NUMERICAL CALCULATION OF THE DISLOCATION BASIS LOOP BIAS IN HEXAGONAL CRYSTAL

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The diffusion fluxes of radiation point defects onto a circular base edge loop of zirconium in a toroidal reservoir are calculated numerically (by the finite difference method). Elastic interaction of point defects and elastic anisotropy of the hexagonal crystal were taken into account. The toroidal geometry of the reservoir seems more acceptable for the loop than spherical or cylindrical since it allows calculations for the loop of any size and without any correction of the elastic field in its influence region. The dependences of the absorption efficiencies and the loop bias on the radius and its nature are obtained. The essential role of the boundary condition on the external surface of the reservoir in the symmetry breaking in the absorption of point defects by loops of different nature is shown.

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INTRODUCTION

Network dislocations and dislocation loops (DL) are usually considered as main extended microstructure defects in metals at the initial phases of irradiation. Their nucleation, diffusion growth, or dissolution directly reflects the processes of generation, migration, and subsequent absorption by various sinks of point defects (PD) caused by irradiation. Understanding the mechanisms controlling the evolution of such objects as dislocation loops is extremely important for describing the phenomena of radiation swelling and growth of structural reactors materials of the modern and future generations [1-3]. Since their main function is that they are sinks for radiation PDs, the problem of correct calculations the diffusion fluxes of the PDs for a specific loop appears. Generally accepted that dislocation loops preferentially absorb their interstitial atoms (ISA) than vacancies, because of their stronger elastic interaction with the ISA. The quantitative expression of this preference is the integral value, called the absorption efficiency of the PD given by the sink, or rather the relative difference between the absorption efficiencies of its interstitial atoms and vacancies, known as bias. As a result, loops absorb more ISA, and vacancies remaining in excess diffuse into other (with a smaller preference factor) sinks: grain boundaries and pores. This is the possible explanation of the phenomenon of vacancy swelling of stainless steel under irradiation. There is a separation of the diffusion fluxes of PD between various types of effluents (loops and pores), which ultimately causes macrodeformation of the material. In this case, interstitial loops should grow, and vacancy loops should dissolve. For steel this conclusion is confirmed by numerous experiments [4]. As for HCP metals, under irradiation, along with interstitial ones, vacancy loops of sufficiently large dimensions are also observed [5]. In particular, in zirconium interstitial loops mainly grow on prismatic planes and vacancy loops in the basal plane. Such distribution of loops is usually considered as a reason for radiation growth. Radiation growth is accompanied by a change in the shape of the material without external load and a noticeable change in volume. Thus, zirconium in the process of growth expands in the <a> direction and narrows along the <c> axe [6]. This means that the diffusion fluxes of radiation PDs are separated, but between the sinks of the same type, but of a different nature: interstitial and vacancy loops. The mechanism of this separation is not completely clear. The fact is that if a crystal, as usual, is modeled elastically with an isotropic medium, it turns out that the loop bias does not depend on its nature, it is determined by its radius and the sinks concentration [8]. This makes impossible for the existence of macroscopic vacancy loops. Therefore, another option was proposed which is associated with the anisotropy of the diffusion coefficients of the PD [8]. However, the conclusions of the authors are based on solving the simplest diffusion-anisotropic problem for a straight-line dislocation and the degree of adequacy of generalization to loops is not clear. The dependence on the radius, the nature of the loop and any of its quantitative characteristics are also unclear. Since there are no works including the elastic anisotropy of HCP metals in the diffusion problem, this option is considered as the best way for a qualitative explanation of the phenomenon of radiation growth. In this paper, the specified gap is eliminated. Diffusion flows of PDs onto a circular basic edge loop of zirconium were calculated numerically (by the finite-difference method) taking into account their elastic interaction and the elastic anisotropy of the crystal. The dependences of the efficiency of capturing PD and the bias on the radius and nature of the loop are obtained. The role of the boundary conditions in the formulation of the corresponding diffusion problem is analyzed.

