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FEATURES OF EVOLUTION OF WEDGE-SHAPED TWINS IN BISMUTH SINGLE CRYSTALS SUBJECTED TO POLYSYNTHETIC TWINNING

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Features of evolution of wedge-shaped twins in bismuth single crystals with polysynthetic twins are examined. Polysynthetic twins are found to promote an increase in number, and a decrease in length, of indentation-induced wedge-shaped twins. The latter quantities depend on the density of twins in a polysynthetic twin. Based on the dislocation model, stress fields in the vicinity of wedge-shaped and polysynthetic twins are calculated at a mesoscopic level.

Key words: *wedge-shaped twins, single crystals, twinning.*

Groups of twins usually arise in strained twinning single crystals and polycrystals. The resultant twinned crystals exhibit physical properties that differ from those observed prior to deformation under conditions favorable for twinning [1].

The influence of twin groups on physicomechanical characteristics of materials is presently a matter of much controversy. There exist two opinions: 1) twin boundaries, known to be efficient stress concentrators, promote microcrack nucleation, thus, enhancing the crystal fracture; 2) twinning provides the material with additional plasticity, because twin boundaries act as surmountable (under high strains) potential barriers for moving full dislocations whose path increases, which leads to a lower microcrack nucleation probability [1].

Thus, an investigation into the effect of twin groups on evolution of plastic strains in twinning materials is a challenging problem worth to attack.

The purpose of the present work was to study experimentally the twinning processes in polysynthetic-twin hardened bismuth single crystals during local controlled deformation of their surface and to calculate the stress fields in the vicinity of wedge-shaped and polysynthetic twins on the basis of the mesoscopic dislocation model.

Bismuth single crystals used in the present study were grown by the directed crystallization method, also known as the Bridgman method, from a raw material with a bismuth content of 99.999%. The samples by cleaving single crystals along the (111) cleavage plane. The initial density of basis (nucleated in the cleavage plane) dislocations, as determined by the method of selective etching, was 10^9 m^{-2}, and the initial density of pyramidal dislocations (moving along the faces of a pyramid formed by gliding planes) was 10^7 m^{-2}.

The bismuth single crystals were polysynthetically twinned by compression (under a dimensionless strain $\varepsilon = 8\%$) in the direction of high values of the twinning Schmid factor. Specific features of twin development in locally deformed surface layers of the bismuth single crystals with polysynthetic twins were studied with the help of an PMT-3 instrument equipped with a diamond Vickers indenter. The instrument was adjusted so that indentation was provided precisely at a prescribed place on the single crystal surface. The crystal surface was indented both between the twins and on the twins of a polysynthetic twin (Fig. 1).

The linear density of twins ρ in a polysynthetic twin in the OX direction (Fig. 1) was calculated as

$$\rho = N/L, \tag{1}$$

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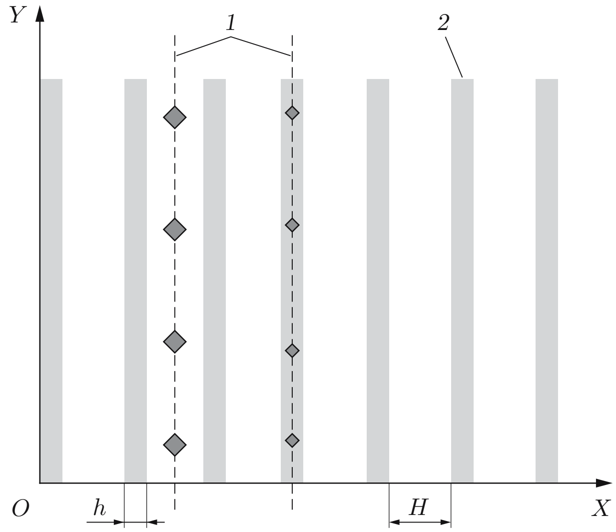

Fig. 1. Polysynthetic twin and directions in which bismuth single crystals were indented with the Vickers indenter: 1) indentation directions; 2) twin.

where N is the number of twins over the segment L on the OX axis. It can be easily shown that $L = N(h + H)$, where h is the twin width and H is the separation between the twins (Fig. 1). As a result, formula (1) can be written as

$$\rho = 1/(h + H).$$

In the present work, we investigated the effect of the parameter ρ on evolution of wedge-shaped twins in the vicinity of the indentation point.

