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$\langle a \rangle$ COMPONENT RADIATION-INDUCED DISLOCATION LOOPS OF DIFFERENT NATURE IN ZIRCONIUM

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A distinctive feature of the microstructure of zirconium under irradiation (electron or neutron) is the coexistence of prismatic loops of different natures. It is believed that classical elastic theory cannot explain this fact. But the theory of anisotropic diffusion is also unable to do this. Note that the conclusion of EID-theory (elastic interaction difference) is based on elastic isotropy. In our calculations in the Green's function formalism, we take into account the specific plane of the loop. It is analyzed whether a loop with a given Bürgers vector can nucleate and grow to visible sizes in a specific plane of zirconium.

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INTRODUCTION

It is well known that zirconium and its alloys submitted to neutron irradiation are subject to irradiation growth, that-is-to-say an anisotropic strain without volume change and without any external stress. From the experimental point of view, irradiation growth (RG) of zirconium and its alloys was extensively studied in the past (see for example [1]). 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. [2, 3] that interstitial loops are formed predominantly on the prismatic planes and vacancy loops on the basic. Although many models based on different mechanisms for irradiation growth have been proposed [4–8], 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. According [9] dislocation loops that form in zirconium under irradiation (electron or neutron) can be classified into two types according to their Bürgers vector. The basal loops or c-loops: they are lying in the (0 0 0 1) plane and their Bürgers vector has a component along the $\langle c \rangle$-axis. These loops are almost always vacancy type. They can be perfect loops ($\vec{\mathrm{b}} = \langle 0\,0\,0\,1 \rangle$) or imperfect loops ($\vec{\mathrm{b}} = 1/2\langle 0\,0\,0\,1 \rangle$). The prismatic loops or a-loops: they have a $\vec{\mathrm{b}} = 1/3\langle 1\,1\,\bar{2}\,0 \rangle$ Bürgers vector (parallel to the $\langle a \rangle$-axis of the lattice structure). They are lying approximately in the prismatic planes $(10\bar{1}0)$. In certain situations, both vacancy and interstitial loops can coexist. During neutron irradiation a-loops form first, c-loops formation is observed only above a certain fluence that depends on solute concentrations and temperature. It has been shown that the 'breakaway growth' of zirconium alloys under neutron irradiation correlates with the appearance of vacancy c-loops that act as vacancy sinks. The latter possibly confirms Buckley's concept. Let us pay attention to the words "*approximately* in the prismatic planes $(10\bar{1}0)$". But it could be prismatic plane $(11\bar{2}0)$. Perhaps they are simply poorly distinguishable. In paper [10] this plane is also is taken in to account: "growth is usually positive along directions normal to a preponderance of $(11\bar{2}0)$ and $(10\bar{1}0)$ planes". So following problem naturally appears: within the framework of classical elastic theory (EID) to calculate bias of a-loops having $\vec{\mathrm{b}} = 1/3\langle 1\,1\,\bar{2}\,0 \rangle$ Bürgers vector and lying in the prismatic plane $(10\bar{1}0)$; to compare it with calculated before for prismatic plane $(11\bar{2}0)$ [11] and analyze the possibility of loop coexistence of different natures in these planes. In addition, in [12] when irradiating samples of pipes made of zirconium alloys E110, E110M, E125 zirconium ions to damaging doses 20…50 dpa (accelerator simulation experiments) the authors talk about a-loops having $\vec{\mathrm{b}} = \langle 1\,1\,\bar{2}\,0 \rangle$ Bürgers vector. Therefore, in this work, for comparison, similar numerical calculations of bias is done for the same loops. The fundamental possibility of the nucleation and growth of prismatic loops of different nature on $(11\bar{2}0)$ and $(10\bar{1}0)$ planes is analized.

