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Cracks as sink of irradiation created point defects

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Abstract

The migration of irradiation produced point defects to a crack under mode I load in hcp Mg is studied in this work. Random diffusion processes and the effect of the long-range elastic field of the crack are considered. A discrete model of the material and a numerical method are used. The crack is considered as an isolated defect and the ‘fictitious’ sink strength of the crack tip (k_{TT}^2) and crack surfaces (k_{TS}^2) for vacancies (v) and interstitials (i) are defined. The dependence of these ‘fictitious’ sink strengths on the anisotropy diffusivity ratio, (D_c/D_a), is studied. © 2001 Elsevier Science B.V. All rights reserved.

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1. Introduction

In a metal under irradiation an equal number of vacancies and self-interstitial atoms, Frenkel pairs, are created out of thermal equilibrium. These point defects migrate by thermal activation in the lattice and they may be trapped by other defects (sinks) like dislocations [1], grain boundaries [2], interfaces [3,4] and voids [5]. Also, the otherwise random walk of point defects is biased by the long-range elastic field induced by the larger defects. The detailed solution to the problem of irradiation produced defects diffusing in a crystal lattice under the combined effects of extended defects, 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 [3,6]. For this approach to be valid, a distribution of each sink type present in the actual material is required to exist, in order to calculate their average properties [7]. Each sink type is identified by the corresponding sink strength. For hcp crystals or uniaxially strained cubic crystals in a

given direction (named c), the anisotropy factor (D_c/D_a) determines the values of the sink strengths for a given metallurgical state of the material [8–11], $D_c(D_a)$ being the diffusivity of vacancies or interstitials parallel (perpendicular) to c-crystal axis. This diffusion anisotropy depends on the intrinsic anisotropy of the lattice and on the elastic strain generated by external and internal stresses. The sink strength behavior allows to analyze the bias for vacancies or interstitials of each sink present in different irradiated materials.

An externally loaded crack in a material under irradiation is also a sink of point defects. However, contrary to other sinks, the evolution of a crack in the material under irradiation 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 to the crack were calculated by Rauh and Bullough [12] assuming that the migration in the vicinity of the crack tip is dominated by the long-range elastic field of stress (pure drift approximation).

In the present work, the vacancy and interstitial fluxes to the crack tip and crack surfaces of a mode I loaded crack are 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 described

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in Section 2.1 are used. Also, from the total defect flow at the crack tip and at the crack surfaces the factors named ‘fictitious’ sink strengths of the crack tip (k_{TT}^2) and crack surfaces (k_{RS}^2) are calculated in a similar way as the strengths of other sinks (Section 2.2). The crack behavior in a hcp Mg crystal is especially considered (Section 4.1).

2. Diffusion of point defects to a crack

In order to calculate the fluxes of irradiation produced point defects to a crack under mode I load, the defect concentration profiles around the crack must be calculated. The crack is considered to be wedge shaped, of length R_e , occupying the negative x -region of the xz -plane with its tip coinciding with the z -axis of a Cartesian coordinate system x, y, z (Fig. 1). The choice of this crack shape facilitates the use of the polar coordinates (r, θ) . The location of a point defect is then defined by (r, θ) , where $x = r \cos \theta$ and $y = r \sin \theta$. At steady state, and when a single point defect type is only present in the crystal, the concentration profiles must fulfil Fick’s law of defect conservation at every representative volume element (RVE) (for a definition see [13])

$$\nabla \cdot J + I_{\text{sc}} = K, \tag{1}$$

where J is the defect current at a point r and its dependence on the concentration $c(r)$ is a function of the crystal and defect symmetry, which will be discussed below for hcp structures (Section 2.1). I_{sc} accounts for

the effect of the alternative sinks and K is the homogeneous defect production rate.

