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MECHANICAL PROPERTIES, PHYSICS OF STRENGTH, AND PLASTICITY

Analytical Methods for the Calculation of the Elastic Interaction of Point Defects with Dislocation Loops in Hexagonal Crystals

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Abstract—The Green's function method for hexagonal crystals within the Lifshitz–Rosenzweig (1947) and Kröner (1953) approaches has been used to obtain analytical expressions for the energy of elastic interaction of radiation-induced point defects with dislocation loops of three types: the basal edge dislocation loop (*c*-loop), the basal shear dislocation loop, and the edge *a*-loop (bedding plane $\{11\bar{2}0\}$, Burgers vector $\mathbf{b}^{\mathbf{D}} = 1/3\langle 11\bar{2}0\rangle$). In the case of the basal edge dislocation loop, a similar expression has been obtained independently by solving the equilibrium equations using the Elliott method. A numerical comparison of the derived expressions for zirconium has demonstrated a complete identity of the results obtained within the approaches considered in this study.

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1. INTRODUCTION

One of the reasons for the evolution of the microstructure in a crystal under irradiation is associated with diffusion fluxes of radiation-induced point defects onto structural elements (pores, dislocations, precipitates of new phases, etc.), which serve as sinks for point defects. The diffusion fluxes themselves are substantially dependent on the gradient of the energy of elastic interaction (drift flow) of point defects with the stress field induced by a sink. Dislocation loops, as a rule, are the first observed extended elements of the microstructure of the material under irradiation. Therefore, the calculation of their elastic fields and the corresponding energy of interaction with point defects is a very important problem in the theory of radiation materials science.

If we know the fictitious distribution of body forces f_i^S, which, in an elastic medium, creates the same stresses as a real source S, then the energy of interaction between two systems of internal stresses $S(\mathbf{u}^S, u_{ij}^S, \sigma_{ij}^S)$ and $T(\mathbf{u}^T, u_{ij}^T, \sigma_{ij}^T)$, according to Eshelby [1], can be represented as the integral of the following form:

$$E_{\text{int}}(S,T) = -\int f_i^S u_i^T dV, \qquad (1)$$

which is taken over the region containing only the source of the system of stresses S. Let this system be determined by a point defect, which, in the theory of elasticity, is described by the volume distribution of dipole forces without a momentum,

$$f_i(\mathbf{r} - \mathbf{r}_0) = -A_{ij}\nabla_j \delta(\mathbf{r} - \mathbf{r}_0), \quad A_{ij} = A_{ji}, \qquad (2)$$

and the system T be determined by a dislocation loop ($T = D$). Then, we have

$$E_{\text{int}}(\mathbf{r}) = -\int f_i(\mathbf{r}' - \mathbf{r}) u_i^D(\mathbf{r}') d\mathbf{r}' = -A_{ij} u_{ij}^D(\mathbf{r}), \qquad (3)$$

and, in the case of a dilatation center, $A_{ij} = P\delta_{ij}$, we can write

$$E_{\text{int}}(\mathbf{r})/P = -Sp\, u_{ij}^D(\mathbf{r}), \qquad (4)$$

where P is the power of the dilatation center; the frame of reference in this case is related to the dislocation, and $\mathbf{r}$ is the coordinate of the point of location of the point defect. In fact, there are two methods for the calculation of an elastic field of a dislocation loop u_{ij}^D. The first method is to solve the equilibrium equations in terms of displacements with the appropriate boundary conditions. In the case of a hexagonal crystal (axial symmetry), the calculation is performed using the Hankel transform [2]. The second method is to use the tensor Green's function G_{ij} of the equilibrium equations of the elastic medium under consideration, which makes it possible to calculate the displacements caused

by a dislocation of any form in any anisotropic elastic medium according to the classical formula [3, 4]:

$$u_i^D(\mathbf{r}) = C_{jklm} b_m^D \int_{S_D} n_l^D \frac{\partial G_{ij}(\mathbf{r}-\mathbf{r}')}{\partial x_k} dS'. \quad (5)$$

The notation used in formula (5) is as follows: C_{jklm} is the tensor of the elastic moduli of the medium simulating the crystal, b_m^D is the mth component of the Burgers vector of the dislocation, n_l^D is the lth component of the normal vector to an arbitrary surface S_D lying on the dislocation line, $\mathbf{r}$ is the coordinate of the point of observation, and $\mathbf{r}'$ is the coordinate of the point on the surface S_D. In the literature, there are two versions of the analytical calculation of the tensor Green's function, namely, within the Lifshitz–Rosenzweig approach (1947) [5] and using the Kröner method (1953) [6] with the correction for the coefficient [7]. The first approach is valid for any unbounded elastic anisotropic medium. In particular, the Lifshitz–Rosenzweig method, as applied to cubic and hexagonal crystals, has been described in sufficient detail in our previous studies [8, 9]. The second method is applicable only to hexagonal crystals.

In order to be able to use all the appropriate analytical methods and to compare the obtained results, in this study, we considered crystals of the hexagonal system (the numerical comparison was performed for zirconium). The point defect was simulated by a dilatation center. Therefore, for dislocation loops of different types, we calculated only the quantity $Spu_{ij}^D(\mathbf{r})$ according to formula (4). This paper is organized as follows. In Sections 2 and 3, we considered basal vacancy dislocation loops with a pure edge component and a pure shear component of the Burgers vector. Since the Burgers vector inclined to the basal plane can always be decomposed into these components, the analytical result can actually be obtained for any basal dislocation loop. Despite the large differences in appearance of the formulas obtained by different methods, the numerical estimates for zirconium demonstrated their complete identity. In Section 4, we considered a more complex object, namely, a dislocation loop lying in the $\{11\bar{2}0\}$ plane. In particular, for zirconium, it is the so-called a-loop with the Burgers vector $\mathbf{b} = 1/3\langle 11\bar{2}0\rangle$. Here, only the tensor Green's function method works fairly well. In this case, again, the numerical estimates obtained for zirconium both within the Lifshitz–Rosenzweig and Kröner approaches showed their complete identity. It should be noted that, in connection with the interpretation of experimentally observed contrasts of dislocation loops, the problems of the calculation of their elastic fields was repeatedly solved in the past (see, for example, [10, 11]). However, usually, the results were presented in the form of fairly cumbersome formulas for elastic stress components. In this study, we are interested only in the quantity $Spu_{ij}^D(\mathbf{r})$. Consequently, all the formulas presented in this paper are not only original, but also, as turned out, are much simpler mathematically.

