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# CALCULATION OF THE STRESS FIELDS IN A POLYSYNTHETIC TWIN LOCATED NEAR THE CRYSTAL SURFACE

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*Without using the thin twin approximation, assuming a continuous distribution of dislocations on the boundaries, a procedure to calculate the stress fields in a polysynthetic twin located near the crystal surface has been developed. It is shown that the stresses in the polysynthetic twin are localized at the boundaries and apices of the twins that enter into the composition of the former twin. Examples of calculations of the cleavage stresses of the polysynthetic twin having rectilinear and curvilinear boundaries with uniform and nonuniform distribution of dislocations at them are given.*

***Keywords:*** *polysynthetic twin, stress fields, twinning dislocation.*

**Introduction.** In deformation of solid bodies the twins usually appear in them in groups [1–3]. Therefore it is of practical interest to study the laws governing the development of twinnings in the stress fields of the groups of twins. On uniaxial compression or extension and twisting, a system of parallel twins called polysynthetic twins [1] is formed in the material.

The study of the stress fields in twins by experimental methods relates to complex problems [1]. Therefore it is advisable to develop theoretical methods of investigations making it possible to predict the behavior of the material liable to twinning under certain operation conditions.

Dislocation models rank among the most developed ones [4]. However, the thin twin approximation used in these models does not allow one to consider a stressed state inside it. This is especially true of those groups of two-dimensional defects, the length of which is commensurable with their width [5, 6].

**Statement of the Problem.** The aim of the present work is the development of the technique of calculation of stress fields of a polysynthetic twin located near the crystal surface.

Figure 1 schematically presents a polysynthetic twin which is located near the crystal surface parallel to the *OY* axis. The wake of the surface coincides with the *OX* axis. The constancy of the parameters of the two-dimensional defects considered does not contradict the generality of the results and mathematical expressions obtained, since one can easily pass to the consideration of any group of polysynthetic twins, the classification of which is given in [7]. Because of the cumbersomeness of the obtainable expressions, it is inadvisable to consider this problem in the present work.

Twinning dislocations are Shockley partial dislocations [8]; therefore their Burgers vector can be expanded into two components: screw ($\mathbf{b}_{sc}$) and edge ($\mathbf{b}_{ed}$) ones. These components are directed so as is shown in Fig. 1.

In the case of a thin twin the following relation is used to calculate stresses [9]:

$$\sigma_{ij}(x, y) = \int_{a_0}^{L} \sigma_{ij}^0 (x, y, y_0)\, \rho (y_0)\, dy_0 . \tag{1}$$

Here $\sigma_{ij}^0(x, y, y_0)$ is defined by the formulas [9]

$$\sigma_{xx}^0 (x, y, y_0) = - D_1 \frac{x [x^2 - (y - y_0)^2]}{[x^2 + (y - y_0)^2]^2} + D_1 \frac{x [x^2 - (y + y_0)^2]}{[x^2 + (y + y_0)^2]^2}$$

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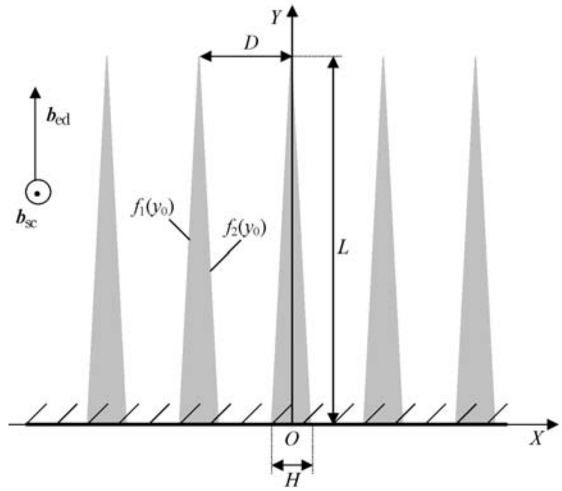


