DIFFUSION GROWTH OF PORES AND PRISMATIC DISLOCATION LOOPS IN THE PRESENCE OF VOLUME SOURCES OF POINT DEFECTS

A. M. KOSEVICH, Z. K. SARALIDZE, and V. V. SLEZOV

Physico-technical Institute, Academy of Sciences, Ukrainian S.S.R.; Institute of Physics, Academy of Sciences, Georgian S.S.R.

Submitted to JETP editor November 28, 1966

J. Exptl. Theoret. Phys. (U.S.S.R.) 52, 1073-1080 (April, 1967)

A method is proposed for determining the rate of diffusion growth of macroscopic defects (pores or prismatic dislocation loops) in the presence of volume sources of point defects (e.g., radiation). It is shown that, accurate to small quantities, the rates formally have the same form as in the absence of volume sources. It is found that the effect or radiation must be taken into account only to determine the mean concentration of defects in the volume on basis of the total balance of matter.

INTRODUCTION

THE question of the flux of vacancies (or flux of interstitial atoms) through the surface bounding a macroscopic defect[1-7] arises in many physical problems connected with diffusion kinetics of macroscopic defects in a crystal. It is precisely this flux which determines the displacement rate or the growth rate of the defect[6], so that its calculation is of great interest in the analysis of such problems. The magnitude of this flux is connected with the gradient of the concentration of the vacancies (or of the interstitial atoms[1)]) at the indicated surface, and is usually obtained by solving a certain stationary diffusion problem for an individual macroscopic defect in an unbounded crystal at a certain effective supersaturation at infinity[6]. The effective supersaturation is determined in turn by reconciling the diffusion fluxes at all the macroscopic defects in the crystal, a reconciliation which follows from the obvious balance of matter within the solid sample. As a rule, the presence of volume sources of vacancies (generated, for example, by radiation) was taken into account only via the described balance of matter, and the direct influence of volume sources on the character of the solution of the corresponding diffusion problem was not ascertained[2,4]. In other words, the vacancy concentration near the defect was calculated by solving the stationary-diffusion equation without sources.

[1)]We shall henceforth speak, for concreteness, of vacancies even though the entire reasoning extends automatically also to the case of interstitial atoms.

In this paper we analyze the solution of the same problem with sources, and discuss the question of reconciling the problem for an individual macroscopic defect with the problem with diffusion kinetics of a large number of single-type defects in the crystal. The concrete physical cause of the volume vacancy sources does not affect the analysis of this problem. However, we think that the greatest interest attaches to the use of our results for a discussion of different diffusion processes occurring in a crystal exposed to radiation.

To simplify the mathematics we consider only two types of defects: spherical pores and flat prismatic dislocation loops. In these two cases, the high symmetry of the single-defect problem makes it possible to obtain all the final formulas in closed form, thus greatly facilitating their physical analysis.

1. RATE DIFFUSION GROWTH OF A PORE

We consider a system of spherical pores homogeneously distributed in an isotropic medium, the average distance l between which greatly exceeds their radii: $l \gg R_i$, where R_i is the radius of the i-th pore. We assume that the medium contains certain volume sources of vacancies, the average strength of which per unit volume is Q. The change in the dimensions of an individual pore is determined generally speaking both by Q and by the intensity of the diffusion exchange of vacancies with the remaining pores.

If $R_i \ll l$, the distribution of the vacancies near each pore can be regarded as spherically symmetrical, so that the pore will change in size without

changing in shape. The rate of growth of the radius of the i-th pore is

$$\frac{dR_i}{dt} = D\frac{\partial c}{\partial r}\Big|_{r=R_i},$$

where c is the vacancy concentration, D their coefficient of diffusion, and r the length of the radius vector measured from the center of the pore.

