https://doi.org/10.46813/2023-147-009

ON THE POSSIBILITY OF COEXISTENCE OF DISLOCATION LOOPS OF DIFFERENT NATURE IN ZIRCONIA WITHIN THE FRAMEWORK OF CLASSICAL ELASTIC THEORY

O.G. Trotsenko, A.V. Babich, P.M. Ostapchuk
Institute of Electrophysics and Radiation Technologies of the NAS of Ukraine, Kharkiv, Ukraine
E-mail: ostapchuk@kipt.kharkov.ua

A distinctive feature of the radiation-induced microstructure of zirconium is, firstly, the coexistence of prismatic loops of different natures, and secondly, the nucleation and growth to large sizes of vacancy basis loops. In the work, within the framework of classical concepts of elastic interaction between a point defect and internal sink the results of numerical calculations of the dependence of bias loops of different natures lying in the basal and prismatic planes of zirconium on their radius are presented. The essential role of the form of the boundary condition on the outer surface of loop area of influence in toroidal geometry is shown. Possibilities, both the coexistence of prismatic loops of different natures and the growth of vacancy basis loops are discussed.

PACS: 62.20Dc;62.20.Fc

INTRODUCTION

In a given microstructure, absorption efficiency of a sink for a given mobile defect quantifies the effect of interaction energy (usually elastic energy) between the sink and the defect on the absorption rate of the defect. It has been recognized that some phenomena occurring under irradiation, such as void swelling [1] or irradiation creep [2], could be rationalized in terms of absorption efficiencies of the different sinks present in the microstructure. More precisely, the relative difference between the absorption efficiencies of interstitials and vacancies, known as the bias, plays a key role in understanding these radiation induced phenomena. Therefore, it was natural to apply the standard elastic ideology (EID – elastic interaction difference) to qualitatively describe another phenomenon – radiation growth (RG) of zirconium and its alloys [3, 4]. Irradiation growth is the volume conserved shape deformation of crystalline materials when subjected to particle irradiation. It has been found that zirconium during growth expands in the $\langle a \rangle$-direction and shrinks along the $\langle c \rangle$-axis. Such its behavior is associated with the idea of Buckley S.N. [5, 6] that interstitial loops are formed predominantly on the prismatic planes of zirconium and vacancy loops on the basic. Although the physics of the RG mechanism has changed over the years, Buckley's general concept has remained the same: vacancy loops nucleating and growing on the base planes "eating" the crystal along the $\langle c \rangle$-axis, while growing interstitial loops, forming additional extra planes in the $\langle a \rangle$-direction, increase its size.

The main difference between the radiation-induced microstructure of zirconium and other hcp metals is, firstly, the coexistence of prismatic loops (Burgers vector $b = 1/3\langle 11\bar{2}0 \rangle$) of different kind, and , secondly, nucleation and growth to large sizes of vacancy basis loops (Burgers vector $b = 1/2[0001]$) [4, 7]. The latter possibly confirms Buckley's concept. Frequently quoted version of the cause of RG of zirconium is anisotropic diffusion of radiation point defects (PD) between its planes (DAD theory – diffusional anisotropy difference) [4, 8]. However, as the authors themselves note, it cannot explain the fact of the coexistence of vacancy and interstitial loops. As for the basal loops, DAD theory provides only a fundamental possibility separating PD flows between straight dislocations lying in the basal and prismatic planes of zirconium. And only under a certain condition on the PD diffusion coefficients in $\langle a \rangle$- and $\langle c \rangle$-directions. However, there is no experimental confirmation of this condition. And, as numerical calculations show, it is precisely not true in the region of reactor temperatures [9]. Therefore, a physical cause of RG associated only with anisotropic diffusion of radiation PD seems poorly substantiated.

The goal of this work is to analyze, within the framework of classical elastic theory (EID), both possibilities, both the coexistence of prismatic loops of different natures and the growth of vacancy basis loops.