1. BIAS OF STRAIGHT LOOP

This classic example, analytically precisely solved problem is given here for two reasons. Firstly, to show how the form of the boundary conditions affects the result. And secondly, for formal testing of the numerical solution of the diffusion equation by the finite difference method [9]. So, in the case of diffusion $D_{ik} = D\delta_{ik}$ and elastic isotropy of the medium, the flow of point defects per unit length of a straight edge dislocation is found by solving the following diffusion problem in the quasistationary approximation:

$$\omega div\, \boldsymbol{j}_{str}(\boldsymbol{r}) = 0; \qquad \boldsymbol{j}_{str}(\boldsymbol{r}) = -\frac{DC(\boldsymbol{r})}{\omega}\beta\,\nabla\mu(\boldsymbol{r}); \qquad \beta \equiv 1/k_B T\ , \tag{1}$$

$$\beta\,\mu(\boldsymbol{r}) = \ln\left(\frac{C(\boldsymbol{r})}{C^e}\exp\left(E_{\text{int}}^{str}(\boldsymbol{r})\right)\right); \qquad E_{\text{int}}^{str}(\boldsymbol{r}) = \frac{L}{r}\sin\varphi, \qquad L \equiv b\frac{1+\nu}{1-\nu}\frac{\Delta V \beta G}{3\pi}.$$

Here E_{int}^{str} – energy (measured in $k_B T$) of the elastic interaction of the dislocation with the PD in the model of the dilatation center; ΔV – dilatation volume of PD; G – shear modulus; ω – volume per atom of the crystal; φ – the angle between the radius vector of the defect location point $\boldsymbol{r}$ and the Burgers vector $\boldsymbol{b}$ in a plane perpendicular to the dislocation line (the axis "z" is directed along the dislocation line, and the Burgers vector is along the "z" axis, so $b_x = b$, $b_y = b_z = 0$); ν – Poisson's ratio; $C(\boldsymbol{r})$ – PD concentration. Equation (1) should be supplemented with boundary conditions, which are proposed to be formulated in the form:

$$C(\boldsymbol{r})\exp\left(E_{\text{int}}^{str}(\boldsymbol{r})\right)|_{r=r_c} = C^e;$$
$$C(\boldsymbol{r})\exp\left(E_{\text{int}}^{str}(\boldsymbol{r})\right)|_{r=R_{ext}} = \bar{C}, \tag{2}$$

Here C^e – thermally equilibrium concentration of PD in a crystal in the absence of a stress field; r_c – dislocation core radius; R_{ext} – the external radius of the diffusion problem (the radius of its influence region). The first condition on the core is standard and corresponds to the value of the chemical potential of the PD for a free flat surface $\beta\,\mu(r_c) = 0$. The second is less obvious. Usually [7] it is formulated as $C(\boldsymbol{r})|_{r=R_{ext}} = \bar{C}$, where $\bar{C}$ – average concentration of PD in an effective medium simulating the influence of the entire ensemble of effluents. In this paper, the point of view is different. The boundary condition is formulated for the chemical potential at the external boundary, namely: $\beta\,\mu(R_{ext}) = \ln(\bar{C}/C^e)$. This is the standard type of chemical potential of TD in an effective environment where the influence of a specific sink is leveled by the entire ensemble. For the desired flow in a cylindrical coordinate system, we have:

$$J_{str}(r_c) = -r_c\int_0^{2\pi}(\boldsymbol{n}\,\boldsymbol{j}_{str}(r_c,\varphi))\,d\varphi, \tag{3}$$

Here is the unit vector of the external normal to the boundary of the dislocation core (coincides with the unit radius vector of the cylindrical coordinate system). The technical details of the solution of the system (1-3) are described in detail in [10, 11]. The result is as follows:

$$J_{str}(r_c) = \frac{D}{\omega}(\bar{C} - C^e)Z_{str}; \qquad Z_{str}(z_c, z_{ext}) = Z_0(z_c, z_{ext}) + 2\sum_{k=1}^{\infty} Z_k(z_c, z_{ext}); \tag{4}$$

$$Z_n(z_c, z_{ext}) = \frac{2\pi\, I_n(z_c)I_n(z_{ext})}{I_n(z_c)K_n(z_{ext}) - I_n(z_{ext})K_n(z_c)}; \quad n = 0;1;.... \qquad z_c \equiv L/2r_c;$$
$$z_{ext} \equiv L/2R_{ext}.$$