2. ELASTIC FIELD OF A PRISMATIC DISLOCATION LOOP LYING IN THE BASAL PLANE OF THE HEXAGONAL CRYSTAL

Let us consider a circular vacancy dislocation loop with a radius R, lying in the plane $z = 0$ (basal plane) of the cylindrical coordinate system (r, φ, z), the Burgers vector of which is perpendicular to the plane of the loop and has only the z-component $(0, 0, b^D)$. The normal vector to the plane of the loop coincides with the positive direction of the "z" axis, which is also the symmetry axis of the crystal. Since the problem is axially symmetric, there is no angular dependence, so that $u_\varphi = 0$ and $\sigma_{r\varphi} = \sigma_{\varphi z} = 0$, and the stress state is uniquely determined by the four components of the stress tensor σ_{rr}, $\sigma_{\varphi\varphi}$, σ_{zz}, and σ_{rz}, which in terms of the displacements have the form

$$\begin{aligned}
\sigma_{rr} &= C_{11}\frac{\partial u_r}{\partial r} + C_{12}\frac{u_r}{r} + C_{13}\frac{\partial u_z}{\partial z},\\
\sigma_{\varphi\varphi} &= C_{12}\frac{\partial u_r}{\partial r} + C_{11}\frac{u_r}{r} + C_{13}\frac{\partial u_z}{\partial z},\\
\sigma_{zz} &= C_{13}\left(\frac{\partial u_r}{\partial r} + \frac{u_r}{r}\right) + C_{33}\frac{\partial u_z}{\partial z},\\
\sigma_{rz} &= C_{44}\left(\frac{\partial u_r}{\partial z} + \frac{\partial u_z}{\partial r}\right)
\end{aligned} \quad (6)$$

and satisfy the equilibrium equations

$$\begin{aligned}
\frac{\partial \sigma_{rr}}{\partial r} + \frac{\partial \sigma_{rz}}{\partial z} + \frac{\sigma_{rr} - \sigma_{\varphi\varphi}}{r} = 0,\\
\frac{\partial \sigma_{rz}}{\partial r} + \frac{\partial \sigma_{zz}}{\partial z} + \frac{\sigma_{rz}}{r} = 0,
\end{aligned} \quad (7)$$

where C_{11}, C_{12}, C_{13}, C_{33}, and $C_{44} = C_{55}$ are six (minimum number) necessary nonzero elastic moduli. An example of this type of objects is provided by the so-called c-loops with the Burgers vector $\mathbf{b} = 1/2[0001]$, which are observed in zirconium under the electron irradiation at the temperature $T = 715$ K. As was shown by Elliott [12], the problem of the calculation of the elastic field of a dislocation loop, which is determined by expressions (6) and (7), can be solved in terms of two stress functions Φ_α ($\alpha = 1, 2$) that satisfy the equations

$$\begin{aligned}
\left(\nabla^2 + v_a\frac{\partial^2}{\partial z^2}\right)\Phi_\alpha(r,z) = 0,\\
\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r},
\end{aligned} \quad (8)$$

and the coefficients v_α are the roots of the quadratic equation

$$C_{44}C_{11}v^2 + (C_{13}^2 + 2C_{44}C_{13} - C_{33}C_{11})v + C_{44}C_{33} = 0. \quad (9)$$

In this case, we have

$$u_r = \frac{\partial}{\partial r}(\Phi_1 + \Phi_2), \quad u_z = \frac{\partial}{\partial z}(k_1\Phi_1 + k_2\Phi_2),$$
$$k_\alpha = \frac{C_{11}v_\alpha - C_{44}}{C_{13} + C_{44}} = \frac{v_\alpha(C_{13} + C_{44})}{C_{33} - C_{44}v_\alpha}. \quad (10)$$

Substitution of expressions (10) into equalities (6) gives the stress field of a dislocation loop in terms of the stress functions Φ_α, and the desired quantity Spu_{ij}^D takes the form

$$Spu_{ij}^D = \sum_{\alpha=1}^{2}(k_\alpha - v_\alpha)\frac{\partial^2}{\partial z^2}\Phi_\alpha. \quad (11)$$

By means of the Hankel transform $G(\xi, z) = \int_0^\infty r\Phi(r, z)J_0(\xi r)dr$ [2], equalities (8) can be reduced to the ordinary differential equations of the form

$$\left(v_\alpha\frac{d^2}{dz^2} - \xi^2\right)G_\alpha(\xi, z) = 0, \quad (12)$$

which have the trivial solution $G_\alpha(\xi, z) = A_\alpha(\xi) \times \exp(-\xi z/\sqrt{v_\alpha}) + B_\alpha(\xi)\exp(\xi z/\sqrt{v_\alpha})$. Since all the components of the displacements and stresses should vanish at $z \to \infty$, we obtain $B_\alpha = 0$ and the coefficients A_α are determined from the boundary conditions of the problem. In our case, these conditions can be written as follows [13]:

$$u_z(r,0) = -\frac{1}{2}b^D, \quad 0 \le r < R,$$
$$u_z(r,0) = 0, \quad r > R, \quad \sigma_{rz}(r,0) = 0. \quad (13)$$

The second condition in formulas (13) follows from the pure edge nature of the dislocation loop. The sign for the z-component of the displacements u_z was chosen positive for the interstitial dislocation loop and negative for the vacancy loop. Using the Hankel inversion theorem [2] and the expression for the function $G_\alpha(\xi, z)$, we obtain

$$\sigma_{rz}(r,z) = C_{44}\int_0^\infty \xi^3\sum_{\alpha=1}^{2}\left[\frac{(1+k_\alpha)}{\sqrt{v_\alpha}}A_\alpha(\xi)\exp(-\xi z/\sqrt{v_\alpha})\right]J_1(r\xi)d\xi. \quad (14)$$

And then, from the second boundary condition, we have the relation

$$A_2(\xi) = -A_1(\xi)\frac{(1+k_1)}{(1+k_2)}\frac{\sqrt{v_2}}{\sqrt{v_1}}.$$

Similarly, for the z-component of the displacements u_z, we obtain

$$u_z(r,z) = -\int_0^\infty \xi^2\sum_{\alpha=1}^{2}\left[\frac{k_\alpha}{\sqrt{v_\alpha}}A_\alpha(\xi)\exp(-\xi z/\sqrt{v_\alpha})\right]J_0(r\xi)d\xi \quad (15)$$

and in the dimensionless variables $t = \xi R$ and $\rho = r/R$, according to the first boundary condition, we have two integral equations

$$\int_0^\infty t^2A_1(t/R)J_0(t\rho)dt = \sqrt{v_1}\frac{1+k_2}{k_1-k_2}\frac{b^DR^3}{2}, \quad 0 \le \rho \le 1,$$
$$\int_0^\infty t^2A_1(t/R)J_0(t\rho)dt = 0, \quad \rho > 1.$$

These equations are satisfied under the condition

$$t^2A_1(t/R) = \sqrt{v_1}\frac{1+k_2}{k_1-k_2}\frac{b^DR^3}{2}J_1(t).$$

As a result, the stress functions Φ_α take the form

$$\Phi_1(r,z) = \sqrt{v_1}\frac{1+k_2}{k_1-k_2}\frac{b^DR}{2} \times \int_0^\infty \frac{1}{\xi}J_1(\xi R)J_0(r\xi)\exp(-\xi z/\sqrt{v_1})d\xi,$$
$$\Phi_2(r,z) = (-1)\sqrt{v_2}\frac{1+k_1}{k_1-k_2}\frac{b^DR}{2} \times \int_0^\infty \frac{1}{\xi}J_1(\xi R)J_0(r\xi)\exp(-\xi z/\sqrt{v_2})d\xi. \quad (16)$$