1. MAIN ELEMENTS OF THE EID – THEORY

1.1. ELASTIC INTERACTION ENERGY

Main element of EID – theory ($D_{ij} = D\delta_{ij}$) is the expression for interaction energy between a PD and source of the inner deformation field $u_{ij}(\boldsymbol{r})$. For PD of the dipole type it has the following form:

$$E(\boldsymbol{r}) = -P_{ij}u_{ij}(\boldsymbol{r})\,; \qquad P_{ij} = P_{ji}\,. \qquad (1)$$

If the elastic dipole has an axis of symmetry which coincides with $\langle c \rangle$-axis of hpc crystal, then tensor P_{ij} has only diagonal components, which in the abbreviated description can be written as $P_i = P(1,1,\varepsilon)$, $P = P_a$, $\varepsilon = P_c/P_a$. Here P_c and P_a – strength of the force-dipoles in $\langle c \rangle$ - and $\langle a \rangle$ -directions. Note that in crystal with non-cubic symmetry quantities P_a and P_c do not have a simple physical meaning. Therefore, in papers [10, 11], by analogy with $P_i=P(1,1,\varepsilon)$, displacement dipoles $Q_i=Q(1,1,\delta)$, $Q = Q_a$, $\delta = Q_c/Q_a$ were introduced. They are connected with force-dipoles by relation $P_i=C_{ij}Q_j$. Here C_{ij} is the crystal elastic moduli. It was assumed that the change in the volume ΔV of the finite crystal caused by a PD is related to the displacement dipoles by the relation $\Delta V = Q\,(2+\delta)$. As a result:

$$P = \Delta V \frac{C_{11}+C_{12}+\delta(\varepsilon)C_{13}}{2+\delta(\varepsilon)};$$

$$\delta(\varepsilon) = \frac{\varepsilon(C_{11}+C_{12})-2C_{13}}{C_{33}-\varepsilon C_{13}}. \qquad (2)$$

In case of dilatation center (ε=1) for hexagonal crystal:

$$E(\boldsymbol{r}) = -\Delta V \frac{2C_{13}{}^2-(C_{11}+C_{12})C_{33}}{4C_{13}-2C_{33}-(C_{11}+C_{12})} Spu_{i\,j}(\boldsymbol{r}) \equiv$$

$$\equiv -P^{hex} Spu_{i\,j}(\boldsymbol{r}). \qquad (3)$$

In the approximation of an elastically isotropic medium $C_{11}=C_{22}=C_{33}=\lambda+2\mu$; $C_{12}=C_{13}=\lambda$ so that

$$E(\boldsymbol{r}) = -\frac{\Delta V}{3}\, 2\mu \frac{1+\nu}{1-2\nu} Spu_{i\,j}(\boldsymbol{r}) \equiv -P^{is} Spu_{i\,j}(\boldsymbol{r}). \qquad (4)$$

Here $\nu = 0.33$ is the Poisson ratio; $\mu = 33\,\text{GPa}$ is the matrix shear modulus. Experimental values of the elastic moduli of zirconium according to [12] ($\text{Mbar} = 10^{11}\,\text{J/m}^3$): C_{11} = 1.154; C_{12} = 0.672; C_{13} = 0.646; C_{33} = 1.725; C_{44} = C_{55} = 0.363. Other values: $\Delta V_i = 1.2\omega$, $\Delta V_v = -0.6\omega$ are the interstitial and vacancy relaxation volume, $\omega = 2.36\cdot 10^{-29}\,\text{m}^3$ is the atomic volume of the lattice. So that in dimensionless variables

$$P_i^{hex}/k_BT = 348.1,\quad P_i^{is}/k_BT = 308.2,$$

$$P_v^{hex}/k_BT = -174.05,\quad P_v^{is}/k_BT = -154.1,\quad T = 573\,\text{K}.$$

As can be seen, the difference in the absolute values of the coefficients is not large.

In the approximation of an elastically isotropic medium equation (4) for circular edge vacancy loop of radius R in cylindrical coordinates (r,z) in units k_BT looks like [13]:

$$E(r,z) = -\frac{P^{is}}{k_BT}\frac{1-2\nu}{1-\nu}\frac{b}{2R} I_0^1\left(\frac{r}{R},\frac{z}{R}\right); \qquad I_m^n\left(\frac{r}{R},\frac{z}{R}\right) = \int_0^\infty t^n J_m\left(\frac{r}{R}t\right) J_1(t)\exp\left(-t\frac{z}{R}\right)dt. \qquad (5)$$