Here $I_n(z)$ and $K_n(z)$ – modified Bessel functions. The flow is proportional to the difference $(\bar{C} - C^e)$, and Z_{str} is the absorption efficiency of PD by dislocation. It is invariant under the transformation $L \to -L$, so in (4) one can formally consider $z \equiv |L|/2r$. Thus, the absorption efficiency is sensitive only to the absolute value of L, and not to the sign of the relaxation volume of the PD or the sign of the projection of the Burgers vector onto the "x" axis. In the week interaction limit ($z_c \to 0$; $z_{ext} \to 0$) $Z_{str} \to 2\pi/\ln(z_c/z_{ext})$, In the strong interaction limit ($z_c >> 1$; $z_{ext} \to 0$) $Z_{str} \to 2\pi/\ln(1/z_{ext})$. It is significant that, in both cases, the sum in (4) makes a small (to the extent of smallness z_{ext}) contribution to the absorption efficiency of the TD by the dislocation, which is mainly determined by the first term.

Another approach is related to the formulation of the second boundary condition in (2) in the form $C(\boldsymbol{r})|_{r=R_{ext}} = \bar{C}$. Then, for the desired PD flow per unit dislocation length, we have:

$$J_{str}(r_c) = \frac{D}{\omega}\left(\bar{C}\,Z_{str}^a - C^e Z_{str}^e\right);$$
$$Z_{str}^a(z_c, z_{ext}) = Z_0(z_c, z_{ext}) + 2\sum_{k=1}^{\infty}(-1)^k Z_k(z_c, z_{ext}). \tag{5}$$

Two efficiencies of PD appear in this approach. Absorption efficiency Z_{str}^a and emission efficiency Z_{str}^e [10]. Z_{str}^e exactly coincide with Z_{str} in (4). Sum in (5) is negative value, therefore $Z_{str}^a < Z_{str}^e$, that is, a dislocation should emit PDs more easily than absorb. In our approach, the absorption and emission processes have the same efficiency. From (4), (5) one can see, that the desired absorption efficiency depends on the size of the influence area of the sink R_{ext}, which is determined by the total power of the drains in the system k_{tot}^2, cm^{-2} [7] by the equation:

$$R_{ext}(k_{tot}) = \sqrt{\frac{Z_{str}(k_{tot}^2)}{\pi k_{tot}^2}}. \tag{6}$$

Substitution of (6) to (4) gives the transcendental equation for $Z_{str}(k_{tot}^2)$. Solving it numerically one can obtain *bias* $B_{str}(k_{tot}^2) = 1 - Z_{str,v} / Z_{str,i}$, here indexes "$i$" and "$v$" correspond to CIA vacancy respectively. Dependence of straight dislocation bias on sinks density is shown on Fig. 1. There are three lines. Solid one corresponds to exact solution, dotted one to Margvelashvili-Saralidze approximation, [12], $Z_{str} = Z_0$, ($I_0(z_{ext}) \approx 1$), and dashed one corresponds to strong interaction approximation $Z_{str} = 2\pi / \ln(1/z_{ext})$. One can see that exact solution is between two approximations.

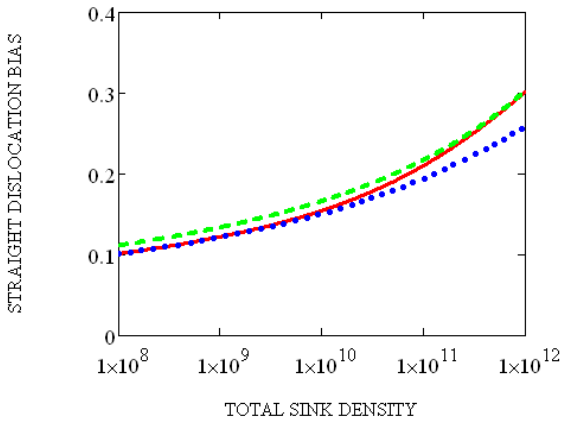


Fig. 1. Dependence of the bias factor of rectilinear dislocation on the density of drains. Solid line - exact solution (4), dotted - approximation [12], dashed – strong interaction approximation. The calculations are done for zirconium at $T = 573\,K$, *material parameters are:* $G = 33\,GPa$; $\nu = 0.33$; $b = 3.23 \cdot 10^{-10}\ m$; $\Delta V_i = 1.2\omega$; $\Delta V_v = -0.6\omega$; $\omega = 2.36 \cdot 10^{-29}\ m^3$; $r_c = 3b$

