

## Elimination of irradiation point defects in crystalline solids: Sink strengths

N. V. Doan and G. Martin

*Service de Recherches de Métallurgie Physique, Commissariat à l'Énergie Atomique, Centre de Saclay,  
91191 Gif sur Yvette Cedex, France*

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The rate theory of irradiation effects in crystalline solids rests on a set of two ordinary differential equations which, for each type of point defect (vacancy and self-interstitial), describe the balance between the production of defects on the one hand and their annihilation on the other. The latter process occurs either by mutual recombination, a bimolecular reaction, or by elimination on point defect sinks, a first-order reaction. The elimination rate is proportional to the defect concentration times the defect diffusion coefficient times a geometrical factor, the “sink strength.” The *classical expression* of sink strengths is obtained by solving the diffusion equation of point defects in a cell, which contains the sink, and ensuring that the *mean value* of the defect concentration in the cell equals the concentration in the rate theory. We propose an *alternative criterion*. Since the amplitude of the irradiation effects of practical relevance is dictated by the *partitioning of the defect annihilation* between mutual recombination and elimination on sinks, we propose that the value of the sink strength should give the correct value for the latter partitioning. The sink strengths so defined, scaled to their classical value, are evaluated for sink geometries of practical interest and expressed as a function of one dimensionless parameter, which is a function of the irradiation flux and temperature. Depending on the irradiation conditions, the correcting factors for individual sink strengths may be large (several orders of magnitude). When several types of sinks compete, we further impose that the partitioning of the elimination among the various types of sinks has the correct value. The sink strengths, as defined in this work, are additive, at variance with the classical ones. According to our definition, the dislocation bias, which measures the relative difference between the sink strengths of dislocations respectively for interstitials and vacancies, is shown to increase with the strength of neutral sinks around the dislocation. It ranges from zero when the dislocations are the only sinks to several  $10^{-1}$  when the neutral sinks have a strength much larger than that of dislocations. The computation of the correcting factor is presented in such a way that it can be easily incorporated into the rate theory of irradiation effects.

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### I. INTRODUCTION

We discuss here “high-temperature irradiation effects,” i.e., effects which take place in crystalline solids under irradiation at temperatures and time scales where the irradiation-produced point defects may migrate for large distances. Such effects result from the competition between the production of Frenkel pairs by nuclear collisions on the one hand and, on the other hand, the annihilation of the point defects by two distinct types of processes: (i) the mutual *recombination* of Frenkel pairs and (ii) the *elimination* of point defects at sinks (surfaces, interfaces, dislocation cores, etc.), the yield of which needs not be the same for both types of defects, e.g., because of distinct interaction energies of the defects with the sink.

The partitioning of defect annihilation among the above two processes is at the origin of a well-known fact: any high-temperature irradiation effect occurs with a maximum intensity in some domain of irradiation flux and temperature. Indeed at high flux and low temperature, freshly created defects cannot migrate a long distance before the creation of a new Frenkel pair and the probability for a defect to encounter another defect is larger than to encounter a sink: mutual recombination dominates. The reverse is true at higher temperature and lower flux. At very high temperature, interstitials recombine with thermal vacancies before reaching sinks: the recombination regime again prevails. Those irradiation effects which imply defect-defect encounter (nucle-

ation of defect clusters, homogeneous irradiation induced precipitation,<sup>1-3</sup> etc.) are favored in the first case. Those which imply the elimination of defects by sinks (swelling, growth, creep, irradiation induced segregation at sinks, etc.<sup>4-7</sup>) are favored in the second case.

The simplest theory of such effects is the so-called “rate theory,” widely used because of its ability to yield very easily orders of magnitudes and to point to basic couplings among various irradiation effects. In its simplest form, the rate theory reduces to the two following coupled nonlinear ordinary differential equations for the concentrations  $c_i$  of interstitials and  $c_v$  of vacancies:

$$\frac{dc_i}{dt} = G - Rc_i c_v - k_i^2 D_i c_i,$$

$$\frac{dc_v}{dt} = G - Rc_i c_v - k_v^2 D_v (c_v - c_v^e). \quad (1)$$

In Eqs. (1),  $G$  is the production rate of Frenkel pairs; in the present study, for the sake of simplicity, we do not consider the clustering of defects which may occur in the core of displacement cascades and which results in distinct production rates for isolated interstitials and vacancies. The term  $-k_\alpha^2 D_\alpha c_\alpha$  represents the rate of loss of  $\alpha$  defects on the sinks, and  $c_v^e$  is the thermal equilibrium vacancy concentration.<sup>28</sup> The geometrical constant  $k_\alpha^2$  is the sink strength for  $\alpha$  defects: the higher the sink strength, the higher

the rate of defect elimination at the sinks. The term  $-Rc_i c_v$  represents the rate of loss of defects because of mutual recombination with the rate constant  $R$  (Ref. 8):

$$R = 4\pi r_r (D_i + D_v) / \Omega, \quad (2)$$

where  $\Omega$  is the atomic volume,  $r_r$  the recombination radius, and  $D_\alpha$  ( $\alpha = i, v$ ), is the diffusion coefficient of  $\alpha$  defects.

Solving Eqs. (1) under steady-state conditions ( $dc_i/dt = dc_v/dt = 0$ ) yields the stationary vacancy and interstitial concentrations under irradiation, from which one may compute the sink elimination yield  $Y_s$ :

$$Y_s = \frac{k_\alpha^2 D_\alpha (c_\alpha - c_\alpha^e)}{G}. \quad (3)$$

Notice that, since the production rates of interstitials and vacancies are equal and since the recombination reaction destroys the same number of vacancies and of interstitials, the defect loss rate to sinks is the same for vacancies and interstitials, under steady-state conditions:  $k_i^2 D_i c_i = k_v^2 D_v (c_v - c_v^e)$ .

In practice, several types of sinks are fed from the defect population, e.g., grain boundaries and other interfaces, dislocations, cavities, and free surfaces. Some sinks may exhibit a bias in favor of one of the defects while some are neutral.<sup>9-12</sup>

For modeling the microstructural evolution under irradiation, one must first write the sink strengths in Eqs. (1) as a function of the microstructural features of interest (grain size, dislocation density, density of voids and dislocation loops, etc.) and complement Eqs. (1) by rate equations for the time evolution of the corresponding partial sink strengths.<sup>2</sup>

The simplest expressions for the sink strengths are obtained by assuming that the rate of defect loss on a sink is diffusion controlled and by neglecting the recombination reaction.

Thus the sink strength of the free surfaces of a thin plate with thickness  $e$  is of the order of  $\pi^2/e^2$ ,<sup>13</sup> and that of dislocations is approximately the dislocation density  $\rho$ . The well-known result for unbiased cavities is

$$k_{ic}^2 = k_{vc}^2 \approx 4\pi N_c r_c = \frac{3}{r_c^2} \frac{\Delta V}{V}, \quad (4)$$

with  $N_c$  the number of cavities per unit volume,  $r_c$  the radius of the cavities, and  $\Delta V/V = r_c^3/R_c^3$  the void volume per unit volume (i.e., the swelling),  $R_c$  being the mean half distance between cavities.

The strength of most sinks has been computed in this manner in the early 1970s [for reviews, see Refs. 14–17]. Moreover, at this level of approximation, the strengths of the various types of sinks are supposed to be additive, so that the two sink strengths entering Eqs. (1) are written as the weighted sum of the sink strengths of each component of the microstructure.

Two main corrections have been done to the simplest expressions: (i) going beyond the hypothesis of additivity of the individual sink strengths<sup>17,18</sup> and (ii) taking into account

the production and mutual recombination of Frenkel pairs in the medium while computing defect fluxes to the sink.<sup>17,19-23</sup>

The way this latter correction has been derived is, however, questionable for reasons to be explained below. In Sec. II, we derive a technique for evaluating the sink strengths, in the presence of a homogeneous defect production and of the vacancy-interstitial recombination reaction. In Sec. III, the technique is applied to most sink geometries, while interference effects among sinks of distinct nature are studied in Sec. IV with special attention to the problem of dislocation bias. The correction factors to the classical sink strengths can be given as a function of *universal parameters* which makes it easy to incorporate the present results into the rate theory of irradiation effects.

