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The effect of the point defects on the behavior of a crack inside of a pressure tube

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Abstract

The effect of the vacancies and interstitials created by irradiation on the macroscopic behavior of a crack in an in-service pressure tube is analyzed in the present work. The isolated crack is considered as a sink of point defects. The vacancy and interstitial total flows to the crack tip and crack surfaces are calculated from the corresponding values of the so-called fictitious sink strengths of the crack tip (k^2_{fT}) and crack surfaces (k^2_{fS}) and from the average defect diffusivity values and the average defect concentrations. From the interatomic potential which were used to describe the material, it is predicted that the crack length and the opening of the crack surfaces will be increased by the irradiation.

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1. Introduction

The textured polycrystals of Zr-2.5 wt% Nb alloy that compose the pressure tubes of CANDU–PHW nuclear reactors, change their shape by irradiation growth and creep [1]. The individual grain distortion is restricted by the geometrical boundaries provided by neighboring grains. Internal stresses are generated which allow the distortion to be accommodated via elastic–plastic and creep deformation within each grain [2,3]. The strain of the lattice has an effect on the thermal migration of vacancies (v) and interstitials (i) produced by irradiation outside thermal equilibrium, and modifies the anisotropy of their diffusivity tensors [4,5]. Those vacancies and interstitials may be trapped by other defects (sinks) like dislocations [6], grain boundaries [7], interfaces [8,9] and voids [10]. Also, the otherwise random walk of point defects is biased by the long-range elastic field induced by the larger defects. The detailed solution of the problem of irradiation-produced defects diffusing in a crystal lattice under the combined effects of extended defects, internal stresses and eventually an externally imposed stress field (σ^{e}), is extremely complex. In order to obtain an approximate solution, the microstructural evolution and the corresponding macroscopic observable phenomena were studied earlier within the framework of the rate theory [8,11]. In this approach, a distribution of each sink type present in the actual material is required to exist, in order to calculate their average properties [12]. In particular, the bias for vacancies or interstitials of each sink type distribution is identified by the corresponding sink strength. For hcp crystals in a given metallurgical state, the anisotropy factor ($D_{\mathrm{c}}/D_{\mathrm{a}}$) determines the value of each sink strength [5,13–15], $D_{\mathrm{c}}(D_{\mathrm{a}})$ being the diffusivity of vacancies or interstitials parallel (perpendicular) to *c*-crystal axis.

An externally loaded crack in a material under irradiation is also a sink of point defects [16]. However, contrary to other sinks, the evolution of the crack cannot be analyzed using the above-mentioned rate theory. In fact, the crack is an isolated defect and the incoming point defect fluxes must be calculated in order to ascertain its evolution. The fluxes of vacancies and interstitials were calculated by Rauh and Bullough [16] within a pure drift approximation: the migration in the

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vicinity of the crack tip was assumed to be dominated by the long-range elastic field of stress of the crack.

In a recent work [17], the vacancy and interstitial fluxes to the crack tip and crack surfaces of a mode I loaded crack [18] in a Mg lattice under irradiation were calculated by considering both the effect of the long-range elastic field of the crack and the random diffusion processes of point defects. A discrete model of the material and a numerical method were used. Also, from the total defect flows to the crack tip and to the crack surfaces the factors named fictitious sink strengths of the crack tip (k^2_{fT}) and crack surfaces (k^2_{fS}) were calculated (these calculations will be briefly reviewed in section 2). From their definition, these fictitious sink strengths allow us to calculate the approximate values of the total flows of vacancies and interstitials to the tip and surfaces of cracks inserted in materials under irradiation in which the corresponding average diffusivities and average concentrations of interstitials and vacancies are known [17]. In the present work, these approximated calculations are used to analyze the effect that the point defects have on the behavior of a mode I loaded subcritical crack inserted in an in-service pressure tube of a CANDU–PHW nuclear reactor. The microstructure of the pressure tube and the internal stresses generated by irradiation growth and creep processes are explicitly included in the calculations.

2. Fictitious sink strengths

The fictitious sink strength of a crack tip (k^2_{fT}) and the fictitious sink strength of crack surfaces (k^2_{fS}) were defined in reference [17] in a similar mathematical way as the strengths of other sinks. In fact, if I_{T} and I_{S} are the total defect flows at the crack tip and at the crack surfaces, respectively, k^2_{fT} and k^2_{fS} can be obtained as (assuming the isolated crack inserted in an unit volume)

$$I_{\mathrm{T}} = k^2_{\mathrm{fT}}\langle D\rangle\langle c\rangle \tag{1}$$

and

$$I_{\mathrm{S}} = k^2_{\mathrm{fS}}\langle D\rangle\langle c\rangle, \tag{2}$$

where $\langle D\rangle$ is the average defect diffusivity and $\langle c\rangle$ the average defect concentration in the material where the crack is inserted. $\langle D\rangle$ is chosen as the invariant of the diffusivity tensor [19], $\langle D\rangle = [D_1D_2D_3]^{1/3}$, where D_j, $j = 1, 2, 3$ are the eigenvalues of the diffusivity tensor in the crystal coordinate axes. The adjective fictitious takes into account the fact that these sink strengths do not measure 'per se' any trapping capability.