ELASTIC INTERACTION ENERGY

Main element of EID-theory ($D_{i\,j} = D\delta_{i\,j}$) is the expression for interaction energy between a point defect (PD) and source of the inner deformation field $u_{i\,j}(\boldsymbol{r})$. In case of dilatation center (ε=1) for hexagonal crystal [11]:

$$E(\boldsymbol{r}) = -\Delta V \frac{2C_{13}{}^2 - (C_{11} + C_{12})C_{33}}{4C_{13} - 2C_{33} - (C_{11} + C_{12})} Spu_{i\,j}(\boldsymbol{r}) \equiv -P\, Spu_{i\,j}(\boldsymbol{r}). \quad (1)$$

Experimental values of the elastic moduli of zirconium according to [13] ($\mathrm{Mbar} = 10^{11}\,\mathrm{J/m^3}$):

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, $\omega = 2.36 \cdot 10^{-29}\,\mathrm{m}^3$ is the atomic volume of the lattice. So that in dimensionless variables $P_i / k_B T = 348.1$, $P_v / k_B T = -174.05$, $T = 573\mathrm{K}$.

For prismatic a-loop in zirconium in the Green's function formalism we have:

$$\vec{b} = a/3\left\langle 11\bar{2}0\right\rangle = a\sqrt{3}/6\,\vec{e}_{\langle 10\bar{1}0\rangle} + a/6\,\vec{e}_{\langle\bar{1}2\bar{1}0\rangle};\quad E = E^{(10\bar{1}0)}_{\langle 10\bar{1}0\rangle} + E^{(10\bar{1}0)}_{\langle\bar{1}2\bar{1}0\rangle}\;;\quad a = 0.323\,\mathrm{nm}; \tag{2}$$

$$E^{(10\bar{1}0)}_{\langle 10\bar{1}0\rangle}(\boldsymbol{r}) = \frac{\sqrt{3}}{24\pi}\frac{P}{k_B T}\left\{\int\limits_{S_D}\frac{d^2 r'}{|\boldsymbol{r}-\boldsymbol{r}'|^3}Q(\tau_3^2) + (C_{11}-C_{12})\int\limits_{S_D}\frac{d^2 r'}{|\boldsymbol{r}-\boldsymbol{r}'|^3}\tau_1^2\left[3Y(\tau_3^2) + 2\tau_3^2\frac{dY}{d\tau_3^2}\right]\right\}; \tag{3}$$

$$E^{(10\bar{1}0)}_{\langle\bar{1}2\bar{1}0\rangle}(\boldsymbol{r}) = \frac{1}{24\pi}\frac{P}{k_B T}(C_{11}-C_{12})\int\limits_{S_D}\left[\frac{\tau_1\tau_2\, d^2 r'}{|\boldsymbol{r}-\boldsymbol{r}'|^3}\left\{2\tau_3^2\frac{\partial Y\left(\tau_3^2\right)}{\partial\tau_3^2} + 3Y\left(\tau_3^2\right)\right\}\right];\quad r = r/a;$$

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

$$\Psi(\tau_3^2) = V(\tau_3^2) + W(\tau_3^2);\quad Y(\tau_3^2) = \mathrm{K}(\tau_3^2) + V(\tau_3^2);\quad \tau_1 = x/|\boldsymbol{r}-\boldsymbol{r}'|;\quad \tau_2 = (y-y')/|\boldsymbol{r}-\boldsymbol{r}'|;\ \tau_3 = (z-z')/|\boldsymbol{r}-\boldsymbol{r}'|.$$

The functions $\mathrm{K}(\tau_3^2)$, $W(\tau_3^2)$, $V(\tau_3^2)$ are quite complicated. Their explicit expressions are given in [14]. Here formula (2) is the expantion of Bürgers vector on normal $\vec{e}_{\langle 10\bar{1}0\rangle}$ and tangential $\vec{e}_{\langle\bar{1}2\bar{1}0\rangle}$ components. Accordingly E in (2) – is the energy of elastic interaction of PD with a loop in the prismatic plane $(10\bar{1}0)$ having $\vec{\mathrm{b}} = 1/3\left\langle 11\bar{2}0\right\rangle$ Bürgers vector. Recall that the a-loop is lying in the “yz” ($(10\bar{1}0)$) plane of Cartesian coordinate system (its normal coincides with the positive direction of the “x” axis). The integration in (3) is carried out over the area of the loop, herefore $x' = 0$. There is a dependence on the azimuthal angle in the loop plane. In Fig. 1 in dimensionless cylindrical coordinates $z = r\sin\varphi$; $z' = r'\sin\varphi'$; $y = r\cos\varphi$; $y' = r'\cos\varphi'$; $|\boldsymbol{r}-\boldsymbol{r}'|^2 = x^2 + r^2 - 2rr'\cos(\varphi-\varphi') + r'^2$ the radial dependence of the interaction energy of the vacancy prismatic loop (2) with the SIA ($P_i / k_B T = 348.1$) is shown for four values of the angle φ.

