Kinetic equation for vacancion pores. Pore lattice as a dissipative structure stable under irradiation conditions

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A closed kinetic equation is obtained for the evolution of vacancion (ion vacancy) pores in dimension space and in coordinate space. The diffusion interaction of pores in an ensemble is considered, with account taken of the microscopic processes that occur near and on the surfaces of the pores. Kinetic equations are calculated for the growth rate and velocity of the pores and for the pore diffusion coefficient in coordinate space and in the pore-dimension space. The influence exterted on these coefficients by deformations of the activation barriers in the pore surface layer is investigated. The obtained kinetic equation is used to determine the region of stability of a lattice of vacancion pores with respect to the growth of the pores and with respect to displacements of the pores from the lattice sites.

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1. INTRODUCTION

Experiment[1] has revealed an interesting physical phenomenon in metals irradiated by particles of sufficiently high energy, namely the formation of vacancion pores in these metals at high irradiation temperatures ($T \gtrsim 0.3T_S$, where T_S is the melting temperature of the metal). Vacancion (ion vacancy) pores are clusters or, as they are frequently called, "negative crystals," consisting of a large number of vacancies and measuring tens and hundreds of periods of the crystal lattice of the metal. Vacancion porosity exerts a substantial influence on various physical properties of metals, particularly on their endurance to radiation. In addition, this phenomenon is of general physical interest as a model system that can be used to develop methods of investigating the kinetics of first-order phase transitions.

To describe the kinetics of the nucleation and growth of vacancion pores it is customary to use the well known Zel'do-vich kinetic equation[2] (see also Ref. 3) used to study the kinetics of condensation of supersaturated vapor and the boiling-up of a superheated liquid. In the theory of formation of vacancion pores, this equation describes the evolution of the change of the pore-dimension distribution in homogeneous space. For a more complete investigation of the kinetics of vacancion pairs in crystals it is necessary to use a kinetic equation capable of describing the variation of the pore distribution not only in size but also in space. The latter is particularly important for the study of the formation kinetics and of the stability of an ordered periodic lattice of vacancion pores, which was experimentally observed in a number of metals.[4] An interesting feature of this dissipative structure is that the pore lattice has a macroscopic period amounting to several hundred angstroms, while the average radius of the pores located at the sites of this lattice is equal to dozens of angstroms. However, no kinetic equation has been derived so far for the description of an inhomogeneous distribution of the pores in space.

We derive in this paper a kinetic equation that describes the kinetics of an ensemble of vacancion pores in an inhomogeneous space, with account taken of the microscopic processes that take place near and on the surfaces of the pores (see also Ref. 5). The latter is particularly important, since it is known[6] that the coefficient of surface diffusion of vacancies exceeds the coefficient of volume diffusion by several orders of magnitude. We consider separately the motion of a selected pore in the inhomogeneous field due to the gradient of the vacancy concentration. In a somewhat different formulation of the problem, a similar motion of pores was considered earlier by Krivoglaz.[6] We consider also in this paper the influence of the diffusion interaction of vacancion pores on the growth rate and displacement of the pores in space.[7] The results are used to investigate the stability of a pore lattice. Diffusion interaction of the pores, as a mechanism that governs the stability of a pore lattice, was proposed in our previous paper,[7] and also independently by Martin and Benoist.[8]

2. KINETIC EQUATION FOR THE EVOLUTION OF VACANCION PORES IN INHOMOGENEOUS SPACE

Vacancion pores in crystals are accumulations of vacancies that form clusters in the form of vacancion cavities that measure up to a thousand periods of the initial crystal lattice. The surface of a pore has in the general case crystalline faceting and possesses a definite structure. In crystals with weak anisotropy, the pore surface can be regarded as close to spherical. In an ensemble of pores, each vacancion pore will be characterized by the position r of its center of gravity and by the number m of vacancies of which it is made up ($m = 4\pi R_m^3/3\omega_v$, where R_m is the radius of the pore and ω_v is the volume per vacancy), and we shall designate this pore by the symbol $A(\mathbf{r}, m)$. In the derivation of the kinetic equation, we shall consider for simplicity the evolution of an ensemble of pores in a space in which is located a supersaturated gas of point defects, of only one type namely vacancies. Allowance for the interstitial atoms in the derivation of the kinetic equation, as can be easily seen does not change the qualitative picture of the pore evolution, but this allowance would greatly encumber the physical model. Therefore interstitial atoms will be disregarded in the present paper. We shall denote hereafter a free vacancy by the symbol V.