## II. COMPUTATIONAL METHOD OF SINK STRENGTHS

Interstitial-vacancy recombination in the medium between the sinks affects the shape of the defect concentration profiles in the vicinity of each sink and therefore modifies the flux of defects to the sink. This fact was recognized in the early 1970s by Foreman<sup>19</sup> who computed the defect concentration profiles in a thin foil under irradiation, with and without internal sinks in the foil. The purpose of the study was to estimate to which extent the free surfaces do affect the defect concentration in the bulk of the foil, in order to assess the experimental conditions under which an irradiation of the thin foil is representative of that of a bulk sample. Later on, Lam *et al.*<sup>20</sup> addressed the same problem, in both finite and semi-infinite media. They focused on the defect concentration profile, the value of the maximum defect concentration and of the average concentration in the medium, as a function of the sink density. In a most comprehensive paper, Brailsford and Bullough<sup>18</sup> showed that the concentrations entering the rate equations [Eqs. (1)] can be viewed as average concentrations in the medium between the sinks,  $\langle C_\alpha \rangle$ , provided that the product  $\langle C_i \rangle \langle C_v \rangle \approx \langle C_i C_v \rangle$  on the right-hand sides of Eqs. (1). The authors named  $I$  the difference between the two quantities. The paper, however, does not discuss the conditions under which  $I$  is small. If such is the case, the procedure to compute the strength of a sink is simple: (i) solve the diffusion equation in the cell around the sink, (ii) compute the average defect concentration  $\langle C_\alpha \rangle$  in the cell, and (iii) the value to be given to the sink strength in Eqs. (1) is that which yields a defect concentration  $c_\alpha$  equal to the latter average  $\langle C_\alpha \rangle$ .

The above procedure requires that, once the computation is done, the value of  $I$  be checked and that the result is correct only in the case where  $I$  is small.

The present work introduces an alternative definition of the sink strengths, which avoids the latter difficulty and which is based on the following remark. As discussed in Sec. I, the quantity of interest, for practical issues, is the sink elimination yield  $Y_s$ , i.e., the fraction of the produced defects which eliminate at the sinks. This quantity can be computed exactly in a cell around a given sink, taking into account the homogeneous production of defects by irradiation and the mutual recombination. In doing so, we solve the set of coupled partial derivative of equations:

$$\begin{aligned}\frac{dC_i}{dt} &= G - RC_i C_v + D_i \nabla^2 C_i, \\ \frac{dC_v}{dt} &= G - RC_i C_v + D_v \nabla^2 C_v,\end{aligned}\quad (5)$$

where  $C_\alpha$  is the *space-dependent* concentration of the  $\alpha$ -type defect at variance of  $c_\alpha$  in Eqs. (1), which is space independent. Equations (5) require, to be solved, the specification of boundary conditions: these are the defect concentrations at the sink, which are fixed to their thermal equilibrium value ( $C_i^e=0$ ;  $C_v^e$ ), and the zero-flux condition at the cell boundary in the case of a regular array of sinks. The initial condition should also be specified. In the present paper, we restrict ourselves to stationary regimes ( $dC_\alpha/dt=0$ ). Solving Eqs. (5) with appropriate boundary conditions, under steady-state conditions, yields the steady defect flux at the sink. The sink elimination yield  $Y_s$  is simply

$$Y_s = \frac{\int_A -D_\alpha \nabla C_\alpha dA}{GV}, \quad (6)$$

where the integral is taken over the surface of the sink,  $dA$  is the elementary surface area with its normal pointing toward the sink core, and  $V$  is the volume of the cell around the sink.

On the other hand, the sink elimination yield is straightforwardly obtained solving Eqs. (1) in the stationary regime:

$$\begin{aligned}0 &= G - Rc_i c_v - k_i^2 D_i c_i, \\ 0 &= G - Rc_i c_v - k_v^2 D_v (c_v - c_v^e).\end{aligned}\quad (7)$$

Simple algebra shows that a given value of  $Y_s$  yields a relationship between  $k_i^2$  and  $k_v^2$ :

$$Y_s = \frac{k_i^2 D_i c_i}{G} = \frac{k_v^2 D_v (c_v - c_v^e)}{G}. \quad (8)$$

Since we focus on  $Y_s$  rather than on  $c_\alpha$ , we may impose that the sink strength be the same for vacancies and interstitials,  $k_i^2 = k_v^2 = k^2$ , which results in  $D_i c_i = D_v (c_v - c_v^e)$ . Equation (7) then gives the sink strength as a function of  $Y_s$  [the value of which is given by Eq. (6)]:

$$\begin{aligned}k^2 &= \frac{Y_s}{2(1-Y_s)} [A + \sqrt{A^2 + 4f_0(1-Y_s)}], \\ A &= \frac{f_0 y_0}{G}; \quad y_0 = D_v c_v^e; \quad f_0 = \frac{RG}{D_i D_v}.\end{aligned}\quad (9)$$

Notice that, in the case where  $A^2 \ll 4f_0(1-Y_s)$ , a very simple expression holds for  $k^2$ :

$$k^2 = Y_s \sqrt{\frac{f_0}{1-Y_s}}. \quad (10)$$

Notice that, since the value of  $k^2$  given by Eq. (9) ensures that  $Y_s$  has the correct value, the recombination yield  $Y_r = 1 - Y_s$  also has its correct value.

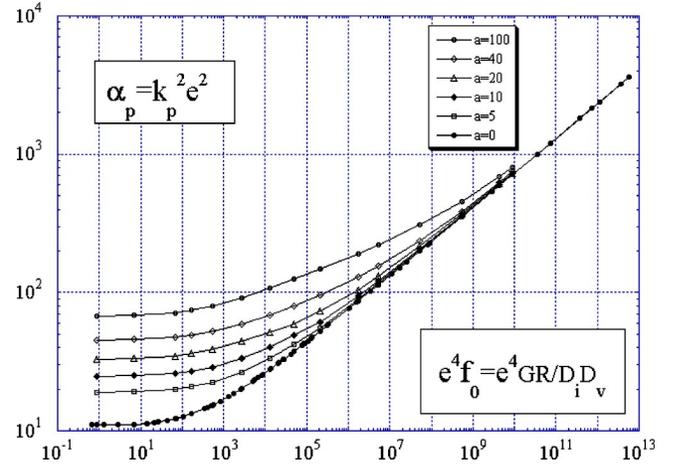


FIG. 1. Reduced sink strength of thin films. In the absence of internal sinks ( $a=0$ ), the fitted curve is  $\alpha_p = 2.7174x^{0.24311}$  for  $x = e^4 f_0 > 5 \times 10^3$ .

### III. SINK STRENGTH REEXAMINED

We now apply the novel technique to the most common sink geometries: the free surfaces of a thin foil, the grain boundary of a grain described as a plain sphere, a cavity described as a spherical hole at the center of a spherical cell, and a dislocation described as a hollow cylinder along the axis of a cylindrical cell. In the latter case, the drift of the point defects towards the dislocation, as the result of defect-dislocation interaction, is taken into account.

#### A. Free surfaces of a thin plate

Equations (5) are solved under stationary conditions in a slab bounded by two parallel planes, a distance  $e$  apart. The concentrations are fixed to their equilibrium value on the planes (0 for interstitials,  $c_v^e$  for vacancies). The integration is performed either with a Runge-Kutta algorithm or a shooting method of our own.  $Y_s$  is then computed according to Eq. (6), and the value of the sink strength of the foil surfaces is obtained from Eq. (9). In the parameter range we studied, which covers most cases of interest, Eq. (10) is an excellent approximation, so that the sink strength is function of a single parameter  $f_0$ . In Fig. 1, the curve labeled  $a=0$  depicts the variation of the sink strength (scaled to  $e^{-2}$ ) as a function of  $f_0$  scaled to  $e^{-4}$ . The reduced sink strength ( $k_p^2 e^2 = \alpha_p$ ) ranges from an asymptotic value of about 11 at low values of the dimensionless parameter  $e^4 f_0$  ( $< 10$ ), to a power dependence with the latter beyond about  $10^5$ . Low values of  $e^4 f_0$  correspond to a small recombination yield (high temperature, low irradiation flux, small foil thickness); it is not surprising that, in this range, we find  $\alpha_p$  close to its classical value  $\pi^2$ , since the latter is computed neglecting the recombination reaction. High values of  $e^4 f_0$  correspond to a large recombination yield: the sink strength when given its classical value can be underestimated by several orders of magnitude. Beyond  $e^4 f_0 > 10^5$ , the surface foil sink strength  $k_p^2$  varies approximately as  $f_0^{1/4}/e$  (see Table I).

