THE METHODS FOR THE CALCULATION OF THE ELASTIC INTERACTION OF POINT DEFECTS WITH A DISLOCATION LOOPS IN HEXAGONAL CRYSTALS

O.G. Trotsenko, P.N. Ostapchuk
Institute of Electrophysics and Radiation Technologies,
National Academy of Sciences of Ukraine, Kharkov, Ukraine
E-mail: ostapchuk@kipt.kharkov.ua

Green's function method is used for hexagonal crystals according to Lifshitz-Rosenzweig and Kröner. Analytical expressions have been derived for the energy of elastic interaction of radiation point defects with dislocation edge loops of two types: c-loop (in the basal plane; the Burger's vector $\mathbf{b^D} = 1/2\langle 0001\rangle$) and a-loop (in the plane $\{11\bar{2}0\}$, the Burger's vector $\mathbf{b^D} = 1/3\langle 11\bar{2}0\rangle$). In the case of the basal loop an analogous expression is obtained by the independent solution of the equilibrium equations by the Eliot's method. Numerical comparison of the expressions for zirconium showed complete identity of these approaches.

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1. INTRODUTION AND THE BASIC

Irradiation by high-energy particles of the constructions of nuclear facilities significantly change their physical properties and entails a number of phenomena that limit the duration of their operation [1] (radiation embrittlement, radiation growth and creep, radiation swelling). They adversely affect on the performance of the elements of the reactors designs, disabling them in unscheduled time. The physical mechanisms underlying these phenomena are connected with the evolution of the defect structure of the original material, which is caused by diffusion fluxes of radiation point defects (PD) (SIAs, vacancies) for specific components of this structure. Density of flow of PD to internal sinks S, which are the elements of the defect structure of the material, contains two terms at a constant temperature T and an isotropic coefficient of diffusion D:

$$\boldsymbol{j}^S(\boldsymbol{r}) = -\frac{D}{\omega}\nabla C(\boldsymbol{r}) - \frac{DC(\boldsymbol{r})}{\omega}\nabla\frac{E^S_{\text{int}}(\boldsymbol{r})}{kT}. \quad (1)$$

The first (stochastic) connected with the gradient of the concentration $C(\boldsymbol{r})$ of PD in the material volume and at the sink boundary, the second (drift current) – connected with the interaction of PD with the sink elastic field $E^S_{\text{int}}(\boldsymbol{r})$. Therefore, the theoretical description of the sinks system evolution implies the ability to calculate the value $E^S_{\text{int}}(\boldsymbol{r})$. The most important element of the defect structure of any metal is a system of dislocations in the form of single loops or clusters (network in cubic and rows or layers in hexagonal close-packed crystals). With regard to clusters, it is the task of the future, but the version of a single loops is quite observable today. We are interested, first of all zirconium, so the proposed material is focused on hcp crystals. Thus, the purpose of the article is to show how we can analytically calculate the energy of the elastic interaction of PD with the specific dislocation loops in real hexagonal crystal. As an example, we considered the edge dislocation loops of two types: c-loop (in the basal plane, the Burger's vector $\mathbf{b^D} = 1/2\langle 0001\rangle$) and – a-loop (in the plane $\{11\bar{2}0\}$, the Burger's vector $\mathbf{b^D} = 1/3\langle 11\bar{2}0\rangle$). In addition, for c-loop required energy directly calculated by solution of the equilibrium equations.

In the theory of elasticity PD is described by the volume distribution of dipole forces without moments, i. e. by the expression of the form:

$$f_i(\boldsymbol{r}) = -P_{ij}\nabla_j\delta(\boldsymbol{r}),\ P_{ij} = P_{ji}. \quad (2)$$

According Eshelby [2], the energy of interaction of such an object with a source of stress S ($\boldsymbol{u}^S, u^S_{ij}, \sigma^S_{ij}$) in an elastic medium is given by

$$E_{\text{int}}(\boldsymbol{r}) = -P_{ij}u^S_{ij}(\boldsymbol{r}), \quad (3)$$

where $\boldsymbol{r}$ is coordinate of PD. If $P_{ij} = P\delta_{ij}$, i. e. PD is modeled by the dilation center, and source of stress S is dislocation loop, for the energy of their interaction finally we have:

$$E_{\text{int}}(\boldsymbol{r})/P = -Spu^D_{ij}(\boldsymbol{r}), \quad (4)$$

where P is the power of dilatation center; and the coordinate system is associated with dislocation. Our task is the calculation of the value Spu^D_{ij} for a particular dislocation loop.