2. BIAS PF BASE DISLOCATION LOOP IN HCP-METALS

Let us consider a basic (plane *Z=0* of a cylindrical coordinate system) vacancy loop of radius R, located in a toroidal reservoir which is coaxial to dislocation loop [7]. External radius of reservoir is R_{ext}, inner is r_c. The Burgers vector of the loop is perpendicular to its plane and has only a *Z*-component ($0, 0, b^D$).The normal vector to the loop plane coincides with the positive axis direction «z», which is also the axis of the crystal symmetry. The problem is formulated in terms of a variable $\psi(r,z) = \left[C(r,z)\exp E_{\text{int}}^D(r,z) - C^e\right]/(\bar{C} - C^e)$. The quasistationary diffusion equation in dimensionless cylindrical coordinates has the form:

$$\frac{\partial^2\psi}{\partial r^2} + \frac{\partial^2\psi}{\partial z^2} + \left(\frac{1}{r} - \frac{\partial E_{\text{int}}^D}{\partial r}\right)\frac{\partial\psi}{\partial r} - \frac{\partial E_{\text{int}}^D}{\partial z}\frac{\partial\psi}{\partial z} = 0, \quad (7)$$

the interaction energy of the loop with the PD in the HCP crystal is given by [13]:

$$E_{\text{int}}^D(r,z) = -\frac{G\Delta V}{3k_BT}\frac{1+\nu}{1-2\nu}\frac{b^D}{R}\left[\frac{1+k_2}{k_1-k_2}\frac{k_1-\nu_1}{\sqrt{\nu_1}}I_0^1\left(\frac{r}{R},\frac{z}{R\sqrt{\nu_1}}\right) - \frac{1+k_1}{k_1-k_2}\frac{k_2-\nu_2}{\sqrt{\nu_2}}I_0^1\left(\frac{r}{R},\frac{z}{R\sqrt{\nu_2}}\right)\right], \quad (8)$$

$$I_m^n\left(\frac{r}{R},\frac{z}{R}\right) = \int_0^\infty t^n J_m\left(\frac{r}{R}t\right)J_1(t)\exp\left(-t\frac{z}{R}\right)dt, \qquad k_\alpha = \frac{C_{11}\nu_\alpha - C_{44}}{C_{13}+C_{44}} = \frac{\nu_\alpha\left(C_{13}+C_{44}\right)}{C_{33}-C_{44}\nu_\alpha}.$$

Here C_{11} and so on – crystal elastic moduli; $J_m(t)$ – Bessel function, ν_α ($\alpha = 1,2$) – roots of the quadratic equation $C_{44}C_{11}\nu^2 + \nu\left(C_{13}{}^2 + 2C_{44}C_{13} - C_{33}C_{11}\right) + C_{44}C_{33} = 0$. The boundary conditions for (7) are set on the inner and outer toroidal surfaces.

$$\psi(r,z) = 0 \quad \text{on} \quad \left(r^2+z^2+R^2-r_c^2\right)^2 = 4R^2r^2, \quad R - r_c \le r \le R + r_c, \quad (9)$$

$$\psi(r,z) = 1 \quad \text{on} \quad \left(r^2+z^2+R^2-R_{ext}{}^2\right)^2 = 4R^2r^2,$$

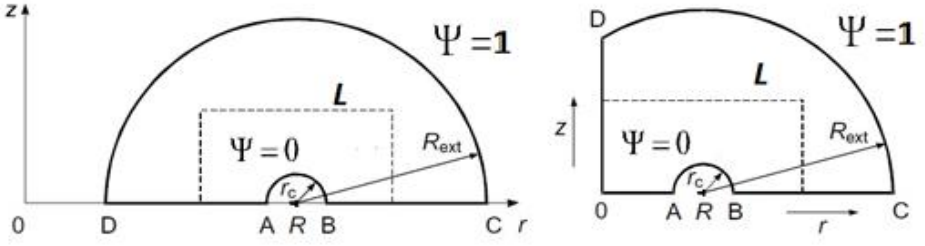
$$R - R_{ext} \le r \le R + R_{ext} \quad \text{for} \quad R > R_{ext}, \quad 0 \le r \le R + R_{ext} \quad \text{for} \quad R < R_{ext}.$$

They correspond to similar conditions for a straight dislocation (2). The desired absorption efficiency of the dislocation loop has the form:

$$\frac{J^D}{2\pi R\frac{D}{\omega}\left(\bar{C}-C^e\right)} = Z\left(r_c,R,R_{ext}\right) = \frac{1}{2\pi R}\iint_S \exp\left(-E_{\text{int}}^D(r,z)\right)\left[\vec{n}\ \vec{\nabla}\psi(r,z)\ \right]d\sigma, \quad (10)$$

Here J^D – full PD flow per loop; the integral is taken over an arbitrary surface containing a loop, $\vec{n}$ – its external normal.