TABLE I. Some values of the reduced sink strength,  $\alpha_p = k_p^2 e^2$ , of the surfaces of a plate with thickness  $e$ , as a function of the dimensionless parameter  $e^4 f_0$ , in the presence of secondary sinks with strength  $K^2 = ak_p^2(0)$ .

$e^4 f_0 \backslash a \rightarrow$	0	5	10	20	40	100
0.8873	11.01	20.28	25.92	34.30	46.39	70.62
33.761	11.67	20.73	26.54	35.16	47.62	72.57
$2.734 \times 10^{+3}$	20.24	27.26	34.08	45.07	61.35	94.20
$5.066 \times 10^{+4}$	37.67	42.96	49.35	61.93	82.91	127.17
$1.068 \times 10^{+6}$	77.06	81.31	86.43	98.13	122.26	181.68
$5.402 \times 10^{+7}$	200.71	204.38	208.43	217.53	238.68	308.95
$9.121 \times 10^{+9}$	716.45	719.89	723.44	730.85	746.88	803.21
$3.70 \times 10^{+11}$	1805.3	1808.8	1812.3	1819.4	1834.1	1882.2

**B. Boundary of a spherical grain**

We describe a grain as a plain sphere of radius  $r_g$ . The spherical surface represents the grain boundary along which the defect concentrations are given their equilibrium values. The procedure is identical to that in the above section, but the integration is performed in spherical geometry. Figure 2 shows the result, with the radius of the spherical grain,  $r_g$ , instead of the thickness of the foil,  $e$ , in the scaling factors (curve  $a=0$ ). Much in the same way as for the thin plate, the reduced sink strength ( $k_{gb}^2 r_g^2 = \alpha_{gb}$ ) ranges from an asymptotic value of about 12 at low values of the dimensionless parameter  $r_g^4 f_0 (< 10)$  to a power dependence with the latter beyond about  $10^3$ :  $k_{gb}^2$  shifts from  $\pi^2/r_g^2$  to  $f_0^{1/4}/r_g$ . When the recombination reaction becomes dominant, the same qualitative trends are observed as in the plate, but with a slightly different amplitude.

**C. Cavity**

The computational cell is now a hollow sphere. The inner cavity has a radius  $r_c$ , the outer sphere a radius  $R_c$ , such

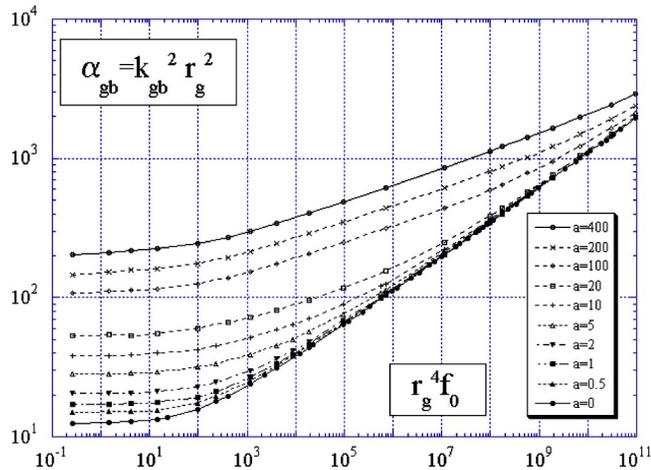


FIG. 2. Reduced sink strength of grain boundaries. In the absence of internal sinks ( $a=0$ ), the fitted curve is  $\alpha_{gb} = 12.661x^{0.015067}$  for  $x=r_g^4 f_0 < 14.5$ ,  $\alpha_{gb} = 8.463x^{0.14225}$  for  $14.5 < x < 1.197 \times 10^3$ , and  $\alpha_{gb} = 3.886x^{0.24463}$  for  $x > 1.197 \times 10^3$ .

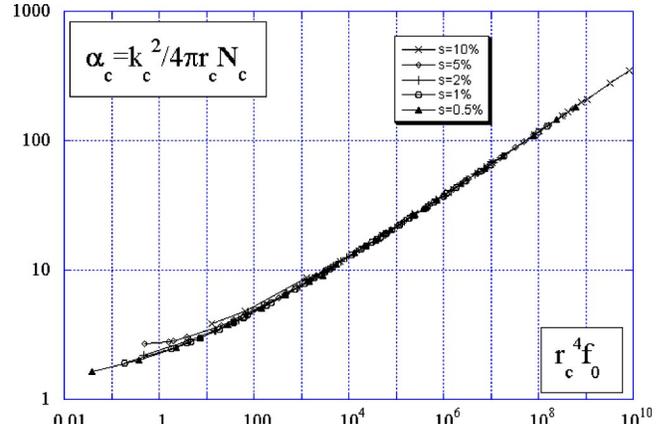


FIG. 3. Reduced sink strength of cavities. The fitted curve is  $\alpha_c = 2.366x^{0.15956}$  for  $x=r_c^4 f_0 < 1.461 \times 10^3$  and  $\alpha_c = 1.3595x^{0.24113}$  for  $x > 1.461 \times 10^3$  where  $\alpha_c$  is independent of the swelling ( $s \leq 10\%$ ).

that the number of cavities per unit volume is  $N_c = 3/4 \pi R_c^3$ . Note that the void volume fraction, i.e., the swelling, is  $\Delta V/V = (r_c/R_c)^3$ . Equations (5) are solved in spherical geometry. The defect concentrations are fixed at their thermal equilibrium values at  $r_c$ ; for the sake of simplicity, we have ignored the Gibbs-Thompson effect on the thermal equilibrium vacancy concentration. The defect flux is set to zero at  $R_c$ .

In the limit of swelling values of practical interest ( $\Delta V/V < 10\%$ ), the void sink strength, scaled to its classical value [ $\alpha_c = k^2/4\pi N_c r_c = k^2 r_c^2 / (3\Delta V/V)$ ], mainly depends on the dimensionless parameter  $r_c^4 f_0$ , as shown in Fig. 3. Again, the classical value ( $\alpha_c = 1$ ) is recovered for low values of  $r_c^4 f_0$ . The latter is underestimated by more than two orders of magnitude in the high-recombination regime. Notice that the void sink strength depends both on the radius of the cavity and on the void volume fraction, but the scaling factor  $\alpha_c$  only depends on the dimensionless parameter  $r_c^4 f_0$ , in a broad range of void volume fraction (up to 10%), at least for large values of the former ( $r_c^4 f_0 > 10^4$ ).

