M. Y. BOSIN, Y. P. GOMOZOV, T. G. DRYGACH

MATHEMATICAL MODEL OF THE DEVELOPMENT OF A SINGLE TWIN LAYER IN METAL CRYSTALS

By analyzing the experimental data available in the scientific literature, a mathematical model of the development of a single twin layer in metal crystals has been obtained. The model has the form of a differential equation, the order of which is determined by the required accuracy of obtaining the results associated with the solution of this equation. Even in the linear approximation of one of the main parameters of the phenomenological model, the latter gives qualitatively the same dependences of the development of single twins under different loading conditions compared to the experiment. Despite a large number of experimental works devoted to twinning, there is still no rigorous quantitative theory of the development of twinning layers in different media and under different conditions. However, in these works, the mathematical approach was demonstrated only in relation to elastic twins. This work is an introduction to the creation of a quantitative theory of twinning in metal crystals. Comparisons with the experimental results of the proposed phenomenological model were limited in this work to the task of demonstrating the performance of the model in the sense of predicting the most specific effects of the development of twins under various conditions and loading modes. In particular, the model implies the effect of loss and subsequent restoration of hardening by twin boundaries during stress pulsations, the Bauschinger effect upon a change in the sign of the applied voltage, and a number of other effects observed experimentally on a number of different metal crystals.

Key words: model, twin, crystal, loading mode, differential equation, forest dislocations.

М. Є. БОСІН, Є. П. ГОМОЗОВ, Т. Г. ДРИГАЧ
МАТЕМАТИЧНА МОДЕЛЬ РОЗВИТКУ ОДИНИЧНОГО ДВІЙНІКОВОГО ПРОШАРКУ В МЕТАЛИЧНИХ КРИСТАЛАХ

За останні десять років двійникування почало досить активно використовуватися при створенні наноструктур та нанотехнологій. За допомогою аналізу експериментальних даних, які знаходяться у науковій літературі, отримана математична модель розвитку одиничного двійникового прошарку в металевих кристалах. Модель має вид диференціального рівняння, порядок якого визначається необхідною точністю отримання результатів, пов'язаних з розв'язком цього рівняння. Навіть у лінійному наближенні одного із основних параметрів феноменологічної моделі, остання дає якісно однакові із експериментом залежності розвитку одиничних двійників при різних режимах навантаження. Незважаючи на велику кількість експериментальних робіт, присвячених двійникуванню, строгої кількісної теорії розвитку двійникових прошарків у різних середовищах та в різних умовах поки що немає. В деяких роботах описувався розвиток двійників в термінах дислокаційних взаємодій. Однак, в цих роботах математичний підхід продемонстрований тільки стосовно пружних двійників. Ця робота є вступом до створення кількісної теорії двійникування в металевих кристалах. Порівняння з експериментальними результатами запропонованої феноменологічної моделі були обмежені у цій роботі задачею демонстрації працездатності моделі в сенсі передбачення найбільш специфічних ефектів розвитку двійникові за різних умов та режимів навантаження. Зокрема, з моделі слідує ефект втрати та подальшого відновлення зміцнення межами двійників при пульсації прикладеної напруги, ефект Баушингера при зміні знаку прикладеної напруги та ряд інших ефектів, що спостерігаються експериментально на ряді різних металевих кристалів.

Ключові слова: модель, двійник, кристал, режим навантаження, диференціальне рівняння, дислокації лісу.

М. Е. БОСИН, Е. П. ГОМОЗОВ, Т. Г. ДРЫГАЧ
МАТЕМАТИЧЕСКАЯ МОДЕЛЬ РАЗВИТИЯ ЕДИНИЧНОЙ ДВОЙНИКОВОЙ ПРОСЛОЙКИ В МЕТАЛЛИЧЕСКИХ КРИСТАЛЛАХ

С помощью анализа имеющихся в научной литературе экспериментальных данных получена математическая модель развития единичной двойниковой прослойки в металлических кристаллах. Модель имеет вид дифференциального уравнения, порядок которого определяется необходимой точностью получения результатов, связанных с решением этого уравнения. Даже в линейном приближении одного из основных параметров феноменологической модели, последняя дает качественно одинаковые с экспериментом зависимости развития единичных двойников при разных режимах нагружения. Несмотря на большое количество экспериментальных работ, посвященных двойникованию, строгой количественной теории развития двойниковых прослоек в разных средах и в разных условиях пока нет. В некоторых работах описывалось развитие двойников в терминах дислокационных взаимодействий. Однако, в этих работах математический подход был продемонстрирован только применительно к упругим двойникам. Данная работа является вступлением к созданию количественной теории двойникования в металлический кристаллах. Сравнения с экспериментальными результатами предложенной феноменологической модели были ограничены в данной работе задачей демонстрации работоспособности модели в смысле предсказания наиболее специфических эффектов развития двойников при различных условиях и режимах нагружения. В частности, из модели следует эффект потери и последующего восстановления упрочнения границами двойников при пульсации напряжений, эффект Баушингера при изменении знака приложенного напряжения и ряд других эффектов, наблюдаемых экспериментально на ряде различных металлических кристаллов.