Fig. 1. Schematic representation of a polysynthetic twin near the crystal surface.

$$+ 4D_1 \frac{xy_0 \,[x^2 (3y + 2y_0) - (y + y_0)^2 (y - 2y_0)]}{[x^2 + (y + y_0)^2]^3},$$

$$\sigma^0_{yy} (x, y, y_0) = - D_1 \frac{x \,[x^2 + 3\,(y - y_0)^2]}{[x^2 + (y - y_0)^2]^2} + D_1 \frac{x \,[x^2 + 3\,(y + y_0)^2]}{[x^2 + (y + y_0)^2]^2} - 4D_1 \frac{xyy_0 \,[x^2 - 3\,(y + y_0)^2]}{[x^2 + (y + y_0)^2]^3}, \tag{2}$$

$$\sigma^0_{xy} (x, y, y_0) = - D_1 \frac{(y - y_0)\,[x^2 - (y - y_0)^2]}{[x^2 + (y - y_0)^2]^2} + D_1 \frac{(y + y_0)\,[x^2 - (y + y_0)^2]}{[x^2 + (y + y_0)^2]^2}$$

$$- 2D_1 y_0 \frac{x^4 - 6x^2 y\,(y + y_0)\,(y - y_0)\,(y + y_0)^3}{[x^2 + (y + y_0)^2]^3},$$

$$\sigma^0_{xz} (x, y, y_0) = D_2 \left[ \frac{y - y_0}{x^2 + (y - y_0)^2} - \frac{y + y_0}{x^2 + (y + y_0)^2} \right],$$

$$\sigma^0_{yz} (x, y, y_0) = - D_2 \left[ \frac{x}{x^2 + (y - y_0)^2} - \frac{x}{x^2 + (y + y_0)^2} \right],$$

where $D_1 = \dfrac{\mu \mathbf{b}_{ed}}{2\pi(1 - \nu)}$; $D_2 = \dfrac{\mu \mathbf{b}_{sc}}{2\pi}$.

The problem of calculation of the stress fields inside a twin can be solved if instead of (1) we use

$$\sigma_{ij} (x, y) = \sigma^{(1)}_{ij} (x, y) + \sigma^{(2)}_{ij} (x, y)\,, \tag{3}$$

where $\sigma^{(1)}_{ij}(x, y)$ and $\sigma^{(2)}_{ij}(x, y)$ are the stresses created by each boundary of the twin and determined by the curvilinear integrals:

$$\sigma_{ij}^{(1)} = \int_{L_1} \rho_1 \sigma_{ij}^{(1,0)} \, ds \,, \tag{4}$$

$$\sigma_{ij}^{(2)} = \int_{L_2} \rho_2 \sigma_{ij}^{(2,0)} \, ds \,. \tag{5}$$

In the above relations $\sigma_{ij}^{(1,0)}$ and $\sigma_{ij}^{(2,0)}$ are defined by the formulas