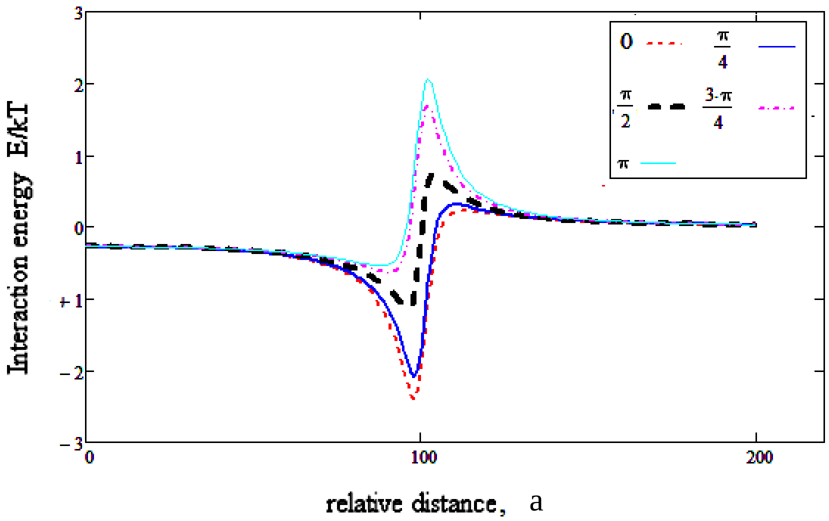

Fig. 1. The radial dependence of the interaction energy of the vacancy prismatic loop (2,3) with the SIA for different values of the angle φ: $\varphi = 0$; $\varphi = \pi/4$; $\varphi = \pi/2$; $\varphi = 3\pi/4$; $R = 100a$ (~ 32 nm) and $x = 5a$ (~ 2 nm)

We note a slight dependence on the azimuth angle φ near the loop boundary, which however 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 ($r < 100a$) to the outer one ($r > 100a$). But this dependence greatly complicates numerical calculations. Therefore, we will eliminate it by averaging the (3) over the angle φ, making the problem isotropic in the “ yz ” plane.

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 [11] 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. In terms of a variable $\psi(r,\xi)=C(r,\xi)\exp E/\bar{C}$ after averaging in (2) 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:

$$\frac{\partial^2\psi}{\partial r^2}+\frac{\partial^2\psi}{\partial\xi^2}+\left(\frac{1}{r}-\frac{\partial E}{\partial r}\right)\frac{\partial\psi}{\partial r}-\frac{\partial E}{\partial\xi}\frac{\partial\psi}{\partial\xi}=0\,. \qquad (4)$$

Coordinate "ξ" coincides with "x", because loop is lying in "yz" plane; 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 $C\exp E(\boldsymbol{r})|_{Sc}=C^e=0$: $\psi(r,\xi)=0$. 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: $\psi(r,\xi)=\exp E(r,\xi)$; and $\psi(r,\xi)=1$; one corresponds to the boundary condition in the form $C(\boldsymbol{r})|_{S_{ext}}=\bar{C}$, where $\bar{C}$ is the average PD concentration in an effective medium that simulates the influence of all sinks. Second one corresponds to $C\exp E(\boldsymbol{r})|_{S_{ext}}=\bar{C}$.