There are two methods for calculating the elastic field of the loops u^D_{ij}. The first method is the solution of the quilibrium equations in the terms of displacements with appropriate boundary conditions. The second method is the Green's function method allowing to calculate the displacement caused by the dislocation of any form in an arbitrary anisotropic elastic medium, according to the classical formula [3, 4]

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

where C_{jklm} is the tensor of the elastic moduli of the medium simulating the crystal; b_m^D is mth component of the Burger's vector of the dislocation; n_l^D is l th component of the normal vector to any surface S_D, lying on the dislocation line; $\boldsymbol{r}'$ is the coordinate of the point on the surface S_D; $\boldsymbol{r}$ is the coordinate of the point of observation and G_{ij} is the tensor Green's function (TFG) of the elastic medium. According Elliott [5], the equilibrium equations are solved in terms of two stress functions. As for the TFG, two approaches are cited in the literature: Lifshitz-Rosenzweig (1947) [6] and Kröner (1953) [7] with a modified coefficient [8]. The first approach is valid for any unlimited elastic anisotropic medium, and the second is valid seemingly only for the hexagonal system.

2. EDGE LOOP IN THE BASAL PLANE OF THE HEXAGONAL CRYSTAL

We consider a circular vacancy loop of radius R lying in the plane $z = 0$ (basal plane) of the cylindrical coordinate system (r , φ , z), the Burger's vector which is perpendicular to the plane of the loop and has the only z-component $\mathbf{b^D} = (0,0,\mathrm{b^D})$. The normal vector to the plane of the loop $\mathbf{n} = (0,0,1)$ coincides with the positive direction of the axis "z", which is also the axis of symmetry of the crystal. An example of such an object can serve, according to [9], the so-called c-loop $\mathrm{b} = 1/2[0001]$ in zirconium under electron irradiation at the temperature $T = 715\,K$.

2.1. SOLUTION OF THE EQUILIBRIUM EQUATIONS (ELLIOTT'S APPROACH)

Since the problem is axially symmetric, the angular dependence is absent, and the stress state is uniquely determined by four components of the stress tensor: $\sigma_{rr}, \sigma_{\varphi\varphi}, \sigma_{zz}, \sigma_{rz}$, which satisfy the equations of equilibrium

$$\frac{\partial \sigma_{rr}}{\partial r} + \frac{\partial \sigma_{rz}}{\partial z} + \frac{\sigma_{rr} - \sigma_{\varphi\varphi}}{r} = 0 \ ; \quad (6)$$

$$\frac{\partial \sigma_{rz}}{\partial r} + \frac{\partial \sigma_{zz}}{\partial z} + \frac{\sigma_{rz}}{r} = 0 . \quad (7)$$

In terms of displacement, taking into account the substitution $u_r = \frac{\partial \Phi}{\partial r}$; $u_z = k\frac{\partial \Phi}{\partial z}$ they take the form

$$\frac{\partial}{\partial r}\left[\nabla^2\Phi + \frac{C_{44} + k(C_{13}+C_{44})}{C_{11}} \frac{\partial^2 \Phi}{\partial z^2}\right] = 0;$$

$$\frac{\partial}{\partial z}\left[\nabla^2\Phi + \frac{C_{33}k}{C_{44}k + (C_{13}+C_{44})} \frac{\partial^2 \Phi}{\partial z^2}\right] = 0 , \quad (8)$$

where $\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r}$ and $C_{11}, C_{12}, C_{13}, C_{33}$, $C_{44} = C_{55}$ is the minimum number of non-zero elastic moduli of hexagonal crystal. Equations (8) have a solution under the condition

$$\frac{C_{44} + k(C_{13}+C_{44})}{C_{11}} = \frac{C_{33}k}{C_{44}k + (C_{13}+C_{44})} = \nu .$$