$$\begin{aligned}
\sigma_{xx}^{(1,0)} &= -D_1 \frac{(x-f_1(y_0))\,[(x-f_1(y_0))^2-(y-y_0)^2]}{[(x-f_1(y_0))^2+(y-y_0)^2]^2} + D_1 \frac{(x-f_1(y_0))\,[(x-f_1(y_0))^2-(y+y_0)^2]}{[(x-f_1(y_0))^2+(y+y_0)^2]^2} \\
&+ 4D_1 \frac{(x-f_1(y_0))\,y_0\,[(x-f_1(y_0))^2(3y+2y_0)-(y+y_0)^2(y-2y_0)]}{[(x-f_1(y_0))^2+(y+y_0)^2]^3}, \\
\sigma_{yy}^{(1,0)} &= -D_1 \frac{(x-f_1(y_0))\,[(x-f_1(y_0))^2+3(y-y_0)^2]}{[(x-f_1(y_0))^2+(y-y_0)^2]^2} + D_1 \frac{(x-f_1(y_0))\,[(x-f_1(y_0))^2+3(y+y_0)^2]}{[(x-f_1(y_0))^2+(y+y_0)^2]^2} \\
&- 4D_1 \frac{(x-f_1(y_0))\,yy_0\,[(x-f_1(y_0))^2-3(y+y_0)^2]}{[(x-f_1(y_0))^2+(y+y_0)^2]^3}, \\
\sigma_{xy}^{(1,0)} &= -D_1 \frac{(y-y_0)\,[(x-f_1(y_0))^2-(y-y_0)^2]}{[(x-f_1(y_0))^2+(y-y_0)^2]^2} + D_1 \frac{(y+y_0)\,[(x-f_1(y_0))^2-(y+y_0)^2]}{[(x-f_1(y_0))^2+(y+y_0)^2]^2} \\
&- 2D_1 y_0 \frac{(x-f_1(y_0))^4-6(x-f_1(y_0))^2\,y(y+y_0)+(y-y_0)(y+y_0)^3}{[(x-f_1(y_0))^2+(y+y_0)^2]^3}, \\
\sigma_{xz}^{(1,0)} &= D_2 \left[ \frac{y-y_0}{(x-f_1(y_0))^2+(y-y_0)^2} - \frac{y+y_0}{(x-f_1(y_0))^2+(y+y_0)^2} \right], \\
\sigma_{yz}^{(1,0)} &= -D_2 \left[ \frac{x-f_1(y_0)}{(x-f_1(y_0))^2+(y-y_0)^2} - \frac{x-f_1(y_0)}{(x-f_1(y_0))^2+(y+y_0)^2} \right],
\end{aligned} \tag{6}$$

$$\begin{aligned}
\sigma_{xx}^{(2,0)} &= -D_1 \frac{(x-f_2(y_0))\,[(x-f_2(y_0))^2-(y-y_0)^2]}{[(x-f_2(y_0))^2+(y-y_0)^2]^2} + D_1 \frac{(x-f_2(y_0))\,[(x-f_2(y_0))^2-(y+y_0)^2]}{[(x-f_2(y_0))^2+(y+y_0)^2]^2} \\
&+ 4D_1 \frac{(x-f_2(y_0))\,y_0\,[(x-f_2(y_0))^2+(3y+2y_0)(y+y_0)^2(y-2y_0)]}{[(x-f_2(y_0))^2+(y+y_0)^2]^3}, \\
\sigma_{yy}^{(2,0)} &= -D_1 \frac{(x-f_2(y_0))\,[(x-f_2(y_0))^2+3(y-y_0)^2]}{[(x-f_2(y_0))^2+(y-y_0)^2]^2} + D_1 \frac{(x-f_2(y_0))\,[(x-f_2(y_0))^2+3(y+y_0)^2]}{[(x-f_2(y_0))^2+(y+y_0)^2]^2}
\end{aligned}$$

$$-4D_1 \frac{(x - f_2(y_0))\, y y_0 \,[(x - f_2(y_0))^2 - 3\,(y + y_0)^2]}{[(x - f_2(y_0))^2 + (y + y_0)^2]^3} \,,$$

$$\sigma_{xy}^{(2,0)} = -D_1 \frac{(y - y_0)\,[(x - f_2(y_0))^2 - (y - y_0)^2]}{[(x - f_2(y_0))^2 + (y - y_0)^2]^2} + D_1 \frac{(y + y_0)\,[(x - f_2(y_0))^2 - (y + y_0)^2]}{[(x - f_2(y_0))^2 + (y + y_0)^2]^2} \qquad (7)$$

$$-2D_1 y_0 \frac{(x - f_2(y_0))^4 - 6\,(x - f_2(y_0))^2\, y\,(y + y_0) + (y - y_0)\,(y + y_0)^3}{[(x - f_2(y_0))^2 + (y + y_0)^2]^3} \,,$$