By substituting function (16) into formulas (10) and (6), we obtain all the components of the elastic stresses. We will not write out them in the explicit form. This was done in [10]. Here, we are interested only in the quantity Spu_{ij}^D. From expressions (11) and (16), we have

$$Spu_{ij}^D = \frac{b^D}{2R}\left[\frac{1+k_2}{k_1-k_2}\frac{k_1-v_1}{\sqrt{v_1}}I_0^1\left(\frac{r}{R}, \frac{z}{R\sqrt{v_1}}\right) - \frac{1+k_1}{k_1-k_2} \times \frac{k_2-v_2}{\sqrt{v_2}}I_0^1\left(\frac{r}{R}, \frac{z}{R\sqrt{v_2}}\right)\right] \equiv \frac{b^D}{4\pi R}I\left(\frac{r}{R}, \frac{z}{R}\right), \quad (17)$$

where

$$I_m^n\left(\frac{r}{R}, \frac{z}{R}\right) = \int_0^\infty t^nJ_m\left(\frac{r}{R}t\right)J_1(t)\exp\left(-t\frac{z}{R}\right)dt.$$

Thus, the problem of the calculation of the elastic interaction energy of a dilatation center with the prismatic dislocation loop under consideration is solved.

Next, we consider the same problem, but within the formalism of the tensor Green's function (5):

$$Spu_{ij}^{D}(\mathbf{r}) = b^{D}\int_{S_D} d^2r'\left[C_{13}\sum_{\alpha=1}^{2}G_{i\alpha,\alpha i}(\mathbf{r}-\mathbf{r}')+C_{33}G_{i3,3i}(\mathbf{r}-\mathbf{r}')\right], \quad (18)$$

$$G_{ij,km}\equiv\frac{\partial^2 G_{ij}}{\partial x_k\partial x_m}.$$

The first method, as applied to our problem, was described in sufficient detail in the authors' recent paper [14]. Therefore, below the obtained results will be presented in a concise manner. The Kröner method was used in the work of Yoo [15] for the calculation of the energy of interaction between two point defects within the force dipole model, and his original method of presentation is also relevant in our case. We introduce the following notation:

$$K_1=\sum_{\gamma=1}^{2}\sum_{\alpha=1}^{2}G_{\gamma\alpha,\alpha\gamma},\quad K_2=G_{33,33},\quad K_3=\sum_{\alpha=1}^{2}G_{3\alpha,\alpha3}.$$

Then, from expression (18), it follows that

$$Spu_{ij}^{D}=\frac{b^{D}}{4\pi}\int_{S_D} d^2r'[C_{13}K_1+C_{33}K_2+(C_{33}+C_{13})K_3]. \quad (19)$$

According to Kröner, we can write

$$G_{11}=\sum_{k=1}^{3}\frac{1}{[v_k r^2+z^2]^{1/2}}\left[A_k\frac{x^2z^2-y^2(v_k r^2+z^2)}{r^4}+B_k\right],$$

$$r^2=x^2+y^2,$$

$$G_{22}=\sum_{k=1}^{3}\frac{1}{[v_k r^2+z^2]^{1/2}}\left[A_k\frac{y^2z^2-x^2(v_k r^2+z^2)}{r^4}+B_k\right],$$

$$G_{33}=\sum_{k=1}^{3}\frac{D_k}{[v_k r^2+z^2]^{1/2}},$$

$$G_{12}=\frac{xy}{r^4}\sum_{k=1}^{3}A_k\frac{[v_k r^2+2z^2]}{[v_k r^2+z^2]^{1/2}}, \quad (20)$$

$$G_{31}=\frac{xz}{r^2}\sum_{k=1}^{3}\frac{C_k}{[v_k r^2+z^2]^{1/2}},$$

$$G_{32}=\frac{yz}{r^2}\sum_{k=1}^{3}\frac{C_k}{[v_k r^2+z^2]^{1/2}}.$$

It turns out that all the functions K_i ($i=1, 2, 3$) in our case can be written in a compact form as follows (slightly different from that used in [15]):

$$K_i=\frac{1}{|\mathbf{r}-\mathbf{r}'|^3}T_i(\tau_3^2),\quad T_1=\sum_{\alpha=1}^{2}A_\alpha v_\alpha^2 F_\alpha(\tau_3^2),$$

$$T_2=\sum_{\alpha=1}^{2}D_\alpha F_\alpha(\tau_3^2),\quad T_3=\sum_{\alpha=1}^{2}C_\alpha v_\alpha F_\alpha(\tau_3^2), \quad (21)$$

$$F_\alpha(\tau_3^2)\equiv\frac{2\tau_3^2-v_\alpha(1-\tau_3^2)}{[\tau_3^2+v_\alpha(1-\tau_3^2)]^{5/2}},$$

where v_α are the roots of the same quadratic equation (9), and the coefficients appearing in expressions (21) have the form

$$\begin{aligned}A_\alpha&=[(C_{66}-C_{11})(C_{33}-v_\alpha C_{44})+(C_{13}+C_{44})^2]/E_\alpha,\\ C_{66}&=(C_{11}-C_{12})/2,\\ D_\alpha&=(C_{44}-v_\alpha C_{11})(C_{44}-v_\alpha C_{66})/E_\alpha,\\ C_\alpha&=(C_{13}+C_{44})(C_{44}-v_\alpha C_{66})/E_\alpha,\\ E_1&=C_{11}C_{44}C_{66}(v_1-v_3)(v_1-v_2),\\ E_2&=C_{11}C_{44}C_{66}(v_2-v_3)(v_2-v_1).\end{aligned} \quad (22)$$

Here, τ_k are the components of the unit vector $\boldsymbol{\tau}=(\mathbf{r}-\mathbf{r}')/|\mathbf{r}-\mathbf{r}'|$, and the obvious equality $\sum_k\tau_k^2=1$ is taken into account. Thus, the problem is reduced to the integration of expression (19) (with due regard for formulas (21) and (22)) over the plane of the circular dislocation loop (recall that $z'=0$, because the dislocation loop lies in the basal plane of the crystal):

$$Spu_{ij}^{D}(\mathbf{r})=\frac{b^{D}}{4\pi}\int_{S_D}\frac{d^2r'}{|\mathbf{r}-\mathbf{r}'|^3}\times[C_{13}T_1(\tau_3^2)+C_{33}T_2(\tau_3^2)+(C_{13}+C_{33})T_3(\tau_3^2)]. \quad (23)$$