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Since the pore dimension $R_m \gtrsim \lambda$ (where $\lambda \approx a$ is the vacancy mean free path and is close to the period a of the crystal lattice), it follows that near each pore there exists an inhomogeneous vacancy distribution that can be represented in the form of a vacancy-gas cloud. The vacancy distribution in this inhomogeneous cloud is characterized by the quantity $C(\mathbf{R}, \mathbf{r}, m)$, which determines the probability of finding the vacancy at the point $\mathbf{R}$ near the pore $A(\mathbf{r}, m)$. The vacancy concentration $C(\mathbf{R}, \mathbf{r}, m)$ is normalized in such a way, that the quantity

$$\int \frac{d^3R}{\omega_v} C(\mathbf{R}, \mathbf{r}, m)$$

represents the total number of vacancies in the volume over which the integration is carried out ($\omega_v \approx a^3$ is the volume per vacancy). The vacancy density near each pore depends in a self-consistent manner on the arrangement and on the evolution of the distribution of the pores in space.

We shall describe an ensemble of vacancion pores with the aid of a distribution function $f(\mathbf{r}, m, t)$ that determines the number density, at the point $\mathbf{r}$, of pores consisting of m vacancies at the instant of time t. The distribution function $f(\mathbf{r}, m, t)$ is normalized to the total number $N(t)$ of the pores in the crystal:

$$\int d^3r \int dm f(\mathbf{r}, m, t) = N(t).$$

To obtain a kinetic equation that describes the evolution of an ensemble of pores it is necessary to formulate a model of the processes that occur near and on the surfaces of the pores. The displacement of the pores in space and their growth as a whole are determined by microscopic processes that take place in near-surface layers of the pores and are analogous to the processes that take place in crystal growth.

The pore surface is crystalline and has, like a crystal surface, a structure in the form of an essembly of terraces with steps and breaks on them.[9] On the surface of the terraces are located surface vacancies and adsorbed atoms, which diffuse over this surface. For simplicity we shall henceforth neglect the influence of the adsorbed atoms on this process, although it is not difficult to take them into account.

The diffusion of the vacancies towards the pore and their settling on the pore lead to displacement and to growth of the pores. For large pores this process proceeds in several stages. The vacancies land first on the surface of the terrace by volume diffusion. Next, they land on the steps by surface diffusion over the terrace, and from there, by linear diffusion along the steps, they settle on the breaks of the steps and vanish. In addition, the inverse process of fluctuation detachment of vacancies from the break at the steps takes place. The principal processes that lead to a change in the distribution of the pores in a supersaturated vacancy gas are the following: condensation I_P, evaporation I_Q, and surface diffusion I_S of the vacancies as well as, generally speaking, pore coagulation I_C. We therefore have

$$\partial f(\mathbf{r}, m, t)/\partial t = -I_P - I_Q - I_S - I_C. \tag{2.1}$$

We consider now these processes separately.

In condensation, a vacancy from the near-surface layer lands on the surface of the pore. This process leads to an increase in the number of vacancies in the pore $A(\mathbf{r}, m)$ by unity and to a displacement of the center of gravity of the pore by an amount $\delta\mathbf{r}$. This process can be schematically represented in the form

$$A(\mathbf{r}, m) + V \rightarrow A(\mathbf{r} + \delta\mathbf{r}, m+1),$$

where $\delta\mathbf{r} = \mathbf{R}_s/m$, $\mathbf{R}_s$ is a vector directed from the center to the surface of the pore and characterizing the position of the vacancies on the surface of the pore ($|\mathbf{R}_s| = R_m$).