This condition reduces (8) in the form

$$\left(\nabla^2 + \nu_\alpha \frac{\partial^2}{\partial z^2}\right)\Phi_\alpha(r,z) = 0 , \quad \alpha = 1, 2 , \quad (9)$$

where coefficients ν_α are the roots of a quadratic equation

$$C_{44}C_{11}\nu^2 + \left(C_{13}{}^2 + 2C_{44}C_{13} - C_{33}C_{11}\right)\nu + \\ + C_{44}C_{33} = 0. \quad (10)$$

Meanwhile,

$$u_r = \frac{\partial}{\partial r}\sum_{\alpha=1}^{2}\Phi_\alpha \ ; \quad u_z = \frac{\partial}{\partial z}\sum_{\alpha=1}^{2} k_\alpha \Phi_\alpha \ ;$$

$$k_\alpha = \frac{C_{11}\nu_\alpha - C_{44}}{C_{13}+C_{44}} = \frac{\nu_\alpha (C_{13}+C_{44})}{C_{33} - C_{44}\nu_\alpha} \quad (11)$$

and the desired quantity Spu_{ij}^D in terms of the functions Φ_α is given by the expression

$$Spu_{ij}^D = \sum_{\alpha=1}^{2}(k_\alpha - \nu_\alpha)\frac{\partial^2}{\partial z^2}\Phi_\alpha \ . \quad (12)$$

Hankel's transform [10] reduces (9) to ordinary differential equations

$$\left(\nu_\alpha \frac{d^2}{dz^2} - \xi^2\right) G_\alpha(\xi, z) = 0 , \quad (13)$$

whose solution is trivial

$$G_\alpha(\xi, z) = A_\alpha(\xi)\exp(-\xi z/\sqrt{\nu_\alpha}) + \\ + B_\alpha(\xi)\exp(\xi z/\sqrt{\nu_\alpha}).$$

In our case we consider the solutions when all components of the displacement and stress converges to zero, when $z \to \infty$. Then we have $B_\alpha = 0$, and the coefficients A_α are determined from the boundary conditions of the problem in the plane $z = 0$. They are as follows [11]:

$$u_z(r,0) = -\frac{1}{2}b^D,\ 0 \le r < R;$$

$$u_z(r,0) = 0,\quad r > R,\ \sigma_{rz}(r,0) = 0. \qquad (14)$$

Using Hankel's inversion theorem [10], we obtain for shear stress:

$$\sigma_{rz}(r,z) =$$

$$= C_{44}\int_0^\infty \xi^3 \sum_{\alpha=1}^{2}\left[\frac{1+k_\alpha}{\sqrt{\nu_\alpha}} A_\alpha(\xi)\exp(-\xi z/\sqrt{\nu_\alpha})\right] J_1(r\xi)d\xi, \qquad (15)$$

where J_0, J_1 are Bessel functions of the first kind. And then the second boundary condition (14) gives the relationship $A_2(\xi) = -A_1(\xi)\frac{1+k_1}{1+k_2}\frac{\sqrt{\nu_2}}{\sqrt{\nu_1}}$. Acting in a similar way for z-component of the displacement we receive the following expression

$$u_z(r,z) =$$

$$= -\int_0^\infty \xi^2 \sum_{\alpha=1}^{2}\left[\frac{k_\alpha}{\sqrt{\nu_\alpha}} A_\alpha(\xi)\exp(-\xi z/\sqrt{\nu_\alpha})\right] J_0(r\xi)d\xi. \qquad (16)$$

It is convenient to use dimensionless variables $t = \xi R$; $\rho = r/R$. Then the first boundary condition (14) gives two integral equations

$$\int_0^\infty t^2 A_1(t/R) J_0(t\rho)dt =$$

$$= \sqrt{\nu_1}\frac{1+k_2}{k_1-k_2}\frac{b^D R^3}{2},\quad 0 \le \rho < 1;$$

$$\int_0^\infty t^2 A_1(t/R) J_0(t\rho)dt = 0\ ,\ \rho > 1,$$

which are satisfied under the condition $t^2 A_1(t/R) = \sqrt{\nu_1}\frac{1+k_2}{k_1-k_2}\frac{b^D R^3}{2} J_1(t)$. As a result, the function Φ_α takes the form:

$$\Phi_1(r,z) =$$

$$= \sqrt{\nu_1}\frac{1+k_2}{k_1-k_2}\frac{b^D R}{2}\int_0^\infty \frac{1}{\xi} J_1(\xi R) J_0(r\xi)\exp(-\xi z/\sqrt{\nu_1})d\xi; \qquad (17)$$

$$\Phi_2(r,z) =$$

$$= -\sqrt{\nu_2}\frac{1+k_1}{k_1-k_2}\frac{b^D R}{2}\int_0^\infty \frac{1}{\xi} J_1(\xi R) J_0(r\xi)\exp(-\xi z/\sqrt{\nu_2})d\xi.$$