To obtain well-documented data concerning the effect of basis gliding on the twinning pattern of bismuth single crystals, these crystals were deformed by compression in a direction parallel to the (111) crystal plane, favorable for the basis gliding (gliding in the cleavage plane, i.e., in the most densely packed crystal plane in which the dislocation Burgers vector has the least value).

A typical deformation pattern arising on the (111) crystal face of a bismuth single crystal indented with the Vickers pyramid is shown in Fig. 2. A specific feature here is the presence of indentation-induced $\{110\}\langle 001\rangle$ wedge-shaped twins, which normally develop at the intersection points of pyramidal-gliding shear strips, where the stress attains its highest values. The pyramidal gliding traces at the point of indentation form a hexagon.

Evolution of wedge-shaped twin ensembles in bismuth single crystals, as dependent on deformation conditions, can be predicted rather accurately with the dependences plotted in Fig. 3 (the single crystals were indented between the twins). Compressive strain of bismuth single crystals ($\varepsilon = 8\%$) induced under conditions of orientation-forbidden twinning (at a low value of the Schmid factor) leads to an increased number of indentation-induced wedge-shaped twins and a decreased length of these twins. With the indenter load increasing in the examined range of loads, the number of twins around the indenter increases; in the initial sample, given no pre-treatment with pressure, an increasing indenter load leaves the total number of twins approximately unchanged. This fact provides evidence that pre-compression increases the density of basis and pyramidal dislocations in the sample. As a result, the stress concentration around the stoppers increases because of an increased number of dislocations in the vicinity of the stoppers. Dislocation clusters present a kind of twinning-dislocation sources, because splitting of perfect dislocations into partial twinning dislocations is energetically beneficial under these conditions [2]. In turn, the latter promotes an increase in the number of active sources of twinning dislocations in bismuth single crystals strained with a concentrated load. As the indenter load increases, the material in the vicinity of the indentation point becomes more strained, and the stress increases; as a result, those sources of twinning dislocations that could not be activated at lower stresses become now activated. This fact is manifested in an increase in the number of twins with increasing indenter load (Fig. 3a).

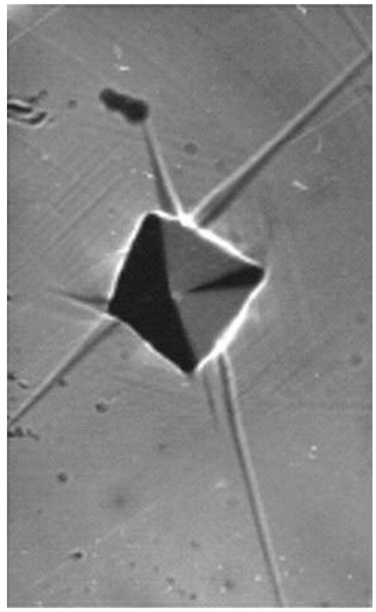

Fig. 2. Deformation pattern on the (111) face of a bismuth single crystal indented with the Vickers pyramid.