This form of writing expression (23) was not chosen randomly. The Lifshitz–Rosenzweig method gives the analogous result in a similar form [14] in the same variables

$$Spu_{ij}^{D}(\mathbf{r})=-\frac{b^{D}}{4\pi}\int_{S_D}\frac{d^2r'}{|\mathbf{r}-\mathbf{r}'|^3}\times\left[(1-3\tau_3^2)Q(\tau_3^2)+2\tau_3^2(1-\tau_3^2)\frac{dQ}{d\tau_3^2}\right], \quad (24)$$

$$Q(\tau_3^2)=C_{13}K(\tau_3^2)+C_{33}W(\tau_3^2)+(C_{13}+C_{33})V(\tau_3^2).$$

The functions $K(\tau_3^2)$, $W(\tau_3^2)$, and $V(\tau_3^2)$ are very cumbersome; therefore, they are given in the Appendix. It is important that we have three versions of the solution of the same problem. It is reasonable to compare them. The numerical evaluations were performed for zirconium. The experimental values of the elastic moduli for zirconium according to [16] are as follows

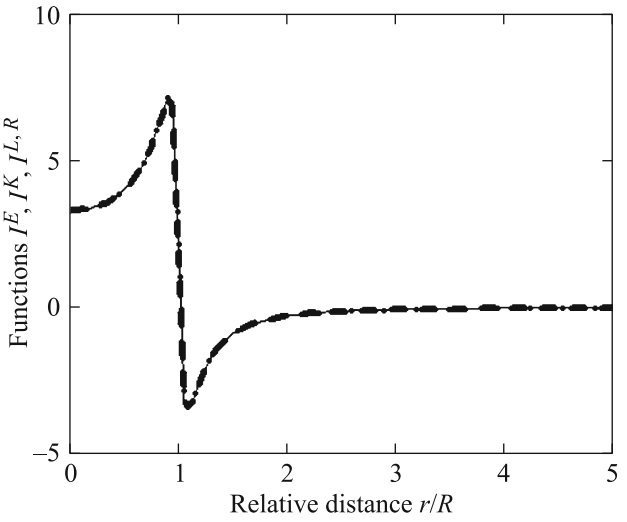

Fig. 1. Dependences of the functions $I^E(\rho, \zeta)$ (solid line), $I^K(\rho, \zeta)$ (dotted line), and $I^{L,R}(\rho, \zeta)$ according to formulas (17), (23), and (24) on the relative distance $\rho = r/R$ in the plane $\zeta = 0.1$ of the zirconium crystal.

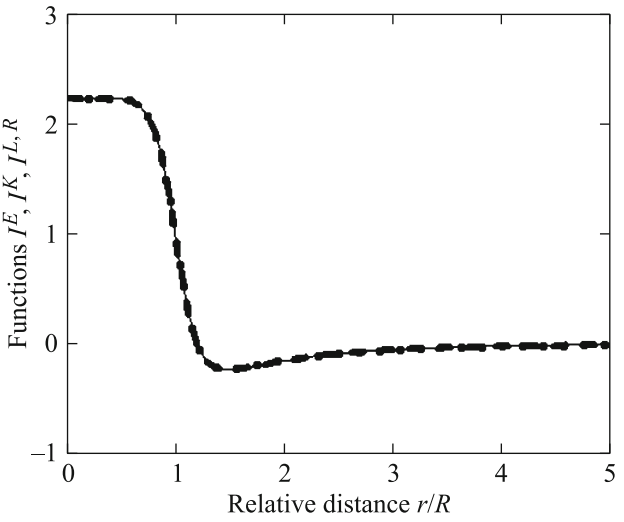

Fig. 2. Dependences of the functions $I^E(\rho, \zeta)$ (solid line), $I^K(\rho, \zeta)$ (dotted line), and $I^{L,R}(\rho, \zeta)$ according to formulas (17), (23), and (24) on the relative distance $\rho = r/R$ in the plane $\zeta = 0.5$ of the zirconium crystal.

(in Mbar): $C_{11} = 1.554$, $C_{12} = 0.672$, $C_{13} = 0.646$, $C_{33} = 1.725$, and $C_{55} = C_{44} = 0.363$. The results of the comparison are presented in Figs. 1 and 2 in the dimensionless cylindrical coordinates $\rho = r/R$ and $\zeta = z/R$. In this case, we have $\tau_3^2 = \zeta^2/|\mathbf{r} - \mathbf{r}'|^2$ and $|\mathbf{r} - \mathbf{r}'|^2 = \rho^2 + \zeta^2 - 2\rho\rho'\cos(\varphi - \varphi') + \rho'^2$. Because of the isotropy in the basal plane, the result naturally does not depend on the azimuthal angle φ. Therefore, it was assumed to be zero. Formulas (17), (23), and (24) are reduced to a single form: $Spu_{ij}^D = \dfrac{b^D}{4\pi R} I(\rho, \zeta)$. Consequently, the function $I^E(\rho, \zeta)$ in Figs. 1 and 2 corresponds to formula (17) (H.A. Elliott), the function $I^K(\rho, \zeta)$—to formula (23) (Kröner), and the function $I^{L,R}(\rho, \zeta)$—to formula (24) (Lifshitz–Rosenzweig). The figures show the dependences of the functions I^E, I^K, and $I^{L,R}$ on the relative distance ρ for two planes $z = 0.1R$ and $z = 0.5R$. It can be seen from these figures that there is a perfect agreement of all three versions of solving the problem. In our previous study [14], the function $I^{L,R}(\rho, \zeta)$ was compared with the isotropic approximation. It was found that there was a difference, even though small, but it was. Here, we did not find any difference. But, this is only a special case. The majority of dislocation loops have the Burgers vector inclined to the plane of the loop. Since the Burgers vector can always be decomposed into the prismatic component (perpendicular to the loop plane) and the shear component (lying in the loop plane), it was appropriate to consider the similar problem for the pure shear component.

3. ELASTIC FIELD OF A SHEAR DISLOCATION LOOP LYING IN THE BASAL PLANE OF THE HEXAGONAL CRYSTAL

Since the axial symmetry of the problem in this case is broken, the Hankel transform method is not applicable. It remains now to use the Green's function method. Let the "x" axis of the basal plane "xy" be directed along the shear component b^S of the Burgers vector of the dislocation loop. Then, from formula (5), we obtain the following equation for the components of the displacement vector:

$$u_i^S(\mathbf{r}) = b^S C_{44} \int_{S_D} [G_{i3,1}(\mathbf{r} - \mathbf{r}') + G_{i1,3}(\mathbf{r} - \mathbf{r}')] d^2 r', \quad (25)$$

where the integration, as before, is performed over the dislocation loop area. And again, we will continue to be interested only in the quantity Spu_{ij}^S; that is,

$$Spu_{ij}^S(\mathbf{r}) = b^S C_{44} \int_{S_D} [G_{i3,i1}(\mathbf{r} - \mathbf{r}') + G_{i1,i3}(\mathbf{r} - \mathbf{r}')] d^2 r', \quad (26)$$

where the summation is performed over the index "i" running from 1 to 3. After the necessary calculations, according to Kröner, we obtain

$$Spu_{ij}^S(\mathbf{r}) = \frac{b^S}{4\pi} C_{44} \int_{S_D} d^2 r' \frac{\tau_3 \tau_1}{|\mathbf{r} - \mathbf{r}'|^3} \times \left[3 \sum_{\alpha=1}^{2} \frac{(C_\alpha - A_\alpha) v_\alpha^2 + (D_\alpha - C_\alpha + B_\alpha) v_\alpha}{[v_\alpha (1 - \tau_3^2) + \tau_3^2]^{5/2}} \right], \quad (27)$$