For the same loop in the basal plane of zirconium equation (4) has following form:

$$E(r,z) = -\frac{P^{hex}}{k_BT}\frac{b}{2R}\left[\frac{1+k_2}{k_1-k_2}\frac{k_1-\nu_1}{\sqrt{\nu_1}} I_0^1\left(\frac{r}{R},\frac{z}{R\sqrt{\nu_1}}\right) - \frac{1+k_1}{k_1-k_2}\frac{k_2-\nu_2}{\sqrt{\nu_2}} I_0^1\left(\frac{r}{R},\frac{z}{R\sqrt{\nu_2}}\right)\right]. \qquad (6)$$

Here $k_\alpha = \dfrac{C_{11}\nu_\alpha - C_{44}}{C_{13}+C_{44}} = \dfrac{\nu_\alpha\left(C_{13}+C_{44}\right)}{C_{33}-C_{44}\nu_\alpha}$; $J_m(t)$ – Bessel function; ν_α ($\alpha = 1,2$) – roots of the quadratic equation $C_{44}C_{11}\nu^2 + \nu\left(C_{13}{}^2 + 2C_{44}C_{13} - C_{33}C_{11}\right) + C_{44}C_{33} = 0$; $b = 3.23\cdot 10^{-10}\,m$ – magnitude of the Burgers vector of loop. Instead of I_0^1 its expression in terms of complete elliptic integrals of the first and second kind $K(k)$, $E(k)$ is often used:

$$I_0^1(r,z) = \frac{1}{\pi}\frac{R}{\sqrt{(R+r)^2+z^2}}\left[\frac{R^2-r^2-z^2}{(R-r)^2+z^2}E(k)+K(k)\right]; \qquad k^2 = \frac{4Rr}{(R+r)^2+z^2}. \qquad (7)$$

Then the radius of the loop in (5), (6) is reduced, and the transition to dimensionless variables $r \to r/b$; $z \to z/b$; $R \to R/b$ allows one to reduce parameter b. Note that there is no angular dependence here due to symmetry with respect to rotation around z-axis, perpendicular to the loop plane. It should also be noted, that formulas (5), (6) were obtained by solving the equilibrium equations of an elastic medium in terms of displacements [14, 15]. But their analogues can also be obtained in the formalism of Green's functions [16]. It should be remembered that (r,z) – these are the coordinates of the observation point.

For prismatic a-loop in zirconium the situation is different. The axial symmetry in this case is absent so well-developed methods for solving equilibrium equations are not applicable. But the Green's function formalism remains applicable [17]:

$$E(\boldsymbol{r}) = \frac{P^{hex}}{k_BT}\frac{b}{4\pi}\left\{\int_{S_D}\frac{d^2r'}{\left|\boldsymbol{r}-\boldsymbol{r}'\right|^3}Q(\tau_3^2) + (C_{11}-C_{12})\int_{S_D}\frac{d^2r'}{\left|\boldsymbol{r}-\boldsymbol{r}'\right|^3}\tau_1^2\left[3Y(\tau_3^2)+2\tau_3^2\frac{dY}{d\tau_3^2}\right]\right\}; \qquad (8)$$

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

$$\Psi(\tau_3^2) = V(\tau_3^2)+W(\tau_3^2);\quad Y(\tau_3^2) = \mathrm{K}(\tau_3^2)+V(\tau_3^2);\quad \tau_1 = x/\left|\boldsymbol{r}-\boldsymbol{r}'\right|;\quad \tau_3 = (z-z')/\left|\boldsymbol{r}-\boldsymbol{r}'\right|.$$

The functions $K(\tau_3^2)$, $W(\tau_3^2)$, $V(\tau_3^2)$ are quite complicated. Their explicit expressions are given in [16]. All dependence on τ_3^2 is in the first integral (8), and additional terms associated with the contribution of τ_1^2 are in the second integral. Recall that the vacancy a-loop is in the "yz" plane of Cartesian coordinate system. Its normal coincides with the positive direction of the "x"-axis. The integration in (8) is carried out over the area of the loop, therefore $x'=0$. There is a dependence on the azimuthal angle in the loop plane here, in contrast to (5), (6). In Fig. 1 in dimensionless cylindrical coordinates $z=r\sin\varphi$; $z'=r'\sin\varphi'$; $y=r\cos\varphi$; $y'=r'\cos\varphi'$; $|\mathbf{r}-\mathbf{r}'|^2=x^2+r^2-2rr'\cos(\varphi-\varphi')+r'^2$ the radial dependence of the interaction energy of the vacancy prismatic loop (8) with the SIA ($P_i^{hex}/k_BT=348.1$) is shown for four values of the angle φ.

