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CRYSTALLOGEOMETRIC ANALYSIS OF DISLOCATION REACTIONS AND TRANSFORMATIONS OF "FOREST" DISLOCATIONS AT TWIN BOUNDARIES IN hcp CRYSTALS

Interaction reactions of basal, pyramidal, and prismatic dislocations with twinning dislocations in hcp *crystals have been considered. The corresponding information is necessary for evaluating the phenomenological parameters of the mathematical model for the development of single twin layers. The density of gliding dislocations ("forest" dislocations) of each type in the vicinity of twin boundaries determines the nature of dislocation reactions at twin boundaries and, in essence, the development of twins. All possible interactions between twinning and forest dislocations in hcp crystals have been analyzed. The results are presented in a form that is convenient for further analysis of the development of twin layers under various loading conditions.*
K e y w o r d s: twin, twin boundary, dislocation structure, basal dislocation, pyramidal dislocation, prismatic dislocation, "forest" dislocation.

1. Introduction

In paper [1], a mathematical model for the development of twin layers in metal crystals under sharp loading regimes and under various conditions has been proposed. Paper [1] was published much later than the works by I.M. Lifshits [2], A.H. Cottrell [3], A.M. Kosevich [4], and O.M. Ostrikov [5], which constituted the classical theory of twinning until recent years. After the publication of those classical works, quite a few interesting experiments were conducted to study the properties of single twins in metal crystals and the behavior of twin boundaries under various specimen loading regimes. A number of very interesting phenomena in twins during loading were discovered. In particular, the Bauschinger effect under alternating loads, the effect of strengthening loss and subsequent recovery at twin boundaries under pulsating loads, some features of twin behavior under creep and shock loading, and so forth, were revealed. All those effects and phenomena in various aspects were described in detail in our Refs [6–15].

In Ref. [1], a mathematical model was proposed, from which the aforementioned phenomena follow. However, in order to clarify the physical meaning of the parameters of this model, it is necessary to un-

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derstand not only the interaction of twin dislocations with each other, but also the interaction of these dislocations with other obstacles. The main objects in the path of twin dislocation motion are forest dislocations. So the main current task is the analysis of dislocation reactions between twin and forest dislocations. The task is quite cumbersome, so in this work, we will solve it only for hcp crystals.

2. Types of Slip in HCP Crystals

The most easily activated slip system for all metals with hcp lattices is the slip in the system $\{0001\}\,\langle 11\bar{2}0\rangle$. This type of slip is called basal. A more difficult slip occurs in the system $\{\bar{1}\bar{1}22\}\,\langle 11\bar{2}3\rangle$ and is called pyramidal. It is characterized by a higher yield strength than the basal one and is activated mainly when the latter is hindered. Slip in the system $\{1\bar{1}00\}\,\langle 11\bar{2}0\rangle$ in most hcp metals is observed only at high temperatures. This type of slip is called prismatic.

To predict the results of interaction between twinning and slip, it is necessary, first, to identify the active slip systems by taking into account geometric factors and yield strengths for various slip systems and, second, to analyze the reactions between twinning dislocations and the corresponding slip dislocations.

3. Penetration of "Forest" Dislocations into Twins. Dislocation Reactions

All cases of the penetration of undissociated dislocations from the matrix into the twin can be divided into three groups.

1. The Burgers vector of undissociated dislocation $b \parallel \eta_1$, where η_1 is the twin shear direction. In this case, the undissociated dislocations pass into a twin as screw dislocations that slide transversely without dislocation reactions at the boundaries.

2. If $b \parallel \eta_2$, where η_2 is the associated shear direction, an undissociated dislocation decays at the boundary into two twinning dislocations and one undissociated dislocation in the twin lattice. Such reactions should contribute to the growth of the twin-layer thickness.

3. The Burgers vector of undissociated dislocation b is parallel neither to the twinning shear direction η_1 nor to the associated shear direction η_2. In this case, an undissociated dislocation splits into one partial dislocation and one undissociated dislocation in the twin. Such an interaction should inhibit the development of the twin.

An analysis of all possible dislocation interactions in hexagonal crystals, taking dislocation reactions and emerging thresholds into account, allows some general conclusions to be drawn.

