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INTERNAL STRESSES IN A SOLID WITH DISLOCATIONS

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Formulas for calculating internal stresses in a material, generated by continuously distributed dislocations, are found on the basis of the gauge theory of defects. It is shown that internal stresses are self-balanced and satisfy the equilibrium equations and boundary conditions in the absence of external loads.

Key words: *internal stresses, dislocations, elasticity, boundary conditions, equilibrium equations, gauge theory of dislocations.*

Internal stresses generated by defects reach significant magnitudes and can appreciably affect physicomechanical properties of materials. For this reason, calculation of internal stresses is an urgent problem, which is extensively investigated. One of the first methods of calculating stresses induced by a point defect, which was proposed by Eshelby, consists in adding a bulk force proportional to the derivative from the plastic strain tensor to the right side of the equilibrium equations [1]. Later, this method was generalized to calculate stresses from a single dislocation and a set of continuously distributed dislocations [1]. This method is incomplete, however, because it ignores the vortex component of the stress tensor, which identically satisfies the equilibrium equations. The vortex component of the stress tensor was discussed in [2–4] in the general case and as applied to a continuous field of defects in [5, 6].

Internal stresses generated by continuously distributed dislocations are considered in the present work on the basis of the gauge theory of defects.

Following [7], we write the equilibrium equations of a solid body with a continuously distributed field of dislocations:

$$\frac{\partial \sigma_{ij}}{\partial x_j} = 0, \qquad \tilde{S}_{ij} - S^r_{ij} = 0, \qquad \tilde{S}_{ij}\tilde{S}_{ij} < \frac{2}{3}\,Y_s^2,$$

$$\sigma_{ij} = -p\delta_{ij} + S_{ij}, \quad p = -K\varepsilon^e_{kk}, \quad S_{ij} = 2\mu e^e_{ij}, \quad K = \lambda + 2\mu/3,$$

$$e^e_{ij} = \varepsilon^e_{ij} - \frac{1}{3}\,\varepsilon^e_{kk}\delta_{ij}, \qquad \varepsilon^e_{ij} = \frac{1}{2}\Big(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\Big) - \varepsilon^p_{ij}, \qquad \varepsilon^p_{ij} = \frac{1}{2}\,(\beta_{ij} + \beta_{ji}), \tag{1}$$

$$\tilde{S}_{ij} = S_{ij} + S'_{ij}, \qquad S'_{ij} = \sigma'_{ij} - \frac{1}{3}\,\sigma'_{kk}\delta_{ij}, \qquad \sigma'_{ij} = -C\varepsilon_{jkl}\,\frac{\partial \alpha_{li}}{\partial x_k}, \qquad \alpha_{ji} = \varepsilon_{jsp}\,\frac{\partial \beta_{pi}}{\partial x_s}.$$

Here u_i are the components of the displacement vector, σ_{ij}, ε_{ij}, β_{ij}, α_{ij}, S_{ij}, and e_{ij} are the tensors of stresses, strains, plastic distortion, dislocation density, stress deviator, and strain deviator, respectively, ε_{ijk} is the absolutely antisymmetric Levi-Civita tensor, δ_{ij} is the Kronecker symbol, p is the pressure, and K and μ are the bulk compression and shear moduli; the subscripts "e" and "p" refer to elastic and plastic strains, respectively; summation is performed over repeated subscripts. The boundary conditions for system (1) have the following form (see [7]):

$$f_i = \sigma_{ij}n_j, \qquad \varepsilon_{kjl}n_j\alpha_{li} = 0. \tag{2}$$

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It follows from the third inequality of system (1) that the steady solutions of this system exist under the condition that the stress deviator $\tilde{S}_{ij}$ does not go out to the yield surface. In this case, the stresses $\tilde{S}_{ij}$ are balanced by the stresses of "dry" friction S^r_{ij} [see the second equation in (1)]. The stresses of "dry" friction S^r_{ij} are similar to the averaged absolute value of the Peierls force [8]; they have inelastic origin and are related to the atomic structure of the crystal.