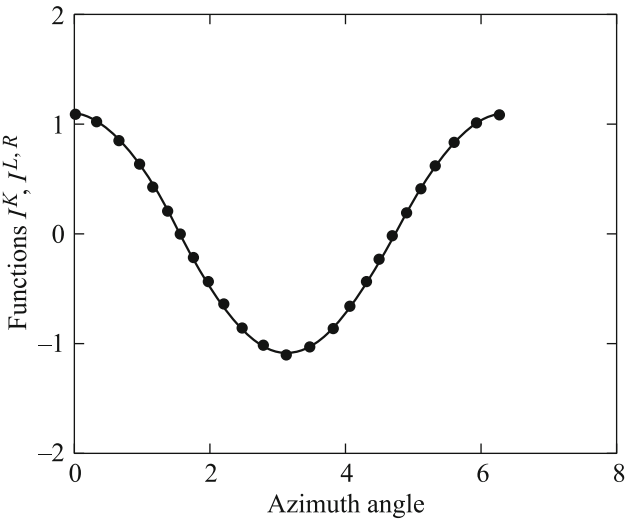

Fig. 3. Dependences of the functions $I^K(\rho, \zeta, \varphi)$ (dotted line) and $I^{L,R}(\rho, \zeta, \varphi)$ (solid line) according to formulas (27) and (28) on the azimuthal angle φ in the plane $\zeta = 0.5$ of the zirconium crystal for the relative distance $\rho = 1.5$.

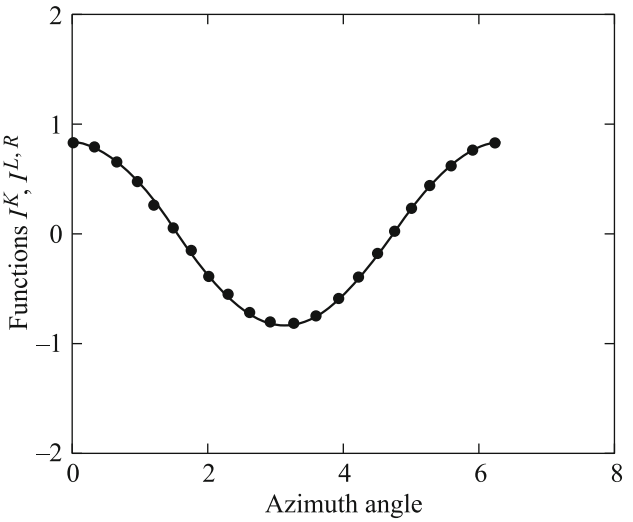

Fig. 4. Dependences of the functions $I^K(\rho, \zeta, \varphi)$ (dotted line) and $I^{L,R}(\rho, \zeta, \varphi)$ (solid line) according to formulas (27) and (28) on the azimuthal angle φ in the plane $\zeta = 0.5$ of the zirconium crystal for the relative distance $\rho = 0.5$.

where

$$B_\alpha = [(C_{44} - v_\alpha C_{11})(C_{33} - v_\alpha C_{44}) + v_\alpha (C_{13} + C_{44})^2]/E_\alpha,$$

and all other quantities are defined above (see formulas (22)) ($\tau_k = (x_k - x_k')/|\mathbf{r} - \mathbf{r}'|$). A similar problem was solved in [11] in connection with the interpretation of experimentally observed contrasts of dislocation loops. The results obtained in [11] are presented in the form of formulas for elastic stress components. They are very cumbersome and expressed in terms of the integrals I_m^n (17). Our formula is quite different. It is fairly compact and easily perceptible. Hence, we believe that this formula is absolutely original.

A similar expression to the same variables, according to Lifshitz and Rosenzweig, has the form

$$Spu_{ij}^D(\mathbf{r}) = \frac{b^S}{4\pi} C_{44} \int_{S_D} d^2 r' \frac{\tau_3 \tau_1}{|\mathbf{r} - \mathbf{r}'|^3} \times \left[3\{\Psi(\tau_3^2) - Y(\tau_3^2)\} + 2\tau_3^2 \frac{d\Psi}{d\tau_3^2} + 2(1 - \tau_3^2) \frac{dY}{d\tau_3^2} \right], \quad (28)$$

$$\Psi(\tau_3^2) = V(\tau_3^2) + W(\tau_3^2), \quad Y(\tau_3^2) = K(\tau_3^2) + V(\tau_3^2).$$

The functions $K(\tau_3^2)$, $W(\tau_3^2)$, and $V(\tau_3^2)$ are given in the Appendix. In the dimensionless cylindrical coordinates $\rho = r/R$ and $\zeta = z/R$, formulas (27) and (28) for a circular dislocation loop, again, are reduced to the form $Spu_{ij}^S = \frac{b^S}{4\pi R} I(\rho, \zeta, \varphi)$. Then, we numerically compare the corresponding expression (27) for the function I^K according to Kröner and expression (28) for the function $I^{L,R}$ according to Lifshitz and Rosenzweig. The obtained results are presented in Figs. 3–5. First, we should note the complete coincidence of the results in both approaches, which indicates their equivalence. But, in contrast to the case of a pure prismatic dislocation loop, here, there is a dependence on the azimuthal angle φ in the basal plane of the hexagonal crystal. Figures 3 and 4 show such dependences

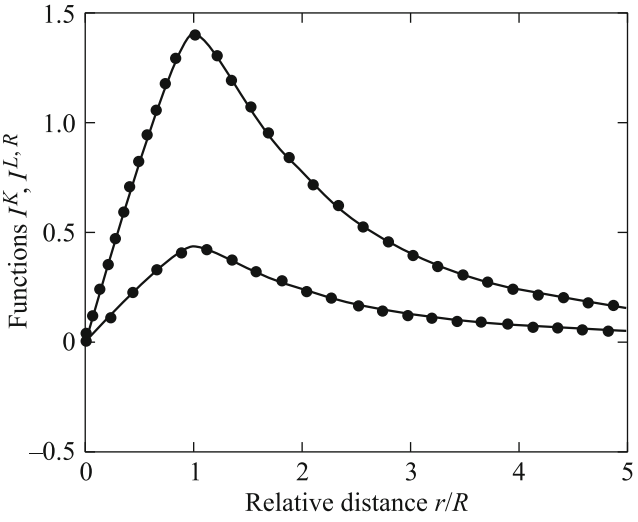

Fig. 5. Dependences of the functions $I^K(\rho, \zeta, \varphi)$ (dotted line) and $I^{L,R}(\rho, \zeta, \varphi)$ (solid line) according to formulas (27) and (28) on the relative distance $\rho = r/R$ in the plane $\zeta = 0.5$ of the zirconium crystal for two azimuthal angles $\varphi = 0$ and $\varphi = 2\pi/5$.