1. Sliding thresholds are always formed at dislocations responsible for basal slip when crossing any other dislocations existing in hexagonal crystals. Those thresholds do not represent serious obstacles to dislocation movement. Therefore, in the case of basal slip, there is no strengthening due to the formation of thresholds when dislocations are crossed. Perhaps, such circumstances can explain, to some extent, the ease of basal slip. Whence it also follows that plastic deformation along the (0001) plane, as a rule, should not be accompanied by the formation of vacancies.

2. In hexagonal close-packed crystals, there are favorable conditions for the formation of fixed sites on dislocation lines, which can contribute to the dislocation multiplication according to the Frank–Read mechanism. On the other hand, the resistance to dislocation movement in the planes of prisms and pyramids of the I and II kinds substantially exceeds the resistance to the movement in the basal planes, which complicates transverse slip. All those circumstances should lead to a strong localization of slip bands in hcp crystals, which is observed experimentally.

3. When sliding in the planes of a pyramid of the II kind, dislocation configurations capable of working as Frank–Read sources can be easily formed. Perhaps, this is one of the reasons why Frank–Read sources are most frequently observed in crystals with a hexagonal structure.

4. In hexagonal crystals, the formation of sessile dislocations due to the intersection of dislocations in the pyramid's planes is possible. Those dislocations should significantly affect the development of the dislocation structure during deformation under conditions that exclude basal slip. Thus, the maximum strengthening in hcp crystals should occur at pyramidal slip.

It should be noted that the slip of undissociated dislocations is random and depends on whether the dislocation in the active slip plane encounters another dislocation in its own or another slip plane. During twinning, all dislocations in the parent crystal, in the region of motion of twin boundaries, interact with partial twinning dislocations and, depending on the character of this interaction (attraction or repulsion), undissociated dislocations are either incorporated into the twin or repelled by the twin boundary. The repulsive interaction of twinning and undissociated dislocations leads to the removal of the latter from the twin boundaries, and the near-boundary region acquires the orientation of the parent crystal, with a substructure created by the interaction between undissociated dislocations.

The character of dislocation reactions at twin boundaries depends not only on the type of dislocation, but to a large extent on the crystal orientation with respect to the applied stress, which determines the type of "forest" dislocations that are activated during the twinning process. At stresses exceeding the yield stress, sliding in crystals occurs inhomogeneously, namely, at places of local stress concentrators. Incoherent twin boundaries are stress concentrators; therefore, in their vicinity, sliding is more intensive than in other crystal regions. In this case, a transition of dislocations from the matrix into a twin is possible, which is accompanied by the generation of twinning dislocations. Let us consider a possible transition of "forest" dislocations from the parent crystal into a twin. A visual representation of the transition of the basal and pyramidal "forest" dislocations is depicted in Fig. 1, where the lattices of the parent crystal and the twin are tinted light and dark gray, respectively.

From the schematic diagram in Fig. 1, one can see that the transition of two basal dislocations is accompanied by the formation of two twinning dislocations and one pyramidal dislocation in the twin lattice. Analytically, this transformation can be represented in the form

$$\text{(B)} \quad \frac{2}{3}\,[1\bar{2}10]^{(0001)}_{4,00} \rightarrow \frac{1}{3}\,[2\bar{1}\bar{1}3]^{*(\bar{2}112)^*}_{4,46} + \\ + \frac{\left[\left(\frac{C}{a}\right)^2 - 3\right]}{\left[\left(\frac{C}{a}\right)^2 + 3\right]}\,[01\bar{1}\bar{1}]^{(01\bar{1}2)}_{0,03}\,.$$

The indices of the planes and directions in the twin lattices are marked with asterisks, and the superscripts near the Burgers vectors show the planes of the dislocations. The subscripts near the Burgers vectors show the dislocation energies in relative units (the ratio between the squared dislocation Burgers vector and the squared lattice parameter).