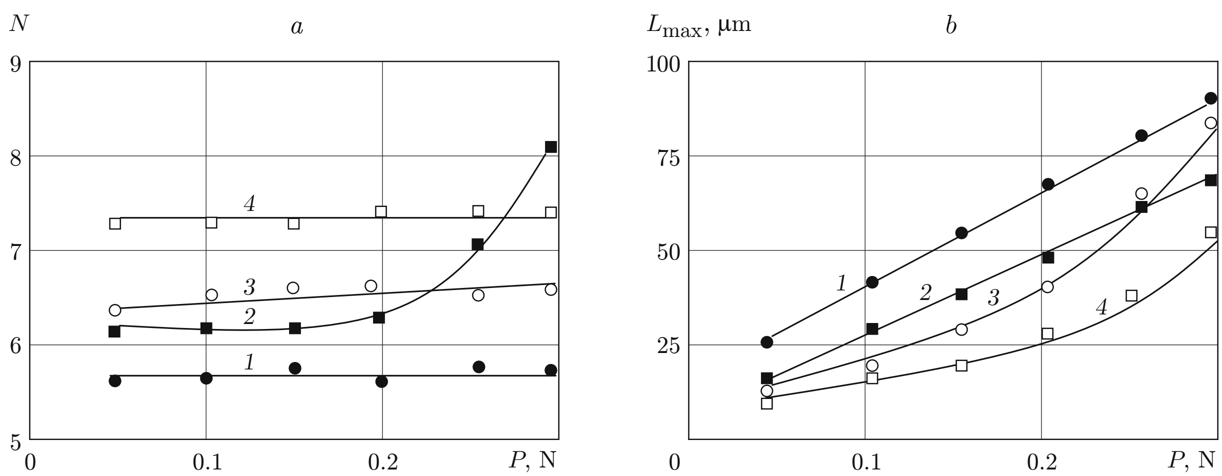

Fig. 3. Mean number N of indentation-induced twins (a) and the maximum twin length L_{max} (b) versus the indenter load P: curves 1 refer to the initial sample, curves 2 to sample deformed by compression ($\varepsilon = 8\%$) under conditions of orientation-forbidden twinning, and curves 3 and 4 refer to polysynthetically twinned samples ($\varepsilon = 8\%$) with $\rho = 0.005\ \mu m^{-1}$ and $0.02\ \mu m^{-1}$, respectively.

Acting as additional sources of twinning dislocations, clusters of basis and pyramidal dislocations simultaneously impede the development of twins from the viewpoint of formation of the twin–host crystal interface and translation of twinning dislocations along twin boundaries. This results in a decreased length of indentation-induced wedge-shaped twins in compression-strained bismuth single crystals. Yet, the twin boundaries themselves act as concentrators of high internal stresses, and their interaction with clusters of basis or pyramidal dislocations generates favorable conditions for twin branching [3]. In a strained single crystal, the number of branching twins exceeds the number of branching twins in a non-strained single crystal.

Polysynthetic twins affect the development of indentation-induced wedge-shaped twins (see Fig. 3), which leads to an increased number of wedge-shaped twins and to a decreased twin length. A similar situation emerges with indentations made along a single interlayer between twins in a polysynthetic twin. The influence of polysynthetic

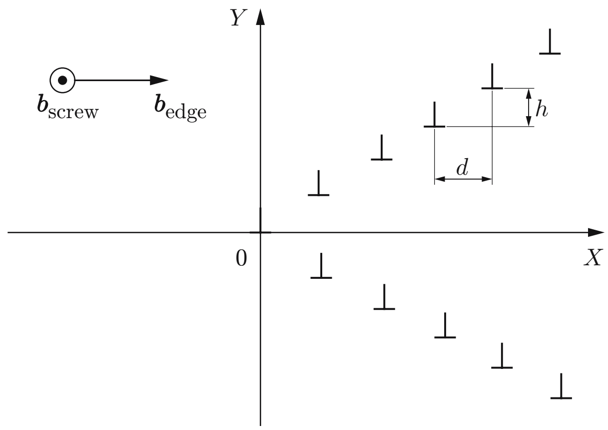

Fig. 4. Dislocation model of the wedge-shaped twin.

twins on the strain pattern near the indentation point is caused by the action of the stressed state in the space between the twins and also by the high density of basis and pyramidal dislocations. As a result, generation of twinning dislocations during indentation begins at a lower external stress, those sources of twinning dislocations being active for which the indenter-induced stress was insufficiently high to generate dislocations in a bismuth single crystal without polysynthetic twins. Because of accumulation of basis and pyramidal dislocations, the total number of sources of twinning dislocations increases owing to splitting of non-dissociated dislocations into partial twinning dislocations. All these factors ensure an increased number of indentation-induced wedge-shaped twins.

Simultaneously, polysynthetic twins impede the development (increase in length) of wedge-shaped twins; that is why the twin length in bismuth single crystals subjected to polysynthetic twinning is shorter than in initial samples, and also in samples deformed under conditions with orientationally forbidden twinning (see Fig. 3b). At the same time, the mouth width of wedge-shaped twins in bismuth single crystals with polysynthetic twins increases by a factor of 1.5–2, as compared with the same quantity in initial samples. The increased twin mouth width is indicative of enhanced generation of twinning dislocations.

It follows from Fig. 3 that the quantitative characteristics of wedge-shaped twins depend on the parameter ρ. As the density of parallel twins increases, the length of wedge-shaped twins introduced into the crystal near the indenter decreases and the number of these twins increases.

It is of interest to investigate the crack nucleation mechanism in locally strained bismuth single crystals with polysynthetic twins. In brittle materials, in regions with dislocation clusters near the twin boundaries, the crack nucleation probability is high. In plastic bismuth single crystals, such clusters initiate secondary gliding. Accumulation of secondary pyramidal dislocations of various crystallographic directions generates favorable conditions for nucleation of indenter-induced microcracks.