of the functions I^K and $I^{L,R}$ in the plane $z = 0.5R$ of the zirconium crystal for two values of r: $r = 1.5R$ (outside the dislocation loop) and $r = 0.5R$ (inside the loop). It can be seen that, in both cases, the interaction changes the sign at angles $\varphi = \pi/2$ and $\varphi = 3\pi/2$. The dilatation center is attracted in one half of the shear dislocation loop and repelled in the other half. Figure 5 shows the dependences of the functions I^K and $I^{L,R}$ in the plane $z = 0.5R$ of the zirconium crystal for two angles $\varphi = 0$ and $\varphi = 2\pi/5$ on the relative distance $\rho = r/R$. The interaction has the same sign, because the azimuthal angle lies in the range $0 \le \varphi \le \pi/2$, and the interaction itself decreases in absolute value to zero at $\varphi = \pi/2$. Thus, the question of the elastic interaction of a basal dislocation loop in a hexagonal crystal with a dilatation center can be considered as closed.

4. ELASTIC FIELD OF AN *a*-LOOP IN ZIRCONIUM

The next object of our investigation is an *a*-loop in zirconium with the Burgers vector $\mathbf{b} = 1/3\langle 11\bar{2}0\rangle$, which lies in the $\{11\bar{2}0\}$ plane. This form of dislocation loops dominates under neutron irradiation. Such dislocation loops, both vacancy-type and interstitial in their nature, are perfect prismatic [17]. For a vacancy *a*-loop, the direction of the Burgers vector coincides with the direction of the normal to the plane of the loop. Therefore, it is natural to choose the "*x*" axis of the Cartesian coordinate system in the same direction. Then, the displacement defined by expression (5) is convenient to write in the form

$$u_i^D(\mathbf{r}) = b^D \int_{S_D} [C_{12}G_{i\alpha,\alpha} + C_{13}G_{i3,3}]d^2r' + b^D(C_{11} - C_{12})\int_{S_D} G_{i1,1}(\mathbf{r} - \mathbf{r}')d^2r', \quad (29)$$

$$Spu_{ij}^D(\mathbf{r}) = b^D \int_{S_D} [C_{12}G_{i\alpha,\alpha i} + C_{13}G_{i3,3i}]d^2r' + b^D(C_{11} - C_{12})\int_{S_D} G_{i1,1i}(\mathbf{r} - \mathbf{r}')d^2r'. \quad (30)$$

The summation on the right-hand side of formula (30) is performed over the index "α" running from 1 to 2 and over the index "*i*" running from 1 to 3. The convenience of this representation is that the first term in formula (30) coincides, up to coefficients, with expression (18), for which the result has already been known both according to Kröner (formula (23)) and according to Lifshitz–Rosenzweig (formula (24)). Therefore, we should calculate only the sum $G_{i1,1i}$. The result of the calculations according to the Kröner method is as follows:

$$Spu_{ij}^D(\mathbf{r}) = \frac{b^D}{4\pi}\int_{S_D}\frac{d^2r'}{|\mathbf{r} - \mathbf{r}'|^3} \times [C_{12}T_1(\tau_3^2) + C_{13}T_2(\tau_3^2) + (C_{12} + C_{13})T_3(\tau_3^2)] + \frac{b^D}{4\pi}(C_{11} - C_{12})\int_{S_D}\frac{d^2r'}{|\mathbf{r} - \mathbf{r}'|^3}T(\tau_1^2, \tau_3^2), \quad (31)$$

$$T(\tau_1^2, \tau_3^2) = \sum_{\alpha=1}^{2}\frac{[A_\alpha v_\alpha^2 + (C_\alpha - B_\alpha)v_\alpha]}{[v_\alpha(1 - \tau_3^2) + \tau_3^2]^{3/2}} \times \left[1 - \frac{3\tau_1^2 v_\alpha}{v_\alpha(1 - \tau_3^2) + \tau_3^2}\right],$$

where all the functions and constants were defined above by formulas (21) and (22). A similar result of the calculations according to the Lifshitz–Rosenzweig method is given by the expressions

$$Spu_{ij}^D(\mathbf{r}) = -\frac{b^D}{4\pi}\int_{S_D}\frac{d^2r'}{|\mathbf{r} - \mathbf{r}'|^3}Q(\tau_3^2) - \frac{b^D}{4\pi}(C_{11} - C_{12})\int_{S_D}\frac{d^2r'}{|\mathbf{r} - \mathbf{r}'|^3}\tau_1^2\left[3Y(\tau_3^2) + 2\tau_3^2\frac{dY}{d\tau_3^2}\right], \quad (32)$$

$$Q(\tau_3^2) = (1 - 3\tau_3^2)[C_{12}Y(\tau_3^2) + C_{13}\Psi(\tau_3^2)] + 2\tau_3^2(1 - \tau_3^2) \times \frac{d}{d\tau_3^2}[C_{12}Y(\tau_3^2) + C_{13}\Psi(\tau_3^2)] - (C_{11} - C_{12})Y(\tau_3^2),$$

$$\Psi(\tau_3^2) = V(\tau_3^2) + W(\tau_3^2), \quad Y(\tau_3^2) = K(\tau_3^2) + V(\tau_3^2).$$

The functions $K(\tau_3^2)$, $W(\tau_3^2)$, and $V(\tau_3^2)$ are given in the Appendix. Here, it should be kept in mind that the dislocation loop lies in the "*yz*" plane; i.e., $\tau_1 = x/|\mathbf{r} - \mathbf{r}'|$ and $\tau_3 = (z - z')/|\mathbf{r} - \mathbf{r}'|$. Therefore, the dimensionless cylindrical coordinates used for a visual comparison of formulas (31) and (32) for a circular dislocation loop are as follows: $\zeta = x/R$ and $\rho = r/R$ ($r^2 = y^2 + z^2$, $y = r\cos\varphi$, $z = r\sin\varphi$; i.e., φ is still the azimuthal angle, but in the "*yz*" plane of the loop). As was done above, expressions (31) and (32) are reduced to the standard form $Spu_{ij}^D = \frac{b^D}{4\pi R}I(\rho, \zeta, \varphi)$. Then, we numerically compare the corresponding expression (31) for the function I^K according to Kröner and expression (32) for the function $I^{L,R}$ according to Lifshitz and Rosenzweig. For zirconium, the obtained results are presented in Fig. 6 for the parameters $\zeta = 0.5$ and $\rho = 1.5$ (the region outside the dislocation loop). And again, as can be seen, there is a complete coincidence of the results obtained within both approaches. In contrast to the case of a basal prismatic dislocation loop, here, the functions I^K and $I^{L,R}$ have a weak dependence on the