Ключевые слова: модель, двойник, кристалл, режим нагружения, дифференциальное уравнение, дислокации леса.

Introduction. *Twinning deformation* has become the subject of close study in connection with the development of cryogenic technology, which is necessary both for space research and for the development of technologies requiring low-temperature conditions. Over the past decade, twinning has begun to be used in the creation of *nanostructures* and *nanotechnology*. Despite a large number of experimental works devoted to twinning, there is still no rigorous quantitative theory of the development of twinning layers in different media and under different conditions.

Analysis of recent research. The development of twins in terms of dislocation interactions is described in [1]. The work [2] is also of some interest in this sense. However, in these works, the mathematical approach was demonstrated only in relation to elastic twins. The experimental results that we used in this work were obtained, firstly, on different materials (primarily on metals): zinc [3, 5, 7, 8, 9, 11], beryllium [6,12], bismuth [10], iron and its alloys [4], etc.; sec-

ondly, under different loading conditions: under creep [9], under shock loads [11], under cyclic loads [12], under uniform loads [4; 7], under stress pulsations [8]. It was also interesting to take into account the presence of defects in crystals, for example, the type and density of forest dislocations [7], radiation defects [10].

Formulation of the problem. In this work, an attempt is made to obtain an *isotropic mathematical model* of the behavior of twinning layers, the conclusions of which would correspond to the experimental results. We emphasize that so far we are not talking about the creation of a rigorous mathematical theory; only after clarifying the exact meaning of the phenomenological parameters can we talk about the transformation of the phenomenological model into *a physical* and *mathematical theory*.

Mathematical model. Fig. 1 shows a particular case of the arrangement of a twinning layer in the parent crystal. Particularly, firstly, the twin is plane-parallel (most of the twins are wedge-shaped, and the top of the twinned wedge can be located inside the crystal), and secondly, twin boundaries are perpendicular to the faceting of the sample only at a certain orientation of the latter. The initial thickness of the twin is indicated in Fig. 1 through «b_0». After the load P is
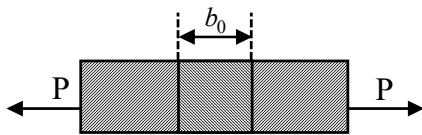

Fig. 1 – particular case of arrangement of twinning layer in parent crystal.

applied (as shown in Fig. 1), the thickness of the twin increases and reaches the value Δb. We denote the relative thickening of the twin by ε:

$$\varepsilon = \frac{\Delta b}{b_0}. \tag{1}$$

Taking into account the property of twin boundaries to accumulate and possibly lose hardening which is irreversibility and reversibility observed during the development of twins, we represent the relative thickening of the

twin in the form:

$$\varepsilon = \varepsilon_e + \varepsilon_P, \tag{2}$$

where ε_e – is the elastic part of the thickening, which disappears after stress relief, and ε_P – the plastic (irreversible) part of the thickening.

For ε_e by analogy with *Hooke's law*, we write

$$\varepsilon_e = \frac{\sigma}{G_2}, \tag{3}$$

here G_2 plays the role of an elastic modulus for a single twin.

For ε_P, using the concept of *viscous resistance forces* that cause irreversibility of the displacement of twin boundaries, we can write by analogy with the well-known *Newton's law* (the stress of resistance to plastic shear is proportional to the strain rate):

$$\frac{d\varepsilon_P}{dt} \equiv \dot{\varepsilon}_P = \frac{\sigma}{\eta}, \tag{4}$$

here η is a parameter that has the dimension of the usual viscosity coefficient.

With the growth of the twin, the value of η changes in connection with a change in the dislocation structure in the vicinity of the twin boundaries and, consequently, with a change in the "viscous resistance" forces. That's why

$$\eta = \eta(\varepsilon_P). \tag{5}$$

Restricting ourselves to the linear part of the expansion of $\eta(\varepsilon_P)$ in *the Maclaurin series*, we write:

$$\eta(\varepsilon_P) \approx \eta_0 + \frac{d\eta}{d\varepsilon_P}\varepsilon_P, \tag{6}$$

here η_0 is the value of η at $\varepsilon_P = 0$. From (6) and (4) we find:

$$\sigma = \left(\eta_0 + \frac{d\eta}{d\varepsilon_P}\varepsilon_P\right)\dot{\varepsilon}_P = \eta_0\dot{\varepsilon}_P + \frac{d\eta}{d\varepsilon_P}\times\frac{d\varepsilon_P}{dt}\varepsilon_P = \eta_0\dot{\varepsilon}_P + \dot{\eta}\varepsilon_p. \tag{7}$$