A great body of information on elastic properties of twins can be gained by considering the configurations of stress fields in the vicinity of the twins. According to the dislocation theory of elastic twins, their boundary is formed by either edge or screw dislocations [1, 4], and the stress fields produced by such dislocation clusters are superpositions of stresses induced by individual dislocations. Information on particular stress-field configurations in the vicinity of wedge-shaped twins, however, is lacking at the moment, because the twin boundaries are formed by numerous dislocations whose density at the twin boundaries reaches 10^4–10^6 cm^{-2} [5]), and summation of stresses induced by individual dislocations is a labor-consuming problem.

Based on the theory of Fourier series, an attempt was made in [6, 7] to reduce the sums to functions whose analysis somewhat simplifies the task. As was noted in [6, 7], however, summation can be reduced to functional dependences only for one twin boundary, so that the result of [6, 7] can only be used in the approximation of a sufficiently large twin width for the influence of the second boundary to be neglected.

Computer simulations performed in the present study on the basis of the dislocation model of the twin boundary can solve this problem.

Nucleation of wedge-shaped twins in single crystals usually occurs in regions of external stress localization.

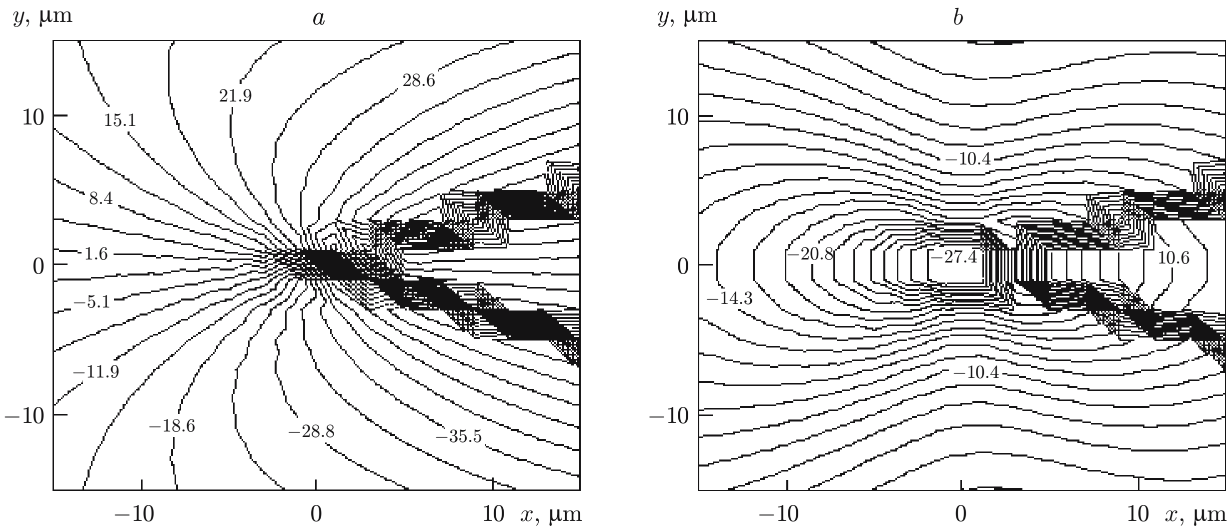

Fig. 5. Stress distribution around a wedge-shaped twin ($-15\ \mu$m $< x <$ 15 μm, $-15\ \mu$m $< y <$ 15 μm, $N = 100$, $M = 99$, $d = 0.15\ \mu$m, and $h = 0.05\ \mu$m): (a) $\sigma_{xx}/(b_{\rm edge}A(x,y))$; (b) $\sigma_{xy}/(b_{\rm edge}A(x,y))$.