On the other hand, the total defect flows I_{T} and I_{S} are calculated in [17] by solving the diffusion equations for vacancies and interstitials, assuming (see Fig. 1(a)): a wedge shaped crack inside purely elastic ideal hcp materials characterized by different intrinsic anisotropy factors; the crack tip as an ideal sink of radius R_{i} ($c_{\mathrm{v,i}}(R_{\mathrm{i}}, \pm\theta) = 0$, $c_{\mathrm{v,i}}$ being the vacancy or interstitial concentration, respectively); the crack surfaces as ideal sinks as well ($c_{\mathrm{v,i}}(r, \pm(\pi - \Phi)) = 0$). Also, R_{i} is taken equal to 10 in units of the lattice parameter and 2Φ, the angle of the crack, is assumed to be equal to 5°. Finally, for modeling the migration of irradiation produced defects towards the crack, it is assumed that a source of constant concentration $c_{\mathrm{ev,i}}$ exists at a radius R_{e} from the crack tip. Within the latter assumption, $\langle c\rangle$ is given by $c_{\mathrm{ev,i}}$ [5]. R_{e} is considered to be the length of the crack and is taken equal to $50R_{\mathrm{i}}$. From this distance onwards, the influence of the long-range elastic field of the crack could be neglected. From these considerations

$$I_{\mathrm{T}} = 2/A\int_0^{\pi-\Phi} J_{\mathrm{r}}(R_{\mathrm{i}},\theta)R_{\mathrm{i}}\,\mathrm{d}\theta \tag{3}$$

and

$$I_{\mathrm{s}} = 2/A\int_{R_{\mathrm{i}}}^{R_{\mathrm{e}}} J_\theta(r,\Phi)\,\mathrm{d}r, \tag{4}$$

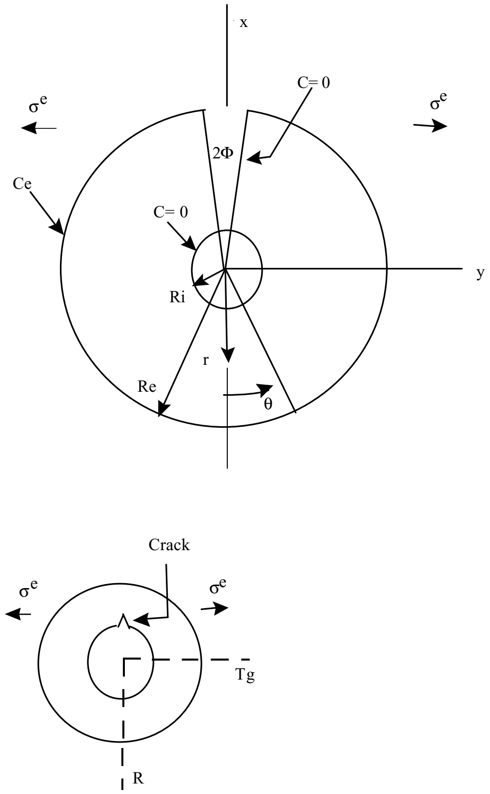

Fig. 1. (a) Geometrical description of a wedge shaped crack under mode I load (used in [17]) and their influence area. $R_{\mathrm{i}} = 10$ in units of the α-Zr lattice parameter and $R_{\mathrm{e}} = 50R_{\mathrm{i}}$. $2\Phi = 5°$. (b) Schematic representation of a crack in a pressure tube (radial–tangential plane).

where J_r is the defect current component normal to the surface of radius R_i around the crack tip and J_θ is the corresponding to the crack surfaces. A is equal to the area $(\pi - \Phi)(R_e^2 - R_i^2)$ and an unit length in the z-direction (perpendicular to the xy-plane) is considered. The calculations of J_r and J_θ are based on a point defect diffusion model which takes into account the discrete character of the defect jump [20,21].

3. Evolution of the anisotropy factors

In hexagonal strained materials, the diffusion anisotropy (D_c/D_a) of vacancies and interstitials depends on the intrinsic anisotropy of the lattice and on the elastic strain generated by external and internal stresses. The effect of the induced strain field (ε) on the defect diffusivity can be obtained for small elastic deformations explicitly as [4,22]

$$D_{ij}^{\varepsilon} = d_{ijkl}\varepsilon_{kl}, \tag{5}$$

where d is the elastodiffusion tensor for vacancies or interstitials. Therefore, the total diffusivity tensor D results

$$D_{ij} = D_{ij}^{\circ} + d_{ijkl}\varepsilon_{kl}, \tag{6}$$

where D° is the point defect diffusion tensor in the strain free crystal. In most cases, by the effect of the strain, the tetragonal symmetry is lost and both diagonal basal components (D_{11} and D_{22}) of D are different. When they are close enough, the anisotropy of the diffusion could be approximated by D_c/D_a' where $D_a' = (D_{11} + D_{22})/2$ and $D_c = D_{33}$ [23].