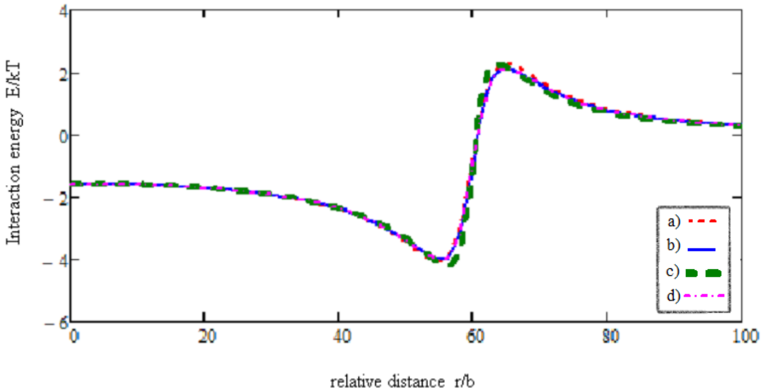


Fig. 1. The radial dependence of the interaction energy of the vacancy prismatic loop (8) with the SIA for different values of the angle φ: a – $\varphi=0$; b – $\varphi=\pi/4$; c – $\varphi=\pi/2$; d – $\varphi=3\pi/4$; $R=60b$ and $x=5b$

We note a very weak dependence on the azimuth angle φ, which does not change the nature of the interaction (sign) in each region. The interaction changes sign only when passing from the inner region of the loop ($r<60b$) to the outer one ($r>60b$). However, this dependence greatly complicates numerical calculations. Therefore, we will eliminate it by averaging the right side of (8) over the angle φ, making the problem isotropic in the "yz" plane [19]. In the expression (8), the dependence on the variable "x" is quadratic, i.e. replacement $x\to -x$ doesn't change anything. Therefore, as in the case of the basic loop, numerical calculations can be carried out only in one part of the half-space.

1.2. DIFFUSION PROBLEM

Having the interaction energy, the corresponding diffusion problem is then solved – the diffusion equation in a quasi-stationary approximation with boundary conditions on the inner and outer surfaces of the loop influence region. Following [18] we accept the toroidal geometry of the area of influence. Toroidal geometry seems more suitable for a loop than spherical or cylindrical one, because it allows one to perform the calculations for a loop of any size and without any correction of the elastic field in its area of influence. Since the angular dependence in (5), (6), and after averaging in (8) is absent, in terms of a variable $\psi(r,\xi)=C(r,\xi)\exp E/\bar{C}$ the diffusion problem in the cross section of coaxial toroids in the area of influence of the loop in dimensionless cylindrical coordinates has the form:

$$\frac{\partial^2\psi}{\partial r^2}+\frac{\partial^2\psi}{\partial\xi^2}+\left(\frac{1}{r}-\frac{\partial E}{\partial r}\right)\frac{\partial\psi}{\partial r}-\frac{\partial E}{\partial\xi}\frac{\partial\psi}{\partial\xi}=0. \qquad (9)$$

Coordinate "ξ" coincides with "z", if loop is in "xy" plane (formulas (5), (6)), and with "x" in case (8); coordinate r is a radial coordinate of the observation point in the loop plane. For us, only absorption of PD is important, so on the inner toroidal surface S_C that contains a dislocation line (r_c is the dislocation core radius) we use conventional boundary condition $C\exp E(\mathbf{r})|_{Sc}=C^e=0$:

$$\psi(r,\xi)=0;\ \left(r^2+\xi^2+R^2-r_c^{\,2}\right)^2=4R^2r^2;$$
$$R-r_c\le r\le R+r_c. \qquad (10)$$

