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 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.

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Немає летакії десять десять дійсних, які знаходяться у науковій літературі, отримана математична модель розвитку однієї двойникової прослойки 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, отримання дає якісно однакові із експериментом залежності розвитку однієї двойникової прослойки при різних режимах навантаження. Незва- жаючи на велику кількість експериментальних робіт, присвячених двойниковій прослойці, 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 продемонстровано тільки стосовно пружних двійників. Ця робота є вступом до створення кількісної теорії двойників 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 розвит-ку двойників за різних умов та режимів навантаження. Зокрема, з моделі слідує ефект втрати та подальшого відновлення зміцнення межами двойників при пульсації прикладеної напруги, ефект Башингера при зміні знаку прикладеної напруги та ряд інших ефектів, що спостерігаються експериментально на ряді різних металевих кристалів.

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

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

У 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 однієї двойникової прослойки 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, отримання дає якісно однакові із експериментом залежності розвитку однієї двойникової прослойки при різних режимах навантаження. Незважаючи на велику кількість експериментальних робіт, присвячених двойниковій прослойці, 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 продемонстровано тільки стосовно пружних двійників. Ця робота є вступом до створення кількісної теорії двойників 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 двойників за різних умов та режимів навантаження. Зокрема, з моделі слідує ефект втрати та подальшого відновлення зміцнення межами двойників при пульсації прикладеної напруги, ефект Башингера при зміні знаку прикладеної напруги та ряд інших ефектів, що спостерігаються експериментально на ряді різних металевих кристалів.

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

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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 «b₀». After the load P is 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:

$$\varepsilon = \frac{\Delta b}{b_0}. \quad (1)$$

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:

$$\varepsilon = \varepsilon_e + \varepsilon_p, \quad (2)$$

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

For \(\varepsilon_e\) by analogy with *Hooke's law*, we write

$$\varepsilon_e = \frac{\sigma}{G_2}, \quad (3)$$

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

For \(\varepsilon_p\), 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):

$$\frac{d\varepsilon_p}{dt} = \dot{\varepsilon}_p = \frac{\sigma}{\eta}, \quad (4)$$

here \(\eta\) is a parameter that has the dimension of the usual viscosity coefficient.

With the growth of the twin, the value of \(\eta\) 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

$$\eta = \eta(\varepsilon_p). \quad (5)$$

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

$$\eta(\varepsilon_p) \approx \eta_0 + \frac{d\eta}{d\varepsilon_p}\varepsilon_p, \quad (6)$$

here \(\eta_0\) is the value of \(\eta\) at \(\varepsilon_p = 0\). From (6) and (4) we find:

$$\sigma = \left(\eta_0 + \frac{d\eta}{d\varepsilon_p}\varepsilon_p\right)\dot{\varepsilon}_p = \eta_0\dot{\varepsilon}_p + \frac{d\eta}{d\varepsilon_p}\varepsilon_p\dot{\varepsilon}_p = \eta_0\dot{\varepsilon}_p + \eta_\dot{\varepsilon}_p. \quad (7)$$

The parameter \(\eta\) has the dimension of the elastic modulus, so we introduce the notation:

$$\eta = G_1. \quad (8)$$

From (2), (3), (7) and (8) we obtain a differential equation connecting \(\sigma\) and \(\varepsilon\):

$$\sigma + \tau_\varepsilon \dot{\varepsilon} = G\left(\varepsilon + \tau_\varepsilon \dot{\varepsilon}\right), \quad (9)$$

here

$$\tau_\varepsilon = \frac{\eta}{G_1 + G_2}, \quad G = \frac{G_1 G_2}{G_1 + G_2}, \quad \tau_\sigma = \frac{\eta_0}{G_1}. \quad (10)$$
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*, $\tau_\varepsilon$ and $\tau_\sigma$ 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 $G_1$, $G_2$, $\eta_0$ (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 $\varepsilon_p$. Then instead of equation (6) we get the formula:

$$
\eta(\varepsilon_p) \approx \eta_0 + \frac{d\eta}{d\varepsilon_p} \varepsilon_p + \frac{1}{2} \frac{d^2\eta}{d\varepsilon_p^2} \varepsilon_p^2,
$$

and instead of (9), the equation

$$
\sigma = \eta_0 \left( \dot{\varepsilon} - \frac{\dot{\varepsilon}}{G_2} \right) + G_1 \left( e - \frac{\varepsilon}{G_2} \right) + \frac{1}{2} \left( \dot{\varepsilon} - \frac{\dot{\varepsilon}}{G_2} \right)^2 \left( \dot{\varepsilon} - \frac{\dot{\varepsilon}}{G_2} - G_1 \left( e - \frac{\varepsilon}{G_2} \right) \right).
$$

Here $\xi$ 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 $\sigma = \text{const}$:

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

   The solution of this equation under the initial condition $\varepsilon(0) = 0$ has the form:

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

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

   We put $\sigma = \xi$, that is,

   $$
   \sigma = \xi t.
   $$

   Equation (9) then takes the form

   $$
   \dot{\varepsilon} + \frac{1}{\tau_\varepsilon} \varepsilon = \frac{\xi}{G \tau_\sigma} (t + \tau_\varepsilon).
   $$

   The solution to this equation under the initial condition $\varepsilon(0) = 0$ is the function

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

   The relaxation times $\tau_\varepsilon$ and $\tau_\sigma$ 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:
\[ \varepsilon = \frac{C}{2\eta_0} t^2. \]  

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

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

(20)

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

\[ \ddot{\varphi} = 2 \left( \frac{\varphi}{t} \right) \left[ \frac{\eta_0}{G_1} \varphi + \varphi - \frac{C}{G_2} t \right] + \frac{\ddot{\varphi}}{G_1} \ddot{\varphi}. \]  

(21)

Recall that \( \frac{C}{G_2} t = \sigma \) 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 \( \varepsilon = \text{const} \).