**D. Dislocation**

The computational cell is a hollow cylinder. The inner cylinder with radius  $r_d$  represents the dislocation core; the outer radius  $R_d$  is fixed by the dislocation density  $\rho$ :  $\rho = 1/\pi R_d^2$ . The defect concentrations are given their thermal equilibrium values at  $r_d$ ; the defect flux is set to zero at  $R_d$ . In a first step, the sink strength of the medium in the cylindrical cell is set to zero, and any defect-dislocation interaction is ignored. Equations (5) are solved in the stationary regime with cylindrical geometry. In the stationary regime, since the cell contains a single sink, the dislocation core, vacancies, and interstitials are captured in equal amount at the dislocation core. The result is depicted Fig. 4(a) where the dislocation sink strength, scaled to its classical value  $\rho$  ( $\alpha_d = k^2/\rho$ ), is shown as a function of  $r_d^4 f_0$  for typical values of the dislocation density. Up to a dislocation density of  $10^{12} \text{ cm}^{-2}$ , the reduced sink strength  $\alpha_d$  is uniquely de-

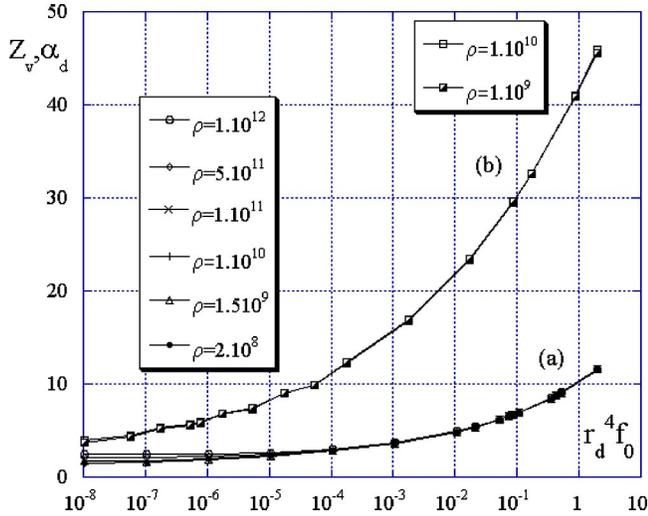


FIG. 4. Reduced sink strength of dislocations: (a)  $\alpha_d$  where the defect-dislocation interaction is omitted; (b)  $Z_v$  where the defect-dislocation interaction is taken into account (see Sec. IV F). The fitted curves for densities  $\rho \leq 10^{11}$  are  $\alpha_d = 5.2155x^{0.070912}$  for  $x = r_d^4 f_0 < 10^{-4}$  and  $\alpha_d = 9.708x^{0.14368}$  for  $x > 10^{-4}$ .

finied by the value of  $r_d^4 f_0$ . For higher dislocation densities,  $\alpha_d$  also depends on the dislocation density, at least at smaller values of  $r_d^4 f_0$ . Depending on the irradiation conditions and on the dislocation density, the classical value ( $\alpha_d = 1$ ) overestimates or underestimates the actual sink strength by a factor which can reach one order of magnitude.

The dislocation defect interaction introduces a drift term in the expression of the defect flux towards the dislocation. This term will be dealt with in Sec. IV where the effect of internal sinks will be considered.

#### IV. MULTIPLE SINKS

The competition between several types of sinks is of particular interest, i.e., cavities and dislocations. One cavity at the center of a sphere approximates a regular array of cavities with a given radius and a given spacing, while a cavity population contains a spectrum of these.<sup>29</sup>

One might suppose that a random array could give a rather different sink strength. Similarly, in the absence of other sinks, dislocations alone, despite their stronger interaction with interstitials compared to vacancies, eliminate equal numbers of interstitials and vacancies under stationary conditions. For estimating the bias factor of dislocations for eliminating interstitials, one must embed the dislocation population among other sinks.

In the case where several types of sinks are present in the cell, an effective medium approach is used:<sup>18</sup> the lossy medium around the primary sink is modeled adding a first-order elimination reaction on the RHS's of Eqs. (5):

$$\begin{aligned} \frac{dC_i}{dt} &= G - RC_i C_v - K_i^2 D_i C_i + D_i \nabla^2 C_i, \\ \frac{dC_v}{dt} &= G - RC_i C_v - K_v^2 D_v (C_v - c_v^e) + D_v \nabla^2 C_v. \end{aligned} \quad (11)$$

In Eqs. (11), we treat the defect elimination on the primary sink (e.g., a grain boundary) by a diffusion equation [Eqs.

(11)], while the effect of the secondary sinks (e.g., cavities in the grain) is approximated by a lossy medium in the computation cell. The rate constant of the elimination reaction in the lossy medium is written  $K_\alpha^2 D_\alpha$ , by mere analogy with the rate theory. We use a capital  $K$ , for the sink strength of the effective medium, to remind us that the loss rate is proportional to the *local* defect concentration  $C$  in the medium. One important question is as follows: would we get the same result exchanging the primary and secondary sinks in the computation procedure—i.e., smearing out the grain boundary into the computation cell around the cavity rather than smearing out the cavities in the grain? This will be discussed in Secs. IV D and IV E.

#### A. Computational procedure

We first present the technique we use, taking cavities as an example. The cavity population is treated as the primary sink, the strength of which is named  $k_{1\alpha}^2$  ( $\alpha = i, v$ ) in the rate theory. The secondary sinks, or sinks inside the cell surrounding each primary sink, are given a strength  $k_{2\alpha}^2$  in the rate theory, so that  $k^2$  in Eqs. (1) now represents the sum of two contributions:  $k_t^2 = k_{1\alpha}^2 + k_{2\alpha}^2$  (the subscript  $t$  on the LHS stands for “total” sink strength). As discussed in Sec. II, we chose  $k_t^2$  to be independent of the type of defect  $\alpha$ . Once created, a defect either recombines or eliminates on a sink; the latter belongs either to the primary sink population or to the secondary one. Thus, the sink elimination yield is the sum of two partial yields  $Y_{st} = Y_{s1\alpha} + Y_{s2\alpha}$ . Notice that the *partial* yields may depend on the type of defect  $\alpha$ , because of some preferential interaction of one sink with one type of defect, while the *total* sink elimination yield does not. Each partial sink elimination yield can be computed according to the procedure used in Sec. III. For doing so, we solve Eqs. (11) with a cell geometry corresponding to the primary sink (here the cavity) and with the secondary sink smeared out in the cell [third term on the RHS's of Eqs. (11)].  $Y_{s1\alpha}$  is given by Eq. (12), deduced from Eq. (6),

$$Y_{s1\alpha} = \frac{\int_A -D_\alpha \nabla C_\alpha dA}{GV} \quad (12)$$

and  $Y_{s2\alpha}$  by

$$Y_{s2\alpha} = \frac{\int_V K_\alpha^2 D_\alpha (C_\alpha - c_\alpha^e) dV}{GV}. \quad (13)$$

In Eq. (13), the integral is taken over the volume of the cell  $V$  and  $C_\alpha$  is the concentration of defect  $\alpha$  at point  $\mathbf{r}$ .

For finding the value to be given to the two sink strengths  $k_{1\alpha}^2$  and  $k_{2\alpha}^2$  in the rate theory, we impose the following condition: the *total* sink elimination yield given by the rate theory should be equal to  $Y_{st}$  as computed from Eqs. (12) and (13):

TABLE II. Some values of the reduced sink strength,  $\alpha_{gb} = k_{gb}^2 r_g^2$ , of the grain boundaries with radius  $r_g$ , as a function of the dimensionless parameter  $r_g^4 f_0$ , in the presence of secondary sinks with strength  $K^2 = a k_{gb}^2$ .

$r_g^4 f_0 \setminus a \rightarrow$	0	0.5	2	5	20	100	200	400
0.2557	12.50	15.00	20.40	28.10	53.41	106.91	146.28	204.66
4.0918	12.79	15.16	20.69	28.50	53.36	113.18	156.90	217.89
96.669	15.74	17.50	22.89	31.53	59.79	125.25	174.48	244.15
1197.0	24.06	25.30	29.76	38.87	72.43	153.37	214.26	300.42
96 958.0	64.15	65.03	68.07	75.43	117.31	246.75	346.01	486.65
$1.126 \times 10^7$	203.46	204.25	206.73	212.20	248.05	441.31	613.89	862.83
$5.641 \times 10^8$	536.35	537.10	539.42	544.43	572.82	791.55	1018.5	1406.6
$7.037 \times 10^9$	1005.1	1006.1	1008.4	1013.1	1038.7	1218.4	1479.4	1960.1
$9.696 \times 10^{10}$	1932.2	1933.4	1935.7	1940.3	1964.2	2120.7	2360.0	2880.7

$$\frac{k_t^2 D_i c_i}{G} = \frac{k_t^2 D_v (c_v - c_v^e)}{G} = Y_{st} = Y_{s1i} + Y_{s2i} = Y_{s1v} + Y_{s2v}. \quad (14)$$

We find

$$k_t^2 = \frac{Y_{st}}{2(1 - Y_{st})} [A + \sqrt{A^2 + 4f_0(1 - Y_{st})}],$$

$$k_{j\alpha}^2 = \frac{Y_{sj\alpha}}{2} [A_j + \sqrt{A_j^2 + 4f_0}], \quad j = 1, 2,$$

$$A_i = A + k_t^2, \quad (15)$$

with  $A$  and  $f_0$  defined in Eqs. (9). The expression of  $k_{j\alpha}^2$  as given in Eqs. (15) does indeed yield the correct partitioning of sink elimination among the primary and secondary ones:

$$\frac{k_{1\alpha}^2}{k_{2\alpha}^2} = \frac{Y_{s1\alpha}}{Y_{s2\alpha}}, \quad \frac{k_{1\alpha}^2}{Y_{s1\alpha}} = \frac{k_{2\alpha}^2}{Y_{s2\alpha}} = \frac{k_t^2}{Y_{st}}. \quad (16)$$

The above relationships [Eqs. (16)] are important in describing the rate of microstructural evolution under irradiation, since the latter depends on the detailed partitioning of the defect elimination among competing sinks.