We denote by $W_{VS}(\mathbf{R} \rightarrow \mathbf{R}_s, \mathbf{r}, m)$ the probability, per unit time, of a vacancy hopping over from the point $\mathbf{R}$ to the point $\mathbf{R}_s$ on the surface of the pore via volume diffusion. Actually, the motion of the vacancies proceeds in discrete fashion: the vacancies hop over from one side to another. However, bearing in mind the probabilistic character of the description of the vacancy motion and of the evolution of the pore ensemble, which shall hereafter by regarded as continuous the medium through which the vacancies move, implying throughout averaging over the microscopic fluctuations of the crystal structure and of the pore surface.

For convenience in the subsequent calculations, we shall hereafter represent the integration of a certain function $F(\mathbf{R}_s)$ over the surface of a pore in one of three forms:

$$\int d^2R_s F(\mathbf{R}_s) = \int d^3R F(\mathbf{R}) \delta(R - R_m) = \int dx^1 dx^2 g^{1/2} F(\mathbf{R}_s),$$

where $(d\mathbf{R}_s)^2 = g_{\alpha\beta} dx^\alpha dx^\beta$, $g_{\alpha\beta}$ is a metric covariant tensor ($\alpha, \beta = 1, 2$).[10] The probability of condensation of one vacancy by the pore $A(\mathbf{r}, m)$ then takes the form

$$\int d\Gamma_P = \int \frac{d^2R_s}{\omega_s} \int \frac{d^3R}{\omega_v} C(\mathbf{R}, \mathbf{r}, m) W_{VS}(\mathbf{R} \rightarrow \mathbf{R}_s, r, m), \tag{2.2}$$

where ω_s is the area per vacancy ($\omega_s \approx a^2$). In this and the following expressions, the integration over d^3R extends over the region $R > R_m$.

The distortions of the near-surface layer can be due, e.g., to the pore's own dilatation or to a deformation due to impurity atoms that can settle on the surface of the pore.[11] These distortions alter substantially the activation barriers of the volume diffusion of the vacancies. The thickness of the near-surface layer can amount to several lattice periods.[6] For simplicity, however, we shall consider a surface layer in the form of one monolayer, inasmuch as the use of excessive details of the model increases the number of the parameters without changing the qualitative picture of the phenomenon. The integration over d^3R in (2.2) is therefore over a surface layer of thickness on the order of the vacancy mean free path.

The process of condensation of the vacancies leads to the following change, per unit time, of the density of pores consisting of m vacancies:

$$\begin{aligned} I_P = \int \frac{d^3R}{\omega_v} \int \frac{d^3R'}{\omega_v} \{ & C(\mathbf{R}', \mathbf{r}, m) W_{VS}(\mathbf{R}' \rightarrow \mathbf{R}, \mathbf{r}, m) \delta(R - R_m) \\ \times & (\mathbf{r}, m) - C(\mathbf{R}', \mathbf{r} - \delta\mathbf{r}, m-1) W_{VS}(\mathbf{R}' \rightarrow \mathbf{R}, r - \delta\mathbf{r}, m-1) \\ & \times \delta(R - R_{m-1}) f(\mathbf{r} - \delta\mathbf{r}, m-1) \}. \end{aligned} \tag{2.3}$$

The last term in this expression describes the condensation of one vacancy on a pore consisting of $m-1$ vacancies, with arrival of the pore in the state $A(\mathbf{r}, m)$:

$$A(\mathbf{r}-\delta\mathbf{r}, m-1)+V\to A(\mathbf{r}, m).$$

We shall assume that the pore distribution $f(\mathbf{r}, m)$ is weakly inhomogenous and changes little when the number of vacancies in the pore changes by unity. Then the expression (2.3) is reduced in the usual manner to the Fokker-Planck form:

$$I_P=\frac{\partial}{\partial m}(J_Pf)+\nabla(\mathbf{v}_Pf)-\frac{1}{2}\frac{\partial^2}{\partial m^2}(J_Pf)-\frac{\partial}{\partial m}\nabla(\mathbf{v}_Pf)-\nabla_i\nabla_k(\mathscr{D}^{ik}f). \quad (2.4)$$