4. Evolution of the point defects in an in-service cold-work pressure tube

The microstructure of cold-work Zr-2.5 wt% Nb pressure tubes consists of two phases: a hcp α-phase formed by large sized in the axial-tube direction α-grains, containing about 1 wt% Nb and a homogeneous dislocation density of about 7×10^{14} m^{-2}, and a bcc β-phase containing about 20 wt% Nb at the α-grain boundaries [24,25]. From Cheadle et al. [26], the texture of the pressure tube can be represented by three different grain orientations [27]: c on the radial (R)-tangential (Tg) plane of the tube, ±80° from R axis (volume density 0.6); c on R-Tg plane, ±70° from R axis (0.2); c on R-Tg plane, ±90° from R axis (0.2). The above-mentioned density of dislocations, assumed to be prismatic edge dislocations, and the grain boundaries of the α-grains (assumed to be parallelepiped shaped grain of 35×10^{-6} m in the axial-tube direction (A), 7×10^{-6} m in the tangential-tube direction and 0.7×10^{-6} m in the radial-tube direction), are considered in this work as point defect sinks and thermal sources of vacancies when the tube is under neutron irradiation. Their sink strengths (function of the diffusion anisotropy) are introduced in a code, based on the model proposed by Savino and Laciana [2], in order to calculate the macroscopic change of shape (due to the creep and irradiation growth) of the irradiated pressure tube under an external below-yield-stress field, as a function of the fluence. The induced intergranular stresses, coming out from the different grain distortions, are also obtained from the code for different times. These intergranular stresses and eventually present external stresses, introduced in the developed explicit expressions for the vacancy and interstitial elastodiffusivity tensors, allow us to calculate each D_{ij} (Eq. (6)). Then, the anisotropy factors (D_c/D_a') and $\langle D\rangle$ for vacancies and interstitials present in the pressure tube, can be obtained as a function of the neutron fluence at the in-service reactor temperature, $T \cong 560$ K.

For the steady-state case, the vacancy concentrations $\langle c\rangle_v$, and the corresponding interstitials concentrations $\langle c\rangle_i$ in a pressure tube under irradiation (in the case of anisotropic diffusion [28]), can be described by the rate equations [29]

$$\langle c\rangle_v = (k_i^2\langle D\rangle_i/2\alpha)\{-(1-\xi) + [(1+\xi)^2 + \eta]^{1/2}\} \tag{7}$$

and

$$\langle c\rangle_i = (k_v^2\langle D\rangle_v/2\alpha)\{-(1+\xi) + [(1+\xi)^2 + \eta]^{1/2}\}, \tag{8}$$

where

$$\xi = \alpha c_v^{\circ}/k_i^2\langle D\rangle_i \tag{9}$$

and

$$\eta = 4\alpha K/k_v^2\langle D\rangle_v k_i^2\langle D\rangle_i, \tag{10}$$

by assuming the same production rate K for free interstitials and vacancies. α is the mutual recombination constant ($\alpha \cong 21\langle D\rangle_i/a_{Zr}^2$ [30], a_{Zr} being the α-Zr lattice parameter) and c_v° the equilibrium vacancy concentration at a given temperature. k_v^2 and k_i^2 are the total sink strengths for vacancies and interstitials considering all sinks present in the material, i.e. dislocations and grain boundaries.

For the high dislocation density case of cold-work pressure tubes, and from the behavior of the grain boundary sink strengths versus dislocation density [13], the total sink strengths for vacancies and interstitials are approximately equal to the dislocation sink strengths for vacancies and interstitials, respectively [14]. An approximate expression for prismatic dislocation sink strengths as a function of the anisotropy factors $(D_c/D_a)_{v,i}$, can be obtained as follows (see Fig. 3 in [15]):

$$k^2_{\mathrm{dv,i}} = [4.85 - 2.83(D_\mathrm{c}/D_\mathrm{a})_{\mathrm{v,i}} + 1.05(D_\mathrm{c}/D_\mathrm{a})^2_{\mathrm{v,i}} - 0.13(D_\mathrm{c}/D_\mathrm{a})^3_{\mathrm{v,i}}] \times 10^{14}\ \mathrm{m}^{-2}. \qquad (11)$$

As it is shown in Eq. (11), the dislocation sink strength will change with the fluence and temperature: (i) through the corresponding change in the $(D_\mathrm{c}/D_\mathrm{a})$ factors; (ii) through the corresponding change in the dislocation density. In this work, the last change will not be considered and the dislocation density will be taken as the above mentioned constant value. In Section 6, it will be analyzed how this assumption could affect the results. Thus, from the evolution of $(D_\mathrm{c}/D_\mathrm{a})_{\mathrm{v,i}}$, and $\langle D\rangle_{\mathrm{v,i}}$ with the neutron fluence, the corresponding evolution of $\langle c\rangle_{\mathrm{v,i}}$, can also be obtained.

