Journal of Applied Mechanics and Technical Physics, Vol. 45, No. 6, pp. 871–877, 2004

CALCULATION OF THE FIELD OF INTERNAL STRESSES FOR A PLANE-STRAINED STATE OF AN ELASTIC BODY WITH DISLOCATIONS

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UDC 539.3

Results of numerical calculations of internal stresses in a material for the case of a plane strain are presented. The dependence of the stress distribution on the spatial structure of dislocations is demonstrated.

Key words: *internal stresses, strains, dislocations, elasticity.*

It is known that mechanical characteristics of metals, such as strength, plasticity, and creep, depend on internal stresses in a material. The level of internal stresses can be increased by material quenching or decreased by annealing. In this aspect, calculation of internal stresses is an important problem. One of the main sources of internal stresses are dislocations whose number in the material can be rather high. In the present paper, the internal stresses generated by dislocations are calculated with the help of a mathematical model of plasticity based on the gauge theory of defects with allowance for energy dissipation [1].

Let us consider the problem of determining stresses in an elastic body with dislocations in the absence of external loads for a plane-strained state. In this case, the equations from [1] acquire the form

$$\alpha_{zx} = \frac{\partial \beta_{yx}}{\partial x} - \frac{\partial \beta_{xx}}{\partial y}, \qquad \alpha_{zy} = \frac{\partial \beta_{yy}}{\partial x} - \frac{\partial \beta_{xy}}{\partial y},$$

$$\beta_{xx} + \beta_{yy} = 0, \qquad (\beta_{xy} + \beta_{yx})/2 = \varepsilon^p_{xy}, \qquad \beta_{xx} = \varepsilon^p_{xx},$$

$$\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} = 0, \qquad \frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} = 0,$$

$$\sigma_{xx} = -P + S_{xx}, \qquad \sigma_{yy} = -P + S_{yy}, \qquad \sigma_{xy} = S_{xy}, \tag{1}$$

$$P = K(\rho/\rho_0 - 1), \qquad \rho/\rho_0 = \varepsilon_{xx} + \varepsilon_{yy},$$

$$S_{ij} = 2\mu e^e_{ij}, \qquad e_{ij} = e^e_{ij} + e^p_{ij}, \qquad e^p_{ij} = \varepsilon^p_{ij}, \qquad ij = \{xx, yy, xy\},$$

$$e_{xx} = \varepsilon_{xx} - (\varepsilon_{xx} + \varepsilon_{yy})/3, \qquad e_{yy} = \varepsilon_{yy} - (\varepsilon_{xx} + \varepsilon_{yy})/3, \qquad e_{xy} = \varepsilon_{xy},$$

$$\varepsilon_{xx} = \frac{\partial u_x}{\partial x}, \qquad \varepsilon_{yy} = \frac{\partial u_y}{\partial y}, \qquad \varepsilon_{xy} = \frac{1}{2}\Big(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x}\Big),$$

where α_{zx} and α_{zy} are the components of the tensor of density of dislocations, β_{ij} is the tensor of plastic distortion, ε^p_{xx} and ε^p_{xy} are the components of the tensor of plastic strain, σ_{ij} is the stress tensor, P is the pressure, S_{ij} is

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the stress deviator, K is the volume compression modulus, μ is the shear modulus, ρ is the density of the strained material, ρ_0 is the density of the nonstrained material, ε_{ij} and ε_{ij}^p are the tensors of strain and plastic strain, e_{ij}, e_{ij}^e, and e_{ij}^p are the deviators of strain, elastic strain, and plastic strain, respectively, and u_x and u_y are the components of the displacement vector.

As was shown in [2], the total stresses $\tilde{\sigma}_{ij}$ in the material in the two-dimensional case are determined by the formulas

$$\tilde{\sigma}_{xx} = \sigma_{xx} + \sigma'_{xx}, \qquad \tilde{\sigma}_{yy} = \sigma_{yy} + \sigma'_{yy}, \qquad \tilde{\sigma}_{xy} = \sigma_{xy} + \sigma'_{xy},$$
$$\tilde{\sigma}_{yx} = \sigma_{yx} + \sigma'_{yx}, \qquad \sigma'_{xx} = -C\,\frac{\partial \alpha_{zx}}{\partial y}, \qquad \sigma'_{yy} = C\,\frac{\partial \alpha_{zy}}{\partial x}, \tag{2}$$
$$\sigma'_{xy} = C\,\frac{\partial \alpha_{zx}}{\partial x}, \qquad \sigma'_{yx} = -C\,\frac{\partial \alpha_{zy}}{\partial y},$$