If the average pore dimension $\overline{R}$ changes little during the time $\tau \sim l^2/D$ of establishment of the stationary distribution of the vacancies in the system under consideration ($a^3Ql^3\tau \ll \overline{R}^3$), we can assume that the diffusion growth of the pores is a stationary process. Then the function c is the solution of the following diffusion problem:

$$\Delta c = -a^3Q/D, \quad c|_{r=R_i} = c_i, \tag{1}$$

where a is the lattice constant and c_i is the equilibrium concentration of the vacancies at the surface of the i-th pore. As is well known, c_i can always be written in the form

$$c_i = c(R_i) = c_\infty + \alpha/R_i, \tag{2}$$

where c_∞ is the equilibrium concentration at the flat surface and α is a constant connected with the surface tension[1].

When $l \ll \overline{R}$, problem (1) can be approximately reduced to a certain problem involving an individual isolated pore.

By assuming that the diffusion conditions are stationary in the presence of "external" volume sources of vacancies, we assume by the same token that the pores "manage to absorb" all the vacancies created in the volume. But the latter means that it is possible to separate around each pore a certain region (the region of its "influence") possessing the following property: all the vacancies created by the volume sources within this region are absorbed by the given pore, and the vacancies which appear outside this region are absorbed by all the remaining pores. The regions of "influence" of all the pores, naturally, constitute the entire volume of the crystal.

Let us consider now a certain pore of radius R, assuming for simplicity that its region of influence is bounded by a sphere of radius R_0. We can then assume that the concentration of the vacancies around this pore is determined by the solution of the following problem:

$$\begin{array}{ll} \Delta c = -a^3Q/D, & R < r < R_0; \\ \Delta c = 0, & R_0 < r < \infty, \\ c|_{r=R} = c(R), & c_{r=\infty} = \bar{c}, \end{array} \tag{3}$$

where $\bar{c}$ is the average vacancy concentration in the crystal. It is determined both by the stationary distribution of the pore dimensions, and by the magnitude of Q (see[2] concerning this question). In the problem (3), the value of $\bar{c}$ is assumed specified.

By putting $\Delta c = 0$ when $r > R_0$, we have effectively taken into account the fact that outside the sphere of radius $r = R_0$ there are situated regions of influence of the remaining pores, ensuring absorption of all the vacancies created there by the volume sources.

In order to make clear the physical meaning of R_0, we subdivide the problem (3) into two parts, representing the sought-for concentration in the form of the sum

$$c = c_0 + c_1.$$

The first term c_0 describes the distribution of the vacancies around the pores in the absence of volume sources and at a certain effective concentration at infinity:

$$\Delta c_0 = 0, \quad c_0|_{r=R} = c(R), \quad c_0|_{r=\infty} = \bar{c} - c^*. \tag{4}$$

The quantity c_1 is that part of the vacancy concentration which is completely created in the volume. When $r > R_0$ it is constant ($c_1 = c^* = \text{const}$), and when $r < R_0$ it is a solution of the equation

$$\Delta c_1 = -\frac{a^3Q}{D}, \quad c_1|_{r=R} = 0, \quad c_1|_{r=R_0} = c^*. \tag{5}$$

The radius R_0 of the region of influence of the pore is obtained from the condition

$$\frac{dc_1}{dr}\Big|_{r=R_0} = 0. \tag{6}$$

Formally (6) is the requirement of continuity of the flux through the surface $r = R_0$, and physically it reflects the assumption formulated above, that the vacancies created inside the sphere $r = R_0$ are totally absorbed by the pore under consideration.

The solution of the spherically-symmetrical problems (4) and (5) entails no difficulty, so we present the final result for the rate of growth of the pore under the assumption that $R_0 \gg R$:

$$\frac{dR}{dt} = \frac{D}{R}\left[\bar{c} - c(R) + \frac{1}{2}\frac{a^3}{D}QR_0^2(R)\right]. \tag{7}$$