It is of interest to note that, in addition to the "conventional" stresses σ_{ij} determined from Hooke's law, the stresses $\tilde{S}_{ij}$ involve the stresses σ'_{ij}, though the latter do not enter the equilibrium equations [first equation in (1)] and boundary conditions (2). This allows us to assume that the stresses σ'_{ij} identically satisfy the equilibrium equation and zero boundary conditions (2), where the surface force at each point of the boundary equals zero $f_i = 0$. Since the stresses σ'_{ij} are expressed via the rotor of the dislocation-density tensor, they will be referred to as vortex and self-balanced stresses below. On the basis of the assumption made, the total stresses in an elastic material with dislocations are described by the expression $\tilde{\sigma}_{ij} = \sigma_{ij} + \sigma'_{ij}$, where the stresses σ_{ij} are determined similar to [1] from the equilibrium equations and Hooke's law, and the vortex self-balanced stresses σ'_{ij} are found by the formula

$$\sigma'_{ij} = -C\varepsilon_{jkl}\,\frac{\partial \alpha_{li}}{\partial x_k} = -C\varepsilon_{jkl}\varepsilon_{lsp}\,\frac{\partial^2 \beta_{pi}}{\partial x_k\,\partial x_s}. \tag{3}$$

It follows from formula (3) that the tensor σ'_{ij} is not symmetric. The sequence of subscripts in the asymmetric tensors σ'_{ij} and α_{ij} in formula (3) is uniquely determined from the condition of invariance of system (1) with respect to the group of gauge transformations

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

where $h_i(x_k)$ is an arbitrary function of coordinates. The subscript i related to the function $h_i(x_k)$ is called the group subscript, and j is called the space subscript.

Let us prove the above-made assumptions concerning the stress σ'_{ij}.

The validity of the first assumption is verified by a direct substitution of expression (3) into the equilibrium equation [first equation in system (1)]:

$$\frac{\partial \sigma'_{ij}}{\partial x_j} = -C\varepsilon_{jkl}\,\frac{\partial^2 \alpha_{li}}{\partial x_j\,\partial x_k} = -C\varepsilon_{kjl}\,\frac{\partial^2 \alpha_{li}}{\partial x_k\,\partial x_j} = C\varepsilon_{jkl}\,\frac{\partial^2 \alpha_{li}}{\partial x_k\,\partial x_j} = 0.$$

The third term in this chain of equalities is obtained from the second one by replacing the repeated subscripts $k \leftrightarrow j$, and the fourth term is obtained by permutation of the subscripts k and j in the antisymmetric tensor ε_{kjl}. As a result, we find that the fourth term equals the second term with the opposite sign and, hence, equals zero. Thus, it is shown that the equilibrium equation is identically satisfied if we substitute stresses determined by formula (3) into this equation.

To verify the second assumption, we first consider a particular case where the body has the form of a cube. We introduce a Cartesian coordinate system x_1, x_2, x_3 and place the origin to the center of the cube; then, the equations for the cube faces are $x_i = \pm 1$. Using Eqs. (1) and (2), we find the value of the surface force $f_i = \sigma'_{ij} n_j$ on the face $x_1 = 1$, for which $n_1 = 1$ and $n_2 = n_3 = 0$. Substituting these n_i into the second equation in (2), we obtain that $\alpha_{3i} = \alpha_{2i} = 0$ is valid on the face $x_1 = 1$, and α_{1i} is an arbitrary function of the coordinates x_i. Differentiating the first two relations with respect to x_2, x_3, we rewrite the boundary conditions for α_{ij} on the face $x_1 = 1$ in the form

$$\frac{\partial \alpha_{2i}}{\partial x_2} = \frac{\partial \alpha_{2i}}{\partial x_3} = \frac{\partial \alpha_{3i}}{\partial x_2} = \frac{\partial \alpha_{3i}}{\partial x_3} = 0. \tag{4}$$

Substituting (4) into the first equation in (2), with allowance for (3), we obtain the following relation for the face $x_1 = 1$:

$$f_i = \sigma'_{ij} n_j = \sigma'_{i1} = -C\Big(\frac{\partial \alpha_{3i}}{\partial x_2} - \frac{\partial \alpha_{2i}}{\partial x_3}\Big) = 0.$$

Similar identities are valid for the other faces of the cube; hence, the vortex stresses σ'_{ij} identically satisfy the zero boundary conditions and are self-balanced.