Here

$$J_P=\int d\Gamma_P, \quad \mathbf{v}_P=\int d\Gamma_P\delta\mathbf{r}, \quad \mathscr{D}_P{}^{ik}=\frac{1}{2}\int d\Gamma_P\delta r^i\delta r^k. \quad (2.5)$$

We consider now the contribution of evaporation of vacancies from the surface of the pores to the change of the distribution function $f(\mathbf{r}, m)$. Evaporation of a vacancy changes the pore $A(\mathbf{r}, m)$ over to the state $A(\mathbf{r}-\delta\mathbf{r}, m-1)$:

$$A(\mathbf{r}, m)\to A(\mathbf{r}-\delta\mathbf{r}, m-1)+V.$$

Therefore the probability per unit time of evaporation of one vacancy from the pore $A(\mathbf{r}, m)$ in the surface layer will be written in the form

$$\int d\Gamma_Q=\int\frac{d^2R_s}{\omega_s}\int\frac{d^3R}{\omega_v}C_S(\mathbf{R}_s, \mathbf{r}, m)W_{SV}(\mathbf{R}_s\to\mathbf{R}, \mathbf{r}, m), \quad (2.6)$$

where $W_{SV}(\mathbf{R}_s\to\mathbf{R}, \mathbf{r}, m)$ is the probability of vacancy jump per unit time from the point $\mathbf{R}_s$ of the surface of the pore $A(\mathbf{r}, m)$ to the point $\mathbf{R}$ of its near-surface layer. In the general case, owing to deformations of the surface layer of the pore, the evaporation and condensation probabilities W_{SV} and W_{VS} are not equal.

The arrival of the pores in the state $A(\mathbf{r}, m)$ as the result of evaporation of one vacancy by a pore consisting of $m+1$ vacancies is described by the process

$$A(\mathbf{r}+\delta\mathbf{r}, m+1)\to A(\mathbf{r}, m)+V.$$

The change, per unit time, of the distribution function $f(\mathbf{r}, m)$ as a result of evaporation of vacancies from the surface of the pores is expressed in the form

$$\begin{aligned}I_Q=\int\frac{d^3R}{\omega_s}\int\frac{d^3R'}{\omega_v}\{&C_S(\mathbf{R}, \mathbf{r}, m)W_{SV}(\mathbf{R}\to\mathbf{R}', \mathbf{r}, m)\delta(R-R_m)f(\mathbf{r}, m)\\ &-C_S(\mathbf{R}, \mathbf{r}+\delta\mathbf{r}, m+1)W_{SV}(\mathbf{R}\to\mathbf{R}', \mathbf{r}+\delta\mathbf{r}, m+1)\cdot\\ &\cdot\delta(R-R_{m+1})f(\mathbf{r}+\delta\mathbf{r}, m+1)\}.\end{aligned} \quad (2.7)$$

For pores consisting of a large number of vacancies ($m\gg1$) and having small center-of-gravity displacements ($\delta r/r\ll1$), expression (2.7) can be simplified to

$$I_Q=-\frac{\partial}{\partial m}(J_Qf)+\nabla(\mathbf{v}_Qf)-\frac{1}{2}\frac{\partial^2}{\partial m^2}(J_Qf)+\frac{\partial}{\partial m}\nabla(\mathbf{v}_Qf)-\nabla_i\nabla_k(\mathscr{D}_Q{}^{ik}f), \quad (2.8)$$

where the coefficients J_Q, $\mathbf{v}_Q$, and $\mathscr{D}_Q^{ik}$ are given by

$$J_Q=\int d\Gamma_Q, \quad v_Q=-\int d\Gamma_Q\delta\mathbf{r}, \quad \mathscr{D}_Q{}^{ik}=\frac{1}{2}\int d\Gamma_Q\delta r^i\delta r^k. \quad (2.9)$$

The motion of the vacancies over the surface of the pores does not change the dimension of the pores, but causes them to be displaced. This process can be represented in the form

$$A(\mathbf{r}, m)+V(\mathbf{R}_s)\to A(\mathbf{r}+\delta\mathbf{r}_s, m)+V(\mathbf{R}_s'), \quad (2.10)$$

where $\delta\mathbf{r}_s=(\mathbf{R}_s-\mathbf{R}_s')/m$ and $V(\mathbf{R}_s)$ characterizes a vacancy located on the surface of the pore at the point $\mathbf{R}_s$.