In the present work the defect production K is replaced considering a source far away from the crack, which maintains a constant concentration c_e at a radius R_e from the crack tip line. The solutions obtained within this non-fully consistent approximation [7] showed the right trend for dislocations [14] and voids [11]. Then, this approximation is used here in order to obtain the approximate solutions for an isolated crack. The defect conservation equation that describes this model is

$$\nabla \cdot J + I_{\text{sc}} = 0 \tag{2}$$

and the boundary conditions (see Fig. 1) are

$$c(R_i, \pm\theta) = 0, \tag{3}$$

$$c(R_e, \pm\theta) = c_{e,i}, \tag{4}$$

$$c(r, \pm(\pi - \Phi)) = 0 \tag{5}$$

assuming the crack tip as an ideal sink of radius R_i (Eq. (3)) and the crack surfaces as ideal sinks as well (Eq. (5)). Also, the crack is assumed to be inserted in a purely elastic material, and the plastic zone in front of the crack is not considered. 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, R_e is taken as equal to (or greater than) $50R_i$; from this distance onwards, the influence of the long-range elastic field of the crack could be neglected. Elastic isotropy is assumed in order to evaluate the crack and the external strain

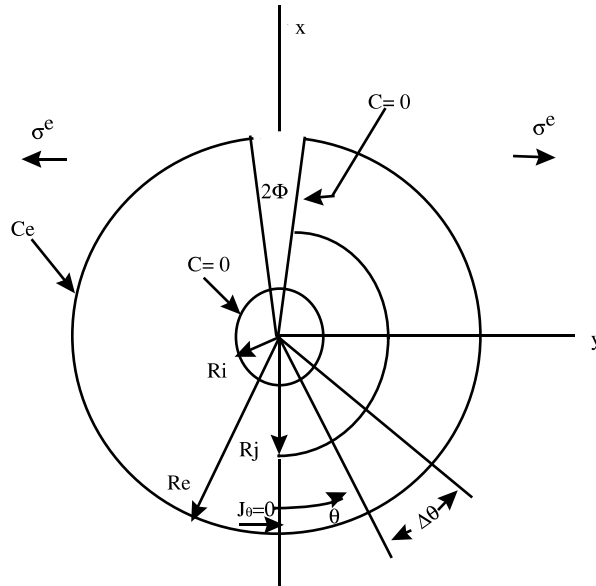


Fig. 1. Wedge shaped crack of length R_e and boundary conditions for the defect concentration around the crack, used in the numerical solution of Eq. (2) by the finite differences method.

field. This assumption was taken following the results previously obtained by Tomé and Savino [15]. In fact, they have shown that the effect of elastic anisotropy in the dislocation and external field on the evaluation of their interaction energy with a point defect is negligible in hcp crystals if the full anisotropy of the defect dipole tensor is consistently considered. Furthermore, the radial and angular dependence of the long-range elastic field of a slit crack [16] was used for the wedge crack as well. This is a good approach when the elastic field is characterized by the stress-intensity factor $K1$ [17]. v , i as in Eq. (4) refers to vacancies and interstitials, respectively.

2.1. Discrete model and numerical method

In the initial work [18] and the following [19–21] the dependence of the defect current J on the crystal and defect symmetry was thoroughly discussed. Within the ‘discrete model’ the current density of defect J at a given equilibrium site i located at r_i in the lattice is evaluated as a sum over all the possible thermally activated migration jump vectors $s_{ij} = r_j - r_i$ to neighbor equilibrium sites j located at r_j . For the particular case of hexagonal symmetry, Eq. (33) in [18] reduces to

$$J(r_i) = \sum_{j=1}^N \frac{v}{2} \exp(-Q^{ij}/kT) [c(r_i) \exp(E(r_i)/kT) - c(r_j) \exp(E(r_j)/kT)] S_{ij}, \quad (6)$$

where $c(r_i)$ and $c(r_j)$ ($E(r_i)$ and $E(r_j)$) are the point defect densities (formation energy) at neighbor sites i and j , respectively, N being the number of sites j that the defect can occupy through a single jump from i in a direction s_{ij} passing a saddle point site with an energy Q^{ij} . v is the frequency associated with the defect vibration in the jump direction.

If the lattice is strained by a field ε , the first-order dependence of the energies $E(r_i)$ and $Q^{ij}(r_s)$ on the induced strain $\varepsilon(r)$ is [18]

$$E(r_i) = E_0 - p^e \cdot \varepsilon(r_i), \quad (7)$$

$$Q^{ij}(r_s) = E_M - p^s \cdot \varepsilon(r_s), \quad (8)$$

E_0 and E_M being the energies of the stress-free lattice with the defect at the equilibrium and at the saddle point configurations, respectively. p^e and p^s are the respective defect dipole tensors as defined by Tomé et al. [20] at the equilibrium and at the saddle-point location. The long-range elastic stress field, a function of r and θ for each $K1$, is explicitly included in calculating the interaction of the crack with the point defects, given by Eqs. (7) and (8). The strain dependence of the energies in these equations implies, in turn, a strain dependence of the defect current in (6).