where C is a constant and σ'_{ij} are self-balanced stresses identically satisfying the equilibrium equations and zero boundary conditions. The stresses σ_{ij} are determined from system (1). In the absence of external loads, system (1), (2), should satisfy zero boundary conditions at the boundary of the body with the normal $\boldsymbol{n}$:

$$\sigma_{xx}n_x + \sigma_{xy}n_y = 0, \qquad \sigma_{yy}n_y + \sigma_{yx}n_x = 0, \qquad \alpha_{zx} = \alpha_{zy} = 0. \tag{3}$$

According to [1], the steady state of the body is possible if the deviator of total stresses $\tilde{S}_{ij}$ satisfies the inequality

$$\tilde{S}_{ij}\tilde{S}_{ij} < (2/3)Y_S^2, \qquad \tilde{S}_{ij} = \tilde{\sigma}_{ij} - (1/3)\tilde{\sigma}_{kk}\delta_{ij},$$

where Y_S is the yield point of the material. In this case, the internal stresses are balanced by the "dry friction force" [1] $\tilde{S}_{ij} = S_{ij}^r$. If this inequality is violated, a plastic flow of the material is observed.

The problem of determining internal stresses is posed as follows. Using system (1), (2) and the boundary conditions (3), we have to find the total stresses $\tilde{\sigma}_{ij}$ for a prescribed field of dislocation density $\alpha_{zx}(x, y)$, $\alpha_{zy}(x, y)$. The self-balanced stresses σ'_{ij} are readily calculated by differentiating the fields α_{ij}. The stresses σ_{ij} are determined by solving the boundary-value problem for the elliptic system (1) with the boundary conditions (3). The solution of this problem can be divided into two stages. At the first stage, we find the components of the distortion tensor $\beta_{ij}(x, y)$ from the first three equations of system (1); after that, the displacements $u_i(x, y)$, strains $\varepsilon_{ij}(x, y)$, and stresses $\sigma_{ij}(x, y)$ are found from the remaining equations of system (1).

The first stage involves a difficulty caused by the fact that the number of equations is smaller than the number of unknowns [there are only three equations in system (1) for determining four unknowns β_{xx}, β_{yy}, β_{xy}, and β_{yx}]. Hence, one component of β_{ij} can be set arbitrarily. Though β_{ij} enter the definition of the deviator of elastic strains in an additive manner $e_{ij}^e = e_{ij} - (\beta_{ij} + \beta_{ji})/2$, the stress tensor $\sigma_{ij} = -P\delta_{ij} + 2\mu e_{ij}^e$ is determined uniquely because system (1) is invariant in the case of the gauge transformation [1]

$$u'_i = u_i + h_i(x_k), \qquad \beta'_{ji} = \beta_{ji} + \frac{\partial h_i}{\partial x_j}. \tag{4}$$

This gauge transformation alters the components of the displacement vector u_i and distortion tensor β_{ij}, whereas the components of the tensors of elastic strains $\varepsilon_{ij}^e = (\partial u_i/\partial x_j + \partial u_j/\partial x_i)/2 - (\beta_{ij} + \beta_{ji})/2$, stresses σ_{ij}, and dislocation density α_{ij} remain unchanged. The components of the distortion tensor $\beta_{ij}(x_k)$ in the general case are determined with accuracy to three arbitrary functions $h_i(x_k)$. Using this arbitrariness, we can show that the distortion tensor can be chosen in the form of a symmetric tensor $\beta_{ij} = \beta_{ji}$.

Let us first consider the general case. Let β'_{ij} be a certain solution of the equation [1] $\varepsilon_{jsp}\,\partial\beta'_{pi}/\partial x_s = \alpha_{ji}$, where $\alpha_{ji} = \alpha_{ji}(x_k)$ are prescribed functions and $\beta'_{ij} \neq \beta'_{ji}$. Since it is assumed that $\beta_{kk} = 0$, according to (4), the functions $h_i(x_k)$ should satisfy the condition $\partial h_k/\partial x_k = 0$. It follows from here that h_i can be presented in the form

$$h_i = -\varepsilon_{ikl}\,\frac{\partial f_l}{\partial x_k}, \tag{5}$$

where $f_l = f_l(x_k)$ are arbitrary functions. Substituting (5) into Eqs. (4), we obtain

$$\beta_{ji} = \beta'_{ji} + \varepsilon_{ikl}\,\frac{\partial^2 f_l}{\partial x_k \partial x_j}. \tag{6}$$