Let us give a similar proof in the general case for a body bounded by an arbitrary surface. We relate the local Cartesian coordinate system to each point of the surface so that the axis ξ^1 at each point is directed along the unit normal vector to the surface $\boldsymbol{n}$. This can be done by parallel transposition and rotation of the Cartesian reference vector $\boldsymbol{e}_i$ when passing from the point ξ^i to the point $\xi^i + d\xi^i$. In this case, the vortex stresses (3) are determined by the formula

$$\hat{\sigma}' = \sigma_i'^j \boldsymbol{e}_j \boldsymbol{e}^i, \qquad \sigma_i'^j = -C\varepsilon^{jkl}\nabla_k \alpha_{li} = -\frac{C}{\sqrt{g}}\Big(\frac{\partial \alpha_{li}}{\partial \xi^k} - \frac{\partial \alpha_{ki}}{\partial \xi^l} - \alpha_{ls}\Gamma^s_{ki} - \alpha_{ks}\Gamma^s_{li}\Big), \tag{5}$$

where Γ^k_{ij} are the Christoffel symbols expressed via the derivatives from the metric tensor g_{ij} [9], $g = \det \|g_{ij}\|$. In the coordinates ξ^i, the boundary condition for α_{ij} [see the second equation in (2)] is written in the form $\varepsilon^{kjl} n_j \alpha_{li} = 0$. At each point of the surface $\xi^1 = 0$, the normal vector has the components $n_1 = 1$ and $n_2 = n_3 = 0$; substituting them into the boundary conditions, we obtain $\alpha_{3i}(\xi^2, \xi^3) = \alpha_{2i}(\xi^2, \xi^3) = 0$, $\alpha_{1i}(\xi^i)$ is an arbitrary function of coordinates. From here, we find the covariant derivatives at the boundary:

$$\nabla_2 \alpha_{3i} = \frac{\partial \alpha_{3i}}{\partial \xi^2} - \alpha_{3s}\Gamma^s_{i2} - \alpha_{si}\Gamma^s_{32} = -\alpha_{1i}\Gamma^1_{32}, \qquad \nabla_3 \alpha_{2i} = -\alpha_{1i}\Gamma^1_{23}.$$

Substituting these derivatives into (5) and taking into account that the Christoffel symbols in the Euclidean space are symmetric with respect to the subscripts $\Gamma^k_{ij} = \Gamma^k_{ji}$ [9], we obtain

$$f_i = \sigma_i'^j n_j = \sigma_i'^1 = -C(\nabla_2 \alpha_{3i} - \nabla_3 \alpha_{2i}) = C\alpha_{1i}(\Gamma^1_{23} - \Gamma^1_{32}) = 0.$$

This identity finalizes the proof of the fact that the stresses σ'_{ij} are self-balanced. It follows from formulas (3), (5) that these stresses depend on nine arbitrary functions α_{ij} or β_{ij}, which should satisfy the second boundary condition in (2). The functions $\alpha_{ij}(x_k)$ are parameters of state, and their form is determined by solving an unsteady problem that describes the process of reaching this steady state or from an experiment. The functions $\beta_{ij}(x_k)$ are not parameters of state because they are changed by gauge transformations. Note, the functions α_{ij} and σ'_{ij} remain unchanged after gauge transformations.

A geometric approach to the description of an elastic body with defects, which is based on the use of non-Euclidean geometry for the distortion field, was developed in [5, 6]. Myasnikov and Guzev [5, 6] proposed a formula for vortex stresses

$$\sigma''_{ij} = A\varepsilon_{jlk}\varepsilon_{isp}\frac{\partial \Gamma_{pl.s}}{\partial x_k}, \tag{6}$$

which identically satisfies the equilibrium equation. We find the surface force generated by stresses (6) on the cube face $x_1 = 1$ for low strains $\beta_{ij} \ll 1$. In this case, $\Gamma_{ij.k} = \partial \beta_{jk}/\partial x_i$ and $\sigma''_{ij} = A\varepsilon_{ilk}\,\partial \alpha_{jk}/\partial x_l$, which, with allowance for Eq. (4), yields $f_i = \sigma''_{i1} = A\varepsilon_{ilk}\,\partial \alpha_{1k}/\partial x_l$. Since α_{1i} is an arbitrary function of coordinates x_i, we have $f_i \neq 0$ in the general case, and stresses (6) σ''_{ij} do not satisfy the zero boundary conditions. To satisfy the boundary conditions, Myasnikov and Guzev [5, 6] introduced elastic stresses generated by the forces on the body surface due to the vortex stresses $f''_i = -\sigma''_{ij} n_j$.