Accordingly, for the desired quantity Spu_{ij}^D from (12) we obtain:

$$Spu_{ij}^D = \frac{b^D}{2R}\left[\frac{1+k_2}{k_1-k_2}\frac{k_1-\nu_1}{\sqrt{\nu_1}} I_0^1\left(\frac{r}{R},\frac{z}{R\sqrt{\nu_1}}\right) - \frac{1+k_1}{k_1-k_2}\frac{k_2-\nu_2}{\sqrt{\nu_2}} I_0^1\left(\frac{r}{R},\frac{z}{R\sqrt{\nu_2}}\right)\right] \equiv \frac{b^D}{4\pi R} I\left(\frac{r}{R},\frac{z}{R}\right), \qquad (18)$$

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

and thus, the problem is solved.

2.2. THE GREEN'S FUNCTIONS METHOD: LIFSHITZ-ROSENZWEIG'S APPROACH

From formula (5) we have:

$$Spu_{ij}^D(\boldsymbol{r}) = b^D \int_{S_D} d^2 r'\left[C_{13}\sum_{\alpha=1}^{2} G_{i\alpha,\alpha i}(\boldsymbol{r}-\boldsymbol{r}') + C_{33} G_{i3,3i}(\boldsymbol{r}-\boldsymbol{r}')\right],\ G_{ij,k} \equiv \frac{\partial}{\partial x_k} G_{ij}\ , \qquad (19)$$

where the index "i" is summation from 1 to 3. Analytical universal expressions for the component of TFG of hexagonal crystal are given in [12]

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

$$G_{\alpha k}(\boldsymbol{r}-\boldsymbol{r}') = \frac{1}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}\left[\mathrm{N}(\tau_3^2)\delta_{\alpha k} - \mathrm{M}(\tau_3^2)\tau_\alpha\tau_\beta\delta_{\beta k} + \Phi(\tau_3^2)\tau_\alpha\tau_3\delta_{3k}\right]. \qquad (20)$$

As a result,

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

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

$$V(\tau_3^2) \equiv (1-3\tau_3^2)\Phi(\tau_3^2) + 2\tau_3^2(1-\tau_3^2)\frac{d\Phi}{d\tau_3^2}; \qquad W(\tau_3^2) \equiv F(\tau_3^2) - 2(1-\tau_3^2)\frac{dF}{d\tau_3^2};$$

$$\mathrm{K}(\tau_3^2) \equiv -\mathrm{N}(\tau_3^2) - 2\tau_3^2\frac{d\mathrm{N}}{d\tau_3^2} - 3\tau_3^2\mathrm{M}(\tau_3^2) + 2\tau_3^2(1-\tau_3^2)\frac{d\mathrm{M}}{d\tau_3^2}. \tag{21}$$

Functions $\Phi(\tau_3^2)$, $F(\tau_3^2)$, $\mathrm{N}(\tau_3^2)$, and $\mathrm{M}(\tau_3^2)$ are quite cumbersom and carried to appendix.

2.3. THE GREEN'S FUNCTIONS METHOD: KRÖNER'S APPROACH

Original formula is (19), but the components of TFG are other here. According to Kröner we have:

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

$$G_{22} = \sum_{k=1}^{3}\frac{1}{\left[\nu_k r^2 + z^2\right]^{1/2}}\left[A_k\frac{y^2z^2 - x^2(\nu_k r^2 + z^2)}{r^4} + B_k\right]; \qquad G_{33} = \sum_{k=1}^{3}\frac{D_k}{\left[\nu_k r^2 + z^2\right]^{1/2}};$$

$$G_{12} = \frac{xy}{r^4}\sum_{k=1}^{3}A_k\frac{\left[\nu_k r^2 + 2z^2\right]}{\left[\nu_k r^2 + z^2\right]^{1/2}}; \quad G_{31} = \frac{xz}{r^2}\sum_{k=1}^{3}\frac{C_k}{\left[\nu_k r^2 + z^2\right]^{1/2}}; \quad G_{32} = \frac{yz}{r^2}\sum_{k=1}^{3}\frac{C_k}{\left[\nu_k r^2 + z^2\right]^{1/2}}. \tag{22}$$

Performing the appropriate summation in (19), we obtain

$$Spu_{ij}^{D}(\boldsymbol{r}) = \frac{b^D}{4\pi}\int_{S_D}\frac{d^2r'}{\left|\boldsymbol{r}-\boldsymbol{r}'\right|^3}\left[C_{13}\mathrm{T}_1(\tau_3^2) + C_{33}\mathrm{T}_2(\tau_3^2) + (C_{13}+C_{33})\mathrm{T}_3(\tau_3^2)\right];$$

$$\mathrm{T}_1 = \sum_{\alpha=1}^{2}A_\alpha\nu_\alpha{}^2F_\alpha(\tau_3^2);\ \mathrm{T}_2 = \sum_{\alpha=1}^{2}D_\alpha F_\alpha(\tau_3^2);\ \mathrm{T}_3 = \sum_{\alpha=1}^{2}C_\alpha\nu_\alpha F_\alpha(\tau_3^2);\ F_\alpha(\tau_3^2) \equiv \frac{2\tau_3^2 - \nu_\alpha(1-\tau_3^2)}{\left[\tau_3^2 + \nu_\alpha(1-\tau_3^2)\right]^{5/2}}, \tag{23}$$

where ν_α are the roots of the same quadratic equation (10), and the coefficients in (22) and (23) have the form

$$A_\alpha = \left[\left(C_{66}-C_{11}\right)\left(C_{33}-\nu_\alpha C_{44}\right) + \left(C_{13}+C_{44}\right)^2\right]/E_\alpha,\ \ C_{66} = \left(C_{11}-C_{12}\right)/2;$$

$$D_\alpha = \left(C_{44}-\nu_\alpha C_{11}\right)\left(C_{44}-\nu_\alpha C_{66}\right)/E_\alpha; \qquad C_\alpha = \left(C_{13}+C_{44}\right)\left(C_{44}-\nu_\alpha C_{66}\right)/E_\alpha;$$

$$E_1 = C_{11}C_{44}C_{66}\left(\nu_1-\nu_3\right)\left(\nu_1-\nu_2\right); \qquad E_2 = C_{11}C_{44}C_{66}\left(\nu_2-\nu_3\right)\left(\nu_2-\nu_1\right). \tag{24}$$

Thus, the problem reduces to the integration of (19) and (23) in a plane of the circular loop of radius R (recall that $z' = 0$ since the loop lies in the basal plane of the crystal).

So, we have three independent variants for solving the same problem. Their numerical comparison was carried out with respect to zirconium. The experimental values of its modulus of elasticity are following [12] (Mbar): $C_{11} = 1.554$; $C_{12} = 0.672$; $C_{13} = 0.646$; $C_{33} = 1.725$; $C_{55} = C_{44} = 0.363$. The comparison results are presented in Figs. 1, 2 in dimensionless cylindrical coordinates; $\rho = r/R$; $\zeta = z/R$.

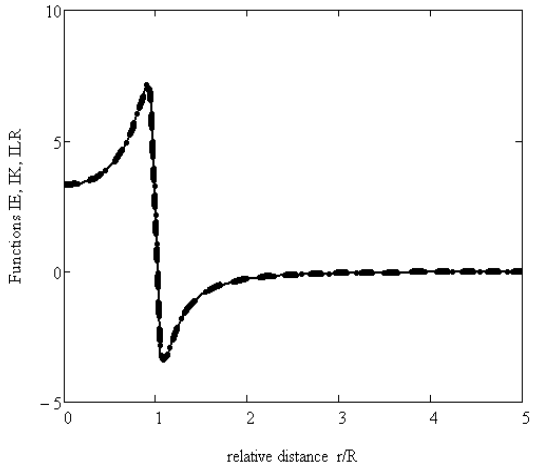

Fig. 1. Dependence of the functions $I^E(\rho,\zeta)$ *(solid line),* $I^{LR}(\rho,\zeta)$ *(dotted line)* $I^K(\rho,\zeta)$ *(points) according (18), (21), and (23) on the relative distance* $\rho = r/R$ *in the plane* $\zeta = 0.1$ *of zirconium*