The diffusion problem (7)–(10) was solved numerically by the finite difference method [7, 9]. Fig. 2 shows a cross section of a toroidal reservoir containing a loop, taking into account the reflection symmetry in the plane *z=0* and the symmetry about rotation around the axis "*oz*".



a *b*

Fig. 2. The coordinate system for the toroidal reservoir: a – $R > R_{ext}$ *; b –* $R < R_{ext}$

For $R > R_{ext}$ the diffusion field was calculated in the region bounded by the surfaces DA, AB, BC, CD, for $R < R_{ext}$ – by the surfaces OA, AB, BC, CD, DO. Above indicated symmetry imposes additional boundary conditions: $\partial\psi / \partial z = 0$ on DA, BC, OA, corresponding to zero flow through the plane $z = 0$, and $\partial\psi / \partial r = 0$ on DO (axis of symmetry) 0. Then the absorption efficiency of the PD was calculated using equation (10) α-type. Arbitrary inner surfase S in (10) was selected in the form of a rectangle of rotation in order to simplify calcculations. On Fig.2 it is line L. The calculations were performed for zirconium, the material parameters of which are given in the previous section.

3. RESULTS AND ITS DISCUSSION

Fig. 3 shows the dependence of the absorption efficiency of the TD dislocation loop α-type $Z_\alpha(R, R_{ext})$ ($\alpha = v, i$; v – vacancy, i – CIA) from it radius in units b (+ – vacancy loop петля, o – interstitial loop; $r_c = 3b$). To simplify the calculations, the radius of the cross section of the outer torus R_{ext} was set the same for vacancies and SIA, which corresponds to the approximation $k^2 \approx 1/\pi R_{ext}^2$. If dislocations are the dominant sink in the system, then the value $R_{ext} = 55b$ corresponds to the density of dislocations $\rho \approx 10^{11} cm^{-2}$ Fig. 3,a,b), and $R_{ext} = 125b$ – to the density of dislocations $\rho \approx 2 \cdot 10^{10} cm^{-2}$ Fig. 3,c,d). The numerical estimation of the bias factor of a straight dislocation is also simplified, since it is not necessary to solve the transcendental equation (4). Absorption efficiency $Z_{str,\alpha}(r_c, R_{ext})$ might be found just by substitution of R_{ext} to (4).