### B. Thin plate containing internal sinks

In order to describe the effect of point defect sinks inside the plate, on the defect loss at the foil surfaces, we solve Eqs. (11) ascribing to the sink strength  $K^2$  of the effective medium an arbitrary value. The latter is scaled to  $k_p^2(0)$ , the sink strength of the foil surfaces of the thin plate, in the absence of internal sinks:  $K^2 = a k_p^2(0)$ . The results obtained with different values of  $a$  are depicted in Fig. 1 (see also Table I). Whenever  $e^4 f_0 < 10^3$ , the value of the sink strength of the foil surfaces is very sensitive to the presence of internal sinks. It increases rapidly with the inner sink strength and can be multiplied by a factor of 7 when the strength of the sinks inside the foil is 100 times of that of the foil surfaces. At larger values of  $e^4 f_0$ , the sink strength of the foil surfaces becomes independent of the internal sinks: indeed, the latter

have a weak contribution to defect balance, compared to the recombination reaction, the effect of which controls the value of  $\alpha_p$ .

### C. Grain boundary containing internal sinks

The same qualitative trends are observed for the effect of internal sinks on the grain boundary sink strength, but with a slightly different amplitude. In particular, the latter recovers its internal sink free value at much larger values of the dimensionless parameter  $r_g^4 f_0$  than the thin plate (see Fig. 2 and Table II).

### D. Cavities together with other cavities

#### 1. One cavity among identical cavities

We first check the consistency of the effective lossy medium procedure for a population of cavities, by computing the sink strength of one cavity by two distinct routes.

(i) Route 1: we consider one cavity of radius  $r_c$  at the center of a sink free sphere of radius  $R_c$ .

(ii) Route 2: we consider the same cavity at the center a large sphere of radius  $R_{c1} > R_c$  (subscript 1 for the primary sink) containing many spheres of radius  $r_c$ , a distance  $2R_c$  apart. The latter are treated as a lossy medium around the central cavity.

As an example, with the parameter values  $r_c = 100a$ ,  $R_{c1} = 5000a$ ,  $R_c = 600a$ ,  $a = 2.87 \times 10^{-8}$  cm, and  $r_c^4 f_0 = 7.038 \times 10^3$ , we find a reduced sink strength of the cavity of 11.66 by route 1 and of 11.63 by route 2. Both values are identical within 0.2%. In other words, if we estimate the sink strength of a single cavity at the center of a sink-free sphere of radius  $R_c$  using the reduced sink strength obtained by route 2, we find  $k^2 = 11.63 \times 3 \times r_c / R_c^3$  instead of  $11.66 \times 3 \times r_c / R_c^3$  computed directly by route 1. For lower values of  $f_0$ , due to higher temperatures, the self-consistency still holds although less accurate. For instance, with parameter values typical of  $\alpha$  iron ( $D_{i0} = 3 \times 10^{-4}$  cm<sup>2</sup> s<sup>-1</sup>,  $E_{mi} = 0.28$  eV for interstitial diffusion,  $D_{v0} = 5.0$  cm<sup>2</sup> s<sup>-1</sup>,  $E_{mv} = 1.36$  eV for vacancy diffusion, and  $E_{fv} = 1.6$  eV for vacancy formation), at a displacement rate of  $10^{-5}$  dPa s<sup>-1</sup> as above and for a temperature of 773 K, we obtain a reduced

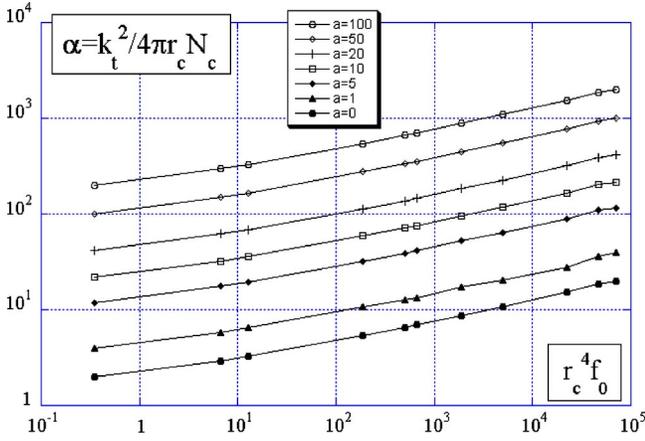


FIG. 5. Total sink strength of cavities in the presence of internal sinks with strength  $K^2 = ak_c^2$ .

sink strength of 1.47 by route 1 and of 1.31 by route 2 (with  $R_{c1}$  up to  $5000a$ ). The sink strength of the cavity is thus 1.3 times larger than the classical value, to a consistency better than 11%. The embedding procedure is thus justified.

### 2. One cavity with other sinks

As discussed above, the sink strengths as defined in this paper are additive. As an example, we consider a cavity of radius  $r_c$ , at the center of a sphere of radius  $R_c$  containing internal sinks, the strength of which is  $K^2$  in Eqs. (11). In the absence of internal sinks, the sink strength of the cavity is

$$k_c^2 = 3\alpha_c(0)r_c/R_c^3, \quad (17)$$

where  $\alpha_c(0)$  refers to the value of  $\alpha_c$  in the absence of internal sinks. Let us write  $K^2$  as  $a \times k_c^2$  and compute the total sink strength in the sphere (cavity + internal sinks), using the procedure described in Sec. IV A. As shown in Fig. 5, in the explored range ( $0 \leq a \leq 100$ ) we find

$$k_t^2 = (1+a)k_c^2, \quad \text{i.e.,} \quad k_t^2 = k_c^2 + K^2. \quad (18)$$

### 3. Cavities with a size distribution

The above additivity makes it easy to compute the sink strength of a population of cavities of various sizes  $r_i$ ; the number of cavities of radius  $r_i$  per unit volume is  $N_i$  ( $i = 1-p$ ). We first embed the cavities of class 1 into the effective medium containing the cavities of class 2 as internal sinks and compute the total sink strength  $k_{1,2}^2$  of this void subpopulation. We then embed class 3 into the effective medium  $k_{1,2}^2$ , etc. It is easily found that the total sink strength of the full cavity population is

$$k_t^2 = \sum_{i=1,p} \alpha_{0i} 4\pi r_i N_i, \quad (19)$$

where  $\alpha_{0i}$  is the internal sink free reduced sink strength of the  $i$ th class of cavities, as given in Fig. 3, i.e., for the value of the dimensionless variable ( $r_i^4 f_0$ ).