The parameter $\dot{\eta}$ has the dimension of the elastic modulus, so we introduce the notation:

$$\dot{\eta} = G_1. \tag{8}$$

From (2), (3), (7) and (8) we obtain a differential equation connecting σ and ε:

$$\sigma + \tau_\varepsilon\dot{\sigma} = G(\varepsilon + \tau_\sigma\dot{\varepsilon}), \tag{9}$$

here

$$\tau_\varepsilon = \frac{\eta}{G_1 + G_2}, \ G = \frac{G_1 G_2}{G_1 + G_2}, \ \tau_\sigma = \frac{\eta_0}{G_1}. \tag{10}$$

4

Вісник Національного технічного університету «ХПІ». Серія: Математичне моделювання в техніці та технологіях, № 1-2 (2) 2021.

Note that equation (9) has a form similar to the equation of the *standard linear body*. The value of G in this model is the *relaxed elastic modulus*, τ_ε and τ_σ – are the stress relaxation times (at constant deformation) and deformation (at constant stress), respectively.

Solving equation (9) with either law $\sigma(t)$ or $\varepsilon(t)$ given, we find the other function. Comparing the curves $\varepsilon(t)$ and $\sigma(t)$, that is, making a formal change in the solution $t \to t(\sigma)$ or $t \to t(\varepsilon)$, one can construct diagrams $\sigma - \varepsilon$. Comparing these diagrams with the experimental curves $\sigma(\varepsilon)$, it is possible to recover the parameters G_1, G_2, η_0 (see below).

Equation (9) is an approximate model of the twin development process. To increase the accuracy, one can take into account the next (quadratic) term in the expansion of $\eta(\varepsilon_P)$ in powers of ε_P. Then instead of equation (6) we get the formula:

$$\eta(\varepsilon_P) \approx \eta_0 + \frac{d\eta}{d\varepsilon_P}\varepsilon_P + \frac{1}{2} \times \frac{d^2\eta}{d\varepsilon_P^2}\varepsilon_P^2, \tag{11}$$

and instead of (9), the equation

$$\sigma = \eta_0\left(\dot{\varepsilon} - \frac{\dot{\sigma}}{G_2}\right) + G_1\left(\varepsilon - \frac{\sigma}{G_2}\right) + \frac{1}{2} \times \frac{\left(\varepsilon - \dfrac{\sigma}{G_2}\right)^2}{\left(\dot{\varepsilon} - \dfrac{\dot{\sigma}}{G_2}\right)^2}\left[\xi\left(\dot{\varepsilon} - \frac{\dot{\sigma}}{G_2}\right) - G_1\left(\ddot{\varepsilon} - \frac{\ddot{\sigma}}{G_2}\right)\right]. \tag{12}$$

Here ξ is a new parameter, the meaning of which, like the meaning of other parameters, can be determined by studying their dependence on various factors (temperature, speed and loading mode, structure, etc.).

Let's consider the main loading modes.

1. *Creep mode.*

Equation (9) can be written under the condition $\sigma = const$:

$$\dot{\varepsilon} + \frac{1}{\tau_\sigma}\varepsilon = \frac{\sigma}{G\tau_\sigma}. \tag{13}$$

The solution of the resulting linear inhomogeneous differential equation with the initial condition $\varepsilon|_{t=0} = 0$ has the form:

$$\varepsilon = \frac{\sigma}{G}\left(1 - e^{-\frac{t}{\tau_\sigma}}\right). \tag{14}$$

Comparison of equation (14) with the experimental creep curve will make it easy to recover the parameters G and τ_σ.

Equation (12) gives a more cumbersome expression for the creep. Substituting $\sigma = const$ into equation (12) and resolving the result obtained with respect to the highest derivative, we obtain:

$$\ddot{\varepsilon} = \frac{2\dot{\varepsilon}^2(\eta_0\dot{\varepsilon} - \sigma)}{G_1\left(\varepsilon - \dfrac{\sigma}{G_2}\right)^2} + \frac{2\dot{\varepsilon}^2}{\varepsilon - \dfrac{\sigma}{G_2}} + \frac{\xi}{G_1}\dot{\varepsilon}. \tag{15}$$

Equation (15) does not explicitly contain the time t and therefore admits a decrease in the order.