The numerical method used in the present work allows to solve the set of Eqs. (2)–(5) by means of a finite differences technique [20]. For the particular case of point defects diffusion in the presence of a crack field, a mesh of nodal points is taken as shown in Fig. 1. A planar grid, composed of a circular sector of angle $\pm(\pi - \Phi - \delta_1)$ centered at the crack tip, is divided by an integer number of angular nodes separated by an angle $\Delta\theta$ and the recursive formula $R_j = (1 + \Delta\theta)R_{j-1}$ applied for the radial nodes. The radial node R_M is fitted to $(R_e - \delta_2)$, $\delta_2 = 3$ being in units of the lattice parameter, and the last node R_{M+1} is taken $R_M + 2\delta_2$. Similarly, the angular node θ_N is fitted to $(\pi - \phi - \delta_1)$, with δ_1 equal to 2° , and the last angular node is $\theta_{N+1} = \theta_N + 2\delta_1$. The values of δ_1 and δ_2 are chosen to make the last elements $R_{M,M+1}$ and $\theta_{N,N+1}$ smaller than the other elements of the mesh. From the described geometry, the problem has reflection symmetry around the x -axis and the size of the mesh is reduced because calculations are made over 1/2 of the associated area. Then, the boundary conditions (5) are replaced by

$$J_\theta(r, 0) = 0 \quad (9)$$

and

$$c(r, (\pi - \Phi)) = 0, \quad (10)$$

where J_θ is the defect current in the θ direction. Finally, for calculations, the concentration at $\theta = \pi - \phi$, $r = R_e$ is assumed to be equal to 0. Then, the considered boundary condition (4) will be valid when $0 \leq \theta \leq \pi - \phi - \delta_1$. Considering the small size chosen for the last elements $R_{M,M+1}$ and $\theta_{N,N+1}$, the error introduced with this assumption is minimized. Therefore, the defect current density as given by (6) is inserted into (2), (3), (4), (9) and (10).

The alternative sinks present in the material are considered to be smeared out at an effective medium within the area $A = (\pi - \Phi)(R_e^2 - R_1^2)$. Their absorption rate (per unit volume) I_{sc} is assumed to depend linearly on the average defect diffusivity $\langle D \rangle$ and concentration $c(r)$,

$$I_{sc}(r) = k_{sc}^2 \langle D \rangle c(r). \quad (11)$$

k_{sc}^2 is the sink strength that measures the trapping capability of the alternative sinks and will be assumed to be a known parameter. The average defect diffusivity is chosen as the invariant of the diffusivity tensor [22],

$$\langle D \rangle = [D_1 D_2 D_3]^{1/3}, \quad (12)$$

where D_j , $j = 1, 2, 3$ are the eigenvalues of the diffusivity tensor in the crystal coordinate axes.

2.2. 'Fictitious' sink strengths

Even if a crack must be considered as an isolated defect, the 'fictitious' sink strengths for vacancies or interstitials are defined in a similar way as the strengths of other sinks [8,9,11,14]. In fact, the 'fictitious' sink strength of a crack tip (k_{IT}^2) and the 'fictitious' sink strength of crack surfaces (k_{IS}^2) are defined from the total defect flows at the crack tip I_{T} and at the crack surfaces I_{S} (assuming the isolated crack insert in an unit volume) as

$$I_{\text{T}} = k_{\text{IT}}^2 \langle D \rangle \langle c \rangle \quad (13)$$

and

$$I_{\text{S}} = k_{\text{IS}}^2 \langle D \rangle \langle c \rangle, \quad (14)$$

where $\langle c \rangle$, when the constant concentration boundary condition is used, is given by $c_{\text{ev},i}$ [11]. The adjective 'fictitious' introduced here takes into account the fact that these sink strengths do not have any special physical meaning. They do not measure 'per se' any trapping capability of the crack.