On the outer toroidal surface (R_{ext} – radius of the generatrix of the coaxial outer torus that corresponds to the radius of the loop influence region) two cases are possible

$$\psi(r,\xi)=\exp E(r,\xi);\ \text{and}\ \psi(r,\xi)=1;$$
$$\left(r^2+\xi^2+R^2-R_{ext}^{\,2}\right)^2=4R^2r^2; \qquad (11)$$
$$R-R_{ext}\le r\le R+R_{ext}\ \text{for}\ R>R_{ext};$$
$$0\le r\le R+R_{ext}\ \text{for}\ R<R_{ext}.$$

First one corresponds to the boundary condition in the form $C(\mathbf{r})|_{S_{ext}}=\bar{C}$, where $\bar{C}$ is the average PD concentration in an effective medium that simulates the influence of all sinks. Second one corresponds to $C\exp E(\mathbf{r})|_{S_{ext}}=\bar{C}$. The sink bias is determined by a relation of the form $B=1-Z_v/Z_i$. Here subscripts v and i correspond to vacancies and SIA respectively. If *B>0*, one says that the loop has a preference to SIA. The dimensionless quantity $Z_{v,i}$ is called the absorption efficiency of the PD by the sink. It is the result of the diffusion problem (9)-(11) solution and looks like:

$$Z(r_c, R, R_{ext}) = \frac{1}{2\pi R} \iint\limits_S \exp(-E(r,\xi))[\boldsymbol{n} \nabla \psi(r,\xi)]\, d\sigma . \quad (12)$$

The integral is taken over an arbitrary surface S with the outer normal $\boldsymbol{n}$ containing the dislocation line. The cross section of this surface is shown in Figure in the form of a line L (Appendix).

2. RESULTS

The diffusion problem (9)–(11) was solved numerically by the finite difference method. Dependence of the loop bias of different nature on their radius for the first version of the boundary condition (11) $\Psi|_{Sext} = \exp E(\boldsymbol{r})|_{Sext}$ and for two values of R_{ext} one can see on Fig. 2. The lower curves (green and yellow) correspond to the isotropic approximation (5); the upper curves (red and blue) correspond to the basal loops of zirconium. The solid horizontal line corresponds to a straight dislocation.

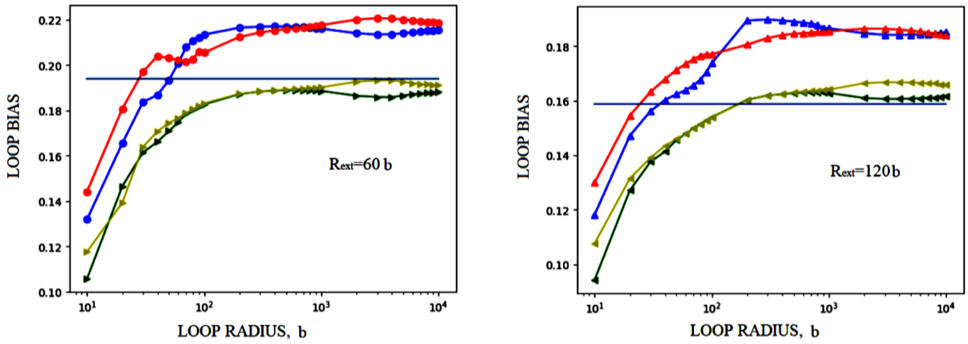


Fig. 2. Dependence of the loop bias of different nature on their radius for the first version of the boundary condition (11) $\Psi|_{Sext} = \exp E(\boldsymbol{r})|_{Sext}$ for two values of R_{ext}

On Fig. 3 similar dependence of loop bias for loops of different natures, but for the second version of the boundary condition (11) $\Psi|_{Sext} = 1$ is illustrated. The colors are the same. Green and yellow correspond to the isotropic approximation (5), red and blue correspond to the basis loops of zirconium.