2. *Active loading mode at $\dot{\sigma} = const$.*

We put $\dot{\sigma} = \mathsf{C}$, that is,

$$\sigma = \mathsf{C}t. \tag{16}$$

Equation (9) then takes the form

$$\dot{\varepsilon} + \frac{1}{\tau_\sigma}\varepsilon = \frac{\mathsf{C}}{G\tau_\sigma}(t + \tau_\varepsilon) \tag{17}$$

The solution to this equation under the initial condition $\varepsilon|_{t=0} = 0$ is the function

$$\varepsilon = \frac{\mathsf{C}}{G}(\tau_\varepsilon - \tau_\sigma)\left(1 - e^{-\frac{t}{\tau_\sigma}}\right) + \frac{\mathsf{C}}{G}t. \tag{18}$$

The relaxation times τ_ε and τ_σ in metals are most often related by the inequality $\tau_\varepsilon \ll \tau_\sigma$ that is, $G_2 \gg G_1$. For a loading duration $t \ll \tau_\sigma$ from equation (18) we obtain:

Вісник Національного технічного університету «ХПІ». Серія: Математичне моделювання в техніці та технологіях, № 1-2 (2)2021.

5

$$\varepsilon = \frac{\mathsf{C}}{2\eta_0} t^2 . \tag{19}$$

Substituting (16) into a more precise equation (12), we get:

$$\ddot{\varepsilon} = 2 \frac{\left(\dot{\varepsilon} - \dfrac{\mathsf{C}}{G_2}\right)^2}{\left(\varepsilon - \dfrac{\mathsf{C}}{G_2} t\right)^2} \left[\frac{\eta_0}{G_1}\left(\dot{\varepsilon} - \frac{\mathsf{C}}{G_2}\right) + \left(\varepsilon - \frac{\mathsf{C}}{G_2} t\right) - \frac{\mathsf{C}}{G_1} t\right] + \frac{\xi}{G_1}\left(\dot{\varepsilon} - \frac{\mathsf{C}}{G_2}\right) . \tag{20}$$

If we introduce an auxiliary function $\varphi(t) = \varepsilon - \dfrac{\mathsf{C}}{G_2} t$, then instead of (20) we can write

$$\ddot{\varphi} = 2\left(\frac{\dot{\varphi}}{\varphi}\right)^2 \left(\frac{\eta_0}{G_1} \dot{\varphi} + \varphi - \frac{\mathsf{C}}{G_1} t\right) + \frac{\xi}{G_1} \dot{\varphi} . \tag{21}$$

Recall that $\dfrac{\mathsf{C}}{G_2} t = \dfrac{\sigma}{G_2}$ is the elastic part of the deformation, so that the function $\varphi(t)$ has the meaning of the irreversible part of the deformation $\varepsilon_P = \varepsilon - \varepsilon_e$.

3. *Active loading mode at $\dot{\varepsilon} = const$.*

Let $\varepsilon = kt$, i.e., the rate of deformation change is

$$\dot{\varepsilon} = k . \tag{22}$$

Equation (9) then takes the form

$$\dot{\sigma} + \frac{1}{\tau_\varepsilon} \sigma = \frac{kG}{\tau_\varepsilon}\left(t + \tau_\sigma\right) . \tag{23}$$

The solution of this equation with the initial condition $\sigma\,|_{t=0} = 0$ leads to the function

$$\sigma = kGt + kG\left(\tau_\sigma - \tau_\varepsilon\right)\left(1 - e^{-\frac{t}{\tau_\varepsilon}}\right) . \tag{24}$$

Expression (24) can be simplified by expanding the exponent in a Maclaurin series and choosing 2 – 3 terms in the expansion. But this requires the fulfillment of the inequality $t \ll \tau_\varepsilon$ which should be dictated by the conditions of the experiment.

Substituting (22) into equation (12), we obtain:

$$\ddot{\varphi} = 2 \frac{G_2}{G_1} \times \frac{\left(k - \dfrac{\dot{\sigma}}{G_2}\right)^2}{\left(kt - \dfrac{\sigma}{G_2}\right)^2}\left[\sigma - \eta_0\left(k - \frac{\dot{\sigma}}{G_2}\right) - G_1\left(kt - \frac{\sigma}{G_2}\right)\right] - \frac{G_2}{G_1}\left(k - \frac{\dot{\sigma}}{G_2}\right)\xi . \tag{25}$$

We introduce an auxiliary function

$$\psi(t) = kt - \frac{\sigma}{G_2} . \tag{26}$$

This function has the same meaning as $\varphi(t)$, introduced earlier, that is, it is the difference between deformation and its elastic part. But since plastic deformation in the modes $\dot{\sigma} = const$ and $\dot{\varepsilon} = const$ proceeds in different ways, the functions $\psi(t)$ and $\varphi(t)$ are significantly different. Taking into account (26), equation (25) can be written in the form:

$$\ddot{\psi} = 2 \frac{\dot{\psi}^2}{\psi^2}\left(\frac{\eta_0}{G_1} \dot{\psi} + \frac{G_1 + G_2}{G_1} \psi - \frac{G_2}{G_1} kt\right) - \frac{G_2}{G_1} \xi \dot{\psi} . \tag{27}$$

The solution of this equation under the initial condition $\sigma\,|_{t=0} = 0$ or, which is the same, $\psi\,|_{t=0} = 0$ gives the dependence $\sigma(t)$ during loading. The latter can be measured experimentally. Comparison, firstly, provides information about the effectiveness of the model, and secondly, it allows to determine the parameters G_1, G_2, η_0, ξ.