The arrival of the vacancy over the surface of the pore at the point $\mathbf{R}_s$ is the inverse of the process (2.10):

$$A(\mathbf{r}+\delta\mathbf{r}_s, m)+V(\mathbf{R}_s')\to A(\mathbf{r}, m)+V(\mathbf{R}_s).$$

The process of surface diffusion of vacancies is described by the combined probability of the hopping of the vacancy from one point on the surface of the pore to another, which is equal to

$$\int d\Gamma_S=\int\frac{d^2R_s}{\omega_s}\int\frac{d^2R_s'}{\omega_s}C_S(\mathbf{R}_s', \mathbf{r}, m)W_{SS}(\mathbf{R}_s'\to\mathbf{R}_s, \mathbf{r}, m), \quad (2.11)$$

where $W_{SS}(\mathbf{R}_s'\to R_s, \mathbf{r}, m)$ is the probability of the hopping of one vacancy per unit time via surface diffusion over the surface of the pore $A(\mathbf{r}, m)$ from the point $\mathbf{R}_s'$ to the point $\mathbf{R}_s$. The contribution of the surface diffusion to the evolution of the distribution function $f(\mathbf{r}, m)$ can then be represented in the form

$$\begin{aligned}I_S=\int\frac{d^2R_s}{\omega_s}\int\frac{d^2R_s'}{\omega_s}\{&C_S(\mathbf{R}_s, \mathbf{r}, m)W_{SS}(\mathbf{R}_s\to\mathbf{R}_s', \mathbf{r}, m)f(\mathbf{r}, m)\\ &-C_S(R_s', \mathbf{r}+\delta\mathbf{r}_s, m)W_{SS}(\mathbf{R}_s'\to\mathbf{R}_s, \mathbf{r}+\delta\mathbf{r}_s, m)f(\mathbf{r}+\delta\mathbf{r}_s, m)\}.\end{aligned}$$

Expanding this expression in terms of $\delta\mathbf{r}_s$, we obtain

$$I_S=\nabla(\mathbf{v}_Sf)-\nabla_i\nabla_k(\mathscr{D}_S{}^{ik}f), \quad (2.12)$$

where the coefficients $\mathbf{v}_S$ and $\mathscr{D}_S^{ik}$ are equal to

$$\mathbf{v}_S=-\int d\Gamma_S\delta\mathbf{r}_s, \quad \mathscr{D}_S{}^{ik}=\frac{1}{2}\int d\Gamma_S\delta r_s{}^i\delta r_s{}^k. \quad (2.13)$$

Finally, we present the known expression for the change of the distribution of the pores as a result of coagulation (see, e.g., Ref. 6):

$$\begin{aligned}I_C=\int dm'\Big\{&W_C(m, m'\to m+m')f(\mathbf{r}, m)f(\mathbf{r}, m')\\ &-\frac{1}{2}f(\mathbf{r}, m-m')f(\mathbf{r}, m')W_C(m-m', m'\to m)\Big\},\end{aligned}$$

where $W_C(m, m'\to m+m')$ is the probability of pore collision per unit time with transition of two pores from dimensions m and m' into a dimension $m+m'$.