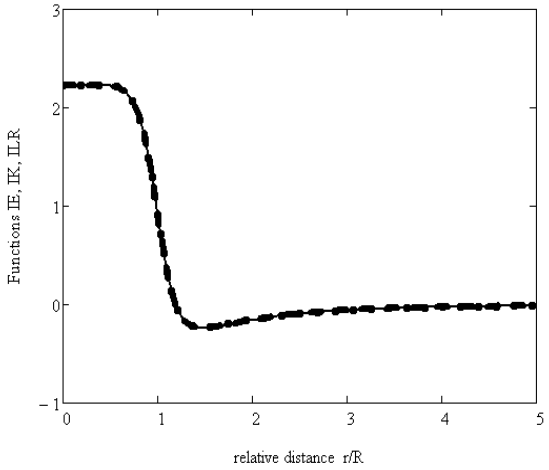

Fig. 2. Dependence of the functions $I^E(\rho,\zeta)$ *(solid line),* $I^{LR}(\rho,\zeta)$ *(dotted line)* $I^K(\rho,\zeta)$ *(points) according (18), (21), and (23) on the relative distance* $\rho = r/R$ *in the plane* $\zeta = 0.5$ *of zirconium*

Formulas (18), (21), (23) are reduced to a united form $Spu_{ij}^D = \frac{b^D}{4\pi R} I(\rho,\zeta)$, so in Figs. 1, 2 the function $I^E(\rho,\zeta)$ (solid line) corresponds to the formula (18), $I^{LR}(\rho,\zeta)$ (dotted line) corresponds to the formula (21) (Lifshitz-Rosenzweig), $I^K(\rho,\zeta)$ (points) corresponds to the formula (23) (Kröner). They show the dependence of the functions I^E, I^{LR}, I^K on the relative distance ρ for the two planes $\zeta = 0.1$ and $\zeta = 0.5$ above the plane of the loop $\zeta = 0$. We see the perfect agreement of all three approaches. The qualitative nature of the interaction does not change (vacancy loop, the formula (4)): vacancy ($P < 0$) is pushed out from the inside of the loop $\rho < 1$, and attracted in the external region $\rho > 1$ (SIA – on the contrary). However, if on a sufficiently large distances from the plane of the loop ($\zeta = 0.5$) interaction smoothly changes its sign at the boundary of the loop $\rho \approx 1$, then with the approaching to the plane of loop ($\zeta = 0.1$) the interaction varies substantially step-wise on its boundary.

3. EDGE LOOP IN PRISMATIC PLANE OF THE HEXAGONAL CRYSTAL

Consider a circular vacancy loop of radius R lying in the plane $x = 0$ of the Cartesian coordinate system (prismatic plane of hexagonal crystal). The Burger's vector is perpendicular to the plane of loop and has only x-component $\mathbf{b^D} = (\mathrm{b}^D, 0, 0)$. The vector of normal to the plane of the loop $\mathbf{n} = (1,0,0)$ coincides with the positive direction of the axis "x". An example of such an object may be, according to [9], the so-called a-loops $\mathbf{b^D} = 1/3\langle 11\bar{2}0\rangle$ in zirconium. It is the dominant form of loops under neutron irradiation as the vacancy as and the interstitial in nature. The axial symmetry in this case is absent so well-developed methods for solving equilibrium equations are not applicable. It remains TFG's method. From (5) we again have:

$$Spu_{ij}^D(\mathbf{r}) = b^D \int_{S_D} \left[C_{12} \sum_{\alpha=1}^{2} G_{i\alpha,\alpha i} + C_{13} G_{i3,3i} \right] d^2r' + \\ + b^D (C_{11} - C_{12}) \int_{S_D} G_{i1,1i}(\mathbf{r} - \mathbf{r}') d^2r', \qquad (25)$$