On the other hand, if an unit length in the z -direction is considered, the total defect flows I_{T} and I_{S} are calculated as

$$I_{\text{T}} = 2/A \int_0^{\pi-\Phi} J_r(R_i, \theta) R_i d\theta \quad (15)$$

and

$$I_{\text{S}} = 2/A \int_{R_i}^{R_c} J_\theta(r, \Phi) dr. \quad (16)$$

$J_r(R_i, \theta)$ is the defect current density component normal to the surface of radius R_i around the crack tip and $J_\theta(r, \Phi)$ is the corresponding defect current density component normal to the crack surfaces.

3. Evolution of the anisotropy factors

In hexagonal strained materials, the diffusion anisotropy (Dc/Da) 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 [19,23]

$$D_{ij}^{\varepsilon} = d_{ijkl} \varepsilon_{kl}, \quad (17)$$

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

$$D_{ij} = D_{ij}^0 + d_{ijkl} \varepsilon_{kl}, \quad (18)$$

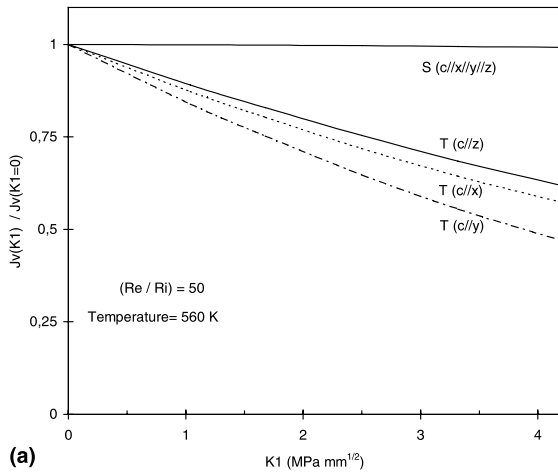
where D^0 is the point defect diffusion tensor in the strain-free crystal. In particular, when the applied external stress is not parallel to c and/or when the inhomogeneous strain field of the crack is considered, the tetragonal symmetry of the hcp lattice is lost and both diagonal basal components (Da_1 and Da_2) of D are different. Then, the anisotropy factor (Dc/Da) cannot be directly defined. However, when Da_1 and Da_2 are closed enough, the anisotropy factor of the diffusion can be approximated by Dc/Da' , where $Da' = (Da_1 + Da_2)/2$ [24]. Each Da_1, Da_2 and Dc component of the diffusivity tensor is evaluated using in Eq. (18) the explicit expressions developed for the vacancy and interstitial elastodiffusivity tensors in a strained hcp lattice, as a function of the defect equilibrium and saddle-point dipole tensors [23].