As an example, we have studied in more detail the total sink strength of a population of cavities defined by the size

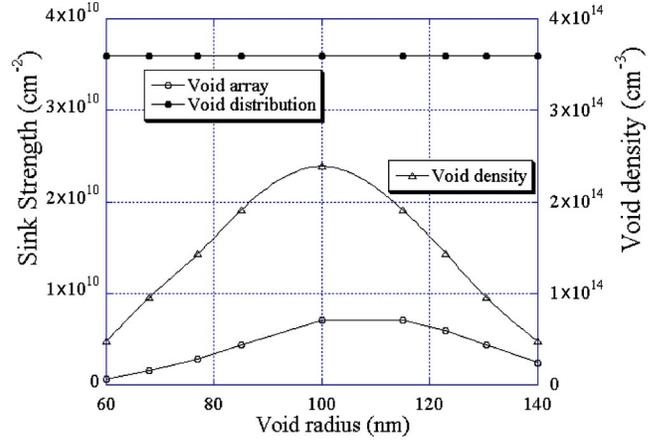


FIG. 6. Sink strength of a cavity population with a size distribution ( $\Delta$ ): (a) Sink strength of each array of identical voids ( $\circ$ ). (b) Total sink strength of the void distribution computed in nine different ways ( $\bullet$ ) (see text).

distribution shown by the open triangles in Fig. 6. The latter shows the number of voids per unit volume, as a function of the radius of the void; nine classes of void radius have been defined. The sink strength of each class of void in the absence of the other classes, has been computed according to the procedure given in Sec. III C (Fig. 3) for  $f_0 = 1.62 \times 10^{24} \text{ cm}^{-4}$ . The result is sketched on Fig. 6 by the open circles (“void array”). The total sink strength has then been computed following the procedure given in Sec. IV A, taking the cavities of class  $i$  as the primary sink and all other cavities (1 to  $i-1$  and  $i+1$  to 9) as the secondary sinks. The secondary sink strength was taken as the sum of the corresponding individual strengths. The total sink strength is thus computed in nine distinct manners, all of which give the same result (solid circles in Fig. 6).

### E. Cavities together with grain boundaries

Consider a spherical grain (with radius  $r_g$ ), containing cavities (with radius  $r_c$ , a distance  $2R_c$  apart). We want to assess whether we get the same sink strengths (total and partial), embedding the grain boundary (primary sink) into the cavities (secondary sink) or doing the reverse, i.e., smearing out the grain boundary sink strength (secondary sink) around the cavity (primary sink).

The sink strength of the cavity *alone* is  $k_{c0}^2 = 3\alpha_c(0) \times r_c/R_c^3$ , where  $\alpha_c(0)$  is the reduced sink strength of the cavity in the absence of internal sinks and is shown on Fig. 3. The sink strength of the grain boundary *alone* is  $k_{gb0}^2 = \alpha_{gb}(0)/r_g^2$ ; here,  $\alpha_{gb}(0)$  is the reduced sink strength of the grain boundary in the absence of internal sinks ( $a=0$ ) (Fig. 2). In a first step (procedure A) we consider the cavity as the primary sink and the grain boundary as the secondary one. This means that we solve Eqs. (11) for the cavity (hollow sphere geometry), giving to the internal sink strength  $K^2$  the grain boundary strength  $k_{gb0}^2$ . From Eqs. (12)–(15), we get the two partial sink strengths  $k_{c1}^2$  and  $k_{gb2}^2$  where the subscripts  $c1$  and  $gb2$  point to the fact that the cavity is the primary sink and the grain boundary is the secondary one. In

TABLE III. Some values of the reduced sink strength,  $\alpha_d = k_d^2/\rho$ , of dislocations as a function of the dimensionless parameter  $r_d^4 f_0$  and of the dislocation density  $\rho$  ( $\text{cm}^{-2}$ ).

$r_d^4 f_0 \setminus \rho \rightarrow$	$1 \times 10^{12}$	$5 \times 10^{11}$	$1 \times 10^{11}$	$1 \times 10^{10}$	$1.5 \times 10^9$	$2.8 \times 10^8$
$1.068 \times 10^{-8}$	0.039	0.079	0.358	0.734	0.718	0.716
$1.068 \times 10^{-7}$	0.124	0.244	0.737	0.831	0.817	0.819
$1.068 \times 10^{-6}$	0.376	0.659	0.990	0.958	0.952	0.955
$1.068 \times 10^{-5}$	0.938	1.154	1.173	1.141	1.139	1.142
$1.068 \times 10^{-4}$	1.486	1.483	1.423	1.406	1.406	1.409
$1.068 \times 10^{-3}$	1.905	1.856	1.814	1.805	1.805	1.808
$1.068 \times 10^{-2}$	2.497	2.461	2.434	2.428	2.429	2.430
$1.068 \times 10^{-1}$	3.497	3.438	3.448	3.443	3.442	3.441
$3.563 \times 10^{-1}$	4.276	4.249	4.228	4.222	4.220	4.216
1.649	5.711	5.649	5.601	5.589	5.585	5.578

a second step (procedure B), we consider the grain boundary as the primary sink and the cavities as the secondary one. We therefore solve Eqs. (11) for the grain geometry (plain sphere with the surface as grain boundary), giving to the internal sink strength  $K^2$  that of the cavities,  $k_{c0}^2$ . Equations (12)–(15) now yield  $k_{gb1}^2$  and  $k_{c2}^2$  where the labels 1 and 2 have been permuted.

We have performed the above calculations for a series of parameter values, varying the relative strength of the cavities versus that of the grain boundary, and for a broad range of reduced sink strengths  $\alpha_{gb}(0)$  and  $\alpha_c(0)$ , i.e., with  $k_{x0}^2$  ( $x = c$  or  $gb$ ) values close to—or far away from—their classi-

cal value. Typical results are given in Tables III and IV. The main result is as follows. In the range where  $0.18 \leq k_{c0}^2/k_{t0}^2 \leq 0.79$  with  $k_{t0}^2 = k_{c0}^2 + k_{gb0}^2$  [see Tables IV(a) and IV(b)], the sink strengths (partial and total) equal their internal sink free values ( $k_{t0}^2$ ) within less than 4%, and the above procedures A and B give the same result within better than 7%. This means that the self-consistency of the embedding procedure is verified to better than 7%. When the grain boundary is the minority sink,  $k_{gb0}^2/k_{t0}^2 \leq 0.1$  [see Table IV(c)], the above conclusion remains valid for the cavity and total sink strengths  $k_c^2$  and  $k_t^2$ , but not for the grain boundary  $k_{gb}^2$ . For the latter, the discrepancy with  $k_{gb0}^2$  as well as between procedures A

TABLE IV. Assessment of the self-consistency of the embedding procedure for cavities together with grain boundaries. The strength of each individual sink alone appears in column 2. The strengths computed embedding the cavity in a lossy medium representing the grain boundary (procedure A) are given in column 3; those obtained embedding the grain boundary in a lossy medium representing the cavities (procedure B) are given in column 4.  $f_0$  and  $y_0$  are computed from the temperature and displacement rate, with parameter values typical of  $\alpha$ -Fe:  $D_{i0} = 3.0 \times 10^{-4} \text{ cm}^2 \text{ s}^{-1}$ ,  $E_{mi} = 0.28 \text{ eV}$  for interstitial diffusion,  $D_{v0} = 5.0 \text{ cm}^2 \text{ s}^{-1}$ ,  $E_{mv} = 1.36 \text{ eV}$  for vacancy diffusion, and  $E_{fv} = 1.6 \text{ eV}$  for vacancy formation.