where the repeated suffix "i", as previously, is summed over the values 1–3. Note that the first term in (25) coincides up to the coefficient with the expression (19), for which the result is already known both Lifshitz-Rosenzweig (21), and by Kröner (23). Therefore, only the sum $G_{i1,1i}$ to be calculated. The result of calculations by Lifshitz-Rosenzweig is following:

$$Spu_{ij}^D(\mathbf{r}) = -\frac{b^D}{4\pi} \int_{S_D} \frac{d^2r'}{|\mathbf{r} - \mathbf{r}'|^3} Q(\tau_3^2) - \frac{b^D}{4\pi} (C_{11} - C_{12}) \int_{S_D} \frac{d^2r'}{|\mathbf{r} - \mathbf{r}'|^3} \tau_1^2 \left[3Y(\tau_3^2) + 2\tau_3^2 \frac{dY}{d\tau_3^2} \right]; \qquad (26)$$

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

$$\Psi(\tau_3^2)=V(\tau_3^2)+W(\tau_3^2)\ ,\qquad Y(\tau_3^2)=\mathrm{K}(\tau_3^2)+V(\tau_3^2).$$

The functions $\mathrm{K}(\tau_3^2), W(\tau_3^2), V(\tau_3^2)$ are the same as in (21). A similar result for Kröner is:

$$\begin{aligned} Spu_{ij}^D(\boldsymbol{r}) &= \frac{b^D}{4\pi}\int\limits_{S_D}\frac{d^2r'}{\left|\boldsymbol{r}-\boldsymbol{r}'\right|^3}\left[C_{12}\mathrm{T}_1(\tau_3^2)+C_{13}\mathrm{T}_2(\tau_3^2)+(C_{12}+C_{13})\mathrm{T}_3(\tau_3^2)\right]+ \\ &+\frac{b^D}{4\pi}(C_{11}-C_{12})\int\limits_{S_D}\frac{d^2r'}{\left|\boldsymbol{r}-\boldsymbol{r}'\right|^3}\mathrm{T}(\tau_1^2,\tau_3^2); \end{aligned} \tag{27}$$

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

All functions and constants are as defined above (23), (24). Here we must remember that the loop lies in the plane «yz» of Cartesian coordinate system, i.e. $\tau_1=x/\left|\boldsymbol{r}-\boldsymbol{r}'\right|$, ($x'=0$), and $\tau_3=(z-z')/\left|\boldsymbol{r}-\boldsymbol{r}'\right|$. Therefore the dimensionless cylindrical coordinates used for the numerical comparison of formulas (26) and (27) are following: $\zeta=x/R$, $\rho=r/R$ ($r^2=y^2+z^2$, $y=r\cos\varphi$, $z=r\sin\varphi$, and φ is an azimuth angle, but in the plane of the loop "yz"). As earlier, formulas (26), (27) are reduced to the standard form $Spu_{ij}^D=\frac{b^D}{4\pi R}I(\rho,\zeta,\varphi)$, however, in order not to overload the article by the pictures, we give them a qualitative description. Firstly, we emphasize again full coincidence of Lifshitz-Rosenzweig's and Kröner's approaches. Secondly, we note that, unlike the base loop the functions I^{LR} (26) and I^K (27) include a weak dependence on the azimuthal angle φ in the plane of the loop, but the character of interaction (their sign on both sides of the conditional boundary loop) from φ is independent. Moreover, the dependence of the functions I^{LR}, I^K on the relative distance ρ for different planes $\zeta=const$ almost coincides with a similar for the base loop (see Figs. 1, 2). It is quite natural in view of the weak sensitivity of these functions to the angle φ.

4. DISCUSSION OF RESULTS

So, the different methods are used to derive analytical expressions for the energy of elastic interaction of PD with the specific dislocation loops in real hexagonal crystal. As an example, we were taken vacancy edge loops of two types: c- and a-loop in zirconium. Simplifies circumstance in cases considered above is that the normal vector to the plane of the loop and its Burgers vector has only one component in a Cartesian coordinate system. In general, it is not. And the initial formula (5) then become much more complicated. However, the method of calculation remains the same and does not contain principal mathematical difficulties.