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 (4), (5) solution and looks like:

$$Z(r_c,R,R_{ext})=\frac{1}{2\pi R}\iint_S \exp(-E(r,\xi))[\boldsymbol{n}\nabla\psi(r,\xi)]\,d\sigma\,. \qquad (5)$$

The integral is taken over an arbitrary surface S with the outer normal $\boldsymbol{n}$ containing the dislocation line [11].

RESULTS

The diffusion problem (4), (5) was solved numerically by the finite difference method for a-loops having $\vec{b}=1/3\langle 11\bar{2}0\rangle$ Bürgers vector and lying in the prismatic planes $(10\bar{1}0)$ (treangles) and $(11\bar{2}0)$ (circles). Dependence of the loop bias of different nature on their radius for the first version of the boundary condition $\Psi|_{Sext}=\exp E(\boldsymbol{r})|_{Sext}$ and for two values of R_{ext} one can see on Fig. 2. The lower curves (blue) correspond to the vacancy; the upper curves (red) correspond to the interstitial loops of zirconium.

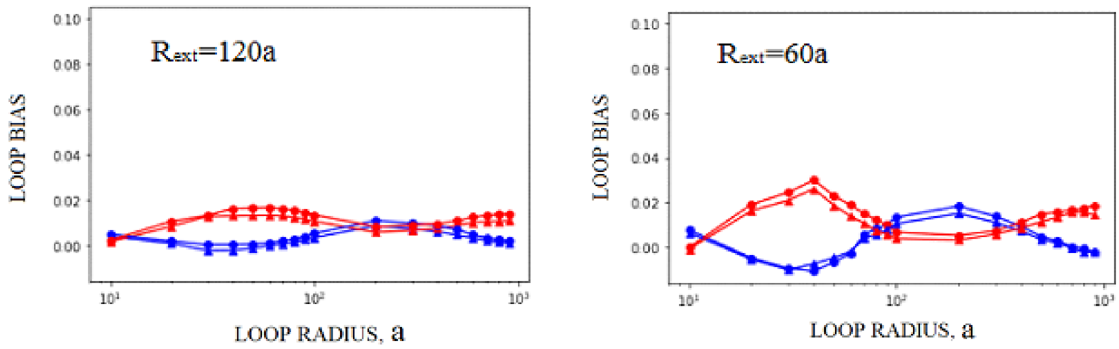

Fig. 2. Dependence of the loop bias of different nature on their radius for the first version of the boundary condition $\Psi|_{Sext}=\exp E(\boldsymbol{r})|_{Sext}$ for two values of R_{ext}

On Fig. 3 the similar dependence of loop bias for loops of different natures, but for the second version of the boundary condition $\Psi|_{Sext}=1$ is illustrated. The colors are the same. Blue correspond to the vacancy and red correspond to the interstitial loops of zirconium.

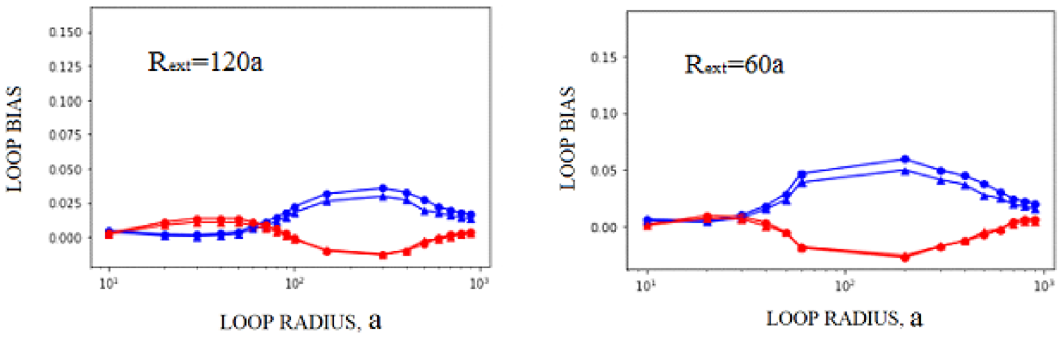

Fig. 3. Dependence of the loop bias of different nature on their radius for the second version of the boundary condition $\Psi|_{Sext}=1$ for two values of R_{ext}

From Figs. 2, 3 one can see, that for a-loops having $\vec{b}=1/3\langle 11\bar{2}0\rangle$ Bürgers vector and lying in the prismatic planes $(10\bar{1}0)$ and $(11\bar{2}0)$ dependence of bias on loop radius is practically indistinguishable.