5. Results

5.1. Fictitious sink strengths of an isolated crack

The already defined fictitious sink strengths obtained from the flow of point defects to the crack tip and crack surfaces in [17] are shown in Fig. 2(a) and (b), for different anisotropy factors, considering $c//y$, $c//x$ or $c//z$ and $R_\mathrm{e}/R_\mathrm{i} = 50$. From these results, each curve can be approximated by cubic polynomials in $(D_\mathrm{c}/D_\mathrm{a})$ (see Appendix A for some examples).

The effect of stresses upon the fictitious sink strength enters via the changes in diffusivity of vacancies and interstitials induced by them. For the sake of illustration, in Fig. 2(a) and (b) $(D_\mathrm{c}/D'_\mathrm{a})$ ranges are indicated for both defects migrating in α-Zr. This phase is assumed to be pure α-Zr and it is described, in all calculations, by a strongly repulsive pair potential adjusted to a vacancy formation energy of 1.8 eV [15]. The value of label 1i (v) corresponds to the intrinsic anisotropy factor for interstitials (vacancies) (strain free crystal lattice) at 560 K. Label 2i (v) corresponds to the anisotropy factor $(D_\mathrm{c}/D'_\mathrm{a})$ for interstitials (vacancies) at the same temperature, calculated assuming $c//y$ and the lattice under a biaxial homogenous stress in the x and y directions (see Fig. 1(a)). Here, the values of these homogenous stresses are obtained by putting in the stress field of the crack [18] $\theta = 0$ and r equal to R_i and $K1 = 2$ MPa mm$^{1/2}$, obtaining an elastic deformation equal to 0.3×10^{-3} for $r \geqslant R_\mathrm{i}$ [17]. D'_a and D_c components of the diffusivity tensor are evaluated as described in Section 4.

5.2. A crack inside a pressure tube

In order to analyze the evolution of a crack inserted in the R-Tg plane of an in-service reactor pressure tube (see Fig. 1(b)) coming out from the trapping of point defects, it will be assumed hereafter that the only effect of the capture of a vacancy at the tip of the crack is to lead the

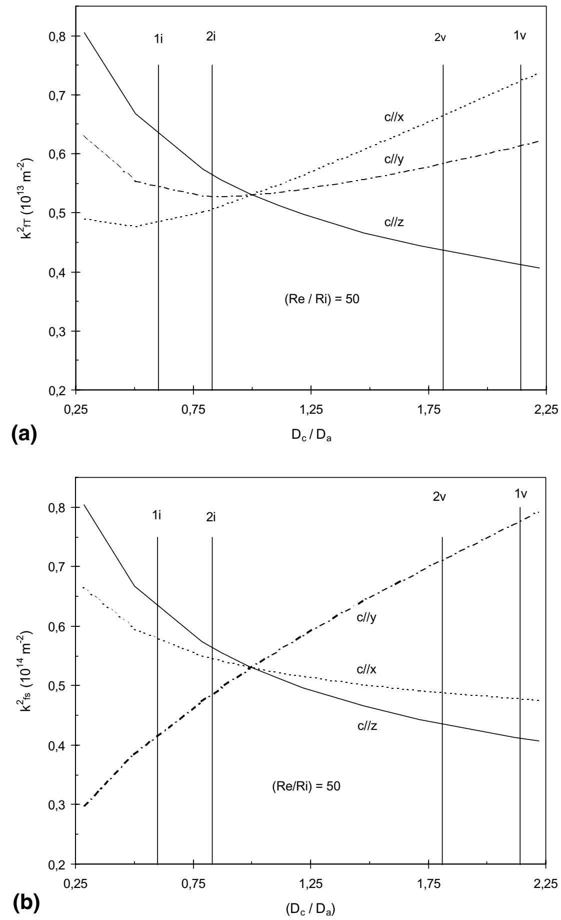

Fig. 2. (a) Fictitious sink strengths of a crack tip (k^2_{fT}), and (b) crack surfaces (k^2_{fS}), as a function of the defect diffusivity ratio $D_\mathrm{c}/D_\mathrm{a}$, for three different crystal orientations and $R_\mathrm{e}/R_\mathrm{i} = 50$ (from [17]). $D_\mathrm{c}/D_\mathrm{a}$ predicted by a repulsive pair potential for vacancies (v) and interstitials (i) in α-Zr at 560 K are shown; labels 1 and 2 correspond to strain free crystal lattice and to the homogenous strained crystal lattice ($\varepsilon = 0.3 \times 10^{-3}$), respectively.

propagation of the crack by an atomic step [31]. The reverse will be assumed if an interstitial is captured. Then, an effective crack propagation will occur when more vacancies than interstitials arrive to the crack tip $((I_\mathrm{v}/I_\mathrm{i})_\mathrm{T} > 1)$. In the same way, the angle (or the opening) of the crack will be increased when more vacancies than interstitials arrive to the crack surfaces $((I_\mathrm{v}/I_\mathrm{i})_\mathrm{S} > 1)$.