We compare the formula for the self-balanced stresses (3) and formula (6) from [5, 6]. For this purpose, first, we extend formula (3) to finite strains. In the case of Cartesian coordinates, the dislocation-density tensor α_{ij} is expressed through the distortion-field torsion tensor $T_{ij.k}$ by the formula [6] $\alpha_{lk} = \varepsilon_{lij} T_{ij.k}$, where $T_{ij.k} = (\Gamma_{ij.k} - \Gamma_{ji.k})/2$. Substituting these relations into Eq. (3), we obtain

$$\sigma'_{ij} = C\varepsilon_{jlk}\varepsilon_{lsp}\frac{\partial \Gamma_{sp.i}}{\partial x_k}. \tag{7}$$

Formulas (6) and (7) differ by the position of the subscripts i, j. Both subscripts are space subscripts in Eq. (6), whereas j is a space subscript and i is a group subscript in Eq. (7).

The formula for vortex stresses can also be determined from the condition that the equilibrium equations remain unchanged if stresses of the form $\sigma'_{ij} = \varepsilon_{jkl}\,\partial F_{il}/\partial x_k$ are added. The generating function F_{il} can be represented in the form of a rotor of another function. The generating function $F'_{il} = \varepsilon_{lsp}\Gamma_{sp.i} = \varepsilon_{lsp}\,\partial \beta_{pi}/\partial x_s$ corresponds to formula (7), and the generating function $F''_{il} = \varepsilon_{isp}\Gamma_{pl.s} = \varepsilon_{ips}\,\partial \beta_{lp}/\partial x_s$ corresponds to formula (6). Representing the distortion tensor β_{ij} as a sum of the symmetric ε_{ij} and antisymmetric ω_{ij} tensors $\beta_{ij} = \varepsilon_{ij} + \omega_{ij}$, we compare these generating functions $F'_{li} = \varphi_{il} - \psi_{il}$ and $F''_{il} = -(\varphi_{il} + \psi_{il})$, where $\varphi_{il} = \varepsilon_{isp}\,\partial \varepsilon_{lp}/\partial x_s$ and

$\psi_{il} = \varepsilon_{isp}\,\partial\omega_{lp}/\partial x_s$. If $\varphi_{il}(x_k) \neq 0$ and $\psi_{il}(x_k) \neq 0$, the generating functions F'_{il} and F''_{il} are different; if one of the functions $\varphi_{il}(x_k)$ or $\psi_{il}(x_k)$ is identically equal to zero, F'_{il} is expressed via F''_{il}. It follows from the comparison that the function F'_{il} should be chosen between the two functions F'_{il} and F''_{il} as a generating function, because F'_{il}, in contrast to F''_{il}, satisfies the zero boundary conditions (2).

We consider the inverse problem of determining the dislocation density α_{ij} from a given field of self-balanced stresses σ'_{ij}. First, we examine a particular case for the stresses σ'_{ij} from [3] and then generalize the result to arbitrary self-balanced stresses σ'_{ij}. Godunov [3] constructed a particular example of self-balanced stresses in a cube ($-1 \leqslant x_i \leqslant 1$, $i = 1, 2, 3$) in the form

$$\begin{gathered}\sigma'_{11} = \cos\pi x_1 \cos\pi x_2 + \cos\pi x_2, \qquad \sigma'_{22} = \cos\pi x_1 \cos\pi x_2 + \cos\pi x_1, \\ \sigma'_{12} = \sigma'_{21} = \sin\pi x_1 \sin\pi x_2.\end{gathered} \tag{8}$$

Assuming that $C = 1$ and $\alpha_{ij} = \alpha_{ij}(x_1, x_2)$ in Eq. (3), we obtain the system

$$\frac{\partial\alpha_{31}}{\partial x_2} = -\sigma'_{11}, \quad \frac{\partial\alpha_{31}}{\partial x_1} = \sigma'_{12}, \quad \frac{\partial\alpha_{32}}{\partial x_1} = \sigma'_{22}, \quad \frac{\partial\alpha_{32}}{\partial x_2} = -\sigma'_{21}. \tag{9}$$

Using the equalities $\partial^2\alpha_{31}/\partial x_1\,\partial x_2 = \partial^2\alpha_{31}/\partial x_2\,\partial x_1$ and $\partial^2\alpha_{32}/\partial x_1\,\partial x_2 = \partial^2\alpha_{32}/\partial x_2\,\partial x_1$ and Eqs. (9), we find the conditions of integrability of Eq. (9), which are the following equilibrium equations:

$$\frac{\partial\sigma'_{11}}{\partial x_1} + \frac{\partial\sigma'_{12}}{\partial x_2} = 0, \qquad \frac{\partial\sigma'_{21}}{\partial x_1} + \frac{\partial\sigma'_{22}}{\partial x_2} = 0. \tag{10}$$