Let the twin be a wedge-shaped cluster of twinning dislocations with a Burgers vector $\boldsymbol{b}$. As twinning dislocations are partial dislocations [1], the Burgers vector of these dislocations can be decomposed into two components, a screw component $\boldsymbol{b}_{\rm screw}$ and an edge component $\boldsymbol{b}_{\rm edge}$. In addition, let the edge component of the Burgers vector be directed along the positive direction of the OX axis (Fig. 4) and the screw component be directed normal to the figure plane along the OZ axis. The medium with dislocations is assumed to be homogeneous and isotropic. Then, using the superposition principle, we can calculate the stress-tensor components for the stress induced by the dislocation cluster of interest as

$$\sigma_{xx} = -b_{\rm edge}A\Big(\sum_{n=0}^{N}\frac{(y+nh)[3(x-nd)^2+(y+nh)^2]}{[(x-nd)^2+(y+nh)^2]^2}+\sum_{m=1}^{M}\frac{(y-mh)[3(x-md)^2+(y-mh)^2]}{[(x-md)^2+(y-mh)^2]^2}\Big),$$

$$\sigma_{yy} = b_{\rm edge}A\Big(\sum_{n=0}^{N}\frac{(y+nh)[(x-nd)^2-(y+nh)^2]}{[(x-nd)^2+(y+nh)^2]^2}+\sum_{m=1}^{M}\frac{(y-mh)[(x-md)^2-(y-mh)^2]}{[(x-md)^2+(y-mh)^2]^2}\Big),$$

$$\sigma_{zz} = \nu(\sigma_{xx}+\sigma_{yy}), \tag{2}$$

$$\sigma_{xy} = b_{\rm edge}A\Big(\sum_{n=0}^{N}\frac{(x-nd)[(x-nd)^2-(y+nh)^2]}{[(x-nd)^2+(y+nh)^2]^2}+\sum_{m=1}^{M}\frac{(x-nd)[(x-md)^2-(y-mh)^2]}{[(x-md)^2+(y-mh)^2]^2}\Big),$$

$$\sigma_{xz} = -b_{\rm screw}B\Big(\sum_{n=0}^{N}\frac{y+nh}{(x-nd)^2+(y+nh)^2}+\sum_{m=1}^{M}\frac{y-mh}{(x-md)^2+(y-mh)^2}\Big),$$

$$\sigma_{yz} = b_{\rm screw}B\Big(\sum_{n=0}^{N}\frac{x-nd}{(x-nd)^2+(y+nh)^2}+\sum_{m=1}^{M}\frac{x-nd}{(x-md)^2+(y-mh)^2}\Big).$$

Here, σ_{xx}, σ_{yy}, σ_{zz} and σ_{xy}, σ_{xz}, σ_{yz} are the normal and shear stresses induced by twinning dislocations, respectively, $A = G/[2\pi(1-\nu)]$ (G is the shear modulus and ν is Poisson's ratio), $B = G/(2\pi)$, n and N are the number of a particular dislocation and the total number of dislocations at the twin boundary in the first quarter of the XOY plane (Fig. 4), m and M are the number of a particular dislocation and the total number of dislocations at the twin boundary in the fourth quarter of the XOY plane, and d and h are the projections of the segment connecting two neighboring twin-boundary dislocations onto the OX and OY axes, respectively.

Some data obtained by computer processing of relations (2) are plotted in Fig. 5 as the contours $\sigma_{xx}/(b_{\text{edge}}A(x,y))$ and $\sigma_{xy}/(b_{\text{screw}}B(x,y))$.

A comparative analysis of graphical data shows that the normal stress components (σ_{xx}, σ_{yy}, and σ_{zz}) and the shear stress components (σ_{xy}, σ_{xz}, and σ_{yz}) in the vicinity of a wedge-shaped twin behave differently. The normal stress is distributed asymmetrically near the twin boundaries, whereas the shear stress is symmetric about the OX axis. Exceptions are the stress components σ_{zz} and σ_{xz}, displaying identical contours. In an immediate vicinity of the twin boundary, however, all the stress components attain their highest values.

Computer simulations showed than an increase in the number of twinning dislocations at the twin boundaries does not leads to any substantial changes in the stress-field configuration. Nonetheless, the value of the stress in the vicinity of the twin varies in proportion to the total number of dislocations in the cluster considered, which, in particular, follows from Eqs. (2).

Note another obvious yet previously not discussed fact: the stress inside a twin is never spatially uniform, increasing in the direction from the twin mouth to the twin tip. This fact cannot be established within the thin-twin model [4].

If the stress-field plotting scale is increased by a factor of three or higher, we can see that the configuration of the stress field in the vicinity of a wedge-shaped twin resembles that in the vicinity of a single dislocation. A similar picture was previously observed for the stress field produced in the vicinity of a dislocation wall [4].