Gathering expressions (2.4), (2.8), and (2.12) into expression (2.1) and taking (2.5), (2.9), and (2.12) to into account, we obtain the general form of the kinetic equation for the pore distribution function

$$\begin{aligned}\frac{\partial f(\mathbf{r}, m)}{\partial t}=&-\frac{\partial}{\partial m}(\dot{m}f)-\nabla(\mathbf{v}f)+\frac{\partial^2}{\partial m^2}(Jf)\\ &+\frac{\partial}{\partial m}\nabla((\mathbf{v}_P-\mathbf{v}_Q)f)+\nabla_i\nabla_k(\mathscr{D}^{ik}f)-I_C.\end{aligned} \quad (2.14)$$

The kinetic coefficients in this equation are equal to

$$\begin{aligned}&\dot{m}=J_P-J_Q, \quad \mathbf{v}=\mathbf{v}_P+\mathbf{v}_Q+\mathbf{v}_S,\\ &J=(J_P+J_Q)/2, \quad \mathscr{D}^{ik}=\mathscr{D}_P{}^{ik}+\mathscr{D}_Q{}^{ik}+\mathscr{D}_S{}^{ik}.\end{aligned} \quad (2.15)$$

What is new in this equation is the term with the mixed derivative. This term can be understood if all the terms with the derivative with respect to m are grouped in the form $-\partial I_m/\partial m$, where

$$I_m=\dot{m}f-\frac{\partial}{\partial m}(Jf)-\operatorname{div}[(\mathbf{v}_P-\mathbf{v}_Q)f].$$

We see that the non-uniform distribution of the pores leads to an additional flux of pores in dimension space, i.e., the number of pores of given dimension at a given point of space changes not only on account of diffusion processes at the given point, but also on account of the spatial displacement of the pores.

It must be stated that in the derivation of the kinetic equation (2.14) we succeeded in obtaining general expressions for the displacement velocity v and for the diffusion coefficient $\mathscr{D}^{ik}$ of the pores. The spatial coefficient of the pores $\mathscr{D}^{ik}$ consists of $\mathscr{D}_S^{ik}$ (the contribution of the surface diffusion of the vacancies) and $\mathscr{D}_V^{ik}=\mathscr{D}_P^{ik}+\mathscr{D}_Q^{ik}$ (the contribution from the random displacements of the pores thanks to the processes of condensation and evaporation of the vacancies). The situation is similar also for the pore displacement velocity v.

3. PORE MOTION IN INHOMOGENEOUS VACANCY FIELDS

The kinetic equation (2.14) is so far only formally closed with respect to $f(\mathbf{r}, m)$, inasmuch as the kinetic coefficients (2.15) are determined by the distribution of the vacancies around each pore. This vacancy distribution depends substantially on the spatial distribution of the pores. Therefore, for a complete description of the evolution of the distributed pores in space we must find the distribution $C(\mathbf{R}, \mathbf{r}, m)$ and calculate the coefficients (2.15). We note also that calculation of the growth rate $\dot{R}$ of a selected pore, of its spatial velocity v, and of the diffusion coefficients J and $\mathscr{D}^{ik}$ under specified external inhomogeneous conditions is also of independent significance.

We obtain now the vacancy distribution $C(\mathbf{R}, \mathbf{r}, m)$ around a selected pore $A(\mathbf{r}, m)$. To this end we write down first, in accord with the vacancy-motion model formulated in the preceding section, the change of the vacancy concentration on the pore surface:

$$\dot{C}_s(\mathbf{R}_s)=\int\frac{d^2R_s'}{\omega_s}\{C_s(\mathbf{R}_s')W_{ss}(\mathbf{R}_s'\to\mathbf{R}_s)-C_s(\mathbf{R}_s)W_{ss}(\mathbf{R}_s\to\mathbf{R}_s')\}$$
$$+\int\frac{d^3R}{\omega_v}\{C(\mathbf{R})W_{vs}(\mathbf{R}\to\mathbf{R}_s)-C(\mathbf{R}_s)W_{sv}(\mathbf{R}_s\to\mathbf{R})\}+\frac{1}{\tau_T}[C_T(R_s)-C_s(\mathbf{R}_s)],\qquad(3.1)$$

where τ_T^{-1} characterizes the probability of attachment and detachment of vacancies from defects on the surface of the pore (breaks on steps, impurity atoms, etc.), while $C_T(R_s)$ is the thermal concentration of the vacancies near the pore surface defects. The first integral in the right-hand side of this expression describes the motion of vacancies over a pore surface by surface diffusion, the second integral describes the processes of condensation and evaporation of the vacanies from the near-surface layer in the volume, while the last term is responsible for the processes of detachment and attachment of vacancies from defects on the surface of the pore.

