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CALCULATION OF THE INTERACTION ENERGY OF THE TWINNING DISLOCATIONS OF A WEDGE TWIN BASED ON THE MESOSCOPIC DISLOCATION MODEL

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The energy of interaction of the twinning dislocations in a wedge crystal twin was calculated based on the mesoscopic dislocation model. It has been established that the interaction energy of the twinning dislocations increases moderately with increase in the length of the twin. It is shown that the dependence of the interaction energy of the twinning dislocations on the width of the twin is near-parabolic.

Keywords: *twinning, twinning dislocation, mesoscopic dislocation model, interaction energy.*

Introduction. The twinning effect should be taken into account in investigating the plastic deformation of metals, such as copper, thin, bismuth, siliceous iron, and titanium. By now voluminous material on experimental investigation of this effect has accumulated in the literature [1–5]. However, a consistent theory on the twinning effect that would make it possible to describe the twinning of crystals in full measure with account for all its features has not been developed to this point. The existing theory of a thin twin [1, 6] gives no way of investigating the stressed state inside a crystal twin and calculating the deformation and stress near its boundaries with a high degree of accuracy [7–9]. Therefore, at present there is a need for further development of the twinning theory. In this connection, the development of the method for calculation of the interaction energy of the twinning dislocations in a wedge twin seems to be a pressing problem. The solution of this problem is the aim of the present work.

Formulation of the Problem and Its Solution. According to the Nabarro formula, the energy of interaction of two dislocations with Burgers vectors $\mathbf{b}_1$ and $\mathbf{b}_2$ per unit length of a dislocation (L_d) can be defined in the following way [10]:

$$\frac{W_{int}}{L_d} = -\frac{\mu (\mathbf{b}_1 \cdot \boldsymbol{\xi}) (\mathbf{b}_2 \cdot \boldsymbol{\xi})}{2\pi} \ln \frac{R}{R_\alpha} - \frac{\mu}{2\pi (1-\nu)} \left[(\mathbf{b}_1 \times \boldsymbol{\xi}) \cdot (\mathbf{b}_2 \times \boldsymbol{\xi}) \right] \ln \frac{R}{R_\alpha}$$

$$- \frac{\mu}{2\pi (1-\nu) R^2} \left[(\mathbf{b}_1 \times \boldsymbol{\xi}) \cdot \mathbf{R} \right] \left[(\mathbf{b}_2 \times \boldsymbol{\xi}) \cdot \mathbf{R} \right] . \quad (1)$$

The twinning dislocations represent partial Shockley dislocations [10]. Therefore, their Burgers vector can be decomposed into two components: the spiral component ($\mathbf{b}_{sp}$) and the boundary one ($\mathbf{b}_b$) [8, 10]. It is easy to show that, in this case, Eq. (1) for two interacting twinning dislocations is transformed into a set of relations:

$$\frac{W_{int}^{b}}{L_d} = -\frac{\mu b_b^2}{2\pi (1-\nu)} \ln \frac{R}{R_\alpha} , \quad (2)$$

$$\frac{W_{int}^{sp}}{L_d} = -\frac{\mu b_{sp}^2}{2\pi} \ln \frac{R}{R_\alpha} . \quad (3)$$

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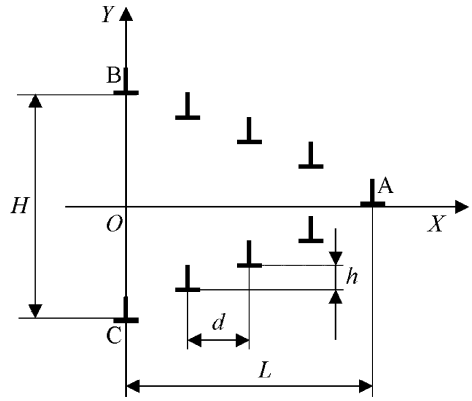

Fig. 1. Diagrammatic representation of a wedge twin in the mesoscopic scale: A denotes the peak of the wedge twin; B and C are the points of its intersection with the axis.