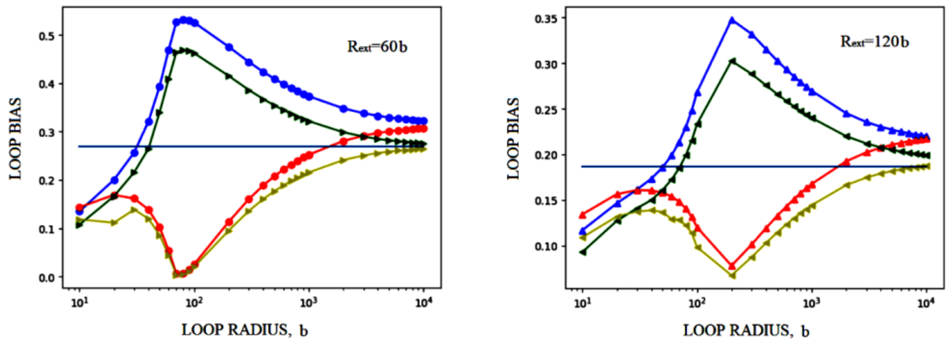


Fig. 3. Dependence of the loop bias of different nature on their radius for the second version of the boundary condition (11) $\Psi|_{Sext} = 1$ for two values of R_{ext}

Fig. 4 shows the bias dependence of prismatic loops ($\{11\bar{2}0\}$ occurrence plane) of different nature on their radius for the first version of the boundary condition (11) $\Psi|_{Sext} = \exp E(\boldsymbol{r})|_{Sext}$ and for two values of R_{ext}. The red curve corresponds to the interstitial loop, the blue curve corresponds to the vacancy loop. The solid horizontal line, as before (see Fig. 2), corresponds to a straight dislocation.

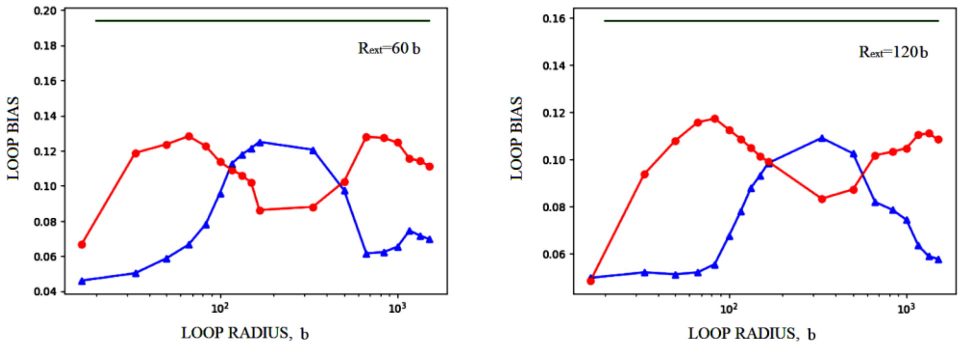


Fig. 4. Dependence of the loop bias of different nature on their radius for the first version of the boundary condition (11) $\Psi|_{Sext} = \exp E(\boldsymbol{r})|_{Sext}$ for two values of R_{ext}

On Fig. 5 similar dependence of bias *призматических* петель of different natures, but for the second version of the boundary condition (11) $\Psi|_{Sext}=1$ is illustrated. The colors are the same.

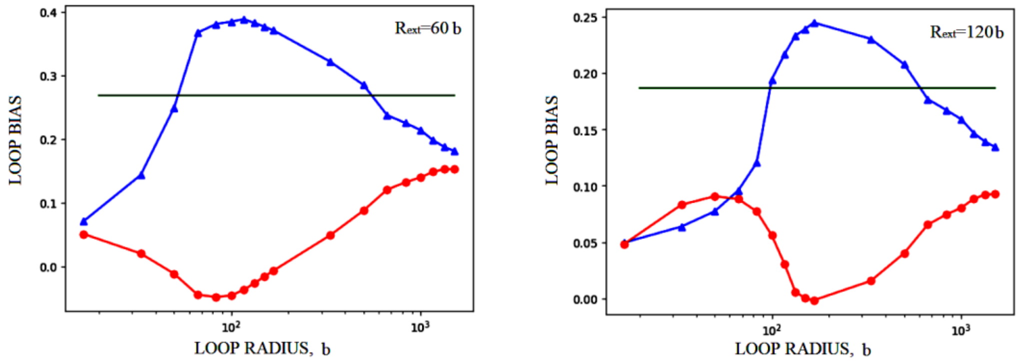


Fig. 5. Dependence of the loop bias of different nature on their radius for the second version of the boundary condition (11) $\Psi|_{Sext}=1$ for two values of R_{ext}