Using now (6), we get in the same approximation:

$$R_0^3(R) = \frac{3D}{a^3Q}c^*R. \tag{8}$$

The average vacancy concentration c*, which is maintained by the work of the volume sources, is not determined in problems (4) and (5) if each is considered separately. However, returning to the

initially formulated general problem, we should stipulate that c* be the same for all pores, that is, that this constant be independent of the radius R of the pore. Then we can write together with (8)

$$\overline{R_0^3} = \frac{3D}{a^3 Q} c^* \bar{R},$$

where $\bar{R}$ is the average radius of the pores. But since the total volume of all the regions of influence of the individual pores is equal to the volume of the body, we have $(4/3)\pi \overline{R_0^3} = l^3$ and we get, eliminating c* from (8),

$$4/3\pi R_0^3 = l^3 R/\bar{R}. \tag{9}$$

Thus, the volume of the region of influence of each pore is proportional to its radius. Formulas (7) and (9) give the approximate solution of our problem of determining the growth rate of the pore in the presence of irradiation. A unique feature is that, regardless of the sign of the difference $\bar{c} - c_\infty$, there can exist pores with radii such that they must grow when exposed to radiation. However, in all problems where the supersaturation of the vacancies is stationary ($d\bar{c}/dt = 0$[2)]), the last term in the right side of (7) is on the average very small. Indeed, we write the condition for conservation of matter:

$$4\pi \int f(R) \frac{dR}{dt} R^3 dR = a^3 Q, \quad N = \int f(R)\, dR, \tag{10}$$

where f(R) is the distribution density of the pore radii and N is the average number of pores per unit volume of the body ($N = l^{-3}$). Substituting (7) in (10) we get

$$\bar{c} - c(\bar{R}) = \frac{a^3}{4\pi D} Q \frac{N}{R} \left[1 - \int f(R) R_0^2(R) R\, dR \right]. \tag{11}$$

Inasmuch as $R \ll \bar{R}_0 \sim l$, it follows from (11) that

$$\bar{c} - c(\bar{R}) = \frac{a^3}{4\pi D} Q \frac{l}{\bar{R}} l^2 \gg \frac{a^3}{4\pi D} Q l^2 \sim \frac{a^3}{4\pi D} Q R_0^2. \tag{12}$$

Thus, when $d\bar{c}/dt = 0$, the average value of the last term in the right side of (7) is indeed small, and the corresponding formula for the growing pores can be written in the usual form[1,2]:

$$\frac{dR}{dt} = \frac{D}{R} [\bar{c} - c(R)],$$

Recalling that the difference $\bar{c} - c(R)$ is determined entirely by the volume sources of the vacancies in accord with formula (12).

[2)]This condition may not be required if the characteristic time of variation of the strength of the sources greatly exceeds the time of establishment of the stationary regime.

2. GROWTH RATE OF PRISMATIC DISLOCATION LOOPS

Analyzing the diffusion development of prismatic dislocations, we confine ourselves to two limiting cases.

A. Loops of small dimensions. We consider a system of circular prismatic dislocations, the radii R of which are small compared with the average distances between loops l ($R \ll l$), and assume that the diffusion fluxes of the vacancies are stationary (the condition for the latter assumption differs somewhat from the similar assumption in the case of spherical pores: $a^3 Q l^3 \tau \ll b\bar{R}^2 = a\bar{R}^2$, where $\bar{R}$ is the average radius of the loop and b = a is the Burgers vector of the dislocation). Then the problem of the diffusion growth of the dislocation loop can be solved in exactly the same manner as the corresponding problem in the preceding section.

For concreteness we assume that the prismatic dislocation encompasses a section of an "unfinished" atomic plane. Then, in the sense of interaction with the vacancies, it will behave like a pore, except that the equilibrium concentration of the vacancies on the dislocation line is[3]

$$c_s(R) = c_\infty + \frac{\Omega}{R} \ln \frac{R}{r_0} + \frac{\beta}{R}, \quad \Omega = \frac{a c_\infty}{4\pi(1-\nu)} \frac{a^3 G}{kT}, \tag{13}$$

where β is a constant that takes into account the linear energy of the dislocation, G is the shear modulus, and ν is the Poisson coefficient.

Repeating the formulation of the problem (3), we must take into account the fact that the "surface" of the dislocation should be regarded to be surface of the toroid enclosing the dislocation loop (its parameters are R and r_0). We shall henceforth denote the surface by S. If we separate c into two parts, $c = c_0 + c_1$, then the internal boundary problem for the problem determining the vacancy distribution c_0 in the absence of volume sources (a problem analogous to (4) in the Sec. 1), should also be specified on the surface S. A similar problem was solved by us earlier[3], so that we shall focus our attention to an approximate determination of the concentration component c_1 due to the volume sources.