Knowing the energy of elastic interaction PD with a loop allows one to calculate the diffusion fluxes of radiation PD on it [13, 14], as well as its bias factor to a specific type of PD. The bias is the most important characteristic of dislocations which made possible to explane such phenomena as swelling, radiation creep, radiation hardening structural materials of nuclear reactors [15–17], etc. Here, however, we should note the following. In all theories bias factor of dislocation was calculated assuming an elastically isotropic crystal when the energy of interaction of PD with a straight dislocation or a loop is harmonic function. For a hexagonal crystal it is not. This follows, for example, from the expression (18) for the base prismatic loop. Therefore, the corresponding diffusion problem [13, 14] is complicated by the presence of the additional term, and the authors' conclusions regarding of the depending of the bias factor from the radius of the loop, the type and ratio of dilatation volume of TD, can change.

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APPENDIX

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

$$\mathrm{N}(\tau_3^2)\equiv\frac{2i}{(z_1+z_2)}\frac{R(\tau_3^2)}{b\,A(\tau_3^2)}-\frac{b\,\tau_3^2}{\sqrt{b\,P(\tau_3^2)}\,(b+\rho)(1-\tau_3^2)};$$

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

$$R(\tau_3^2)=\frac{(a+b)(b+\rho)}{z_1\,z_2}-\frac{A(\tau_3^2)\,P(\tau_3^2)}{2(b+\rho)(1-\tau_3^2)}\left(z_1\,z_2-\frac{b}{P(\tau_3^2)}\right);$$

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

$$A(\tau_3^2)=2\left[k+l(1-\tau_3^2)-m(1-\tau_3^2)^2\right];\quad B(\tau_3^2)=2k+l(1-\tau_3^2)\quad P(\tau_3^2)=b+\rho(1-\tau_3^2);$$

$$k=(a+2b)(b+\rho);\;\; m=(a+b-\rho)\gamma-(\chi+2\rho)^2;\;\; l=(a+2b)\gamma+(2b-\chi)(\chi+2\rho);$$

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

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

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

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МЕТОДЫ РАСЧЕТА УПРУГОГО ВЗАИМОДЕЙСТВИЯ ТОЧЕЧНЫХ ДЕФЕКТОВ С ДИСЛОКАЦИОННЫМИ ПЕТЛЯМИ В ГЕКСАГОНАЛЬНЫХ КРИСТАЛЛАХ

О.Г. Троценко, П.Н. Остапчук

Методом функций Грина для гексагональных кристаллов в подходах Лифшица-Розенцвейга и Кренера получены аналитические выражения энергии упругого взаимодействия радиационных точечных дефектов с дислокационными краевыми петлями двух видов: c-петлей (базисная плоскость залегания, вектор Бюргерса $\mathbf{b^D}=1/2[0001]$) и a-петлей (плоскость залегания $\{11\bar{2}0\}$, вектор Бюргерса $\mathbf{b^D}=1/3\langle11\bar{2}0\rangle$). В случае базисной петли аналогичное выражение получено независимо решением уравнений равновесия методом Элиота. Численное сравнение полученных результатов для циркония показало полное совпадение рассмотренных подходов.

МЕТОДИ РОЗРАХУНКУ ПРУЖНОЇ ВЗАЄМОДІЇ ТОЧКОВИХ ДЕФЕКТІВ З ДИСЛОКАЦІЙНИМИ ПЕТЛЯМИ В ГЕКСАГОНАЛЬНИХ КРИСТАЛАХ

О.Г. Троценко, П.М. Остапчук

Методом функцій Гріна для гексагональних кристалів у підходах Ліфшиця-Розенцвейга і Кренера отримані аналітичні вирази енергії пружної взаємодії радіаційних точкових дефектів з дислокаційними крайовими петлями двох видів: c-петлею (базисна площина залягання, вектор Бюргерса $\mathbf{b}^{\mathbf{D}} = 1/2[0001]$) і a-петлею (площина залягання $\{11\bar{2}0\}$, вектор Бюргерса $\mathbf{b}^{\mathbf{D}} = 1/3\langle 11\bar{2}0\rangle$). У разі базисної петлі аналогічний вираз отримано незалежно рішенням рівнянь рівноваги методом Еліота. Чисельне порівняння отриманих результатів для цирконію показало повний збіг розглянутих підходів.