4. *Mode of pulsating loads.*

Let us choose for the pulsation the regime $\dot{\sigma} = const = \mathsf{C}$ during loading and $\dot{\sigma} = const = \mathsf{C}'$ during unloading. Let also the loading rate be significantly less than the unloading rate $\mathsf{C} \ll \mathsf{C}'$, as it was in the experiments [8]. The voltage ripple amplitude is denoted by σ_0. Solving equation (9) sequentially, first for loading at a rate of $\dot{\sigma} = \mathsf{C}$, then for unloading at a rate of $\dot{\sigma} = \mathsf{C}'$, then for repeated loading at the same rate C and for unloading at a rate C', etc., we obtain a diagram similar to that obtained experimentally in [8]: with each cycle, a certain displacement of twin boundaries is ob-

6

Вісник Національного технічного університету «ХПІ». Серія: Математичне моделювання в техніці та технологіях, № 1-2 (2) 2021.

served, which decays with the number of cycles. For each repeated cycle, the relative displacement of twin boundaries is equal to

$$\beta_k = \varepsilon' e^{-k\frac{G_1\eta_0}{\eta_0 C}}, \tag{28}$$

here $\varepsilon' = \varepsilon_0 - \dfrac{\sigma_0}{G_2}$ is the relative displacement of twin boundaries during the first loading cycle minus the elastic part

$\dfrac{\sigma_0}{G_2}$. Experiments [8, 12] show that the most stable measure of this loss effect and the subsequent restoration of hardening by twin boundaries under voltage pulsations is the value $\delta = \sum \beta_k$. The series with terms given by (28) is convergent, it is easy to calculate its sum:

$$\delta = \sum_{k=1}^{\infty} \beta_k = \varepsilon' \frac{1}{e^{\frac{G_1\sigma_0}{\eta_0 C}} - 1}. \tag{29}$$

Relation (29) is in satisfactory agreement with experiment.

5. Mode of alternating loads.

Let us apply equation (9) to study the behavior of twin boundaries under alternating loading of the sample. Let the second loading, in contrast to the case considered above, be performed at a speed $\dot\sigma = -C$, that is, a load of the opposite sign $\sigma = -Ct$ is applied (the time is counted from the beginning of repeated loading). Under the initial condition $\varepsilon|_{t=0} = \varepsilon'$ for $\varepsilon(t)$ we find:

$$\varepsilon = \left[\varepsilon' + \frac{C}{G}(\tau_\varepsilon - \tau_\sigma) \right] e^{-\frac{t}{\tau_\sigma}} + \frac{C}{G}(\tau_\sigma - \tau_\varepsilon - t). \tag{30}$$

By the time t_0, stress $-\sigma_0$ and deformation ε_2 will be reached, which is calculated by substituting the value $t_0 = \dfrac{\sigma_0}{C}$ into expression (30). If we postpone the $\varepsilon(\sigma)$ curve under loading of the opposite sign in the positive direction of the coordinate axes, as is done in the illustration of *the Bauschinger effect* [13], then for $\sigma = \sigma_0$ the deformation value will be

$$\varepsilon_2' = 2\varepsilon' - \varepsilon_2. \tag{31}$$

The measure of the Bauschinger effect is usually taken as the measure of the discrepancy between the curves of repeated loading in the forward and reverse directions at $|\sigma| = \sigma_0$. Denoting it by β_B, we obtain

$$\beta_B = 2\varepsilon' \left(1 - e^{-\frac{t}{\tau_\sigma}} \right). \tag{32}$$

or, making the substitution $t_0 = \dfrac{\sigma_0}{C}$, instead of (32) we write

$$\beta_B = 2\varepsilon' \left(1 - e^{-\frac{\sigma_0}{C\tau_\sigma}} \right). \tag{33}$$

Expressions (32) and (33) make it possible to estimate the measure of the Bauschinger effect in twinning within the framework of the phenomenological consideration described above. To simplify calculations, consider the limiting case $\tau_\varepsilon \ll \tau_\sigma$ and $t \ll \tau_\sigma$. Moreover, from (32) we find:

$$\beta_B \approx 2\varepsilon' \frac{G_1}{\eta_0} t_0, \tag{34}$$

and from (19) for t_0 we have

$$t_0 \approx \sqrt{\frac{2\eta_0 \varepsilon_0}{C}}, \tag{35}$$

Substituting (35) into (34), we obtain

$$\beta_B \approx 2\varepsilon' G_1 \sqrt{\frac{2\varepsilon_0}{C\eta_0}} \tag{36}$$

or, setting $\varepsilon' \approx \varepsilon_0$ (since for $G_2 \gg G_1$ $\varepsilon_e \ll \varepsilon_P$, $\varepsilon_e \ll \varepsilon$), instead of (36) we can write

$$\beta_B \approx 2\sqrt{2} \frac{G_1}{\sqrt{\eta_0 C}} \varepsilon_0^{\frac{2}{3}}. \tag{37}$$

Вісник Національного технічного університету «ХПІ».Серія: Математичне моделювання в техніці та технологіях, № 1-2 (2) 2021.