We require that the distortion tensor be symmetric, i.e., $\beta_{ij} = \beta_{ji}$. Using Eq. (6), we obtain a system of three equations for three unknown functions f_l:

$$\varepsilon_{ikl}\,\frac{\partial^2 f_l}{\partial x_k \partial x_j} - \varepsilon_{jkl}\,\frac{\partial^2 f_l}{\partial x_k \partial x_i} = \beta'_{ij} - \beta'_{ji}. \tag{7}$$

In the two-dimensional case, we should assume that $i = 1$, $j = 2$, and $l = 3$ in Eqs. (5) and (6). Then, one component $f_3(x, y)$ is other than zero; from Eq. (7), we obtain the Poisson equation for this component:

$$\frac{\partial^2 f_3}{\partial x^2} + \frac{\partial^2 f_3}{\partial y^2} = \omega. \tag{8}$$

Here $\omega = \beta'_{xy} - \beta'_{yx}$ is a specified function of coordinates. Note that f_3 are determined from (8) nonuniquely because Eq. (8) is resolved by the function $f_3 + f_0$, where f_0 is the solution of the Laplace equation

$$\frac{\partial^2 f_0}{\partial x^2} + \frac{\partial^2 f_0}{\partial y^2} = 0.$$

Thus, we have proved that the distortion tensor can be considered as symmetric ($\beta_{xy} = \beta_{yx}$). The nonuniqueness indicated above means that, if there is a certain solution u_x, u_y, β_{xx}, β_{xy}, β_{yx} of system (1), which satisfies the condition $\beta_{xy} = \beta_{yx}$, then, according to (4), another solution is

$$u'_x = u_x + h_1, \qquad u'_y = u_y + h_2, \qquad \beta'_{xx} = \beta_{xx} + \frac{\partial h_1}{\partial x}, \qquad \beta'_{xy} = \beta_{xy} + \frac{\partial h_2}{\partial x},$$

$$\beta'_{yx} = \beta_{yx} + \frac{\partial h_1}{\partial y}, \qquad h_1 = -\frac{\partial f_0}{\partial y}, \qquad h_2 = \frac{\partial f_0}{\partial x}, \qquad h_3 = 0.$$

If the function $f_0(x, y)$ satisfies the equation $\Delta f_0(x, y) = 0$, the components of the distortion tensor are symmetric ($\beta'_{xy} = \beta'_{yx}$). The gauge is fixed by setting the function $f_0(x, y)$ or the distortion-tensor components $\beta_{xx}(x, y)$ and $\beta_{xy}(x, y)$, after which, as is shown below, the displacements u_x and u_y are uniquely determined from the equilibrium equations (1).

With allowance for the information given above, we write the system of equations for determining β_{ij} and e^p_{ij} as

$$\frac{\partial \beta_{xy}}{\partial x} - \frac{\partial \beta_{xx}}{\partial y} = \alpha_{zx}, \qquad \frac{\partial \beta_{xx}}{\partial x} + \frac{\partial \beta_{xy}}{\partial y} = -\alpha_{zy}, \qquad e^p_{ij} = \beta_{ij}. \tag{9}$$

Differentiating the left and right sides of the first two equations in (9), we rewrite them as the Poisson equations:

$$\frac{\partial^2 \beta_{xx}}{\partial x^2} + \frac{\partial^2 \beta_{xx}}{\partial y^2} = -\Big(\frac{\partial \alpha_{zx}}{\partial y} + \frac{\partial \alpha_{zy}}{\partial x}\Big), \qquad \frac{\partial^2 \beta_{xy}}{\partial x^2} + \frac{\partial^2 \beta_{xy}}{\partial y^2} = \frac{\partial \alpha_{zx}}{\partial x} - \frac{\partial \alpha_{zy}}{\partial y}. \tag{10}$$

The computational domain was a square (Fig. 1) whose boundaries were free from loading ($f_i = \sigma_{ij} n_j = 0$), and the components of the dislocation-density tensor α_{ij} at the boundary were assumed to be equal to zero. It is assumed that the distribution of dislocations in the square is nonuniform. The maxima and minima of the dislocation density are located in nodes of square cells and are described by the formulas

$$\alpha_{zx} = A_1 \sin kx \sin ky, \qquad \alpha_{zy} = A_2 \sin kx \sin ky, \qquad kH = 2\pi m. \tag{11}$$