Difference on Figs. 2, 3 associated with different boundary conditions.

The following graphs are for simulation experiments [12]. The upper curves (circles) refer to the loops having $\vec{b} = \langle 11\bar{2}0\rangle$ Bürgers vector and lying in the prismatic plane $(11\bar{2}0)$. The lower curves (triangles) refer to loops having $\vec{b} = 1/3\langle 11\bar{2}0\rangle$ Bürgers vector and lying in the prismatic plane $(10\bar{1}0)$. The red curves corresponds to the interstitial loops, the blue curves corresponds to the vacancy loops. Fig. 4 shows the bias dependence of prismatic loops of different nature on their radius for the first version of the boundary condition $\Psi|_{Sext} = \exp E(\boldsymbol{r})|_{Sext}$ and for two values of R_{ext}.

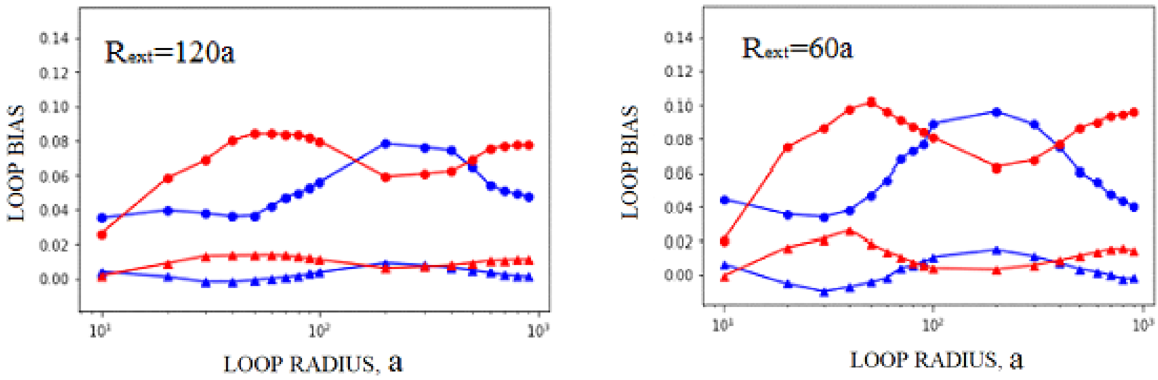

Fig. 4. Dependence of the loop bias of different nature on their radius for the first version of the boundary condition $\Psi|_{Sext} = \exp E(\boldsymbol{r})|_{Sext}$ *for two values of* R_{ext}

On Fig. 5 the similar dependence of prismatic loops bias of different natures, but for the second version of the boundary condition $\Psi|_{Sext} = 1$ is illustrated.