From Eq. (1), the total flow of vacancies to the crack tip/the total flow of interstitials to the crack tip ratio (or the equivalent flux of vacancies to the crack tip/flux of interstitials to the crack tip ratio $(J_\mathrm{v}/J_\mathrm{i})_\mathrm{T}$) can be obtained as

$$(I_\mathrm{v}/I_\mathrm{i})_T = (k^2_{\mathrm{fTv}}\langle D\rangle_\mathrm{v}\langle c\rangle_\mathrm{v})/(k^2_{\mathrm{fTi}}\langle D\rangle_\mathrm{i}\langle c\rangle_\mathrm{i}), \qquad (12)$$

where k^2_{fTv} and k^2_{fTi} depend on $(D_\mathrm{c}/D_\mathrm{a})_\mathrm{v}$ and $(D_\mathrm{c}/D_\mathrm{a})_\mathrm{i}$, respectively. On the other hand, from Eq. (2), the

Table 1
$(D_c/D_a)_{v,i}$, $\langle D\rangle_{v,i}$ and $\langle c\rangle_{v,i}$ for different neutron fluences, $T = 560$ K

Fluence (10^{24} nm^{-2})	$(D_c/D_a)_v$	$(D_c/D_a)_i$	$\langle D\rangle_v$ (10^{-17} m^2 s^{-1})	$\langle D\rangle_i$ (10^{-9} m^2 s^{-1})	$\langle c\rangle_v$ (10^{-5} dpa)	$\langle c\rangle_i$ (10^{-13} dpa)
0	2.02	0.65	0.34	0.15	0.39	0.62
5.9	2.00	0.67	0.34	0.14	0.39	0.63
11.3	1.98	0.68	0.34	0.14	0.39	0.63
16.6	1.96	0.70	0.33	0.14	0.39	0.63
22.0	1.94	0.72	0.33	0.13	0.39	0.64
27.2	1.92	0.74	0.33	0.13	0.39	0.64
32.8	1.90	0.76	0.32	0.12	0.38	0.65

corresponding total flow of vacancies to the crack surfaces/total flow of interstitials to the crack surfaces ratio $(I_v/I_i)_S$ is

$$(I_v/I_i)_S = (k^2_{fSv}\langle D\rangle_v\langle c\rangle_v)/(k^2_{fSi}\langle D\rangle_i\langle c\rangle_i). \quad (13)$$

Therefore, in order to know if $(I_v/I_i)_T$ and $(I_v/I_i)_S$ are greater or smaller than 1 at different neutron fluences, all factors in Eqs. (12) and (13) must be evaluated at different times of irradiation.

From the analysis in Section 4 and from the boundary condition mentioned in Section 2: $c_{v,i}(R_e, \pm\theta) = c_{ev,i} = \langle c\rangle_{v,i}$, $\langle c\rangle_v$ and $\langle c\rangle_i$ in Eqs. (12) and (13) can be taken to be equal to the $\langle c\rangle_v$ and $\langle c\rangle_i$ given by Eqs. (7) and (8). To obtain the corresponding values as a function of the fluence, $(D_c/D_a)_{v,i}$ and $\langle D\rangle_{v,i}$ must be known. $(D_c/D_a)_{v,i}$ at the in-service reactor temperature, calculated as described in Section 4, are shown in Table 1. The internal stresses coming out from the growth and creep processes, the external stress (hoop stress, taken as 136 MPa [32]) and the values of the strain field of the crack in the x and y directions mentioned in Section 5.1, are explicitly included in the calculation. The choice of the value for $r = R_i$ overestimates the effect of the crack. The substitution of the inhomogeneous long-range elastic field of the crack by a homogeneous biaxial stress field, is done to facilitate the attainment of an associated value of $(D_c/D_a)_{v,i}$ from the code that calculates growth and creep under irradiation. This substitution could be considered acceptable since only the average values $\langle c\rangle$ and $\langle D\rangle$ are going to be calculated. Also, a temperature jump of -320 K from a state free of internal thermal stresses at 880 K is imposed as an initial condition in the calculations of the growth and creep processes. This value is assumed considering that the internal thermal stresses generated by the manufacture process could induce plastic deformation in the α-Zr grains above 880 K [33]. Finally, the initial value of $\langle D\rangle_v$ is taken as an adjustable parameter fixed by fitting the axial deformation of the pressure tube calculated using the above mentioned code to the corresponding measured value at a fluence of 32.8×10^{24} nm^{-2} [34]. The obtained values of $\langle c\rangle_{v,i}$ and $\langle D\rangle_{v,i}$ for different fluences are shown in Table 1, also. From the evolution of the anisotropy factors for vacancies and interstitials and the numerical coefficients given in Appendix A, the fictitious sink strengths can be approximated making an interpolation between the values corresponding to the $c//y$ and $c//x$ cases, to take into account the texture of the pressure tube (see Appendix A).