From the results obtained it follows that all loops in zirconia are biased sinks, which absorb SIAs more efficiently than vacancies, since for all $B>0$. In the case of basic loops (see Figs. 2, 3) the role of anisotropy is qualitatively insignificant. The displacement of pairs of curves (red-blue, green-yellow) is associated with the use of a modified coefficient in (6) P^{hex} instead of $P^{is}(1-2\nu)/(1-\nu)$, as in (5). The important fact is that the type of boundary condition on the outer surface of the area of influence of the loop significantly changes the dependence of bias loops on their nature. When $\Psi|_{Sext}=\exp E(\boldsymbol{r})|_{Sext}$ bias does not depend on the nature of the loop [17], for $\Psi|_{Sext}=1$ this is wrong (see Fig. 3). For prismatic loops in case $\Psi|_{Sext}=\exp E(\boldsymbol{r})|_{Sext}$ situation is different (see Fig. 4): bias has a non-monotonic behavior with increasing loop radius and depends on the type of loop; for $\Psi|_{Sext}=1$ nothing changes qualitatively.

SUMMARY

From the point of view of the possibility of coexistence of prismatic loops of different natures, it looks preferable Fig. 4. Bias interstitial loop (red curve) more than vacancy one (blue curve). It absorbs more efficiently SIAs and growth, excess vacancies go to the vacancy loop. However, as one can see Fig. 4, this is only true up to the point of intersection of the curves, which corresponds to $R\simeq 30$ nm for $R_{ext}=60b$ ($\rho_d \approx 8.4\cdot 10^{10}$ cm^{-2}) and $R\simeq 40$ nm for $R_{ext}=120b$ ($\rho_d \approx 2\cdot 10^{10}$ cm^{-2}). Further growth is not possible, since the vacancy loop begins to absorb SIAs more efficiently. It is not clear what causes this non-monotonic behavior of bias. Boundary condition $\Psi|_{Sext}=1$ (see Fig. 5) practically eliminates the possibility of coexistence of prismatic loops of different natures.

Growth of basic vacancy loops, regardless of the type of boundary condition on R_{ext}, is possible only if there is a source of vacancies. It, in case $\Psi|_{Sext}=\exp E(\boldsymbol{r})|_{Sext}$, gives an advantage for survival to vacancy loops of any size (fig.2), and also facilitates to the nucleation and growth of small vacancy loops in the case $\Psi|_{Sext}=1$ (fig.3). Such a source can be straight dislocations and edge elements of the dislocation network, the bias of which is shown by a solid horizontal line.

REFERENCES

1. R. Bullough, R.C. Perrin. The Mechanism and Kinetics of Void Growth During Neutron Irradiation // *ASTM STP*. 484, 1970, p. 317-331.
2. L.K. Mansur // *Philos. Mag. A*. 1979, v. 39, p. 497.
3. M. Griffiths. A review of microstructure evolution in zirconium alloys during irradiation // *J. Nucl. Mater*. 1988, v. 159, p. 190.
4. C.H. Woo. Defect accumulation behaviour in hcp metals and alloys // *J. Nucl. Mater*. 2000, v. 276, p. 90.
5. S.N. Buckley. *Irradiation Growth*. Atomic Energy Research Establishment, Harwell, England, AERE R 3674, 1962.
6. S.N. Buckley. *Irradiation Growth in Uranium*. Atomic Energy Research Establishment, Harwell, England, AERE R 5262, 1966.
7. Sang Il Choi and Ji Hyun Kim. Radiation-induced dislocation and growth behavior of zirconium and zirconium alloys – a review // *Nuclear Engineering and Technology*. 2013, v. 45, N 3, p. 385.
8. C.H. Woo, U. Gosele. Dislocation Bias in an Anisotropic Diffusive Medium and Irradiation Growth // *J. Nucl. Mater*. 1983, v.119, p. 279-228.
9. G.D. Samolyuk, A.V. Barashev, S.I. Golubov, Y.N. Osetsky, R.E. Stoller. Analysis of the anisotropy of point defect diffusion in hcp Zr // *Acta Materialia*. 2014, v. 78, p. 173.
10. E. Kröner // *Zeitschrift fur Phyzik*. 1953, v. 136, p. 402.
11. M.H. Yoo // *Phys. Stat. Sol. (b)*. 1974, v. 61, p. 411.
12. L. Fast, J.M. Wills, B. Johansson, O. Eriksson // *Phys. Rev. B*. 1995, v. 51, p. 17431.
13. F. Kroupa. Circular edge dislocation loop // *Czech. J. Phys. B*. 1960, v. 10, p. 284.