The function c_1 is determined by solving a problem such as (5), in which the internal boundary condition is specified on the surface S. The difficulty of solving the problem of finding the function c_1 is purely technical: the dislocation (circular loop of radius R) and the boundary of its region of influence (sphere of radius R_0) have different symmetries. However, in view of the smallness of the

ratio R/R_0, we can solve this problem approximately. We note first that the contribution of the gradient c_1 to the growth rate of the loop will be determined by the formula

$$\left(\frac{dR}{dt}\right)_1 = \frac{a^2 I}{2\pi R}, \tag{14}$$

where I is the total vacancy flux through the surface S due to the gradient c_1. However, from the Gauss theorem we have on the basis of (5) and (6)

$$I = \frac{4\pi}{3} R_0^3 Q, \tag{15}$$

therefore

$$\left(\frac{dR}{dt}\right)_1 = \frac{2}{3} Q \frac{R_0^3}{R} a^2. \tag{16}$$

Formula (15) contains the still unknown radius R_0 of the influence region. Its connection with the concentration c^*, which is maintained by generation of vacancies by the volume sources, should be obtained from the condition (6). Satisfying this condition, we use a relation, well known from electrostatics, between the field of a charge sphere of radius R and the field of a charged circular filament of the same radius. If the potential of the sphere (and of the filament, respectively) is specified and is equal to φ_0, then at large distances from the field sources ($r \ll R$) the potentials are respectively equal to

$$\varphi_s = \varphi_0 \frac{R}{r}, \quad \varphi_f = \varphi_0 \xi \frac{R}{r}, \quad \xi \equiv \pi / \ln \frac{8R}{r_0},$$

where r_0 is half the thickness of the filament. Thus, for a specified potential on a sphere of radius R or on an annular filament of radius R, the potentials far from them differ by a factor ξ equal to the ratio of the electrostatic capacitances of the filament and of the sphere.

But since the problem (5) for the dislocation loop differs from that for a spherical pore only in the form of the internal surface on which the source-free concentration is specified, the concentration distribution far from the loop (when $r \gg R$) differs from that discussed in Sec. 1 only in that c^* is replaced by $c^*\xi$. Making this substitution and using (8), we can write down immediately

$$\left(\frac{dR}{dt}\right)_1 = \frac{2Dc^*}{a} \xi. \tag{17}$$

Naturally, in such a calculation we neglect all the powers of the small parameter R/R_0.

Combining (17) with the growth rate of the dislocation loop obtained in[3], we write down the final formula

$$\frac{dR}{dt} = \frac{2\pi D}{a \ln (8R/r_0)} [\bar{c} - c_s(R)]. \tag{18}$$

We see that formula (18) does not differ at all from that in[3], apart from the powers of the small parameter R/R_0. Consequently, the entire influence of the irradiation should be taken into account only via the balance of matter, which determines the average concentration c.

B. Loops of large dimensions. We now proceed to consider the case when the distance between the dislocation lines is much smaller than the radii of their curvature: $l \ll \overline{R}$. Such a situation corresponds to a strongly developed diffusion plastic flow of material.

In extending the method developed above to this case, we note that a certain section of the dislocation can be regarded, to some degree, as independent only over a length of the order of l, that is, over the section in which it is linear ($l \ll \overline{R}$). Therefore, in analyzing the diffusion problem we shall assume that the dislocations are straight lines and assume further that each element of the dislocation lines absorbs all the vacancies generated by the volume sources inside a certain cylinder of radius R_0, the axis of which coincides with the center of the dislocation. The radius R_0 should be chosen, as before, to satisfy the condition that the described regions comprise the entire volume of the crystal. We represent, before, the sought-for concentration in the form of a sum, $c = c_0 + c_1$, the first term of which is determined in the same way as in the case of small loops (using the results of[3]), and the second is a solution of a problem analogous to (5). By virtue of the condition $R_0 \ll \overline{R}$, the function of the coordinates c_1 can be regarded as having cylindrical symmetry, therefore the corresponding problem for it will be solved in cylindrical coordinates