Let \( \varepsilon = \dot{\varepsilon} t \), i.e., the rate of deformation change is \( \dot{\varepsilon} = k \).

Equation (9) then takes the form

\[ \sigma + \frac{1}{\tau_e} \sigma = \frac{kG}{\tau_e} (t + \tau_e). \]  

(23)

The solution of this equation with the initial condition \( \sigma(t=0) = 0 \) leads to the function

\[ \sigma = kGt + \frac{kG}{\tau_e} (\tau_e - t) \left( 1 - e^{-\frac{t}{\tau_e}} \right). \]  

(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 \( t \ll \tau_e \) which should be dictated by the conditions of the experiment.

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

\[ \varphi = 2 \frac{G_2}{G_1} \left[ \frac{k - \sigma}{G_2} \right]^2 \left[ \sigma - \eta_0 \left( k - \frac{\sigma}{G_2} \right) - G_1 \left( G_2 - \frac{G_1}{G_2} \right) \right] - \frac{G_2}{G_1} \left( k - \frac{\sigma}{G_2} \right) \xi. \]  

(25)

We introduce an auxiliary function

\[ \psi(t) = kt - \frac{\sigma}{G_2}. \]  

(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 \( \dot{\varepsilon} = \text{const} \) and \( \dot{\varepsilon} = \text{const} \) 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:

\[ \ddot{\psi} = 2 \frac{\psi^2}{\gamma^2} \left[ \frac{\eta_0}{G_1} \psi + \frac{G_2}{G_1} \left( \frac{G_2}{G_1} + \gamma \right) \right] - \frac{G_2}{G_1} \xi \dot{\psi}. \]  

(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 \( G_1 \), \( G_2 \), \( \eta_0 \), \( \xi \).

4. Mode of pulsating loads.

Let us choose for the pulsation the regime \( \dot{\sigma} = \text{const} = \overline{C} \) during loading and \( \dot{\sigma} = \text{const} = \overline{C'} \) during unloading. Let also the loading rate be significantly less than the unloading rate \( \overline{C} \ll \overline{C'} \), as it was in the experiments [8]. The voltage ripple amplitude is denoted by \( \sigma_0 \). Solving equation (9) sequentially, first for loading at a rate of \( \dot{\sigma} = \overline{C} \), then for unloading at a rate of \( \dot{\sigma} = \overline{C'} \), then for repeated loading at the same rate \( \overline{C} \) and for unloading at a rate \( \overline{C'} \), etc., we obtain a diagram similar to that obtained experimentally in [8]: with each cycle, a certain displacement of twin boundaries is ob-
served, which decays with the number of cycles. For each repeated cycle, the relative displacement of twin boundaries is equal to

\[ \beta_k = \varepsilon' e^{-kG\sigma_0/\eta} \]  

(28)

here \( \varepsilon' = \varepsilon_0 - \sigma_0 / G_2 \) is the relative displacement of twin boundaries during the first loading cycle minus the elastic part \( \sigma_0 / G_2 \). 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:

\[ \delta = \sum_{k=1}^{\infty} \beta_k = \varepsilon' \frac{1}{\frac{G\sigma_0}{\eta} - 1}. \]  

(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 \( \sigma = -\sigma_0 \), that is, a load of the opposite sign \( \sigma = -\sigma \) 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:

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

(30)

By the time \( t_0 \), stress \( \sigma_0 \) and deformation \( \varepsilon_2 \) will be reached, which is calculated by substituting the value \( t_0 = \frac{\sigma_0}{\eta} \) 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

\[ \varepsilon'_2 = 2\varepsilon' - \varepsilon_2. \]  

(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 \( B \), we obtain

\[ B = 2\varepsilon' \left( 1 - e^{-\frac{t}{\tau_\sigma}} \right). \]  

(32)

or, making the substitution \( t_0 = \frac{\sigma_0}{\eta} \), instead of (32) we write

\[ B = 2\varepsilon' \left( 1 - e^{-\frac{\sigma_0}{\eta\tau_\sigma}} \right). \]  

(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:

\[ B \approx 2\varepsilon' \frac{G_1}{\eta_0} t_0, \]  

(34)

and from (19) for \( t_0 \) we have

\[ t_0 \approx \sqrt{\frac{2\eta_0\varepsilon_0}{\eta}}. \]  

(35)

Substituting (35) into (34), we obtain

\[ B \approx \frac{G_1}{\eta_0} \sqrt{\frac{2\varepsilon_0}{\eta}} \]  

(36)

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

\[ B \approx 2\sqrt{\frac{G_1}{\eta_0}} \varepsilon_0^\frac{2}{3}. \]  

(37)
Approximate formula (37) is more convenient for analyzing the dependences of $\beta_g$ 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 $\eta_0$. 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 $\eta_0$ 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 $10^5$ cm$^{-2}$, the value of $\eta_0$ increases from 9.10$^3$ to 4.5.10$^4$ MPa·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 $\eta_0$ can be found from the measured values $\delta$ or $\beta_g$ 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 $\varepsilon_e$ using formula (3). The order of this value $G_2 \sim 10^2$ MPa (for Bi) and $G_2 \sim 10^4$ 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.

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