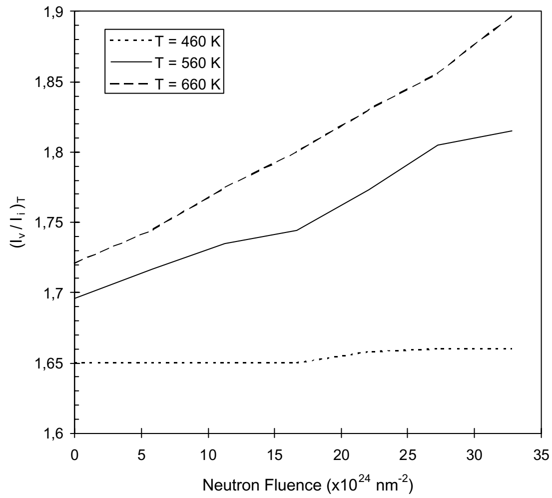

Fig. 3. Total flow of vacancies/total flow of interstitials ratio ($(I_v/I_i)_T$) to the tip of a crack in an in-service pressure tube as a function of the neutron fluence, at different temperatures.

The values of $(I_v/I_i)_T$ obtained for different neutron fluences are presented in Fig. 3. For the sake of comparison, the corresponding values at 460 K (calculated from the values of Table 2) and 660 K (from Table 3) are shown in Fig. 3, also. $(I_v/I_i)_S$ takes the approximate constant values: 2.2, 2.3 and 2.4 at 460, 560 and 660 K, respectively.

6. Discussion and conclusions

The fictitious sink strengths of the crack tip and crack surfaces of a wedge shaped crack were defined and calculated in a previous work [17] as a function of the anisotropy factors (D_c/D_a) (Fig. 2(a) and (b)). The curves obtained can be approximated by cubic

Table 2
$(D_c/D_a)_{v,i}$, $\langle D\rangle_{v,i}$ and $\langle c\rangle_{v,i}$ for different neutron fluences, $T = 460$ K

Fluence (10^{24} nm^{-2})	$(D_c/D_a)_v$	$(D_c/D_a)_i$	$\langle D\rangle_v$ (10^{-20} m^2 s^{-1})	$\langle D\rangle_i$(10^{-10} m^2 s^{-1})	$\langle c\rangle_v$(10^{-3} dpa)	$\langle c\rangle_i$(10^{-13} dpa)
0–16.6	1.98	0.70	0.46	0.39	0.21	0.17
22.0–32.8	1.97	0.70	0.46	0.38	0.21	0.17

Table 3
$(D_c/D_a)_{v,i}$, $\langle D\rangle_{v,i}$ and $\langle c\rangle_{v,i}$ for different neutron fluences, $T = 660$ K

Fluence (10^{24} nm^{-2})	$(D_c/D_a)_v$	$(D_c/D_a)_i$	$\langle D\rangle_v$(10^{-15} m^2 s^{-1})	$\langle D\rangle_i$(10^{-9} m^2 s^{-1})	$\langle c\rangle_v$(10^{-7} dpa)	$\langle c\rangle_i$(10^{-13} dpa)
0	2.05	0.63	0.35	0.38	0.52	0.32
5.9	2.03	0.64	0.34	0.37	0.52	0.32
11.3	2.00	0.66	0.34	0.36	0.52	0.32
16.6	1.98	0.67	0.34	0.34	0.51	0.32
22.0	1.96	0.69	0.33	0.33	0.51	0.33
27.2	1.94	0.71	0.33	0.32	0.51	0.33
32.8	1.92	0.73	0.32	0.30	0.51	0.33

polynomials as it is presented in Appendix A for the particular cases of the *c*-crystal axis//*y*-geometrical crack axis and the *c*-crystal axis//*x*-geometrical crack axis.

From the definition of these fictitious sink strengths, the total flow of vacancies/total flow of interstitials ratio to the crack tip and crack surfaces can be calculated as in Eqs. (12) and (13). Each factor of the right side of these equations, and then $(I_v/I_i)_T$ and $(I_v/I_i)_S$, depends on the strain of the lattice. In particular, when the crack is assumed (as in this work) to be inside an in-service pressure tube, this strain depends on the hoop stress, the elastic stress field around the crack and the internal stresses developed in the tube due to the creep and irradiation growth that, in turn, depend on the neutron fluence. The above-mentioned stresses (the inhomogeneous long-range elastic field of the crack replaced by a homogeneous biaxial field) are explicitly included in the calculation of $(D_c/D_a)_{v,i}$, $\langle D\rangle_{v,i}$ and $\langle c\rangle_{v,i}$ given in Tables 1–3.