For determining the interaction energy of the twinning dislocations in a wedge twin of length L with a width H at the mouth, we will consider this twin as a set of dislocations, the distribution of which along the boundaries of the twin is shown in Fig. 1. In this case, the interaction energy of the twinning dislocations will be determined as the sum of the energies of interaction of the dislocations found at each twin boundary $\left(\frac{W_{\rm int}^{\rm b(1)}}{\sum L_{\rm d}} + \frac{W_{\rm int}^{\rm sp(1)}}{\sum L_{\rm d}}\right)$ and the energies of interaction of the dislocations found at the opposite boundaries of the twin $\left(\frac{W_{\rm int}^{\rm b(2)}}{\sum L_{\rm d}} + \frac{W_{\rm int}^{\rm sp(2)}}{\sum L_{\rm d}}\right)$. Thus, we obtain

$$\frac{W_{\rm int}}{\sum L_{\rm d}} = \frac{W_{\rm int}^{\rm b(1)}}{\sum L_{\rm d}} + \frac{W_{\rm int}^{\rm b(2)}}{\sum L_{\rm d}} + \frac{W_{\rm int}^{\rm sp(1)}}{\sum L_{\rm d}} + \frac{W_{\rm int}^{\rm sp(2)}}{\sum L_{\rm d}}. \tag{4}$$

Assuming that $R_\alpha = b_{\rm b}$, from (2) we have

$$\frac{W_{\rm int}^{\rm b(1)}}{\sum L_{\rm d}} = -\frac{\mu b_{\rm b}^2}{\pi(1-\nu)}\left\{\sum_{i=1}^{N-1} \ln\frac{i\sqrt{d^2+h^2}}{b_{\rm b}} + \sum_{i=1}^{N-2} \ln\frac{i\sqrt{d^2+h^2}}{b_{\rm b}} + \ldots + \sum_{i=1}^{N-M} \ln\frac{i\sqrt{d^2+h^2}}{b_{\rm b}}\right\}, \tag{5}$$

$$\frac{W_{\rm int}^{\rm b(2)}}{\sum L_{\rm d}} = -\frac{\mu b_{\rm b}^2}{2\pi(1-\nu)}\sum_{j=1}^{M}\sum_{i=1}^{N-1} \ln\frac{2jh + \sqrt{(id)^2 + ((2j+i)\,h)^2}}{b_{\rm b}}. \tag{6}$$

Relations (5) and (6) were obtained from (2) on the assumption that $R = \sqrt{d^2+h^2}$. Analogously, assuming that $R_\alpha = b_{\rm sp}$ in (3), we obtain

$$\frac{W_{\rm int}^{\rm sp(1)}}{\sum L_{\rm d}} = -\frac{\mu b_{\rm sp}^2}{\pi}\left\{\sum_{i=1}^{N-1} \ln\frac{i\sqrt{d^2+h^2}}{b_{\rm sp}} + \sum_{i=1}^{N-2} \ln\frac{i\sqrt{d^2+h^2}}{b_{\rm sp}} + \ldots + \sum_{i=1}^{N-M} \ln\frac{i\sqrt{d^2+h^2}}{b_{\rm sp}}\right\}, \tag{7}$$

$$\frac{W_{\rm int}^{\rm sp(2)}}{\sum L_{\rm d}} = -\frac{\mu b_{\rm sp}^2}{2\pi}\sum_{j=1}^{M}\sum_{i=1}^{N-1} \ln\frac{2jh + \sqrt{(id)^2 + ((2j+i)\,h)^2}}{b_{\rm sp}}. \tag{8}$$