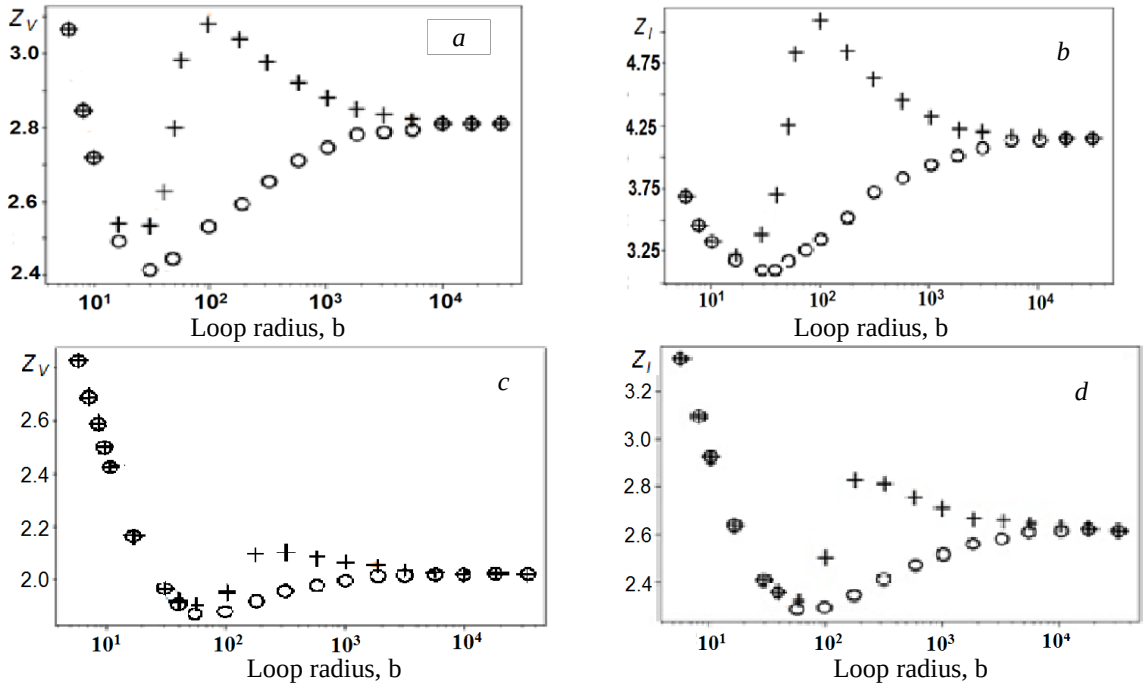


Fig. 3. Vacancy and interstitial absorption efficiency Z_v *(a), (b) and* Z_i *(c), (d) as lopp radius functions, calculated for* $R_{ext} = 55b$ *(a), (b) and* $R_{ext} = 125b$ *(c), (d) ('+' – vacancy loop, 'o' – interstitial loop)*

By definition bias looks like $B = 1 - Z_v / Z_i$. The result of the corresponding calculations is shown in Fig. 4. The dashed line corresponds to the bias factor of the straight dislocation at a given value R_{ext}.

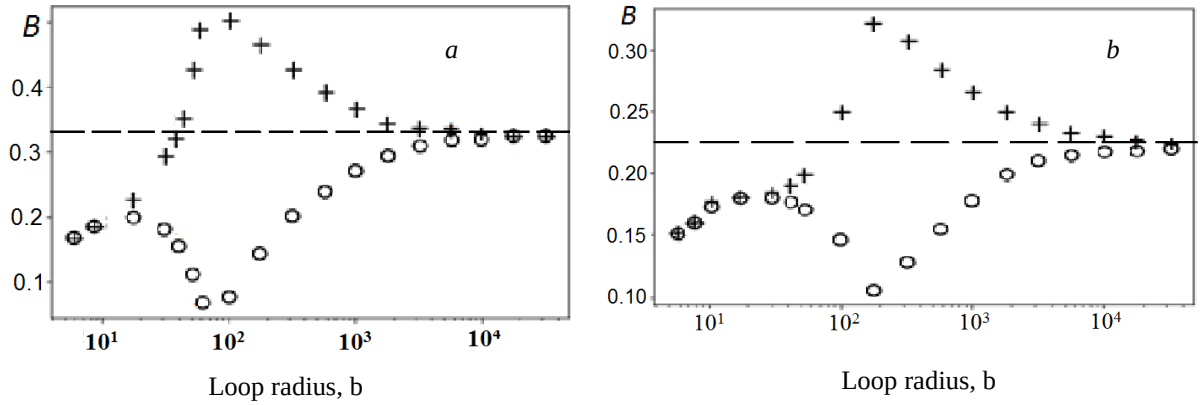


Fig. 4. Biases of vacancy and interstitial loops as functions of loops radiuses for $R_{ext} = 55b$ (a) and $R_{ext} = 125b$ (b). ('+' – interstitial loop, 'o'– interstitial loop)