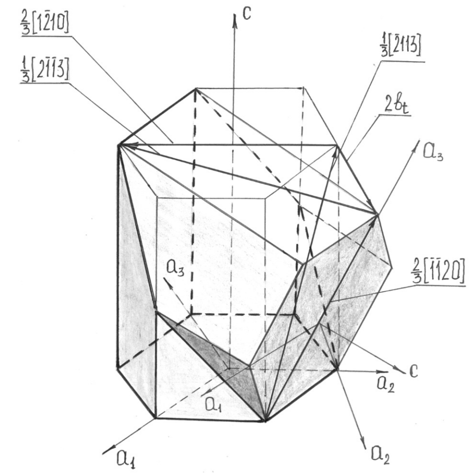

Fig. 1

We see that reaction (B) is energetically unfavorable and occurs only under the action of external shift stresses. In essence, this explains the increase in the yield strength required to initiate twin lattice motion as the density of the basal "forest" dislocations increases. Thus, the transition of basal dislocations from the matrix into a twin is accompanied by the generation of twinning dislocations. In turn, this increases the velocity of twin-boundary motion under the action of a constant external shear stress. The reality of such a mechanism is confirmed by the fact that the products of reaction (B) were experimentally observed in the twin body in the form of pyramidal dislocations, which were absent in the specimen before its twinning.

In Fig. 1, a transition of the pyramidal "forest" dislocation from the matrix into a twin is also shown. In analytical form, this transition is described by the following relationship:

$$\text{(P)} \quad \frac{1}{3}\,[\bar{2}113]^{(2\bar{1}\bar{1}2)}_{4,46} + \frac{\left[\left(\frac{C}{a}\right)^2 - 3\right]}{\left[\left(\frac{C}{a}\right)^2 + 3\right]}\,[01\bar{1}1]^{(01\bar{1}1)}_{0,03} \rightarrow \\ \rightarrow \frac{2}{3}\,[\bar{1}\bar{1}20]^{*0001^*}_{4,0}\,.$$

From reaction (P), one can see that the transition of a pyramidal dislocation from the matrix into a twin is accompanied by the emergence of two twinning dislocations and the inclusion of two basal dislocations into the twin. Therefore, an increase in the density of pyramidal "forest" dislocations in the initial specimen leads to a decrease in the twin-boundary velocity and a substantial increase in the yield stress required to initiate boundary motion, as compared to that for basal "forest" dislocations.

Unlike reaction (B), reaction (P) is energetically favorable. It should be added that pyramidal "forest" dislocations with Burgers vectors, unlike those considered in reaction (P), are not described by the formation of dislocations with known Burgers vectors when transiting from the matrix to a twin. Therefore, an increase of the dislocation density in the system $\{11\bar{2}2\}\,\langle 11\bar{2}3\rangle$ leads to an increase in the yield stress. As a result, the motion of twin boundaries begins, with the inclusion of dislocations with complicated Burgers vectors into the twin. It seems that the presented above crystallogeometric analysis of the transition of "forest" dislocations from the matrix into a twin is a necessary prerequisite for the development of a further analytical description of the transformation reactions of undissociated dislocations when they are included into a twin. This method should be recommended for the consideration of dislocation crystallographic transformations and reactions in crystals with other types of crystal lattices at their twinning.

It is necessary to separately consider the interaction and dislocation reactions of prismatic dislocations with packing defects. When forming prismatic dislocations in the (0001) plane, in addition to the shift by $\frac{1}{3}\langle 10\bar{1}0\rangle$, it is necessary to bring neighboring close-packed planes closer by $\frac{C}{2}$. Then the Burgers vector of prismatic dislocations with packing defects turns out to be equal to

$$\frac{1}{3}\,[10\bar{1}0] + \frac{1}{2}\,[0001] = \frac{1}{6}\,[20\bar{2}3].$$

When removing one close-packed layer, packing defects of two types can be formed. As a result, there are four cases for the interaction of prismatic dislocations.

1) The Burgers vectors of prismatic loops are identical. In this case, the contacting segments of the loops tend to annihilate, resulting in the formation of a single larger loop.

2) The components of the Burgers vectors in the basal plane make an angle of 120°; for example, $\frac{1}{3}\,[\bar{1}100]$ and $\frac{1}{3}\,[10\bar{1}0]$. The types of packing defects of both loops are identical. The coalescence of the dislocation loops will be accompanied by the formation of dislocations having a basal-plane component. In turn, a dislocation with the basal component $\frac{1}{3}\,[\bar{2}110]$ can split according to the reaction

$$\frac{1}{3}\,[\bar{2}101] \to \frac{1}{3}\,[\bar{1}100] + \frac{1}{3}\,[\bar{1}010].$$

A packing defect is formed between the partial dislocations with the components $\frac{1}{3}\,[\bar{2}110]$ and $\frac{1}{3}\,[\bar{1}010]$.