It follows from here that the dislocation density is uniquely determined by the field of self-balanced stresses, since the latter identically satisfy the equilibrium equations. Substituting relations (8) into Eqs. (9), we find the dislocation density

$$\alpha_{31} = -(1/\pi)\sin\pi x_2(\cos\pi x_1 + 1), \qquad \alpha_{32} = (1/\pi)\sin\pi x_1(\cos\pi x_2 + 1). \tag{11}$$

Equations (11) describe the distribution of rectilinear dislocations parallel to the axis x_3. The dislocation density vanishes on the side faces of the cube $x_1 = \pm 1$ and $x_2 = \pm 1$. The dislocation lines are perpendicular to the upper and lower faces of the cube $x_3 = \pm 1$, and the dislocation density on these faces is determined by formulas (11). Integrating Eqs. (11), we find that the total Burgers vector on these faces equals zero:

$$B_1 = \int\limits_{-1}^{1} dx_2 \int\limits_{-1}^{1} \alpha_{31}\,dx_1 = 0, \qquad B_2 = \int\limits_{-1}^{1} dx_2 \int\limits_{-1}^{1} \alpha_{32}\,dx_1 = 0.$$

Let us extend Eq. (11) to the description of a periodic distribution of dislocation density with a zero total Burgers vector $B_1 = B_2 = 0$:

$$\begin{gathered}\alpha_{31} = -A\sin m\pi x_2(\cos n\pi x_1 + 1), \qquad \alpha_{32} = A\sin n\pi x_1(\cos m\pi x_2 + 1), \\ n = 2k + 1, \quad m = 2l + 1.\end{gathered} \tag{12}$$

Substituting (12) into Eqs. (9), we find the self-balanced stresses

$$\begin{gathered}\sigma'_{11} = Am\pi\cos m\pi x_2(\cos n\pi x_1 + 1), \qquad \sigma'_{22} = An\pi\cos n\pi x_1(\cos m\pi x_2 + 1), \\ \sigma'_{12} = An\pi\sin m\pi x_2 \sin n\pi x_1, \qquad \sigma'_{21} = Am\pi\sin m\pi x_2 \sin n\pi x_1, \\ n = 2k + 1, \qquad m = 2l + 1.\end{gathered} \tag{13}$$

By means of direct verification, we can easily see that stresses (13) identically satisfy the equilibrium equations (10) and the boundary conditions $f_1 = \sigma'_{11} = 0$ and $f_2 = \sigma'_{21} = 0$ for $x_1 = \pm 1$ and $f_2 = \sigma'_{22} = 0$ and $f_1 = \sigma'_{12} = 0$ for $x_2 = \pm 1$.

To determine α_{ij} from given σ'_{ij} in the general case, one has to solve a system of three equations in partial derivatives (3): $C\varepsilon_{lkj}\,\partial\alpha_{li}/\partial x_k = \sigma'_{ij}$. Differentiating the left and right sides of this equation with respect to x_j, we obtain

$$C\varepsilon_{lkj}\,\frac{\partial^2\alpha_{li}}{\partial x_j \partial x_k} = \frac{1}{2}\,C\varepsilon_{lkj}\Big(\frac{\partial^2\alpha_{li}}{\partial x_j\,\partial x_k} - \frac{\partial^2\alpha_{li}}{\partial x_k\,\partial x_j}\Big) = \frac{\partial\sigma'_{ij}}{\partial x_j}.$$

Using the identity $\partial^2\alpha_{li}/\partial x_j\,\partial x_k = \partial^2\alpha_{li}/\partial x_k\partial x_j$, we show that, to determine α_{ij}, the stresses σ'_{ij} should satisfy the equilibrium equation $\partial\sigma'_{ij}/\partial x_j = 0$. Since the self-balanced stresses σ'_{ij} identically satisfy the equilibrium equation, the dislocation density α_{ij} is uniquely determined by integrating the equations in partial derivatives (3).

Finally, we note that, though the vortex self-balanced stresses identically satisfy the equilibrium equations and boundary conditions in the absence of external loads, they play an important role in elastoplastic deformation of materials. The reason is that the evolution of the dislocation field in a material occurs under the action of the total stresses $\tilde{\sigma}_{ij}$, which include the self-balanced stresses generated by dislocations.

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