7

Approximate formula (37) is more convenient for analyzing the dependences of β_B on various factors.

6. *Values of phenomenological parameters.*

Thus, the mechanical behavior of twin boundaries under different loading conditions within the framework of the proposed phenomenological consideration is described in terms of three parameters G_1, G_2, and η_0. These parameters are determined both by the characteristics of the twin boundaries themselves and by the defect structure of their surroundings and should, therefore, depend on the degree of incoherence of twin boundaries, the type and density of forest dislocations in crystals, the presence of clusters of point defects, etc.

The parameter η_0 is most easily determined by comparing the experimental dependence $\varepsilon(t)$ during the loading period with the approximate formula (19), which includes only this parameter. The comparison showed that this parameter is sensitive to the density of dislocations of the body in crystals: with an increase in the initial density of the pyramidal forest in Zn crystals from 10^3 to 10^7 cm^{-2}, the value of η_0 increases from $9 \cdot 10^3$ to $4,5 \cdot 10^4$ MPa$\cdot$s. This makes it possible to assume that the viscous deceleration of twin boundaries is largely due to the presence of forest dislocations in the crystal.

The parameter G_1 with a known value of η_0 can be found from the measured values δ or β_B using formulas (29) and (36). The order of this value for twins in Bi and Zn crystals is 10 MPa.

The parameter G_2 is easily estimated from the reverse displacement of the twin boundaries after unloading the crystal, that is, from the value of the elastic part of the relative deformation ε_e using formula (3). The order of this value $G_2 \sim 10^2$ MPa (for Bi) and $G_2 \sim 10^3$ MPa (for Zn), which confirms the condition $G_2 \gg G_1$ used above.

Results of work. Thus, the proposed model predicts the behavior of twin boundaries under various loading conditions. After obtaining a mathematical model by comparing its conclusions and experimental data, some conclusions were made about the meaning of the phenomenological parameters included in the model equation.

In particular, the model implies the effect of loss and subsequent restoration of hardening by twin boundaries during stress pulsations, the Bauschinger effect when the applied voltage changes sign, described in the literature, and a number of other effects observed experimentally on a number of different metal crystals.

Prospects for further research. In the future, the authors intend, by analyzing all the experimental data available in the literature, to clarify the meaning of all the phenomenological parameters of the phenomenological model proposed in the work. Only after this can we talk about the creation of a quantitative theory of twinning.

Conclusions. This work is an introduction to the creation of a quantitative theory of twinning in metal crystals. Comparisons with the experimental results of the proposed phenomenological model were limited in this work to the task of demonstrating the performance of the model in the sense of predicting the most specific effects of the development of twins under various conditions and loading modes.