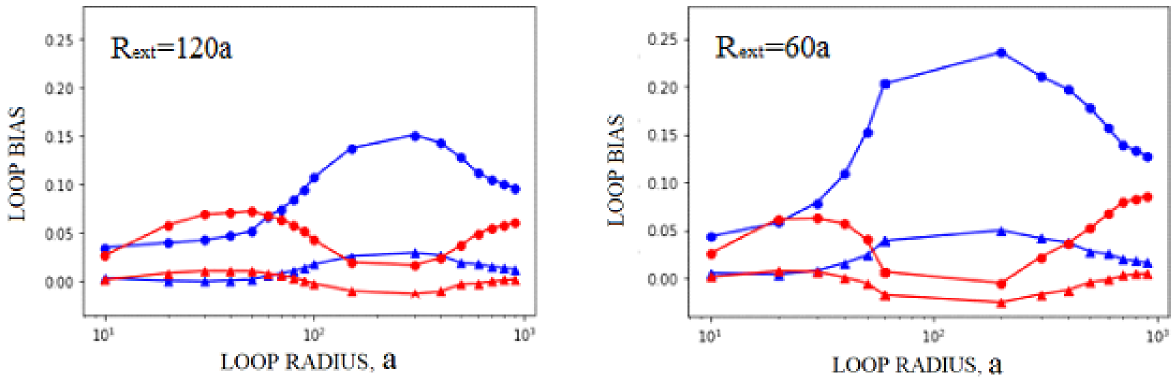

Fig. 5. Dependence of the loop bias of different nature on their radius for the second version of the boundary condition $\Psi|_{Sext} = 1$ *for two values of* R_{ext}

SUMMARY

As noted above, a characteristic feature of the radiation-induced microstructure of zirconium is the coexistence of prismatic loops of different natures. It is believed that classical elastic theory cannot explain this fact. But the theory of anisotropic diffusion is also not able to do this, although it must be admitted that certain successes in modeling the radiation growth of zirconium single crystals using the cluster dynamics method have been achieved [9]. We should note that the conclusion EID - theory are based on the elastic isotropy [15]. We in our calculations using Green's function formalism takes into account the specific plane of the loop. The main question, we are interested in is can a loop with a given Bürgers vector appear and grow to visible sizes in a specific plane. From Figs. 2, 3 one can see, that a-loops of different nature (blue correspond to the vacancy and red to the interstitial loops) having $\vec{b} = 1/3\langle 11\bar{2}0\rangle$ Bürgers vector may arise and grow for $R \simeq 100a \sim 30$ nm in the prismatic planes $(10\bar{1}0)$ (triangles) and $(11\bar{2}0)$ (circles). Dependence of the bias on loop radius practically indistinguishable. Therefore, from the point of view of loops nucleation and growth with such a Bürgers vector, they are practically equivalent. Further growth is problematic, since the vacancy loop begins to absorb SIAs more efficiently. It is not clear what causes this nonmonotonic behavior of bias. Wherein boundary condition $\Psi|_{Sext} = \exp E(\boldsymbol{r})|_{Sext}$ (see Fig. 2) is more preferable. As for simulation accelerator experiments [12], then according to Figs. 4, 5 loops with $\vec{b} = \langle 11\bar{2}0\rangle$ Bürgers vector lying in the prismatic plane $(11\bar{2}0)$ have an advantage. Wherein boundary condition $\Psi|_{Sext} = \exp E(\boldsymbol{r})|_{Sext}$ (see Fig. 4) is also more preferable.

Thus, from the point of view of the classical theory of elasticity, but taking into account the anisotropy of zirconium, it is possible to explain qualitatively the fact of the coexistence of prismatic loops of different natures. It is important to determine correctly the Bürgers vector of the loop and the plane of its occurrence. After all, it may turn out that they lie in different, but very close planes $(10\bar{1}0)$ and $(11\bar{2}0)$ with different Bürgers vectors $\vec{b} = 1/3\langle 11\bar{2}0\rangle$ or $\vec{b} = \langle 11\bar{2}0\rangle$.

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$\langle a \rangle$-КОМПОНЕНТНІ РАДІАЦІЙНО-ІНДУКОВАНІ ДИСЛОКАЦІЙНІ ПЕТЛІ РІЗНОЇ ПРИРОДИ В ЦИРКОНІЇ

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Відмінною рисою мікроструктури цирконію під опроміненням (електронне або нейтронне) є співіснування призматичних петель різної природи. Вважається, що класична пружна теорія не може пояснити цього факту. Але ж і теорія анізотропної дифузії теж неспроможна цього зробити. Зазначимо, що висновок класичної EID-теорії ґрунтується на пружній ізотропії. Ми ж у своїх розрахунках у формалізмі функції Гріна враховуємо конкретну площину залягання петлі. У роботі аналізується, чи може петля з даним вектором Бюргерса зародитись і вирости до видимих розмірів у конкретній площині цирконію.