$$\sigma_{xz}^{(2,0)} = D_2 \left[ \frac{y - y_0}{(x - f_2(y_0))^2 + (y - y_0)^2} - \frac{y + y_0}{(x - f_2(y_0))^2 + (y + y_0)^2} \right],$$

$$\sigma_{yz}^{(2,0)} = -D_2 \left[ \frac{x - f_2(y_0)}{(x - f_2(y_0))^2 + (y - y_0)^2} - \frac{x - f_2(y_0)}{(x - f_2(y_0))^2 + (y + y_0)^2} \right].$$

The curvilinear integrals (4) and (5) are reduced to certain integrals of the form

$$\sigma_{ij}^{(1)}(x, y) = \int_0^L \sqrt{1 + (f_1'(y_0))^2}\, \rho_1(y_0)\, \sigma_{ij}^{(1,0)}(x, y, y_0)\, dy_0 \,, \qquad (8)$$

$$\sigma_{ij}^{(2)}(x, y) = \int_0^L \sqrt{1 + (f_2'(y_0))^2}\, \rho_2(y_0)\, \sigma_{ij}^{(2,0)}(x, y, y_0)\, dy_0 \,. \qquad (9)$$

In relations (3)–(9) we will neglect the magnitude of the step formed by twins on the crystal surface, since it is small as compared to the length of the twin, and allowance for $a_0$ exerts a small influence on the configuration of the stress fields in the given scheme of calculations.

In the case considered we must sum the stresses of all the twins entering into the composition of the polysynthetic twin. Then from Eqs. (8) and (9) we obtain

$$\sigma_{ij}^{(1)}(x, y) = \sum_{n=0}^{N} \int_0^L \sqrt{1 + (f_1'(y_0))^2}\, \rho_1(y_0)\, \sigma_{ij}^{(1,0)}(x - nD, y, y_0)\, dy_0 \,, \qquad (10)$$

$$\sigma_{ij}^{(2)}(x, y) = \sum_{n=0}^{N} \int_0^L \sqrt{1 + (f_2'(y_0))^2}\, \rho_2(y_0)\, \sigma_{ij}^{(2,0)}(x - nD, y, y_0)\, dy_0 \,. \qquad (11)$$

In the case of rectilinear boundaries we have

$$f_1(y_0) = \frac{H}{2}\left(1 - \frac{y_0}{L}\right), \qquad (12)$$

$$f_2(y_0) = -\frac{H}{2}\left(1 - \frac{y_0}{L}\right). \qquad (13)$$

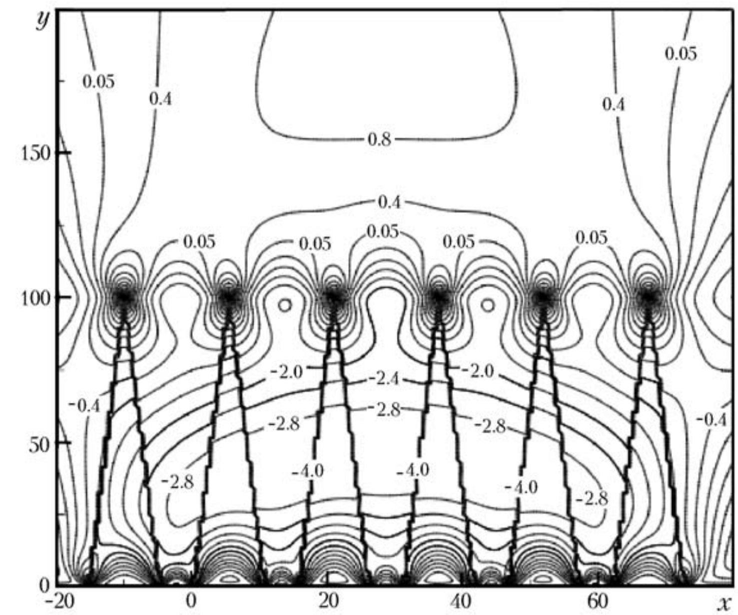


Fig. 2. Results of calculations of the reduced quantity $\sigma^*_{xy}(x, y)$ for the case of rectilinear boundaries of twins with a uniform density of twinning dislocations. $x$, $y$, μm.