From the obtained values of $(I_v/I_i)_T$ and $(I_v/I_i)_S$ shown in Fig. 3 and indicated in Section 5.2 it can be seen that

$$(I_v/I_i)_T > 1 \tag{14}$$

and

$$(I_v/I_i)_S > 1 \tag{15}$$

from the initial fluence up to the last fluence studied. The first result (Eq. (14)) allows us to predict that the trapping of the point defects will lead to the growth of the crack. Therefore, the irradiation will enhance any eventual propagation of a crack inserted in an in-service pressure tube. Also, as it is shown in Fig. 3 this tendency will be accentuated with time and temperature. Finally, it could be seen from Eq. (15), the irradiation will increase the opening of the crack surfaces and, perhaps, an excess vacancy flux to crack surfaces may contribute to crack blunting. Since it is not possible to obtain values for the latter mentioned effects within the static geometrical approximation used, they will not be taken into account in the following analysis.

An approximate value of the crack length increase can be obtained considering the difference (N) between the number of vacancies and the number of interstitials that arrive to the crack tip in the unit time. In fact, taking the larger value of $(I_v/I_i)_T$ at 560 K ($\cong$ equal to 1.8, see Fig. 3), it is (Eq. (1))

$$N = A(I_{Tv} - I_{Ti}) \cong 0.8Ak^2_{fTi}\langle D\rangle_i\langle c\rangle_i. \tag{16}$$

By replacing the value of A (from R_i and R_e values) and taking into account that the atomic volume of the hcp α-Zr matrix is equal to 23.26×10^{-3} nm^3 it results

$$N \cong 0.1 \times 10^{-4}\ \mathrm{s}^{-1}. \tag{17}$$

If every time that one vacancy moves to the tip of the crack, the crack advances a distance a_{Zr} (0.323 nm [24]), during the reactor 30 years lifetime design, the crack tip will advance

$$\Delta x \cong 3 \times 10^{-6}\ \mathrm{m}. \tag{18}$$

The small value obtained (within the approaches used) would indicate that, even if the crack length of a sub-critical crack increases by the effect of the trapping of point defects, this increment will not be significant. In fact, for a crack lying as it is indicated in Fig. 1(b), the increment would be only 7.5×10^{-4} times the thickness of the pressure tube (4×10^{-3} m). If the dislocation density is no longer considered to be constant, i.e. dislocation density increases with fluence, k^2_{fTi} [17] and $\langle c\rangle_i$ would decrease. Then, Δx would result smaller than the value given by Eq. (18). Also, in the model considered here, the crack is assumed to be in a purely isotropic elastic medium. However, as the long-range stress field of the crack in real cases diverges at $r = 0$, a plastic yield will occur at the tip. The slip dislocations formed will themselves act as alternative sinks for interstitials and vacancies. Then, they will screen the crack tip from the point defects [16,17].

From the analysis performed in this work it is clear that all predictions about the macroscopic behavior of a crack in a pressure tube under irradiation (even the qualitative ones about the opening of the crack) depend on the knowledge of the behavior of both the anisotropy factor and the average defect diffusivity of vacancies and interstitials in the α-Zr matrix. Therefore, all predictions have a strong dependence on the interatomic potential used to describe the material. For instance, different potentials may even reverse the diffusional anisotropy and therefore the results [35]. Also, the assumed geometry of the crack may have an influence on the fictitious sink strength values and then on the obtained results [17].

Finally, it must be pointed out that in this work, any eventual effect of the β-phase (which is surrounding the grains of the α-Zr phase) on the diffusion of the point defects was not considered.

7. Summary

- Predictions about the effect of the point defects on the behavior of a wedge shaped crack inserted in an in-service pressure tube were done.
- From the notion of the fictitious sink strengths of the crack tip (k^2_{fT}) and crack surfaces (k^2_{fS}) introduced in a previous work [17], the total flow of vacancies I_{v} and the total flow of interstitials I_{i} to the crack tip (T) and cracks surfaces (S) are approximated (Eqs. (1) and (2)). In fact, k^2_{fTv} and $k^2_{\mathrm{fSv}}(k^2_{\mathrm{fTi}}$ and $k^2_{\mathrm{fSi}})$ are the factors that multiplied by $\langle D\rangle_{\mathrm{v}}(\langle D\rangle_{\mathrm{i}})$ and $\langle c\rangle_{\mathrm{v}}(\langle c\rangle_{\mathrm{i}})$ allow us to calculate $I_{\mathrm{vT}}(I_{\mathrm{iT}})$ and $I_{\mathrm{vS}}(I_{\mathrm{iS}})$ values, respectively. $\langle D\rangle_{\mathrm{v}}(\langle D\rangle_{\mathrm{i}})$ is the vacancy (interstitial) averaged diffusivity and $\langle c\rangle_{\mathrm{v}}(\langle c\rangle_{\mathrm{i}})$ the corresponding averaged concentration.
- Assuming that the crack propagates only if the total flow of vacancies to the crack tip is greater than the corresponding total flow of interstitials ($(I_{\mathrm{v}}/I_{\mathrm{i}})_{\mathrm{T}} > 1$), it is predicted that the crack length of a subcritical crack in a pressure tube in an in-service nuclear reactor will be increased by irradiation. However, this increment will be small in the reactor 30 years lifetime design. Also, an increase of the total opening of the crack is predicted since more vacancies than interstitials arrive to the crack surfaces ($(I_{\mathrm{v}}/I_{\mathrm{i}})_{\mathrm{S}} > 1$).