It was assumed in the calculations that $H = 10^{-2}$ m, $m = 15$, and $A_1 = A_2 = 2.72 \cdot 10^2\ \text{m}^{-1}$, which corresponds to the scalar density of dislocations $n = 8 \cdot 10^{11}\ \text{m}^{-2}$ with the Burgers vector $b = 3.4 \cdot 10^{-10}$ m. The distribution of dislocations (11) models a polycrystalline material where dislocations are concentrated at the boundaries of square crystallites [3]. The total Burgers vector corresponding to distribution (11) equals zero. Substituting relations (11) into the right side of Eqs. (10), we find the components of the distortion tensor β_{ij} and plastic strain tensor ε^p_{ij}:

$$\begin{aligned} \beta_{xx} &= \varepsilon^p_{xx} = (A_2 \cos kx \sin ky + A_1 \sin kx \cos ky)/(2k), \\ \beta_{xy} &= \varepsilon^p_{xy} = (A_2 \sin kx \cos ky - A_1 \cos kx \sin ky)/(2k). \end{aligned} \tag{12}$$

Figure 2 shows the isolines of distortion β_{xy} (plastic strain ε^p_{xy}) plotted by formulas (12). The distribution of the component β_{xx} has a similar form (with the only difference that the bands are parallel to the conjugate

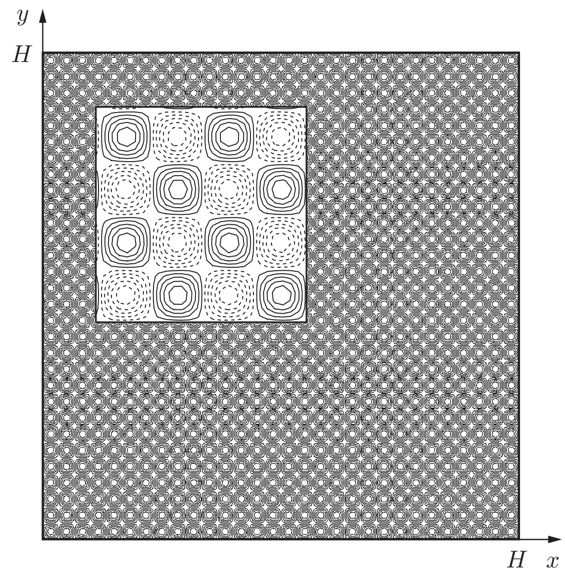

Fig. 1. Computational domain and isolines of the dislocation-density component α_{zx} (the inset shows the inner section: the dashed and solid curves indicate the negative and positive levels, respectively).

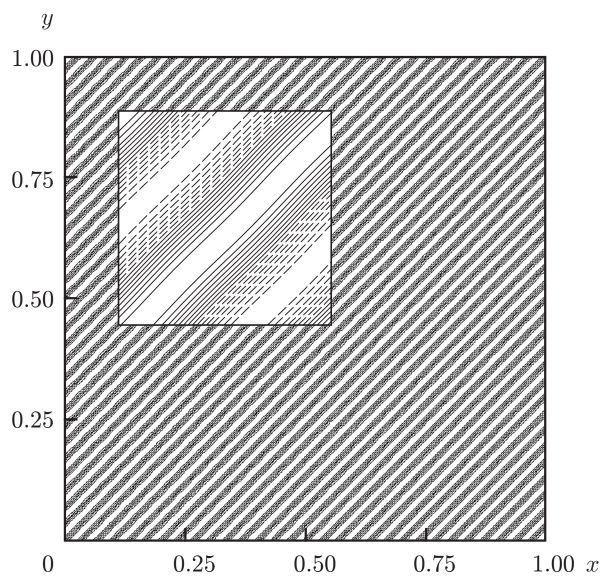

Fig. 2. Isolines of the plastic distortion component β_{xy} (the inset shows the inner section; notation the same as in Fig. 1).

diagonal, i.e., rotated by 90°). Equations (12) describe the banded plastic strain, which leads to the distribution of dislocation density in the form of a square grid (11).