Bibliography

1. *Бойко В. С., Гарбер Р. И., Хосевич А. М.* Обратимая деформация кристаллов. – М. : «Наука», 1991. – 268 с.
2. *Christian I. W., Mahajan S.* Deformation Twinning. Progress in Materials Science. – 1995. – Vol. 39 – P. 157 – 167.
3. *Босін М. Є., Лаврентьєв Ф. Ф., Никифоренко В. Н., Саліта О. П.* Особливості двійникування в ростових бікристалах цинку двійникової орієнтації // УФЖ. – 1995. – Т. 40. – № 6. – С. 559 – 562.
4. *Босин М. Е., Лаврентьев Ф. Ф., Никифоренко В. Н.* О движении ростовой межзеренной границы двойниковой ориентации в бикристалле сплава (Fe+3,5% Si) // ФТТ. – 1996. – Т. 38, – № 12. – С. 3625 – 3627.
5. *Bosin M. E., Lavrentev F. F., Nikiforenko V. N.* On the Motion of a Crown Integranular Boundary with Twin Orientation in Bycrystals of Pure Zine // Physica status solidi (a). – 1996. – Vol. 157. – P. 213 – 216.
6. *Bosin M. E.* Specific features of twin boundaries motion in beryllium single crystals at the twinning and untwining // Functioonal materials. – 1997. – Vol. 4. – № 4 – P. 557 – 559.
7. *Босин М. Е., Лаврентьев Ф. Ф., Никифоренко В. Н.* Область аккомодации – мера релаксации напряжений, локализованных на границах двойников в монокристаллах цинка // The XXI International Conference on Relaxation Phenomena In Solids (RPS-21). – Voronezh, 2004.
8. *Босин М. Е., Лаврентьев Ф. Ф., Никифоренко В. Н.* Дуализм влияния дислокаций леса на развитие двойникования в монокристаллах цинка // The Third International Conference «Deformation and Fracture of Materials and Nanomaterials». – Москва. – 2009. – С. 82 – 83.
9. *Босин М. Е., Русскин В. М.* Особенности влияния дислокаций леса на скорость движения границ двойников в монокристаллах цинка при ползучести // Сб. докладов Международной научной конференции «Актуальные проблемы физики твердого тела» (ФТТ – 2011). – Минск, 2011. – С. 260 – 262.
10. *Босин М. Е., Гомозов Е. П.* Влияние нейтронного облучения на движение границ двойника в монокристаллах висмута // Материалы докладов XX Петербургских чтений по проблемам прочности. – Санкт-Петербург, 2012. – С. 217 – 219.
11. *Босин М. Е., Омельченко Н. В.* Движение границ двойников в монокристаллах цинка при ударном нагружении // Сб. трудов Международной конференции «Актуальные проблемы прочности». – Харьков, 2014. – С. 123 – 124.
12. *Босин М. Е., Русскин В. М.* Закономерности движения двойниковых границ в монокристаллах бериллия и его сплавах с медью при многократном циклическом нагружении // Сб. трудов XIX Международной конференции «Физика прочности и пластичности материалов». – Самара, 2015. – С. 643 – 644.
13. *Башманов В. М., Босин М. Е., Папиров И. И.* Циклический эффект Баушингера на границах механических двойников бериллия // ФММ. – 1973. – Т. 35. – № 1. – С. 220 – 221.

8

Вісник Національного технічного університету «ХПІ». Серія: Математичне моделювання в техніці та технологіях, № 1-2 (2) 2021.

References (transliterated)

1. Boyko V. S., Garber R. I., Khosevich A. M. *Obratimaya deformatsiya kristallov* [Reversible deformation of crystals]. Moscow, Nauka Publ., 1991. 268 p.
2. Christian I. W., Mahajan S. Deformation Twinning. *Progress in Materials Science*. 1995, vol. 39, pp. 157–167.
3. Bosin M. E., Lavrent'ev F. F., Nikiforenko V. N., Salita O. P. Osoblyvi dviynykuvannya v rostovykh bikrystalakh zynku dviynykovoyi ori-yentatsiyi [Features of twinning in growth bicrystals of zinc of twin orientation]. *UFZh* [Ukrainian Journal of Physics]. 1995, vol. 40, no. 6, pp. 559–562.
4. Bosin M. E., Lavrent'ev F. F., Nikiforenko V. N. O dvizhenii rostovoy mezhzyierennoy granitsy dvoynikovoy orientatsii v bikristalle splava (Fe + 3.5% Si) [On the motion of the growth grain boundary of twin orientation in the bicrystal of the alloy (Fe + 3.5% Si)]. *FTT* [Solid State Physics]. 1996, vol. 38, no. 12, pp. 3625–3627.
5. Bosin M. E., Lavrentev F. F., Nikiforenko V. N. On the Motion of a Crown Integranular Boundary with Twin Orientation in Bycrystals of Pure Zine. *Physica status solidi (a)*. 1996, vol. 157, pp. 213–216.
6. Bosin M. E. Specific features of twin boundaries motion in beryllium single crystals at the twinning and untwining. *Functioonal materials*. 1997, vol. 4, no. 4, pp. 557–559.
7. Bosin M. E., Lavrent'ev F. F., Nikiforenko V. N. Oblast' akkomodatsii – mera relaksatsii napryazheniy, lokalizovannykh na granitsakh dvoynikov v monokristallakh tsinka [The accommodation region is a measure of relaxation of stresses localized at the boundaries of twins in zinc single crystals]. *The XXI International Conference on RELAXATION PHENOMENA IN SOLIDS (RPS-21)*. Voronezh, 2004.
8. Bosin M. E., Lavrent'ev F. F., Nikiforenko V. N. Dualizm vliyaniya dislokatsiy lesa na razvitie dvoynikovaniya v monokristallakh tsinka [Dualism of the influence of forest dislocations on the development of twinning in zinc single crystals]. *The Third International Conference «Deformation and Fracture of Materials and Nanomaterials»*. Moscow, 2009, pp. 82–83.
9. Bosin M. E., Russkin V. M. Osobennosti vliyaniya dislokatsiy lesa na skorost' dvizheniya granits dvoynikov v monokristallakh tsinka pri polzuchesti [Features of the influence of forest dislocations on the speed of motion of twin boundaries in zinc single crystals during creep]. *Sb. dokladov Mezhdunarodnoy nauchnoy konferentsii «Aktual'nye problemy fiziki tvyierdogo tela» (FTT – 2011)* [Sat. reports of the International Scientific Conference "Actual Problems of Solid State Physics" (SSP – 2011)]. Minsk, 2011, pp. 260–262.
10. Bosin M. E., Gomozov E. P. Vliyanie neytronnogo oblucheniya na dvizhenie granits dvoynikov v monokristallakh bismuta [Influence of neutron irradiation on the motion of twin boundaries in bismuth single crystals]. *Materialy dokladov XX Peterburgskikh chteniy po problemam prochnost»* [Proceedings of the XX St. Petersburg Readings on Strength Problems]. St. Petersburg, 2012, pp. 217–219.
11. Bosin M. E., Omel'chenko N. V. Dvizhenie granits dvoynikov v monokristallakh tsinka pri udarnom nagruzhenii [Movement of twin boundaries in zinc single crystals under shock loading]. *Sb. trudov Mezhdunarodnoy konferentsii «Aktual'nye problemy prochnosti»* [Sat. Proceedings of the International Conference "Actual Problems of Strength"]. Kharkov, 2014, pp. 123–124.
12. Bosin M. E., Russkin V. M. Zakonomernosti dvizheniya dvoynikovykh granits v monokristallakh berilliya i ego splavakh s med'yu pri mnog-okratnom tsiklicheskom nagruzhenii [Regularities of motion of twin boundaries in single crystals of beryllium and its alloys with copper under multiple cyclic loading]. *Sb. trudov XIX Mezhdunarodnoy konferentsii «Fizika prochnosti i plastichnosti materialov»* [Sat. Proceedings of the XIX International Conference "Physics of Strength and Plasticity of Materials"]. Samara, 2015, pp. 643–644.
13. Bashmanov V. M., Bosin M. E., Papirov I. I. Tsiklicheskiy eyffekt Baushingera na granitsakh mekhanicheskikh dvoynikov berilliya [Cyclic Bauschinger effect on the boundaries of mechanical twins of beryllium]. *FMM* [Physics of Metals and Metal Science]. 1973, vol. 35, no. 1, pp. 220–221.