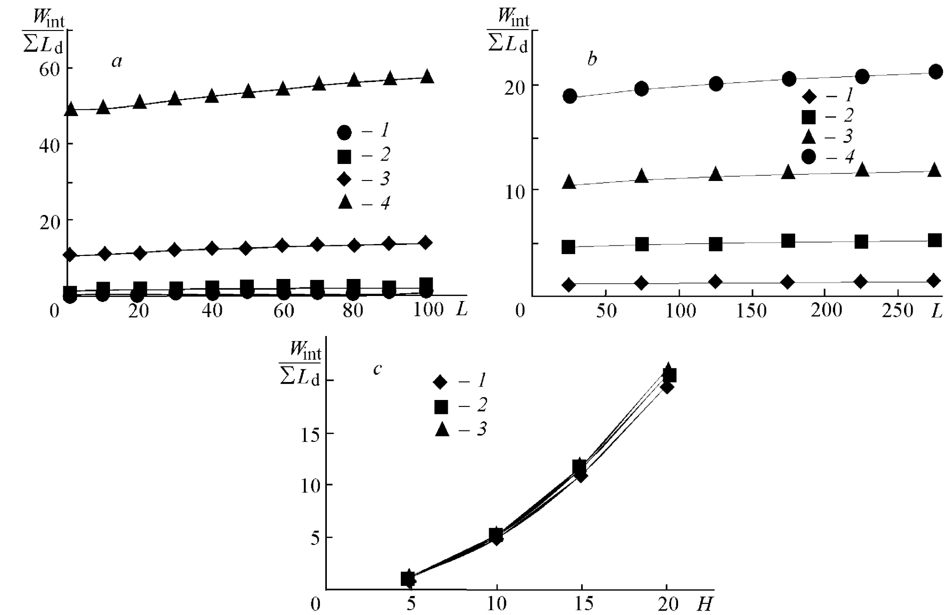

Fig. 2. Dependence of the interaction energy of the dislocations in a wedge nanotwin (a) and in a wedge microtwin (b) on their length and dependence of the interaction energy of the dislocations in a wedge microtwin on its width (c): a) H = 5 nm, N = 10 (1); H = 10 nm (1), N = 20 (2); H = 25 nm, N = 50 (3); H = 50 nm, N = 100 (4); b) H = 5 μm, $N = 1{\cdot}10^4$ (1); H = 10 μm, $N = 2{\cdot}10^4$ (2); H = 15 μm, $N = 3{\cdot}10^4$ (3); H = 20 μm, $N = 4{\cdot}10^4$ (4); c) L = 100 (1), 200 (2), and 300 μm (3). $\left|\frac{W_{int}(L)}{\sum L_d}\right|$, $\frac{\mu J}{m}$; L, nm (a); μm (b); H, μm (c).

Results and Its Discussion. Relations (5) and (7) can be transformed into the form more convenient for analysis

$$\frac{W_{int}^{b(1)}}{\sum L_d} = -\frac{\mu b_b^2}{\pi(1-\nu)} \sum_{i=1}^{N} (N-i) \ln \frac{i\sqrt{d^2+h^2}}{b_b}, \tag{9}$$

$$\frac{W_{int}^{sp(1)}}{\sum L_d} = -\frac{\mu b_{sp}^2}{\pi} \sum_{i=1}^{N} (N-i) \ln \frac{i\sqrt{d^2+h^2}}{b_{sp}}. \tag{10}$$

Then Eq. (4) will take the form

$$\frac{W_{int}}{\sum L_d} = -\left[\frac{\mu}{\pi}\left(\frac{b_b^2}{1-\nu}\sum_{i=1}^{N}(N-i)\ln\frac{i\sqrt{L^2+\frac{H^2}{4}}}{b_b(N-1)} + b_{sp}^2\sum_{i=1}^{N}(N-i)\ln\frac{i\sqrt{L^2+\frac{H^2}{4}}}{b_{sp}(N-1)}\right)\right.$$
$$\left.+\frac{\mu}{2\pi}\left(\frac{b_b^2}{1-\nu}\sum_{j=1}^{N-1}\sum_{i=1}^{N-1}\ln\frac{jH+\sqrt{(iL)^2+\left(\frac{2j+i}{2}H\right)^2}}{b_b(N-1)} + b_{sp}^2\sum_{j=1}^{N-1}\sum_{i=1}^{N-1}\ln\frac{jH+\sqrt{(iL)^2+\left(\frac{2j+i}{2}H\right)^2}}{b_{sp}(N-1)}\right)\right]. \tag{11}$$

In this relation

$$d = \frac{L}{N-1} \quad \text{and} \quad h = \frac{H}{2\,(N-1)}\,. \tag{12}$$

In the majority of experiments, wedge twins were detected; for them the relation $H < L$ is true. However, at the initial stage of development of twins, a situation where $H > L$ can take place.