3) The components of the Burgers vectors in the basal plane form an angle of 60°; for example, $\frac{1}{3}\,[\bar{1}100]$ and $\frac{1}{3}\,[01\bar{1}0]$. In this case, the types of packing defects of both loops are different. Between the contacting loops, the following reaction takes place:

$$\frac{1}{3}\,[\bar{1}100] - \frac{1}{3}\,[01\bar{1}0] = \frac{1}{3}[\bar{1}010].$$

4) The basal components of the Burgers vectors are antiparallel; for example, $\frac{1}{3}\,[\bar{1}100]$ and $\frac{1}{3}\,[1\bar{1}00]$. In this case, the types of packing defects are different. The corresponding reaction between the touching loops looks like

$$\frac{1}{3}\,[\bar{1}100] - \frac{1}{3}\,[1\bar{1}00] = -\frac{2}{3}\,[\bar{1}100].$$

The reaction is energetically unfavorable. Therefore, a dislocation with the basal component $\frac{2}{3}\,[\bar{1}100]$ will tend to split into three dislocations,

$$\frac{2}{3}\,[\bar{1}100] \to \frac{1}{3}\,[01\bar{1}0] + \frac{1}{3}\,[\bar{1}100] + \frac{1}{3}\,[\bar{1}010].$$

Thus, the behavior of all three types of "forest" dislocations in hcp crystals has been considered. This behavior largely determines the mobility of twin boundaries, as well as all effects considered in Ref. [1] (the Bauschinger effect at twin boundaries, the effect of loss and subsequent recovery of twin-boundary strengthening under stress pulsations, and so on).

4. Conclusions

A mathematical model was proposed in Ref. [1], which can describe the behavior of twin boundaries in hcp crystals under various loading regimes: in the active loading regime, in the creep regime, under alternating loads, and under pulsating loads. All those regimes were experimentally implemented with various hcp metals and other materials as well. The obtained results were presented in Refs [6–15], where all the phenomena described in Ref. [1] were detected and measured. The mathematical model allows the model parameters to be determined by fitting the solutions of the corresponding mathematical equation to experimental data. However, the mathematical model does not become theoretical because the physical origin and manifestation of the Bauschinger effect under alternating loads, the effect of strengthening loss at twin boundaries under repeated loads, and other effects under various loading regimes remain unclear. The reason lies in the interaction of twinning and "forest" dislocations with their numerous reaction and dissociation products.

This work is a step toward understanding the origins of such a diverse behavior of twin boundaries under changing loading conditions. "Forest" dislocations are located along the motion path of twinning dislocations, and the interaction with them largely determines the underlying mechanisms. The following steps in this direction are proposed: first, to analyze dislocation reactions between twinning and "forest" dislocations in crystals with other crystal lattice types; second, qualitatively and quantitatively compare the results of dislocation interactions with the parameters of the mathematical model proposed in Ref. [1], in order to transform the mathematical model into a theoretical one.

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КРИСТАЛОГЕОМЕТРИЧНИЙ АНАЛІЗ ДИСЛОКАЦІЙНИХ РЕАКЦІЙ ТА ПЕРЕТВОРЕНЬ ДИСЛОКАЦІЙ "ЛІСУ" НА ДВІЙНИКОВИХ МЕЖАХ У ГПУ-КРИСТАЛАХ

Розглянуто реакції взаємодії базисних, пірамідальних і призматичних дислокацій з двійниковими дислокаціями у ГПУ-кристалах. Результати аналізу таких взаємодій є необхідними для оцінки феноменологічних параметрів математичної моделі розвитку одиничних двійникових прошарків. Щільність кожного виду ковзних дислокацій (дислокацій "лісу") в околі двійникових меж визначає характер дислокаційних реакцій на двійникових межах і, по суті, розвиток двійників. У роботі розглянуто всі можливі взаємодії між двійниковими дислокаціями і дислокаціями "лісу" в ГПУ-кристалах. Результати представлені у вигляді, який є зручним для подальшого аналізу розвитку двійникових прошарків у різних режимах навантаження.

Ключові слова: двійник, двійникова межа, дислокаційна структура, базисна дислокація, пірамідальна дислокація, призматична дислокація, дислокація "лісу".