$k^2$ ( $\text{cm}^{-2}$ ) <sup>a</sup>	Isolated	Procedure A	Procedure B	$(k_B^2 - k_A^2)/k_A^2$
Cavity	$3.112 \times 10^{10}$	$3.115 \times 10^{10}$	$3.015 \times 10^{10}$	-0.032
Grain boundary	$1.457 \times 10^{11}$	$1.414 \times 10^{11}$	$1.457 \times 10^{11}$	+0.030
Total	$1.768 \times 10^{11}$	$1.725 \times 10^{11}$	$1.759 \times 10^{11}$	+0.019
Cavity/total	0.176	0.181	0.171	-0.055
$k^2$ ( $\text{cm}^{-2}$ ) <sup>b</sup>	Isolated	Procedure A	Procedure B	$(k_B^2 - k_A^2)/k_A^2$
Cavity	$3.526 \times 10^9$	$3.527 \times 10^9$	$3.514 \times 10^9$	-0.003
Grain boundary	$9.495 \times 10^8$	$9.156 \times 10^8$	$9.552 \times 10^8$	+0.043
Total	$4.476 \times 10^9$	$4.443 \times 10^9$	$4.469 \times 10^9$	+0.006
Cavity/total	0.788	0.794	0.786	-0.010
$k^2$ ( $\text{cm}^{-2}$ ) <sup>c</sup>	Isolated	Procedure A	Procedure B	$(k_B^2 - k_A^2)/k_A^2$
Cavity	$3.621 \times 10^{10}$	$3.639 \times 10^{10}$	$3.500 \times 10^{10}$	-0.038
Grain boundary	$4.507 \times 10^9$	$4.381 \times 10^9$	$6.622 \times 10^9$	+0.512
Total	$4.072 \times 10^{10}$	$4.077 \times 10^{10}$	$4.162 \times 10^{10}$	+0.021
Cavity/total	0.889	0.893	0.841	-0.058

<sup>a</sup> $r_c = 49.41 \text{ nm}$ ,  $\Delta V/V = 10^{-2}$ ,  $r_g = 1 \text{ }\mu\text{m}$ ,  $f_0 = 3.123 \times 10^{26} \text{ cm}^{-4}$ ,  $r_c^4 f_0 = 1.862 \times 10^5$ ,  $r_g^4 f_0 = 3.123 \times 10^{10}$ .

<sup>b</sup> $r_c = 29.41 \text{ nm}$ ,  $\Delta V/V = 0.005$ ,  $r_g = 10 \text{ }\mu\text{m}$ ,  $f_0 = 5.599 \times 10^{21} \text{ cm}^{-4}$ ,  $r_c^4 f_0 = 0.419$ ,  $r_g^4 f_0 = 5.599 \times 10^5$ .

<sup>c</sup> $r_c = 31.69 \text{ nm}$ ,  $\Delta V/V = 5\%$ ,  $r_g = 1 \text{ }\mu\text{m}$ ,  $f_0 = 2.144 \times 10^{20} \text{ cm}^{-4}$ ,  $r_c^4 f_0 = 2.161 \times 10^{-2}$ ,  $r_g^4 f_0 = 2.144 \times 10^4$ .

and B can be as large as 50%. This is the case when the grain boundary sink strength is close to its classical value ( $r_g^4 f_0$  small): in this case, the grain boundary sink strength is very sensitive to the presence of internal sinks (Fig. 2). However, this discrepancy is of low practical importance, since the contribution of grain boundaries to the defect elimination is small. For large values of  $r_g^4 f_0$ , the self-consistency is improved ( $<13\%$ , for  $k_{gb}^2 \sim 0.06 k_{i0}^2$  and  $r_g^4 f_0 \sim 3 \cdot 10^{12}$ ). The reason for this is that, in this domain, the grain boundary sink strength is less sensitive to the presence of internal sinks.

### F. Dislocations together with other sinks

When dealing with defect elimination on dislocations in the presence of other sinks, one must take into account the dislocation-defect interaction since it has a distinct value for vacancies and interstitials. The diffusion term in Eqs. (11),  $D_\alpha \nabla^2 C_\alpha$ , must be changed into a diffusion and drift term

$$D_\alpha \left( \nabla^2 C_\alpha + \frac{\nabla C_\alpha \nabla E_\alpha + C_\alpha \nabla^2 E_\alpha}{k_B T} \right),$$

where  $E_\alpha$  is the interaction energy of the dislocation with the  $\alpha$  type defect;  $k_B$  is Boltzmann's constant,  $T$  is the temperature, and we have neglected stress effects on the diffusion coefficient  $D_\alpha$ . For simplicity, the dislocation-defect interaction energy is assumed to have cylindrical symmetry,

$$\frac{E_\alpha(r)}{k_B T} = -L_\alpha \left( \frac{1}{r} + \frac{1}{2R_d - r} \right), \quad (20)$$

where  $L_\alpha$  scales the amplitude of the interaction energy:

$$L_\alpha = \frac{\mu b(1+\nu) |v_\alpha^r| \Omega}{3\pi(1-\nu) k_B T}. \quad (21)$$

The latter is proportional to the relaxation volume of the point defect  $v_\alpha^r \Omega$ ;  $\mu$  and  $\nu$  are, respectively, the shear modulus and Poisson's ratio;  $r$  is the position inside the cylindrical cell around the dislocation and  $R_d$  is the radius of the latter cell, i.e., half the spacing between two parallel dislocations. The form given to the interaction energy [Eq. (20)] is taken from Ref. 12 and has the virtue to give zero drift force at the outer surface of the cylindrical computational cell. The fact that  $L_i > L_v$  is at the origin of the "bias" for defect elimination on dislocations. In the classical theory, the sink strengths of dislocations are written as  $Z_i \rho$  and  $Z_v \rho$ , respectively, for interstitials and vacancies, and a "dislocation bias" (in favor of interstitial elimination) is introduced as  $\varepsilon = (Z_i - Z_v)/Z_i$ . We have computed  $Z_i$ ,  $Z_v$ , and  $\varepsilon$  for several sets of parameter values, following the procedure of Sec. IV A. For the sake of definiteness, the dislocation-defect interactions have been evaluated with parameter values typical of  $\alpha$  iron:  $\mu = 8.3 \times 10^{11}$  MPa,  $\nu = 0.29$  (Ref. 24),  $v_v^r = -0.22$ ,  $v_i^r = 1.1$  (Ref. 25), and  $b = 0.202$  nm. Three temperatures have been explored (450, 573, 773 K) with, most of the time, a displacement rate of  $1.5 \times 10^{-5}$  dPa s $^{-1}$ , for three distinct dislocation densities  $10^9$ ,  $10^{10}$ , and  $10^{11}$  cm $^{-2}$  and with a secondary sink strength ranging mostly from 0 to 2 times the dislocation density and in one case ( $\rho = 10^9$  cm $^{-2}$ ,  $T = 773$  K) from

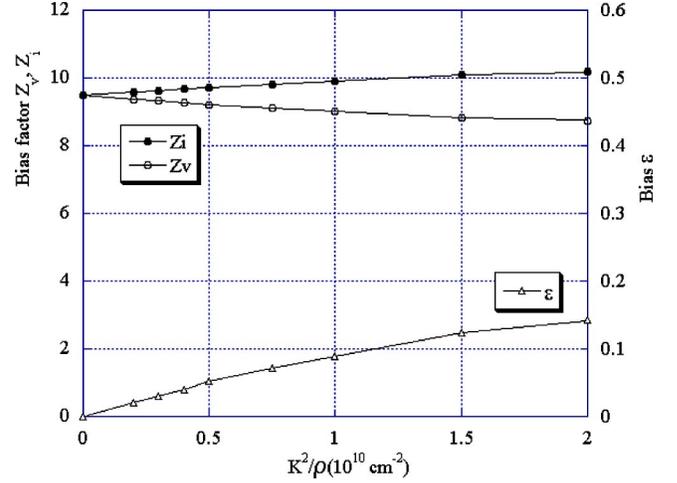


FIG. 7. Sink strength of a dislocation network taking into account the defect-dislocation interaction ( $\rho = 10^{10}$  cm $^{-2}$  and  $r_d^4 f_0 = 0.264 \times 10^{-4}$  at 450 K). Bias factors  $Z_i$  ( $\bullet$ ),  $Z_v$  ( $\circ$ ), and dislocation bias  $\varepsilon$  ( $\triangle$ ) as a function of the internal sink strength  $K^2$ .

0 to 20. The dimensionless parameter  $r_d^4 f_0$  in this study ranges from  $2.64 \times 10^{-5}$  to  $1.14 \times 10^{-11}$ .

Figures 7 and 8 show a typical variation of the bias  $\varepsilon$  and of the bias factors  $Z_i$  and  $Z_v$  as a function of the strength of the internal sinks, scaled to the dislocation density, in two typical cases. The major trends are as follows.