4. Results

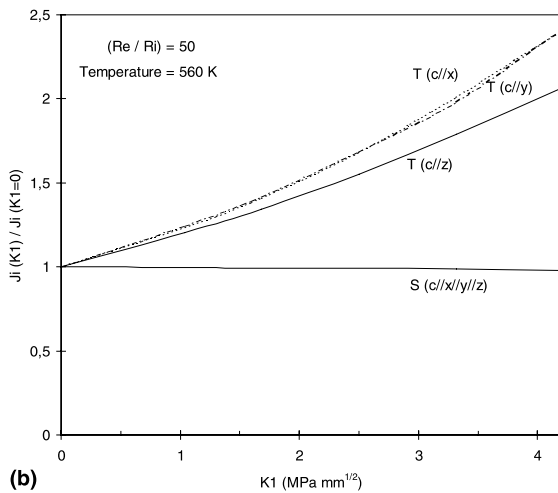
4.1. Vacancy and interstitial flows

The vacancy flow (J_v) and the interstitial flow (J_i) to the tip and surfaces of the crack are calculated (as indicated in Section 2.1) for different intensities of the stress field of the crack. The values used for $K1$ (taken as a parameter) give elastic deformations for $r \geq R_i$. The results are derived using defect configurations corresponding to a hexagonal crystal with a c/a ratio of Mg, where atoms interact via an empirical short-range pair potential fitted to various physical characteristics of the Mg lattice [25]. Also, in Eq. (6) v is assumed to be the same for vacancies and interstitials. The c -crystal axis is taken to be parallel to different geometrical crack-axes. Fig. 2(a) and (b) show the ($J_v(K1)/J_v(K1=0)$) ratio and ($J_i(K1)/J_i(K1=0)$) ratio to the crack tip (T) and crack surfaces (S) as a function of $K1$, considering $c//y$, $c//x$ and $c//z$, for $R_c/R_i = 50$ at 560 K. It can be seen that ($J_v(K1)/J_v(K1=0)$) to the crack tip decreases when the strain field of the crack increases, while the opposite is true for ($J_i(K1)/J_i(K1=0)$). These results are consistent with the calculations of Rauh and Bullough [12] within the 'pure drift' approximation. In fact, they found that when $\Delta V > 0$ (interstitials) the point defects which are not lost in the surrounding microstructure are flowing again only into the precise tip of the crack, whereas when $\Delta V < 0$ (vacancies), they flow due to the strain field effect only into the crack surfaces behind the crack tip (ΔV is the relaxation volume of the elastic material arising from an isolated point defect). The corresponding ($J_v(K1)/J_v(K1=0)$) and ($J_i(K1)/J_i(K1=0)$) values to the crack surfaces are approximately constant. This is a result of the particular strain field of the crack (zero on the crack surfaces).

Finally, if alternative sinks are present in the material, the ($J_v(k_{\text{sc}})/J_v(k_{\text{sc}}=0)$) ratio behaves as it is shown in Fig. 3. While for a relatively large density of single



(a)



(b)

Fig. 2. (a) Flux of vacancies J_v (in units of $J_v(K1 = 0)$) and (b) flux of interstitials J_i (in units of $J_i(K1 = 0)$) to a crack in a Mg crystal modelled with an empirical potential vs. the intensity factor $K1$. Three different crystal orientations are considered. T and S on the curves indicate the crack tip and the crack surfaces, respectively. Temperature = 560 K. $R_c/R_i = 50$.

crystal sinks the calculations predict a decreasing linear dependence of the ratio with the single crystal sink strength, for strengths smaller than 10^{12} m^{-2} the $(J_v(k_{sc})/J_v(k_{sc}=0))$ ratio converges to a constant value. This behavior agrees with the screening effect of the surrounding microstructure mentioned by Bullough [26].

4.2. 'Fictitious' sink strengths of an isolated crack

The already defined 'fictitious' sink strengths are obtained from the flow of point defects to the crack tip and crack surfaces using Eqs. (2)–(4) and (6)–(16) and considering the crack inside of ideal materials characterized by different intrinsic anisotropy factors. Fig. 4(a) and (b)

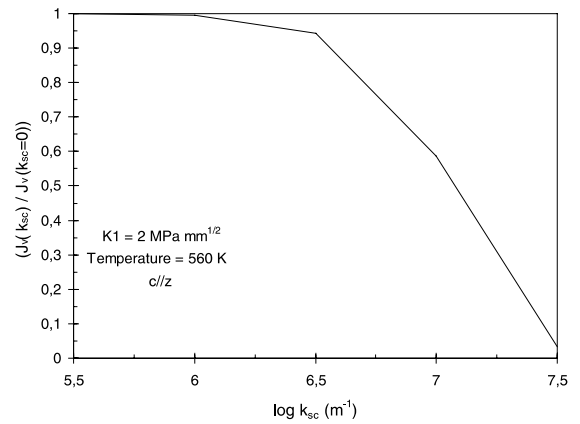


Fig. 3. Ratio between the flux of vacancies to the crack tip in Mg with alternative sinks and the corresponding flux of vacancies in the same material without alternative sinks, as a function of the single crystal sink strength k_{sc} . Temperature = 560 K. $(R_c/R_i) = 50$.

show the values of k_{IT}^2 and k_{IS}^2 for different anisotropy factors, considering $c//y$, $c//x$ or $c//z$ and $R_c/R_i = 50$. If the c -crystal axis is parallel to the crack y -axis or the c -crystal axis is parallel to the crack x -axis, the 'fictitious' sink strength of the crack tip exhibits a minimum value (close to the isotropy in the first case). On the contrary, if the c -crystal axis is parallel to the crack tip (z -axis), k_{IT}^2 decreases as (Dc/Da) increases. The 'fictitious' sink strength of the crack surfaces, k_{IS}^2 , increases or decreases with (Dc/Da) depending on the crystal orientation.