The above predictions about the effect of the point defects on the macroscopic behavior of a crack in an in-service pressure tube, depend on the potential assumed to represent the atomic interactions. In particular, in this work the α-Zr phase was described by a strongly repulsive pair potential.

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Appendix A

Approximate expressions for the fictitious sink strength of the crack tip (Fig. 2(a)) and crack surfaces (Fig. 2(b)) for the cases $c//y$ and $c//x$ as a function of the anisotropy factor $(D_{\mathrm{c}}/D_{\mathrm{a}})$, can be obtained as follows:

If $(D_{\mathrm{c}}/D_{\mathrm{a}}) < 2.12$:

$$k^2_{\mathrm{fTc}//y} = \left[0.50 - 0.02(D_{\mathrm{c}}/D_{\mathrm{a}}) + 0.05(D_{\mathrm{c}}/D_{\mathrm{a}})^2 - 0.01(D_{\mathrm{c}}/D_{\mathrm{a}})^3\right] \times 10^{13}\ \mathrm{m}^{-2}, \tag{A.1}$$

$$k^2_{\mathrm{fSc}//y} = \left[0.32 + 0.21(D_{\mathrm{c}}/D_{\mathrm{a}}) + 0.01(D_{\mathrm{c}}/D_{\mathrm{a}})^2 - 0.01(D_{\mathrm{c}}/D_{\mathrm{a}})^3\right] \times 10^{14}\ \mathrm{m}^{-2}, \tag{A.2}$$

$$k^2_{\mathrm{fTc}//x} = \left[0.48 - 0.03(D_{\mathrm{c}}/D_{\mathrm{a}}) + 0.11(D_{\mathrm{c}}/D_{\mathrm{a}})^2 - 0.02(D_{\mathrm{c}}/D_{\mathrm{a}})^3\right] \times 10^{13}\ \mathrm{m}^{-2}, \tag{A.3}$$

$$k^2_{\mathrm{fSc}//x} = \left[0.63 - 0.14(D_{\mathrm{c}}/D_{\mathrm{a}}) + 0.04(D_{\mathrm{c}}/D_{\mathrm{a}})^2 - 0.01(D_{\mathrm{c}}/D_{\mathrm{a}})^3\right] \times 10^{14}\ \mathrm{m}^{-2} \tag{A.4}$$

and if $(D_{\mathrm{c}}/D_{\mathrm{a}}) < 0.79$:

$$k^2_{\mathrm{fTc}//y} = \left[1.00 - 1.79(D_{\mathrm{c}}/D_{\mathrm{a}}) + 2.28(D_{\mathrm{c}}/D_{\mathrm{a}})^2 - 0.98(D_{\mathrm{c}}/D_{\mathrm{a}})^3\right] \times 10^{13}\ \mathrm{m}^{-2}, \tag{A.5}$$

$$k^2_{\mathrm{fSc}//y} = \left[0.11 + 0.78(D_{\mathrm{c}}/D_{\mathrm{a}}) - 0.59(D_{\mathrm{c}}/D_{\mathrm{a}})^2 + 0.24(D_{\mathrm{c}}/D_{\mathrm{a}})^3\right] \times 10^{14}\ \mathrm{m}^{-2}, \tag{A.6}$$

$$k^2_{\mathrm{fTc}//x} = \left[0.64 - 0.80(D_{\mathrm{c}}/D_{\mathrm{a}}) + 1.17(D_{\mathrm{c}}/D_{\mathrm{a}})^2 - 0.49(D_{\mathrm{c}}/D_{\mathrm{a}})^3\right] \times 10^{13}\ \mathrm{m}^{-2}, \tag{A.7}$$

$$k^2_{\mathrm{fSc}//x} = \left[0.93 - 1.22(D_{\mathrm{c}}/D_{\mathrm{a}}) + 1.42(D_{\mathrm{c}}/D_{\mathrm{a}})^2 - 0.60(D_{\mathrm{c}}/D_{\mathrm{a}})^3\right] \times 10^{14}\ \mathrm{m}^{-2}. \tag{A.8}$$

The values of the fictitious sink strengths used to calculate I_{v} and I_{i} were obtained from the $c//y$ and $c//x$ cases as

$$k^2_{\mathrm{fT,S}} = (8/9)k^2_{\mathrm{fT,S}\ c//y} + (1/9)k^2_{\mathrm{fT,S}\ c//x} \tag{A.9}$$

taken into account the texture of the pressure tube.

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