$$\frac{1}{\rho} \frac{d}{d\rho} \rho \frac{dc_1}{d\rho} = -\frac{a^3}{D} Q, \quad \rho < R_0,$$
$$c_1|_{\rho=r_0} = 0, \quad c_1|_{\rho=R_0} = c^*, \quad \left.\frac{dc_1}{d\rho}\right|_{\rho=R_0} = 0, \tag{19}$$

where ρ is the distance from the dislocation axis. With the aid of the Gauss theorem we can easily find on the basis of (19) the contribution of the gradient c_1 to the vacancy flux per unit length of the dislocation line:

$$j_1 = \frac{2\pi r_0}{a^3} D \left.\frac{dc_1}{d\rho}\right|_{\rho=R_0} = \pi R_0^2 Q. \tag{20}$$

We note that the analogous flux, due to the gradient c_0, is[3,5]

$$j_0 = \frac{2\pi D}{a^3 \ln(8R/r_0)}[\bar{c} - c^* - c_s(R)]. \qquad (21)$$

The summary flux $j = z_0 + j_1$ determines the rate of "climbing" of the corresponding elements of the dislocation line. It is characteristic that the individual terms in the total flux j have generally speaking different dependences on the point on the dislocation line. Whereas j_0 is by definition the same for all points of a circular dislocation, the second term j_1 is in principle different for different sections of the same loop, since R_0 is determined not so much by the radius of the loop as by the surrounding of the element under consideration. We shall, however, take into account, first, the circumstance that during the growth of the loop each of its elements goes over from one surrounding to another, and, second, the fact that the linear diffusion along the dislocation line, which greatly exceeds the volume diffusion, rapidly restores the circular form of the loop, equalizing the rates of motion of its individual elements. These considerations allow us to consider, in lieu of the instantaneous local R_0, an average quantity which is the same for all elements of one dislocation, meaning the same for all the dislocation loops. This quantity can be determined from the condition formulated above, according to which the regions of influence of the dislocations overlap the volume of the entire crystal:

$$R_0^2 = \frac{1}{2\pi^2 \bar{R} N} = \frac{\omega}{2\pi^2 \bar{R}}, \qquad (22)$$

where N is the total number loops per unit volume and ω is the average volume per loop.

Inasmuch as we have already determined the radius R_0, which is the same for all dislocations, then the concentration c^* maintained by the work of the volume sources, should be obtained from the boundary conditions in the problem (19). An elementary calculation leads to the following result:

$$c^* = \frac{a^3 Q}{2D} R_0^2 \ln \frac{\gamma R_0}{r_0}, \quad \ln \gamma = -\frac{1}{2}. \qquad (23)$$

Substituting (23) in (21), we calculate the summary flux of the vacancies per unit dislocation length:

$$j = \frac{2\pi D}{a^3 \ln(8R/r_0)} \left[\bar{c} - c_s(R) + \frac{a^3 Q}{2D} R_0^2 \ln \frac{8R}{\gamma R_0}\right]. \qquad (24)$$

Inasmuch as the last term in (24) has been introduced as a certain effective mean value, we replace in it the radius of the loop by its average value $\bar{R}$, and then we obtain for the flux j the formula

$$j = \frac{2\pi D}{a^3 \ln(8R/r_0)} \{c_{\text{eff}} - c_s(R)\}, \qquad (25)$$

where

$$c_{\text{eff}} = \bar{c} + \frac{a^3 Q}{2D} R_0^2 \ln \frac{8\bar{R}}{\gamma R_0}. \qquad (26)$$

Thus, it turns out that in the presence of volume sources of point defects, the total flux per dislocation has formally the same form as without the sources[3,5], the only difference being that it is determined now by a certain effective concentration, connected with the average concentration by the simple relation (26).