Then at $\rho_1(y_0) = \rho_2(y_0) = \text{const} = \rho$ we obtain

$$\sigma_{ij}^{(1)}(x, y) = \rho \sqrt{1 + \left(\frac{H}{2L}\right)^2} \sum_{n=0}^{N} \int_0^L \sigma_{ij}^{(1,0)}(x - nD, y, y_0)\, dy_0\,, \tag{14}$$

$$\sigma_{ij}^{(2)}(x, y) = \rho \sqrt{1 + \left(\frac{H}{2L}\right)^2} \sum_{n=0}^{N} \int_0^L \sigma_{ij}^{(2,0)}(x - nD, y, y_0)\, dy_0\,. \tag{15}$$

**Results and Their Discussion.** The results of calculations for the given case are presented in Fig. 2 on the example of the shear component $\sigma_{xy}$. For convenience the reduced quantity $\sigma^*_{xy}(x, y) = \sigma_{xy}(x, y)/\rho D_1$ was calculated. It was adopted that $L = 100$ μm; $H = 21$ μm; $D = 31$ μm, and $N = 5$. Since in (14) and (15) the summation is carried out from zero, the total number of twins is by one higher than $N$.

From Fig. 2 it is seen that shear stresses are localized at the boundaries and apices of the twins. A high level of stresses is also observed near the crystal surface. Inside the polysynthetic twin there are regions of equal stresses. The stresses in the twins are negative, but further from their apices in the direction of their development, the stresses are positive.

The procedure suggested allows one to calculate the stress fields of the polysynthetic twin located near the crystal surface not only in the case of a uniform distribution of dislocations on rectilinear boundaries, but also when $\rho_1(y_0) \neq \text{const}$ and $\rho_2(y_0) \neq \text{const}$ at their different forms, if these characteristics are identical for all the twins. As an example, we will consider the case where $\rho_1(y_0) = \rho_2(y_0) = \rho(y_0)$ and

$$\rho(y_0) = \frac{2\sigma(1 - \nu)}{\mu\sqrt{\mathbf{b}_{ed}^2 + \mathbf{b}_{sc}^2}} \sqrt{\frac{L + y_0}{L - y_0}}\,. \tag{16}$$

This expression corresponds to the equilibrium distribution of dislocations in a one-sided cluster pressed toward a barrier by the stress $\sigma$ [8].