In [7], the main results of studies were formulated, in which a similar problem was solved numerically, but in spherical or cylindrical reservoirs, as well as in the approximation of the elastic medium isotropy. Compare them with ours. First, it is noted that dislocation loops are biased sinks that more effectively absorb SIA than vacancies. This conclusion is also confirmed by our calculations, since *B>0* (see Fig. 4). Secondly, the absorption efficiency and the bias depend on the radius of the loop and the density of the sinks but do not depend on the nature of the loop (vacancy or interstitial). In [7], this conclusion remains valid for a toroidal reservoir. In our case, the dependence on the radius and density of the sinks remains, however, the nature of the loops becomes significant. From Figs.3, 4 one can see that radial dependencies of absorption efficiency of sort α PD $Z_\alpha(R, R_{ext})$ and bias $B(R, R_{ext})$ for interstitial loop with fixed external torus radius R_{ext} have minimum and asymptotics which correspond to straight dislocations. Last feature is typical only for toroid reservoir. Similar dependences for the vacancy loop show the presence of a maximum, it means that symmetry of PD absorption by loops of different nature is broken. This is the main result of the paper. Minimum and maximum positions are shifted in region of large loop radius while sink density increases and R_{ext} decreases correspondingly, their absolute values decrease as loop area of influence R_{ext} decrease. Numerical analysis of equations (7), (9), (10) has shown that taking into account of the elastic anisotropy of the crystal (8) for basic edge loops does not play an essential role. Another thing is more important, namely the boundary condition on the external toroidal surface. In our approach on the boundary between the sink influence region and the effective medium, the equality of PD chemical potentials is assumed. As a result we have one absorption efficiency and one flow per loop which are proportional to the difference ($\bar{C} - C^e$), and boundary condition (9) ($\psi = 1$), which does not depend on the loop type. In [7], as in some other works, the equality of PD concentrations is assumed ($C(\vec{r})|_{r=R_{ext}} = \bar{C}$).Then, as in the case of a straight dislocation, two efficiencies appear: absorption and emission, respectively, two flows, and the boundary condition for calculating the absorption flow takes the form $\psi = \bar{C}\exp(E(R_{ext}))$ depending on the loop type. As a result presence of symmetry between PD absorption by loops of different types. It is still impossible to give unequivocal answer to the question which approach is correct. It is encouraging that, in our version, the basic interstitial loops with the smallest biases might be considered as the main sinks for vacancies. Therefore, they have no chance of survival, which is observed experimentally. As for vacancy loops, their fate is ambiguous. Large loops cannot survive because of their larger biases compared to straight dislocations, but they are observed in experiments during crystal growth. Their "accumulation point" can be considered the size where However, if the average bias of the system as a whole is larger than of the straight dislocation, then the "accumulation point" can grow, which means that the size of surviving vacancy loops can increase.

It is shown that the form of the boundary condition on the outer surface of the toroidal reservoir, used in the paper, violates the "traditional" symmetry in the absorption of PD by loops of different nature and leaves no chance for the survival of interstitial base loops in zirconium. But it does not explain the existence of large basic vacancy loops. A source of vacancies in the basal plane is needed. Such may be the interstitial loops nucleating on prismatic planes during the radiation growth of zirconium. But this is a different task.

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ЧИСЛЕННЫЙ РАСЧЕТ ФАКТОРА ПРЕДПОЧТЕНИЯ БАЗИСНОЙ ДИСЛОКАЦИОННОЙ ПЕТЛИ В ГЕКСАГОНАЛЬНОМ КРИСТАЛЛЕ

А.В. Бабич, П.Н. Остапчук

Численно (методом конечных разностей) посчитаны диффузионные потоки радиационных точечных дефектов на круговую базисную краевую петлю циркония в тороидальном резервуаре с учетом их упругого взаимодействия и упругой анизотропии гексагонального кристалла. Тороидальная геометрия резервуара представляется более приемлемой для петли, чем сферическая или цилиндрическая, поскольку позволяет провести расчеты для петли любого размера и без какой-либо коррекции упругого поля в ее области влияния. Получены зависимости эффективностей захвата и «bias»-фактора петли от радиуса и ее природы. Показана существенная роль формы граничного условия на внешней поверхности резервуара в нарушении симметрии в поглощении ТД петлями разной природы.

ЧИСЕЛЬНИЙ РОЗРАХУНОК ФАКТОРА ПЕРЕВАГИ БАЗИСНОЇ ДИСЛОКАЦІЙНОЇ ПЕТЛІ В ГЕКСАГОНАЛЬНОМУ КРИСТАЛІ

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Чисельно (методом кінцевих різниць) пораховані дифузійні потоки радіаційних точкових дефектів на кругову базисну крайову петлю цирконію в тороїдальному резервуарі з урахуванням їх пружної взаємодії і пружної анізотропії гексагонального кристала. Тороїдальна геометрія резервуара є більш прийнятною для петлі, ніж сферична або циліндрична, оскільки дозволяє провести розрахунки для петлі будь-якого розміру і без будь-якої корекції пружного поля в її області впливу. Отримано залежності ефективностей захоплення і «bias»-фактора петлі від радіуса і її природи. Показана суттєва роль форми граничної умови на зовнішній поверхні резервуара в порушенні симетрії в поглинанні ТД петлями різної природи.