The dependence of k_{IT}^2 upon the ratio (Dc/Da) is also analyzed by assuming $(R_c/R_i) = 100$ and 150. In Fig. 4(a) it is shown that the dependence of the 'fictitious' crack sink strength upon (Dc/Da) becomes stronger as the (R_c/R_i) ratio decreases. The same behavior was obtained for the cavity sink strength [11]. These numerical results permit to conclude that, for an assumed c -crystal lattice orientation and a particular (R_c/R_i) ratio, the calculated 'fictitious' sink strength of the crack in a hcp material (in a given metallurgical state) depends only upon the analyzed dimensionless parameter (Dc/Da) .

For Mg, as described by the empirical potential, the $(Dc/Da)^\circ$ corresponding to the intrinsic anisotropy factor for vacancies (values of label v in Fig. 4(a) and (b)) and interstitials (label i in the same figures) are 0.79 and 0.95, respectively. The effect of stresses upon the 'fictitious' sink strengths enters via the changes in diffusivity induced by them. For the mentioned Mg, these changes in diffusivity are larger for interstitials than for vacancies [27].

5. Discussion and conclusions

The present analysis of point defect migration to a wedge-shaped crack under mode I load in a material

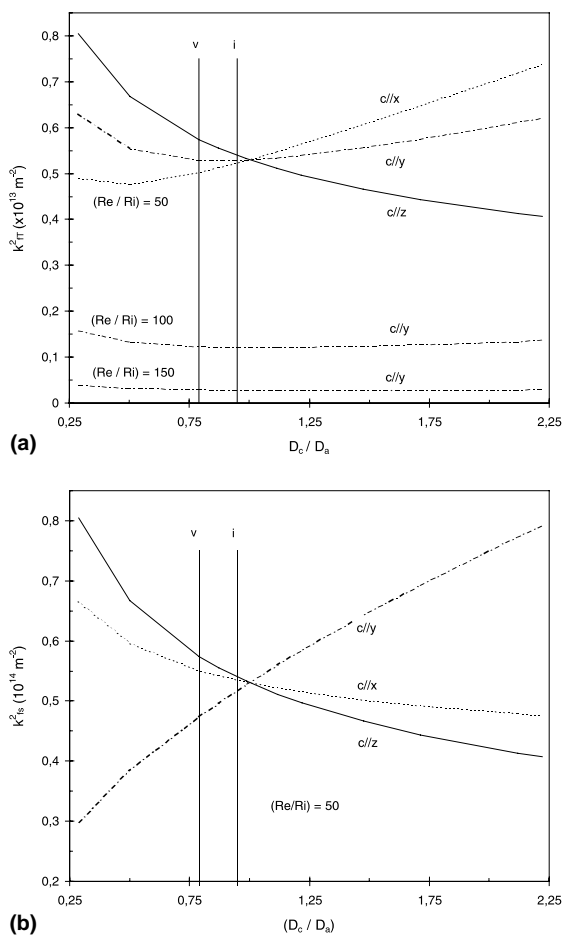


Fig. 4. (a) ‘Fictitious’ sink strengths of a crack tip and (b) crack surfaces, as a function of the defect diffusivity ratio D_c/D_a , for three different crystal orientations. The diffusivities ratio predicted by an empirical potential for vacancies (label v) and interstitials (label i) in a strain-free hcp Mg are shown. $(R_c/R_i) = 50, 100$ and 150 .

under irradiation, completes the studies of ‘pure drift’ approximation previously performed by Bullough and co-workers [7,12,26]. In fact, both the random diffusion process of defects and the effect of the long-range field stress of the crack are included in the present work. The calculations are based on a point defect diffusion model which takes into account the discrete character of the defect jump [18]. A numerical method [20] is used in

order to obtain the fluxes of point defects to a crack, assuming that the latter is inserted in a purely elastic Mg with hexagonal symmetry where atoms interact via an empirical potential [25].

From the results obtained (Fig. 2(a) and (b)), it can be seen that the flux of point defects to the tip of the crack is strongly affected by the long-range elastic field of the crack. In fact, the flux of vacancies is reduced to one-half and the flux of interstitials is increased by $\cong 2.4$ times, when the intensity factor K_I increases from 0 (pure random diffusion processes) to $4.2 \text{ MPa mm}^{1/2}$.