It is easy to show, starting from the condition of conservation of matter ($j \approx \pi R_0^2 Q$) that on the average the ratio is

$$\frac{a^3 Q}{2D} \ln \frac{8\bar{R}}{\gamma R_0} \cdot R_0^2 / (\bar{c} - c_s(R)) \approx \left(\ln \frac{8\bar{R}}{r_0}\right)^{-1} \ll 1,$$

and therefore with the same accuracy we have $c_{\text{eff}} = \bar{c}$, and the same expression as before holds for the growth rate of the loop.

So far we have discussed only the vacancy fluxes per dislocation, without taking into account the interstitial atoms. If we consider the fluxes of defects of both types, then it turns out that the explicit expression for the rate of growth of the dislocation loop is

$$v(R) = a^2 D^* A \left[\Delta^* - \frac{B(R)}{R}\right], \qquad (27)$$

where

$$\Delta^* = \frac{1}{D^*} \{(c^{\text{v}}_{\text{eff}} - c_0{}^{\text{v}}) D^{\text{v}} - (c^{\text{i}}_{\text{eff}} - c_0{}^{\text{i}}) D^{\text{i}}\},$$

$$A = \frac{2\pi}{a^3} \frac{1}{\ln(8\bar{R}/r_0)},$$

$$B(R) = \frac{a}{4\pi(1-\nu)} \frac{a^3 G}{kT} \ln \frac{R}{r_0}, \quad D^* = c_0{}^{\text{v}} D^{\text{v}} + c_0{}^{\text{i}} D^{\text{i}},$$

c_0 are the equilibrium concentrations, and the superscripts "i" and "v" pertain respectively to the interstitial atoms and vacancies.

We note that inasmuch as $c_{\text{eff}} - \bar{c} \sim Q$, the difference between Δ^* and the same quantity in[3] is proportional to the difference $Q^{\text{v}} - Q^{\text{i}}$. In other words, allowance for the volume sources of the point defects in calculating the rate of growth of the dislocations is essential only inasmuch as $Q^{\text{v}} - Q^{\text{i}} \neq 0$.

Let us indicate finally the conditions under which our conclusions are correct. We have assumed that the diffusion is stationary. This is valid when the change in the dimension of the dislocation loop during the time τ of establishment of the stationary fluxes ($\tau \sim l^2/D$) is small compared with its radius. Being interested in the conditions

imposed on the radiation intensity, let us consider the change in the loop radius due to the volume sources. From (27) it follows that

$$\frac{\delta R}{R} = \frac{v\tau}{\bar{R}} \sim \frac{2\pi a^2 R_0^2}{\bar{R}} |Q^v - Q^i| \frac{l^2}{D} \sim \left(\frac{al}{\bar{R}}\right)^2 |Q^v - Q^i| \frac{\omega}{D}.$$

Thus, the intensity of production of point defects should be bounded by the requirement

$$|Q^v - Q^i| \omega \ll D(\bar{R}/al)^2.$$

In conclusion, we thank I. M. Lifshitz for a useful discussion of the work.

[1] I. M. Lifshitz and V. V. Slezov, JETP 35, 479 (1958), Soviet Phys. JETP 8, 247 (1959).

[2] V. V. Slezov and V. B. Shikin, FTT 6, 7 (1964), Soviet Phys. Solid State 6, 5 (1964).

[3] A. M. Kosevich and Z. K. Saralidze, and V. V. Slezov, ibid. 6, 3383 (1964), transl. 6, 2707 (1965).

[4] Z. K. Saralidze and V. V. Slezov, ibid. 7, 904 (1965), transl. 7, 718 (1965).

[5] A. M. Kosevich, I. G. Margvelashvili, and Z. K. Saralidze, FTT 7, 464 (1965), transl. 7, 370 (1965).

[6] I. M. Lifshitz, A. M. Kosevich, and Y. E. Gegusin, J. Phys. Chem. Solids, in press.

[7] A. M. Kosevich, Z. K. Saralidze, and V. V. Slezov, JETP 50, 958 (1966), Soviet Phys. JETP 23, 636 (1966).

Translated by J. G. Adashko
134