The gauge is fixed by choosing the distortion-tensor components in the form (12). Let us show that system (1) yields unique values of the displacements u_x and u_y for prescribed components of the distortion tensor (12). Expressing stresses via displacements and distortions, we write the equilibrium equations in system (1) in the form of the Navier equations:

$$\Delta u_x + \frac{1}{1-2\nu}\frac{\partial}{\partial x}\operatorname{div}\boldsymbol{u} = 2\Big(\frac{\partial \beta_{xx}}{\partial x} + \frac{\partial \beta_{xy}}{\partial y}\Big), \qquad \Delta u_y + \frac{1}{1-2\nu}\frac{\partial}{\partial y}\operatorname{div}\boldsymbol{u} = 2\Big(\frac{\partial \beta_{xy}}{\partial x} - \frac{\partial \beta_{xx}}{\partial y}\Big).$$

Here $\Delta = \partial^2/\partial x^2 + \partial^2/\partial y^2$, $\operatorname{div}\boldsymbol{u} = \partial u_x/\partial x + \partial u_y/\partial y$, and ν is Poisson's ratio. The equilibrium equations in (1)

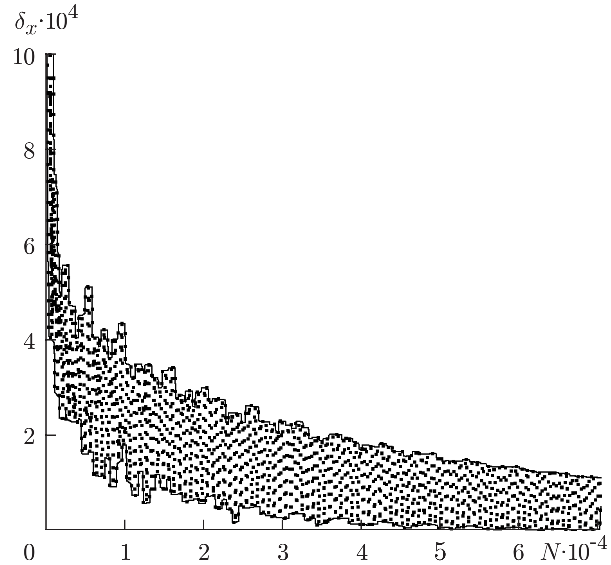

Fig. 3. Norm of the relative error versus the number of the iteration: the points show the calculated values, and the curves show the scatter of numerical data.

reduce to equations of the linear elasticity theory with a volume force, which is expressed via the derivatives of the distortion tensor (12) and is a unique function of coordinates. In this case, the theorems of existence and uniqueness [4] are valid; it follows from these theorems that the displacements in the first boundary-value problem are uniquely determined from system (1).

At the second stage, the equilibrium equations in (1) were solved by the pseudo-transient method. For this purpose, inertial and viscous terms were added:

$$\rho\,\frac{\partial^2 u_x}{\partial t^2} = \frac{\partial \sigma^0_{xx}}{\partial x} + \frac{\partial \sigma^0_{xy}}{\partial y}, \qquad \rho\,\frac{\partial^2 u_y}{\partial t^2} = \frac{\partial \sigma^0_{xy}}{\partial x} + \frac{\partial \sigma^0_{yy}}{\partial y},$$
$$\sigma^0_{ij} = \sigma_{ij} + 2\eta\dot e_{ij}, \qquad \dot e_{ij} = \frac{1}{2}\Big(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\Big) - \frac{1}{3}\,\frac{\partial v_k}{\partial x_k}\,\delta_{ij}, \qquad v_i = \frac{\partial u_i}{\partial t}. \tag{13}$$

Here the quantity σ_{ij} is determined in (1); η is the artificial viscosity. System (13) was solved with fixed ε^p_{ij} and boundary conditions (3) by a finite-difference method by the "cross" scheme [5]. As a result, the solution became steady ($v_i \to 0$, $\partial^2 u_i/\partial t^2 \to 0$, and $\dot e_{ij} \to 0$) and reduced to the corresponding solution of the steady problem ($\sigma^0_{ij} \to \sigma_{ij}$). The solution convergence was determined by the norm of the relative change in the solution during one iteration

$$\delta_i = \|\Delta u_i\|/\|u_i\| = \max_{x,y} |u_i(t+\tau) - u_i(t)|/\max_{x,y} |u_i(t+\tau/2)| < \varepsilon,$$

where $\varepsilon \ll 1$ is a prescribed small number, τ is the time step, and u_i are the values of displacement components in the difference-grid nodes.