The calculations were carried out for iron on the assumption that $b_{sp} = b_b = 0.124$ nm [11], $\mu = 81$ GPa, and $\nu = 0.29$ [12]. The number of dislocations at the twin boundary was determined by the formula

$$N = \frac{H}{2a}\,, \tag{13}$$

where $a = 0.25$ nm [11].

The results of the calculations are shown in Fig. 2. It should be noted that, at the initial stage of development of a twin, an increase in its length ($L < 100$ nm) causes the interaction energy of the twinning dislocations to increase insignificantly. The calculation results shown in Fig. 2a illustrate the situation where $H > L$, typical of nanotwins considered in [13]. In these stages of development of the twin, where $H > L$, the rate of increase in the interaction energy of the dislocations is larger than that at the stages where $H < L$. This manifests itself as a somewhat increased slope of the graph $\left|\frac{W_{\text{int}}(L)}{\sum L_d}\right|$ at the stages where $H > L$ as compared to that at the stages where $H < L$ (see Fig. 2a).

Figure 2b shows the results of calculation of the interaction energy of the twinning dislocations in microtwins detected frequently in experiments [1–9, 14–16]. It should be noted that an increase in the width of a twin at its mouth by three orders of magnitude leads to an increase in the summary energy of interaction of the twinning dislocations by six orders of magnitude (see Fig. 2a and b). As in the case of nanotwins, the interaction energy of the twinning dislocations in wedge microtwins increases with increase in their length. This dependence takes a more and more pronounced nonlinear form as the length of the twins increases. An increase in the width of a twin at its mouth leads to a sharp increase in the interaction energy of the twinning dislocations (Fig. 2c). In this case, the dependence of this energy on the width of the twin has a near-parabolic form. The length of twins markedly influences the difference between the graphs presented in Fig. 2c only in the case where it takes a large value (of the order of 300 μm).

Conclusions. A mesoscopic dislocation model of a wedge twin has been proposed. On the basis of this model, the energy of interaction of the dislocations in this twin was calculated. It has been established that the interaction energy of the twinning dislocations increases insignificantly with increase in the length of the twin. When the width of the twin at its mouth increases by three orders of magnitude, the summary interaction energy of the twinning dislocations increases by six orders of magnitude. The dependence of the interaction energy of the twinning dislocations on the width of the twin has a near-parabolic form.

NOTATION

a, interatomic distance in the twinning plane; b_{sp}, b_b, moduli of vectors; $\mathbf{b}_1$ and $\mathbf{b}_2$, Burgers vectors of two dislocations interacting with each other; $\mathbf{b}_{sp}$, $\mathbf{b}_b$, spiral and boundary components of the Burgers vectors of the twinning dislocations; d, h, projections on the OX and OY axes of the segment connecting two neighboring twinning dislocations; i and j, indices of summation; H, width of a wedge twin at its mouth; L, length of a wedge twin; L_d, length of a unit dislocation; $\sum L_d$, total length of all the dislocations of the wedge twin; N, number of twinning dislocations at the twin boundaries ($M = N - 1$); R, distance between the twinning dislocations; R_α, small parameter having the dimensions of length; W_{int}, energy of interaction of two dislocations; $W_{\text{int}}/\sum L_d$, ratio of the interaction energy of the dislocations in a wedge twin to their summary length; $W_{\text{int}}^{\text{sp}}$, energy of interaction of the spiral components of the twinning dislocations; $W_{\text{int}}^{\text{b}}$, energy of interaction of the boundary component of the twinning dislocations; $W_{\text{int}}^{\text{sp(1)}}$, $W_{\text{int}}^{\text{b(1)}}$, energy of interaction of the twinning dislocations found at one and the same twinning boundary; $W_{\text{int}}^{\text{sp(2)}}$, $W_{\text{int}}^{\text{b(2)}}$, energy of interaction of the twinning dislocations found at different twinning boundaries; ξ, vector directed along the dislocation line; μ, rigidity modulus; ν, Poisson ratio. Subscripts: sp, spiral; b, boundary; d, dislocation; int, interaction; α, distinctive index.