The normal stresses σ_{xx} and σ_{yy} are localized near one of the twin boundaries. This localization implies that there are excess internal stresses at one of the twin boundaries, which is expected to affect the dynamics of twinning dislocations forming a twin wedge as a result of crystal deformation. The normal stresses promote the dislocation climb through obstacles in the form of crystal lattice defects. Hence, the twin boundary with higher normal stresses close to it is less sensitive in the course of its formation to crystal imperfections.

The stresses σ_{xx}, σ_{yy}, and σ_{zz} are responsible for migration of point defects toward the twin boundary. Because of antisymmetry of these stresses (see Fig. 5), the concentration of point defects in the vicinity of one boundary is higher than that at the other boundary with lower normal stresses. For instance, the excess concentration of impurities in the vicinity of the twin boundary favors the formation of clusters consisting of a larger number of atoms that clusters near the boundary with lower normal stresses.

The presence of a nonuniform field of normal stresses inside the twin promotes mass transfer in the twinned volume and migration of atoms toward the twin boundaries.

The shear stresses (see Fig. 5) are responsible for interaction between dislocations and also for generation dislocations. The data obtained by analyzing the field configuration for these stresses indicate that dislocations interacting with the wedge-shaped twin tend to occupy a position in the vicinity of the twin boundaries and near the twin tip, where the shear stresses attain their highest values. Accumulation of dislocations near the twin boundaries gives rise to microcrack formation in these regions, thus, leading to relaxation of internal stresses caused by accumulation of clusters of dislocations that migrated to the wedge-shaped twin.

The shear stress increasing from the twin mouth toward the twin tip promotes generation of twinning dislocations at already formed twin–host crystal interfaces. Apparently, a greater number of twinning dislocations are formed in the vicinity of the tip of the wedge-shaped twin, as compared to its mouth. The dislocations formed near the mouth migrate toward the twin tip, into the region with higher stresses.

The shear-stress nonuniformity in the interlayer between the twins activates dislocation processes in this region.

The stresses near a polysynthetic twin, with its individual twins oriented along the OY axis, can be found from the superposition principle by the formulas

$$\sigma_{xy} = \frac{\mu b_{\text{edge}}}{2D(1-\nu)}\Big(\sum_{n=0}^{N} \frac{\sin 2\pi Y(\cosh\, 2\pi X_n^{(1)} - \cos 2\pi Y - 2\pi X_n^{(1)} \sinh\, 2\pi X_n^{(1)})}{(\cosh\, 2\pi X_n^{(1)} - \cos 2\pi Y)^2} - \frac{\mu b_{\text{edge}}}{2D(1-\nu)} \sum_{n=0}^{N} \frac{\sin 2\pi Y(\cosh\, 2\pi X_n^{(2)} - \cos 2\pi Y - 2\pi X_n^{(2)} \sinh\, 2\pi X_n^{(2)})}{(\cosh\, 2\pi X_n^{(2)} - \cos 2\pi Y)^2}\Big), \quad (3)$$

$$\sigma_{xx} = -\frac{\pi\mu b_{\text{edge}}}{D(1-\nu)}\Big(\sum_{n=0}^{N} \frac{2\pi X_n^{(1)}(\cosh\, 2\pi X_n^{(1)} \cos 2\pi Y - 1)}{(\cosh\, 2\pi X_n^{(1)} - \cos 2\pi Y)^2} - \sum_{n=0}^{N} \frac{2\pi X_n^{(2)}(\cosh\, 2\pi X_n^{(2)} \cos 2\pi Y - 1)}{(\cosh\, 2\pi X_n^{(2)} - \cos 2\pi Y)^2}\Big),$$

where $Y = y/D$, $X_n^{(1)} = (x - n(h + H) - h)/D$, and $X_n^{(2)} = (x - n(h + H))/D$. Equations (3) take into account that the opposite boundaries of an isolated twin of the polysynthetic twin contain dislocations with the opposite Burgers vectors.

Thus, the development of wedge-shaped twins in bismuth single crystals subjected to polysynthetic twinning was studied by the method of local surface straining. Polysynthetic twinning was found to increase the number of active sources of twinning dislocations and to decrease their length. Owing to computer simulations based on the dislocation model of a wedge-shaped twin, it becomes possible to construct the stress field in the vicinity of twin boundaries, which can be used for analyzing the physical features of crystal twinning. Relations for predicting the stress fields in a vicinity of a polysynthetic twin were obtained.

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