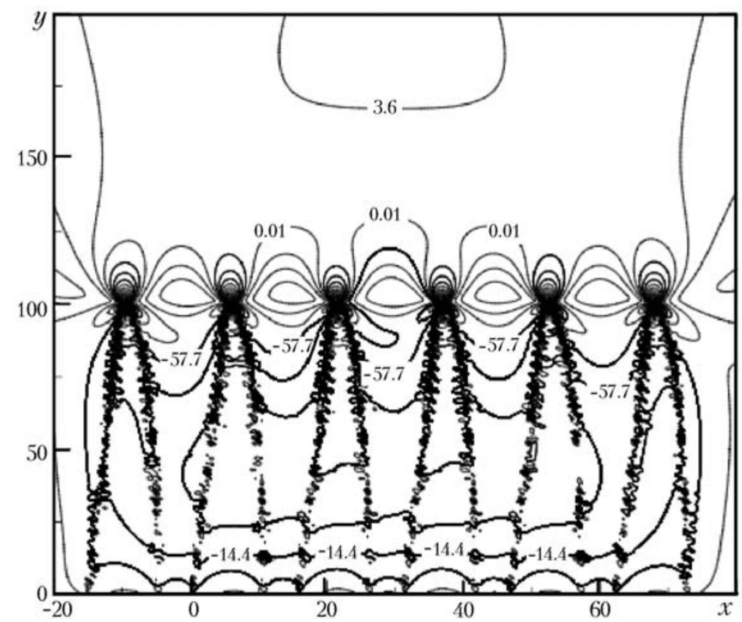


Fig. 3. The form of the distribution of $\kappa_{xy}(x, y)$ for the polysynthetic twin with convex boundaries and nonuniform distribution of dislocations on the boundaries. $x$, $y$, μm.

Let one of the boundaries of the twins of the polysynthetic twin be convex; then we may adopt

$$f_1(y_0) = \frac{H}{2}\sqrt{1 - \left(\frac{y_0}{L}\right)^2}\,. \tag{17}$$

The results of calculations for the example considered are presented in Fig. 3. For convenience of calculations, without loss of generality, we consider the quantity $\kappa_{xy}(x, y) = \sigma_{xy}(x, y)/B_{xy}$, where $B_{xy} = \dfrac{\sigma \mathbf{b}_{ed}}{\pi\sqrt{\mathbf{b}_{ed}^2 + \mathbf{b}_{sc}^2}}$. The remaining calculation parameters were the same as in the previous case.

It is seen from Fig. 3 that stresses are localized at the boundaries and apices of the twins, where the stresses also change their sign. The convexity of one of the boundaries is noticeable.

In [7], a classification of polysynthetic twins is given which is convenient for the physical analysis and makes it possible to follow their evolution depending on the conditions of the deformation of a crystal and means of its working. The procedure suggested in the present work allows one to calculate stresses in various groups of the two-dimensional defects considered. However, the greater the deviation of the structure of a polysynthetic twin from that given in Fig. 1, the more cumbersome are the computational relations.

**Conclusions.** Based on the macroscopic dislocation model of a wedge-like twin, without using the thin twin approximation, a technique of calculation of the stress fields in the polysynthetic twin located near the crystal surface has been developed. It has been established that the stresses are localized at the boundaries and apices of the twins of the polysynthetic twin. The cases of both uniform and nonuniform distribution of twinning dislocations on the twin boundaries, as well as variants of rectangular and curvilinear twin boundaries, are considered.

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## NOTATION

$a_0$, the value of the step formed by the twin on the crystal surface, nm; $\mathbf{b}_{sc}$, $\mathbf{b}_{ed}$, screw and edge components of the Burgers vector, nm; $B_{xy}$, constant, Pa; $D$, distance between neighboring twins of the polysynthetic twin, μm;

$D_1$, $D_2$, constants; $ds$, element of the twin boundary; $f_1(y_0)$, $f_2(y_0)$, functions describing the shape of twin boundaries; $H$, width of a twin at the mouth, μm; $L$, length of a twin, μm; $L_1$, $L_2$, profiles of the twin boundaries along which integration is carried out, μm; $N$, number of twins in the polysynthetic twin; $X$, $Y$, axes of the Cartesian coordinate system; $x$, $y$, $z$, variables; $y_0$, distance from a dislocation to the surface, nm; $\kappa_{xy}(x, y)$, reduced shear stresses, Pa; $\mu$, shear modulus, Pa; $\nu$, Poisson coefficient; $\rho(y_0)$, density of twinning dislocations on the twin boundaries merging into one, $m^{-1}$; $\rho_1$, $\rho_2$, densities of twinning dislocations on twin boundaries, $m^{-1}$; $\sigma$, stress pressing a cluster of dislocations to a barrier, Pa; $\sigma_{ij}$, components of the tensor of stresses, Pa; $\sigma^*_{xy}(x, y)$, dimensionless equivalent of shear stresses. Subscripts: 1, 2, the first and second twin boundaries; ed, edge; sc, screw.

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