REFERENCES

1. M. V. Klassen-Neklyudova, *Mechnical Twinning of Crystals* [in Russian], Izd. AN SSSR, Moscow (1960).
2. V. M. Finkel', V. A. Fedorov, and A. P. Korolev, *Destruction of Crystals in Mechanical Twinning* [in Russian], Izd. Rostov Univ., Rostov-on-Don (1990).
3. O. M. Ostrikov and S. N. Dub, Investigation of the mechanical twinning of antimony single crystals by nanoindentation, *Inzh.-Fiz. Zh.*, **76**, No. 1, 170–172 (2003).
4. O. M. Ostrikov, Use of polyparaxylylene thin films in investigation of plastic deformation of the single crystals of bismuth, *Prikl. Mekh. Tekh. Fiz.*, **47**, No. 4, 162–166 (2006).
5. V. S. Savenko, V. V. Uglov, O. M. Ostrikov, and A. P. Khodoskin, Influence of electric current pulses on the twinning of the single crystals of bismuth irradiated by carbon ions, *Fiz. Metal. Metalloved.*, **85**, No. 5, 96–105 (1998).
6. A. M. Kosevich and V. S. Boiko, The dislocation theory of elastic twinning, *Usp. Fiz. Nauk*, **104**, No. 2, 201–254 (1971).
7. O. M. Ostrikov, Dislocation of the alloy component in polysynthetic twins and the theoretical prediction of the formation of lamellar materials using the phenomenon of polysynthetic twinning, *Mater. Tekhn. Instr.*, **11**, No. 3, 54–56 (2006).
8. O. M. Ostrikov, Dislocation macroscopic model of a wedge twin, *Vestn. GGTU im P. O. Sukhogo*, No. 2, 10–18 (2006).
9. O. M. Ostrikov, Stressed state near the apex of a wedge twin, *Mekh. Tverd. Tela*, No. 2, 104–113 (2004).
10. J. P. Hirth and J. Lothe, *Theory of Dislocations* [Russian translation], Atomizdat, Moscow (1972).
11. I. I. Novikov and K. M. Rozin, *Crystallography and Defects of a Crystal Lattice* [in Russian], Metallurgiya, Moscow (1990).
12. I. E. Irodov, *Problems of General Physics* [in Russian], Nauka, Moscow (1979).
13. O. M. Ostrikov, Nanotwinning of bismuth single crystals, *Izv. Vyssh. Uchebn. Zaved.*, *Chern. Metallurgiya*, No. 3, 51–52 (2002).
14. O. M. Ostrikov, Comparative analysis of the laws governing the development of shear-plastic deformation in amorphous and single-crystal materials under local batched deformation of their surfaces, *Izv. Vyssh. Uchebn. Zaved.*, *Chern. Metallurgiya*, No. 12, 18–21 (2006).
15. O. M. Ostrikov, Shape of wedge twins in locally deformed ion-implanted single crystals of bismuth, *Izv. Vyssh. Uchebn. Zaved.*, *Chern. Metallurgiya*, No. 9, 5–7 (2006).
16. O. M. Ostrikov, Effect of irradiation by boron ions on the character of realization of twinning and slip under prolonged (more than 60 sec) loading of single crystals of bismuth, *Inzh.-Fiz. Zh.*, **72**, No. 5, 967–970 (1999).