*In the absence of internal sinks* ( $K^2 = 0$ ),  $Z_i = Z_v$  and the bias  $\varepsilon$  is zero. Notice that  $Z_v \neq \alpha_d$ , the reduced sink strength of the dislocation discussed in Sec. III D [Fig. 4(a)], since  $\alpha_d$  was computed in the absence of the dislocation-defect interaction. The value of  $Z_v$  as a function of  $r_d^4 f_0$  is given Fig. 4(b). The variation of  $Z_v$  (or  $Z_i$ ) as a function of the temperature and of the displacement rate follows the same qualitative trends as that of  $\alpha_d$  as a function of  $r_d^4 f_0$ . The higher  $f_0$  (i.e., the higher the displacement rate or the lower the temperature), the higher  $Z_v$ .

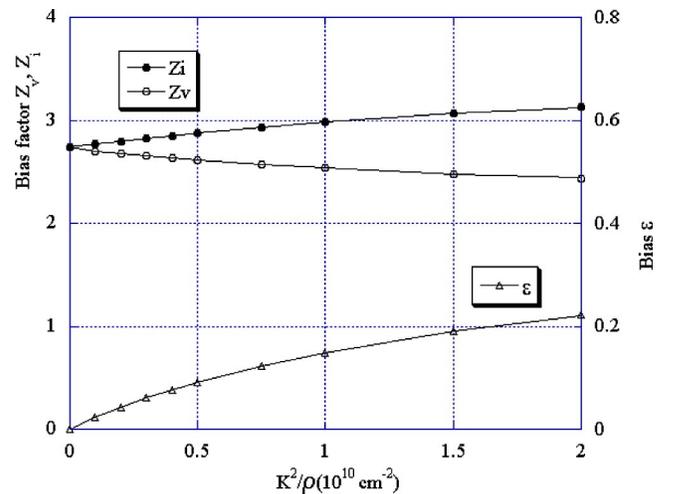


FIG. 8. Same legends as in Fig. 7 ( $\rho = 10^{10}$  cm $^{-2}$  and  $r_d^4 f_0 = 0.1141 \times 10^{-10}$  at 773 K).

In the presence of internal sinks ( $K^2 \neq 0$ ),  $Z_i \neq Z_v$ , the bias  $\varepsilon$  is finite, increases with  $K^2$ , and seems to reach a saturation value only for very large values of  $K^2$  ( $K^2 > 20\rho$ ). At small values of  $K^2/\rho$ , the bias increases linearly with the reduced internal sink strength, with a slope  $\delta\varepsilon/\delta(K^2/\rho)$  which increases from 0.1 at 450 K to 0.2 at 773 K, for  $\rho = 10^{10} \text{ cm}^{-2}$ . For a given dislocation density, the bias increases with the temperature and decreases with the displacement rate.

The bias  $\varepsilon$  thus depends both on the dislocation density and on the internal sink strength and reaches large values (typically 0.10–0.3) when the internal sink strength is twice the dislocation density. On the contrary, the bias is small whenever the internal sink strength is small. As an example, in a material with a grain size of 10  $\mu\text{m}$  and more ( $k_g^2$  of the order of  $10^7 \text{ cm}^{-2}$  or less), with a dislocation density of the order of  $10^9 \text{ cm}^{-2}$  or more, the bias will be negligible: e.g., at 773 K,  $\varepsilon \approx 0.2 k_g^2/\rho = 2 \times 10^{-3}$ . Similarly, at the very early stages of cavity nucleation, the bias is negligible. For instance, for a dislocation density of  $10^{10} \text{ cm}^{-2}$ , if cavities with a radius of 0.1 nm are 15 nm or more apart (i.e.,  $k_c^2$  is of the order of  $10^9 \text{ cm}^{-2}$  and the swelling of the order of  $10^{-3}$ ), the bias will be of the order of  $2 \times 10^{-3}$  at 773 K.

Since we chose the total sink strength in the rate theory to be identical for both defects, the dislocation bias  $\varepsilon$  induces a bias for the cavities. The sink strength of a cavity in the rate theory is now written as:  $k_{c\alpha}^2 = \alpha_{c\alpha}^4 \pi r_c N_c$ . The above discussed low values of the bias point to a possible mechanism of the incubation dose for swelling in cold-worked materials. Indeed the swelling rate is proportional to the bias and the latter is very small for the initial microstructure; it however increases with dose either because the dislocation density decreases (so that  $K^2/\rho$  increases<sup>26,27</sup>) or because the slowly growing void sink strength increases the value of  $K^2/\rho$ . This point deserves further study.

Notice also that, in the classical rate theory, the high values of the bias (0.15–0.25) which are deduced from the elastic theory of dislocation-defect interactions always conflicted with the low values (a few percent) found from empirical fits of swelling rates or defect cluster nucleation rates. The above discussion sheds a new light on this long-standing controversy.

## V. CONCLUSION

We propose that the values to be given to the sink strengths in the rate theory of defect accumulation under irradiation should be such that they give the correct value of the defect elimination yields on each type of sink. Indeed, the latter drive the evolution of the microstructure under irradiation. The sink elimination yields are computed solving, in a cell with appropriate geometry and boundary conditions, the set of coupled nonlinear differential equations which de-

scribe the diffusion of defects, in the presence of a uniform defect production and a local bimolecular recombination reaction, under stationary conditions. When several types of sinks are active, the secondary sinks are modeled by a lossy effective medium in the cell. The study has been performed for the most common sink geometries: thin plates, spherical grains, cavities, and dislocations.

The main results are the following.

(i) The sink strengths, scaled to their classical value, strongly depend on  $l^4 f_0$ , a dimensionless parameter, where  $l$  is a characteristic length (thickness of the plate, radius of the grain, radius of the cavity, core radius of a dislocation) and  $f_0$  depends on the displacement rate and on the temperature via the thermally activated defect diffusion coefficients [Eq. (9)]. The classical values of the sink strengths can be erroneous by several orders of magnitude for large values of  $l^4 f_0$ . Empirical expressions of the reduced sink strengths as a function of  $l^4 f_0$  are given (see captions of Figs. 1–4)

(ii) The presence of secondary internal sinks increases the strength of the primary one. The effect is larger the smaller  $l^4 f_0$ . Typical values are given in Tables I–III.

(iii) The sink strengths as defined are additive.

(iv) The self-consistency of the embedding procedure has been studied in the case of cavities in a spherical grain. Whenever the cavities represent 18%–78% of the overall sink strength, the same values of the sink strengths are obtained, within better than a few percent, smearing out the cavities in the grain or the grain boundary sink strength in the cell around the cavity. The sink strengths so obtained are very close (to better than 1%) to the internal sink-free values of the sink strengths. If the contribution of the grain boundary is very small compared to that of cavities (below 10%), the above result still holds for the cavity and the total sink strength, but not for the grain boundary strength: the discrepancy may reach 50%, at least for small values of  $l^4 f_0$ . For large values of  $l^4 f_0$ , the self-consistency is recovered.

(v) The dislocation bias is computed along the same line. For a given dislocation density, it is found to be an increasing function of the secondary sink strength: in the absence of other sinks, the bias is zero, while it may reach large values (0.1 to 0.4) when the internal sink strength is several times that of the dislocation network. Within the present framework, the dislocation bias induces a bias for the elimination of defects on neutral sinks such as cavities.

The extension of the present method to more complex cases, such as the computation of the sink strengths when several types of biased sinks are competing, remains to be done. The practical implications of the present interpretation of the sink strengths are under study.

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- <sup>28</sup>We assume  $c_i^e = 0$  as is the case in metals. If Frenkel pairs occur at thermal equilibrium,  $c_i^e \neq 0$ , then  $G$  and  $k_i^2 D_i c_i$  on the right-hand sides of Eqs. (1) are replaced, respectively, by  $G + R c_i^e c_v^e$  and  $k_i^2 D_i (c_i - c_i^e)$ .
- <sup>29</sup>It is sometimes claimed that solving the diffusion equation in a hollow sphere yields the sink strength of a void lattice; this is not correct, since the sink strength of a void lattice depends not only on the void radius and the void number density, but also on the lattice geometry [P. Benoist and G. Martin (unpublished)].