14. H.A. Elliott // *Proc. Cambridge Phil. Soc*. 1948, v. 44, p. 522.

15. H.A. Elliott // *Proc. Cambridge Phil. Soc*. 1949, v. 45, p. 621.

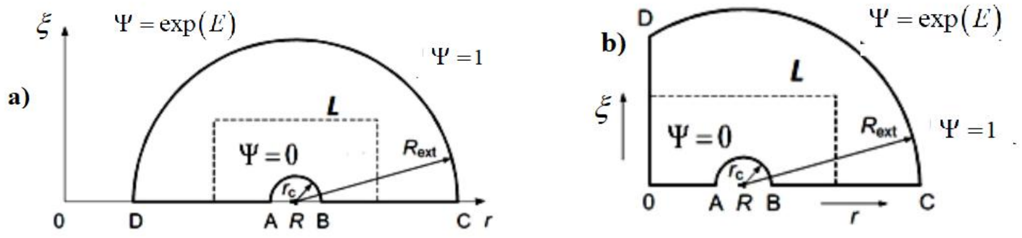
16. O.G. Trotsenko, P.N. Ostapchuk . The methods for the calculation of the elastic interaction of point defects with a dislocation loops in hexagonal crystals // *Problems of Atomic Science and Technology. Series "Physics of Radiation Effect and Radiation Materials Science"*. 2017, N 2(108), p. 83-90.

17. O.G. Trotsenko, A.V. Babich, P.M. Ostapchuk Bias for prismatic dislocation loops in zirconium. Numerical analysis *// Problems of atomic science and technology. Series "Physics of Radiation Effect and Radiation Materials Science"*. 2023, N 2(144), p. 3-7.

18. V.I. Dubinko, A.S. Abyzov, A.A. Turkin. Numerical Evaluation of the Dislocation Loop Bias // *J. Nucl. Mater*. 2005, v. 336, p. 11-21.

19. A.V. Babich, P.N. Ostapchuk. Bias of basal dislocation loop in zirconium // *Problems of atomic science and technology. Series "Physics of Radiation Effect and Radiation Materials Science"*. 2021, N 2(132), p. 29-34.

APPENDIX



a *b*

Coordinate system for a toroidal reservoir: a – $R>R_{ext}$; b – $R<R_{ext}$

For radius $R > R_{ext}$ 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, taking into account the reflection symmetry in the plane $\xi = 0$ and symmetry (after averaging over φ) about rotation around the ξ-axis. The specified symmetry imposes additional boundary conditions: $\partial\psi / \partial\xi = 0$ on DA, BC, OA, corresponding to zero flux through the plane $\xi = 0$, and $\partial\psi / \partial r = 0$ on DO (axis of symmetry). An arbitrary inner surface S in (12) is chosen for the convenience of calculations in the form of a rectangle of rotation. In Figure this is the contour L.

Article received 04.09.2023

ПРО МОЖЛИВІСТЬ СПІВІСНУВАННЯ ДИСЛОКАЦІЙНИХ ПЕТЕЛЬ РІЗНОЇ ПРИРОДИ В ЦИРКОНІЇ У РАМКАХ КЛАСИЧНОЇ ПРУЖНОЇ ТЕОРІЇ

О.Г. Троценко, А.В. Бабіч, П.М. Остапчук

Відмінною рисою радіаційно-індукованої мікроструктури цирконію є, по-перше, співіснування призматичних петель різної природи, а по-друге, зародження та зростання до великих розмірів вакансійних базисних петель. У роботі у рамках класичних уявлень про пружну взаємодію між точковим дефектом та внутрішнім стоком наведено результати чисельних розрахунків залежності фактору переваги петель різної природи, що лежать у базисній та призматичній площинах цирконію, від їхнього радіусу. Показано істотну роль форми граничної умови на зовнішній поверхні області впливу петлі у тороідальній геометрії. Обговорюються можливості як співіснування призматичних петель різної природи, так і ріст вакансій них базисних петель.