Also, it could be seen in Fig. 2(a) and (b) that the presence of the long-range elastic field of the crack splits the flux of point defects to the tip of the crack into three curves. This splitting is a consequence of the dependence of this flux on the stress-induced change in diffusivity given by Eq. (17), which, in turn, is depending on the orientation relationship between the crystal lattice and the crack. The magnitude of the splitting depends on the defect under consideration (it is larger for interstitials than for vacancies) and on the intensity of the field. In the absence of external stresses ($K_I = 0$) is the intrinsic anisotropy of the diffusivity tensor D° which turns the crack more or less effective for defect trapping, depending on the above-mentioned crack orientation (see Table 1).

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 and they will screen the crack tip from the point defects. Then, as it is shown in Fig. 3 by the $J_v(k_{sc})/J_v(k_{sc} = 0)$ ratio, the total defect flow will be decreased from the values obtained in Fig. 2(a) and (b).

The factors ‘fictitious’ sink strengths of the crack tip (k_{IT}^2) and the crack surfaces (k_{IS}^2) are also calculated in this work. They are depending on the dimensionless parameter (D_c/D_a) (Fig. 4(a) and (b)). Then, knowing the anisotropy factors of vacancies and interstitials in a given material the corresponding ‘fictitious’ sink strengths of a crack insert in this material can be determined. From their definitions (Eqs. (13) and (14)), these ‘fictitious’ sink strengths allow to calculate the approximate total flows of vacancies and interstitials to the tip and surfaces of cracks insert in materials where $\langle D \rangle_{v,i}$ and $\langle c \rangle_{i,v}$ are known. Then, could be the behavior

Table 1
Effect of the intrinsic anisotropy on the defect trapping

	$J_v(K_I = 0)/J_v(K_I = 0, c//z)$	$J_i(K_I = 0)/J_i(K_I = 0, c//z)$
$c//z$	1	1
$c//y$	0.93	0.84
$c//x$	0.86	0.82

of a crack in a material under irradiation analyzed without solving the diffusion equations for vacancies and interstitials.

From the analysis performed in this work it is clear that all predictions about the trapping of vacancies and interstitials by a crack in a material under irradiation depend on the knowledge of the behavior of both the anisotropy factor of vacancies and interstitials. Thus, all predictions have a strong dependence on the interatomic potential used to describe the material [28]. Also, the assumed geometry of the crack will have an influence on the results.

6. Summary

- Vacancies and interstitial fluxes to a wedge shaped crack under mode I load in a hexagonal Mg crystal under irradiation are obtained taking into account the effect of the inhomogeneous long-range stress field of the crack and the random diffusion process of point defects. It is assumed that the atoms of Mg interact via an empirical short-range pair potential.
- The long-range stress field of the crack decreases the flow of vacancies and increases the flow of interstitials to the crack tip in Mg. These predictions are depending on the potential assumed to represent the atomic interactions.
- The ‘fictitious’ sink strengths of the crack tip (k_{IT}^2) and the crack surfaces (k_{IS}^2) are defined. $k_{\text{I(T,S)v}}^2$ ($k_{\text{I(T,S)i}}^2$) is the factor that when multiplied by $\langle D \rangle_{\text{v}}$ ($\langle D \rangle_{\text{i}}$) and $\langle c \rangle_{\text{v}}$ ($\langle c \rangle_{\text{i}}$) allows to approximate the total flow of vacancies $I_{\text{(T,S)v}}$ (total flow of interstitials, $I_{\text{(T,S)i}}$) to the crack tip and the crack surfaces. $\langle D \rangle_{\text{v}}$ ($\langle D \rangle_{\text{i}}$) and $\langle c \rangle_{\text{v}}$ ($\langle c \rangle_{\text{i}}$) are the vacancy (interstitial) averaged diffusivity and averaged concentration, respectively. The ‘fictitious’ sink strengths depend on the anisotropy factor ($D_{\text{c}}/D_{\text{a}}$).
- The vacancy and the interstitial flux to the crack tip are decreased by the presence of dislocations around the crack.

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