The numerical calculation was performed for aluminum with the following parameters: $\rho_0 = 2.7\cdot 10^3$ kg/m^3, $K = 7.3\cdot 10^{10}$ Pa, $\mu = 2.48\cdot 10^{10}$ Pa, and $\eta = 4.23\cdot 10^2$ Pa$\cdot$sec. Decaying oscillations were observed during the calculation, and the solution rapidly reached the steady value. The solution-convergence process is illustrated in Fig. 3. The norm of the relative change δ_x oscillates between the minimum value $\delta_{x,\min}$ and maximum value $\delta_{x,\max}$, which tend to zero as the iteration number increases and ensure solution convergence: $\delta_x \to 0$. The solution was assumed to be steady under the condition $\max(\delta_x, \delta_y) < 2\cdot 10^{-4}$.

Figures 4a and 4b show the calculated isolines of stresses σ_{xy} and displacements u_x, respectively. It is seen that the displacements are a superposition of the banded and "staggered" distributions. The distribution of stresses σ_{xy} is similar to the distribution of plastic distortion β_{xy}. We have the stresses $\sigma_{xy} = \sigma_{yx} = 0$ at all boundaries of the square.

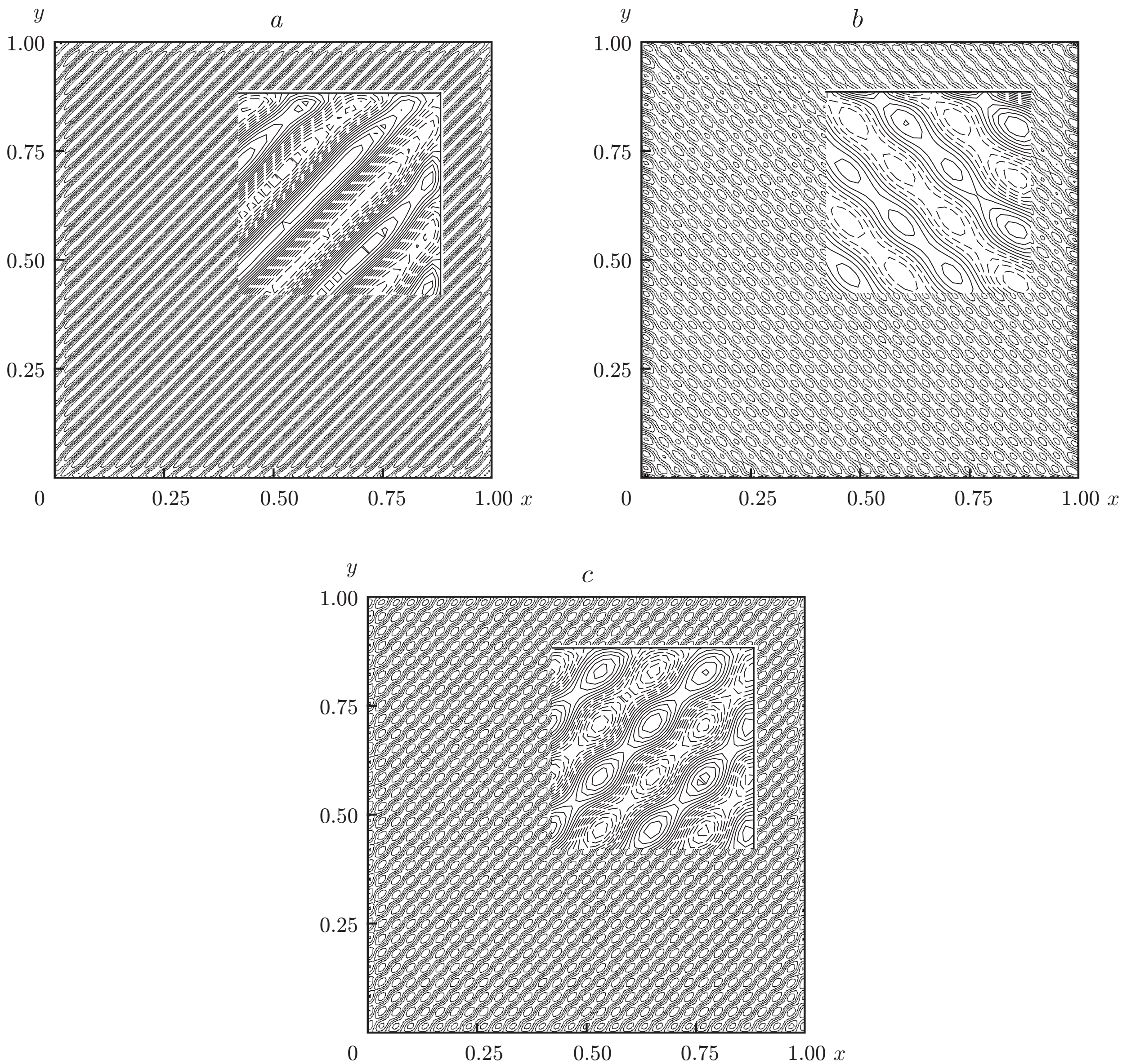

Fig. 4. Isolines of the components of stresses σ_{xy} (a), displacements u_x (b), and total stresses $\tilde{\sigma}_{xy}$ (c) (the insets show the sections in the vicinity of the top right corner: the dashed and solid curves refer to the negative and positive levels, respectively).

The self-balanced stresses σ'_{xy} are determined in accordance with (2) and (12):

$$\sigma'_{xx} = -CA_1 k \sin kx \cos ky, \qquad \sigma'_{yy} = CA_2 k \cos kx \sin ky,$$
$$\sigma'_{xy} = CA_1 k \cos kx \sin ky, \qquad \sigma'_{yy} = -CA_2 k \sin kx \cos ky. \tag{14}$$

Formulas (14) describe the "staggered" distribution of σ'_{ij}. According to (2), the total stresses are determined by the formula $\tilde{\sigma}_{ij} = \sigma_{ij} + \sigma'_{ij}$. Figure 4c shows the isolines of the component $\tilde{\sigma}_{xy}$ of total stresses, constructed for $C = 2.64 \cdot 10^2$ Pa $\cdot$ m^2. Popov et al. [6] proposed the formula $C = \mu l_1 l_2$, where l_1 is the size of the crystallite and l_2 is the distance between the slip lines. The chosen value of C corresponds to the value $l_1 = 1/15$ cm equal to the period of the dislocation structure and to the distance $l_2 = 12$ μm.

