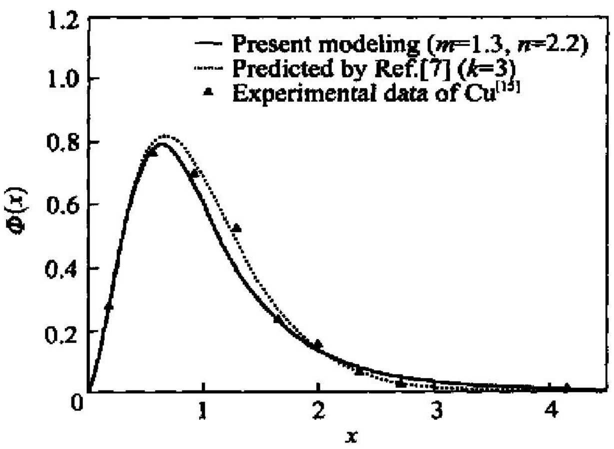

Fig. 4 Comparison of present modeling for Cu with experimental results and modeling by Ref. [7]

3.2 Mobile dislocation density

By using Eqns. (10) and (14), mobile dislocation density could be quantitatively evaluated provided an appropriate critical value x_c is chosen.

In order to verify the correctness of the model, we calculated a set of experimental data for pure copper (in Ref. [15]). Since the plastic deformation is in the range of primary strain and the dislocations are nearly randomly distributed, we can use the following experimental law to calculate the average dislocation velocity[7, 10, 15]:

$$v = v_0 \left(\frac{\tau_e}{\tau_0} \right)^{n'} \qquad (16)$$

The mobile dislocatlon density can be calculated out by using Eqn. (10). The strain rate, $\dot{\varepsilon}$, can also be obtained using Taylor-Orowan equation, $\dot{\varepsilon} = \alpha G b \rho_m v$. The original data used for pure copper are listed in Table 1. The experimental strain rate is about $10^{-4}\ s^{-1}$. The experimentally determined parameters[11] and the calculated results are listed in Table 2. It is obviously that the calculated strain rates are of the order of $10^{-4}\ s^{-1}$, which is consistent with the experiments.

Table 1 Initial data for simulation of pure copper

G/Pa	b/m	v_0/(m·s^{-1})	τ_0	n'
4.11×10^{10}	2.5×10^{-10}	1.0	2.7×10^{5}	1

Table 2 Calculated results for pure copper

τ_a/Pa	ρ/m^{-2}	ρ_m/m^{-2}	v/(m·s^{-1})	$\dot{\varepsilon}$/s^{-1}
8.9×10^{5}	2.3×10^{11}	2.0×10^{6}	3.1	7.3×10^{-4}
6.2×10^{5}	9.2×10^{10}	1.1×10^{6}	2.2	2.7×10^{-4}
4.8×10^{5}	3.4×10^{10}	8.0×10^{5}	1.7	1.6×10^{-4}
3.8×10^{5}	1.1×10^{10}	6.6×10^{5}	1.4	1.1×10^{-4}
3.0×10^{5}	5.4×10^{10}	4.5×10^{5}	1.1	5.8×10^{-5}

4 DISCUSSION

$\Phi(x)$ could be employed to represent the distribution of dislocation segments. The theoretical curves are shown in Figs. 1 and 2. Compared to the description of former researchers, this function is simple and conforms to the experimental points provided appropriate values of m and n are known.

It can be seen from Table 2 that the calculated strain is not exactly equal to $10^{-4}\ s^{-1}$. This might result from the real experimental velocity being larger under lower shear stress but slightly smaller under larger shear stress than that predicted by the theoretical model (Eqn. (16)) for pure copper[16]. Thus the calculated mobile dislocation density might be in the acceptable range.

It should be noted that the real segments must have the maximum and minimum length. While in the present model the maximum value takes infinity and the minimum 0. The assumption may not greatly affect the final results of mobile dislocation density.

Since the area between the curve and the coordinate axis x in the range $(0, x_{\min})$ may be approximately equivalent to that in $(x_{\max}, +\infty)$. Thus their contribution to the assessment of mobile fraction may approximately be canceled.

As shown in Figs. 3 and 4, the distribution of segments may not be the same for different metals. We can get a required distribution by choosing proper m and n. It is expected m and n to be determined by some natural parameters of materials, which is still under investigation.

The model for the prediction of mobile dislocation density is only dependent on the total dislocation density and applied shear stress for a given distribution function. This means that the mobile dislocation density is not relevant to the deformation history in the present model. This does not contradict to the general thought. For any plastic deformation, we can introduce the mechanisms, e. g., dynamic recovery and dynamic recrystallization, to the deformation model. The total dislocation density will vary with strain and the mobile dislocation density could be evaluated.

This model is established on the basis of randomly distributed dislocations. In many plastic deformation of metals, dislocations tend to form cells that are characterized by the alternately appearing of low dislocation density zone (cell interiors) and high density zone (cell walls). In the cell interiors dislocations can be viewed as randomly distributed, thus this model will be assumed to be suitable. While in cell walls, the mobility of dislocation is very small. If the dislocations in cell walls are all immobile, then the strain in these regions will be zero. Therefore, we think that mobile dislocations could also appear in cell walls. Although the dislocation density is very high in cell walls, the mobile density is still in small fraction because of much lower effective stress. This seems to be the real cases.

5 CONCLUSIONS

1) Function $\Phi(x) = (m+1)(n-1)x^m(1+x^{m+1-n})$ can be employed to describe the distribution of dislocation segments by choosing appropriate magnitude of parameters m and n.

2) Eqns. (10) and (14) can be employed to evaluate the mobile dislocation density provided the total dislocation density and applied shear stress are known.

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