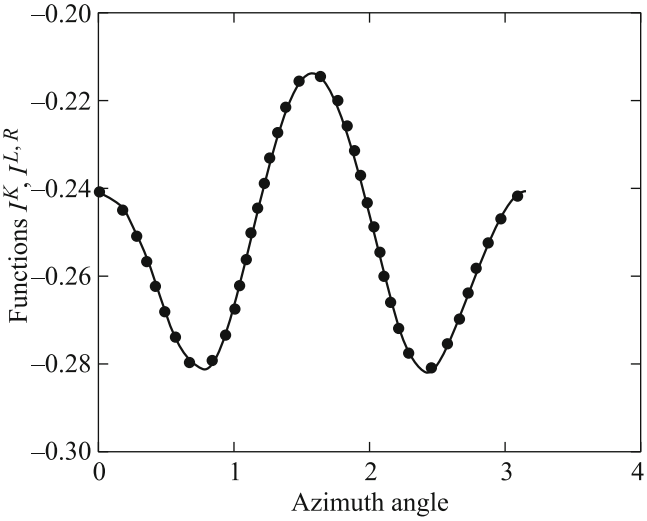

Fig. 6. Dependences of the functions $I^K(\rho, \zeta, \varphi)$ (solid line) and $I^{L,R}(\rho, \zeta, \varphi)$ (dotted line) according to formulas (31) and (32) on the azimuthal angle ϕ for the *a*-loop in the plane $\zeta = 0.5$ of the zirconium crystal for the relative distance $\rho = 1.5$.

azimuthal angle φ, but the character of the interaction (the sign of these functions) does not depend on the angle φ. For the relative distance $\rho = 0.5$ (the region above the dislocation loop), as in the case of a basal dislocation loop, the interaction changes the sign, whereas the weak angular dependence of the functions I^K and $I^{L,R}$ is retained. We did not present here this dependence in order to not overload the figures. It turns out that the dependences of the functions I^K and $I^{L,R}$ on the relative distance ρ for different values of ζ almost completely coincide with the corresponding dependence for the basal prismatic dislocation loop (see Figs. 1, 2). And this is quite natural because of the weak sensitivity of these functions to the angle φ.

5. RESULTS

Thus, this paper concludes a short series of publications [8, 9, 14] concerned with the method of the calculation and with a particular application of the tensor Green's function within the approach proposed by Lifshitz and Rosenzweig [5]. For cubic crystals, this approach implies the expansion in the small anisotropy parameter, and, according to [8, 18], the corrections to [5] are quite significant. For hexagonal crystals, there are two methods for the calculation of the tensor Green's function, namely, the Lifshitz–Rosenzweig method [5, 9] and the Kröner method [6]. In both methods, the tensor Green's function components have a universal form, which is valid for any hexagonal crystal. However, their formulas are so different in appearance that they can be compared with each other only in terms of the results obtained in particular applications. In the literature, the Kröner method is commonly cited in relation to the elastic interaction between two point defects or between a point defect and an infinitesimal dislocation loop. Therefore, the main objective of this study was to compare the results obtained using the two methods with specific examples of the elastic interaction of point defects with dislocation loops of finite sizes in real hexagonal close-packed metals.

We have considered three types of vacancy dislocation loops: the basal prismatic dislocation loop with $\mathbf{n} = (0, 0, 1)$, $\mathbf{b^D} = (0, 0, b^D)$; the basal shear dislocation loop with $\mathbf{n} = (0, 0, 1)$, $\mathbf{b^D} = (b^S, 0, 0)$; and the prismatic *a*-loop in zirconium with $\mathbf{n} = (1, 0, 0)$, $\mathbf{b^D} = (b^D, 0, 0)$ (bedding plane $\{11\bar{2}0\}$, the Burgers vector $\mathbf{b^D} = 1/3\langle 11\bar{2}0\rangle$). For each type of dislocation loops, the analytical expressions for the quantity $Spu_{ij}^D(\mathbf{r})$ (the point defect was simulated by a dilatation center) were obtained by the two methods using expressions (23), (24), (27), (28), (31), and (32). In the case of a basal prismatic dislocation loop, the similar expression was obtained independently by solving the equilibrium equations using the Elliott method [12] (formula (17)). In order to compare the obtained results, we used the circular shape of the dislocation loop. In the dimensionless cylindrical coordinates, they are represented in the form $Spu_{ij}^D = \dfrac{b^D}{4\pi R} I(\rho, \zeta, \varphi)$. The numerical calculations of the curves $I(\rho, \zeta, \varphi)$ were carried out for zirconium. The results of these calculations are presented in Figs. 1–6. The main conclusion is that all the methods used in the calculations are completely equivalent to each other. However, taking into account the limited applicability of the Elliott method [12], the calculation technique is actually the tensor Green's function method within the Lifshitz–Rosenzweig and Kröner approaches.

A simplifying factor in the above-considered cases of dislocation loops is that the normal vector to the plane of the dislocation loop, as well as the dislocation loop Burgers vector, has only one component in the Cartesian coordinate system. In general, this is not the case. And, the initial expressions (5) then become much more complicated. However, the calculation technique remains the same and does not lead to fundamental mathematical difficulties.

With the knowledge of the energy of elastic interaction of a point defect with a dislocation loop, we can calculate the diffusion fluxes of radiation-induced point defects onto the loop [19, 20], as well as the preference (bias) factor for a specific type of point defects. This factor is a very important characteristic of dislocations, in terms of which proper explanations have been found for many phenomena, such as swelling, radiation creep, radiation hardening of structural materials of nuclear reactors [21–24], and others. Here, however, we should note the following. In all the

relevant theories, the dislocation bias factor was calculated under the assumption of an elastically isotropic crystal, when the energy of interaction of point defects with a rectilinear dislocation or a loop is a harmonic function. For a hexagonal crystal, this is not the case. Such a conclusion follows, for example, from expression (17) for a basal prismatic dislocation loop. Therefore, the corresponding diffusion problem [19, 20] is complicated by the presence of the additional term, and the authors' conclusions regarding the dependence of the bias factor on the dislocation loop radius, the type of dislocation loop, and the ratio of the dilatation volumes of point defects can be changed. But, this is already another problem.