It is seen from Fig. 4c that, in contrast to σ_{xy}, the total stresses $\tilde{\sigma}_{xy}$ do not vanish on the left and right boundaries of the computational domain. This is associated with the character of the distribution $\sigma'_{xy}(x, y)$ determined by the third equation in (14). The amplitudes of oscillations $\tilde{\sigma}_{xy}$ and σ'_{xy} for the specified field of dislocations

(11) are 1 GPa and $0.6 \cdot 10^9$ Pa, respectively. It is of interest to note that the distributions of total stresses and displacements are similar to each other. Apparently, this is a random coincidence.

The distribution of total stresses almost in the entire domain is periodic and is determined by the field of dislocations α_{zx} and α_{zy}. The periodicity is violated only in a narrow band near the boundary owing to the influence of zero boundary conditions. The calculations show that the self-balanced stresses σ'_{ij} have the same order as the elastic stresses σ_{ij}; therefore, they have to be taken into account in calculating the total stresses $\tilde{\sigma}_{ij}$.

This work was supported by the Ministry of Education of the Russian Federation (Grant No. EO2-4.0-224) and by the Russian Foundation for Basic Research (Grant No. 04-01-00894).

REFERENCES

1. S. P. Kiselev, "Model of elastoplastic deformation of materials, based on the gauge theory of defects with allowance for energy dissipation," *J. Appl. Mech. Tech. Phys.*, **45**, No. 2, 292–300 (2004).
2. S. P. Kiselev, "Internal stresses in a solid with dislocations," *J. Appl. Mech. Tech. Phys.*, **45**, No. 4, 567–571 (2004).
3. J. Friedel, *Dislocations*, Pergamon Press, Oxford–New York (1967).
4. H. Hahn, *Elastizitatstheorie. Grundlagen der Linearen Theorie und Anwendungen*, Teubner, Stuttgart (1986).
5. M. L. Wilkins, "Calculation of elastoplastic flows," in: B. Alder, S. Fernbach, and M. Retenberg (eds.), *Methods of Computational Physics*, Vol. 3, Academic Press, New York (1964).
6. V. L. Popov, E. E. Slyadnikov, and N. V. Chertova, "Dynamic gauge theory of waves in elastoplastic media," in: *Physical Mesomechanics and Computer Design of Materials* (collected scientific papers) [in Russian], Vol. 1, Nauka, Novosibirsk (1995), pp. 113–129.