Відомості про авторів / Сведения об авторах / Information about authors

Босін Марк Євгенович – доктор фізико-математичних наук, професор, завідувач кафедри математики та фізики, Харківська гуманітарна-педагогічна академія, м. Харків; тел.: (057) 732-87-33; e-mail: kafedramath.ph36@gmail.com.

Босин Марк Евгеньевич – доктор физико-математических наук, профессор, заведующий кафедры математики и физики, Харьковская гуманитарно-педагогическая академия, г. Харьков; тел.: (057) 732-87-332; e-mail: kafedramath.ph36@gmail.com.

Bosin Mark Yevgenovych – Doctor of Physical and Mathematical Sciences, Professor, Head of the Department of Higher Mathematics and Physics, Ukrainian Engineering Pedagogics Academy, Kharkiv; tel.: (057) 732-87-33; e-mail: kafedramath.ph36@gmail.com.

Гомозов Євген Павлович – кандидат фізико-математичних наук, доцент, Національний технічний університет «Харківський політехнічний інститут», м. Харків; тел.: (057) 707-63-51; e-mail: Yevgen.Gomozov@khpi.edu.ua.

Гомозов Евгений Павлович – кандидат физико-математических наук, доцент, Национальный технический университет «Харьковский политехнический институт», г. Харьков; тел.: (057) 707-63-51; e-mail: Yevgen.Gomozov@khpi.edu.ua.

Gomozov Yevgen Pavlovych – PhD in Physics and Mathematics, Associate Professor of Computer Mathematics and Data Analysis, National Technical University "Kharkiv Polytechnic Institute", Kharkiv; tel.: (057) 707-63-51; e-mail: Yevgen.Gomozov@khpi.edu.ua.

Дригач Тетяна Григорівна – кандидат педагогічних наук, старший викладач, Харківська гуманітарна-педагогічна академія, м. Харків; тел.: (057) 732-87-33; e-mail: kafedramath.ph36@gmail.com.

Дрыгач Татьяна Григорьевна – кандидат педагогических наук, старший преподаватель кафедры математики и физики, Харьковская гуманитарно-педагогическая академия, г. Харьков; тел.: (057) 732-87-33; e-mail: kafedramath.ph36@gmail.com.

Drygach Tetyana Grygorivna – Candidate of Pedagogics Sciences, Senior Lecturer at the Department of Higher Mathematics and Physics, Ukrainian Engineering Pedagogics Academy, Kharkiv; tel.: (057) 732-87-33; e-mail: kafedramath.ph36@gmail.com.

Вісник Національного технічного університету «ХПІ».Серія: Математичне моделювання в техніці та технологіях, № 1-2 (2) 2021.

9