APPENDIX

$$V(\tau_3^2) \equiv (1-3\tau_3^2)\Phi(\tau_3^2) + 2\tau_3^2(1-\tau_3^2)\frac{d\Phi}{d\tau_3^2},$$

$$W(\tau_3^2) \equiv F(\tau_3^2) - 2(1-\tau_3^2)\frac{dF}{d\tau_3^2},$$

$$K(\tau_3^2) \equiv -N(\tau_3^2) - 2\tau_3^2\frac{dN}{d\tau_3^2} - 3\tau_3^2 M(\tau_3^2) + 2\tau_3^2(1-\tau_3^2)\frac{dM}{d\tau_3^2},$$

where the functions $\Phi(\tau_3^3)$, $F(\tau_3^3)$, $N(\tau_3^3)$, and $M(\tau_3^3)$ are related to the tensor Green's function components by the following expressions:

$$G_{3k}(\mathbf{r}-\mathbf{r}') = \frac{1}{4\pi|\mathbf{r}-\mathbf{r}'|}[\Phi(\tau_3^2)\tau_3\tau_\beta\delta_{\beta k} + F(\tau_3^2)\delta_{3k}],$$

$$\Phi(\tau_3^2) \equiv \frac{2i}{(z_1+z_2)}\frac{a+b+\chi+\rho}{A(\tau_3^2)},$$

$$F(\tau_3^2) \equiv \frac{2i}{(z_1+z_2)A(\tau_3^2)} \times\left((b+\rho)+(a+b-\rho)\tau_3^2 - \frac{a+2b}{z_1z_2}\right),$$

$$G_{\alpha k}(\mathbf{r}-\mathbf{r}') = \frac{1}{4\pi|\mathbf{r}-\mathbf{r}'|} \times[N(\tau_3^2)\delta_{\alpha k} - M(\tau_3^2)\tau_\alpha\tau_\beta\delta_{\beta k} + \Phi(\tau_3^2)\tau_\alpha\tau_3\delta_{3k}],$$

$$N(\tau_3^2) \equiv \frac{2i}{(z_1+z_2)}\frac{R(\tau_3^2)}{bA(\tau_3^2)} - \frac{b\tau_3^2}{\sqrt{bP(\tau_3^2)}(b+\rho)(1-\tau_3^2)},$$

$$M(\tau_3^2) \equiv \frac{2i}{(z_1+z_2)}\frac{S(\tau_3^2)}{(1-\tau_3^2)bA(\tau_3^2)} - \frac{P(\tau_3^2)+b\tau_3^2}{\sqrt{bP(\tau_3^2)}(b+\rho)(1-\tau_3^2)^2},$$

$$R(\tau_3^2) = \frac{(a+b)(b+\rho)}{z_1z_2} - \frac{A(\tau_3^2)P(\tau_3^2)}{2(b+\rho)(1-\tau_3^2)}\left(z_1z_2 - \frac{b}{P(\tau_3^2)}\right),$$

$$S(\tau_3^2) = (a+b)(b+\rho)\left[\frac{1}{z_1z_2}+\tau_3^2\right] - \frac{A(\tau_3^2)P(\tau_3^2)}{2(b+\rho)(1-\tau_3^2)} \times\left[\left(z_1z_2 - \frac{b}{P}\right) + \left(z_1^2z_2^2 + \frac{b}{P}\left[z_1z_2 - \frac{2B}{A}\right]\right)\tau_3^2\right],$$

$$A(\tau_3^2) = 2[k + l(1-\tau_3^2) - m(1-\tau_3^2)^2],$$

$$B(\tau_3^2) = 2k + l(1-\tau_3^2), \quad P(\tau_3^2) = b + \rho(1-\tau_3^2),$$

$$k = (a+2b)(b+\rho),$$

$$m = (a+b-\rho)\gamma - (\chi+2\rho)^2,$$

$$l = (a+2b)\gamma + (2b-\chi)(\chi+2\rho),$$

$$a = C_{12}, \quad b = \frac{1}{2}(C_{11}-C_{12}) = C_{66}, \quad \chi = C_{13}-C_{12},$$

$$\rho = C_{44} - \frac{1}{2}(C_{11}-C_{12}), \quad \gamma = C_{11}+C_{33}-4C_{44}-2C_{13},$$

$$z_1z_2 = -\sqrt{\frac{2k}{A(\tau_3^2)}}, \quad z_1+z_2 = i\sqrt{2}\left(\sqrt{\frac{2k}{A(\tau_3^2)}} + \frac{B(\tau_3^2)}{A(\tau_3^2)}\right)^{1/2}.$$

REFERENCES

1. *Progress in Solid State Physics*, Ed. by F. Seitz and D. Turnbull, Vol. 3: J. D. Eshelby, *The Continuum Theory of Lattice Defects* (Academic, New York, 1956, Nauka, Moscow, 1963).
2. Ian. N. Sneddon, *Fourier Transforms* (McGraw-Hill, New York, 1951).
3. L. D. Landau and E. M. Lifshitz, *Course of Theoretical Physics*, Vol. 7: *Theory of Elasticity* (Nauka, Moscow, 1987, Butterworth–Heinemann, Oxford, 1995).
4. J. P. Hirth and J. Lothe, *Theory of Dislocations* (McGraw-Hill, New York, 1968, Atomizdat, Moscow, 1972).
5. I. M. Lifshitz and L. N. Rosenzweig, Zh. Eksp. Teor. Fiz. **17**, 783 (1947).
6. E. Kröner, Z. Phys. **136**, 402 (1953).
7. J. R. Willis, Quart. J. Mech. Appl. Math. **18**, 419 (1965).
8. P. N. Ostapchuk, Phys. Solid State **54** (1), 98 (2012).
9. P. N. Ostapchuk, Phys. Solid State **55** (1), 109 (2013).
10. S. M. Ohr, J. Appl. Phys. **43**, 1361 (1973).
11. S. M. Ohr, Phys. Status Solidi B **58**, 613 (1973).
12. H. A. Elliott, Proc. Cambridge Philos. Soc. **44**, 522 (1948); H. A. Elliott, Proc. Cambridge Philos. Soc. **45**, 621 (1949).
13. F. Kroupa, Czech. J. Phys. B **10**, 284 (1960).

14. P. N. Ostapchuk and O. G. Trotsenko, Phys. Solid State **58** (9), 1810 (2016).
15. M. H. Yoo, Phys. Status Solidi B **61**, 411 (1974).
16. L. Fast, J. M. Wills, B. Johansson, and O. Eriksson, Phys. Rev. B: Condens. Matter **51** (24), 17431 (1995).
17. C. H. Woo, J. Nucl. Mater. **276**, 90 (2000).
18. S. A. Kukushkin, A. V. Osipov, and R. S. Telyatnik, Phys. Solid State **58** (5), 971 (2016).
19. V. I. Dubinko, A. S. Abyzov, and A. A. Turkin, J. Nucl. Mater. **336**, 11 (2005).
20. T. Jourdan, J. Nucl. Mater. **467**, 286 (2015).
21. V. F. Zelenskii, I. M. Neklyudov, and T. P. Chernyaeva, *Radiation-Induced Defects and Swelling of Metals* (Naukova Dumka, Kiev, 1988) [in Russian].
22. P. T. Heald and M. V. Speight, Philos. Mag. **29**, 1075 (1974).
23. L. K. Mansur, Philos. Mag. A **39**, 497 (1979).
24. V. I. Dubinko, S. A. Kotrechko, and V. F. Klepikov, Rad. Eff. Defects Solids **164**, 647 (2009).

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