The evolution of the distribution of the vacancies in the vicinity of the pore $(R>R_s)$ will be described by the equation

$$\dot{C}(\mathbf{R})=\int\frac{d^3R'}{\omega_v}\{C(\mathbf{R}')W_v(\mathbf{R}'\to\mathbf{R})-C(\mathbf{R})W_v(\mathbf{R}\to\mathbf{R}')\}$$
$$+\int\frac{d^2R_s}{\omega_s}\{C_s(\mathbf{R}_s)W_{sv}(\mathbf{R}_s\to\mathbf{R})-C(\mathbf{R})W_{vs}(\mathbf{R}\to\mathbf{R}_s)\}-\gamma[C(\mathbf{R})-C_0]+G.\qquad(3.2)$$

Here C_0 is the thermal concentration of the vacancies in the volume; γ and G are the effective rates of absorption and generation of vacancies. The first integral in this expression describes the volume diffusion of the vacancies, the second the evaporation and condensation of vacancies from the surface layer of the pore into the volume, while the third term describes effectively the capture of vacancies by other volume defects (dislocations, impurity atoms) and the fourth term describes the production of vacancies by the irradiation. We note that the probabilities $W_{SV}(\mathbf{R}_s\to\mathbf{R})$ and $W_{VS}(\mathbf{R}\to\mathbf{R}_s)$ in Eqs. (3.1) and (3.2) do not coincide, generally speaking, with the limits

$$\lim_{R'\to R_s}W_v(\mathbf{R}'\to\mathbf{R}),\quad\lim_{R'\to R_s}W_v(\mathbf{R}\to\mathbf{R}').$$

We are interested in a weakly inhomogeneous distribution of the vacancies. In this case we can change over from the integral form of Eqs. (3.1) and (3.2) to a differential form. We first simplify for this purpose in (3.1) the integral corresponding to the surface motion of the vacancies. The calculations yield

$$\int\frac{d^2R_s'}{\omega_s}\{C_s(\mathbf{R}_s')W_{ss}(\mathbf{R}_s'\to\mathbf{R}_s)-C_s(\mathbf{R}_s)W_{ss}(\mathbf{R}_s\to\mathbf{R}_s')\}=-\operatorname{div}_s\mathbf{j}_s,\qquad(3.3)$$

$$\operatorname{div}_s\mathbf{j}_s=g^{-1/2}\frac{\partial}{\partial x^\alpha}(g^{1/2}j_s^\alpha),\qquad j_s^\alpha=V_s^\alpha C_s-D_s^{\alpha\beta}\frac{\partial C_s}{\partial x^\beta},\qquad(3.4)$$

$$V_s^\alpha(x)=\int\frac{d^2x'}{\omega_s}g^{1/2}W_{ss}^{(-)}(\mathbf{x}\to\mathbf{x}')(x'^\alpha-x^\alpha),\qquad(3.5)$$

$$D_s^{\alpha\beta}(x)=\frac{1}{2}\int\frac{d^2x'}{\omega_s}g^{1/2}W_{ss}^{(+)}(\mathbf{x}\to\mathbf{x}')(x^\alpha-x'^\alpha)(x^\beta-x'^\beta)\approx D_sg^{\alpha\beta},\qquad(3.6)$$

where V_S^α is the surface "hydrodynamic" vacancy velocity, D_S is the coefficient of surface diffusion of the vacancies; $W_{SS}^{(-)}$ and $W_{SS}^{(+)}$ are respectively the antisymmetrical and symmetrical parts of the probability of vacancy hopping from the surface point x to the point x′ $(\alpha,\beta=1,2)$.

It is important that the expression for the surface flux of the vacancies j_s^α contains the hydrodynamic drift (3.5), with V_S^α different from zero if the hopping probability W_{SS} has an antisymmetrical part $W_{SS}^{(-)}$ that can be produced by a temperature or stress gradient on the surface of the pore.

The final equation (3.1), which describes the change of the vacancy concentration in the surface layer takes, with allowance for (3.3)—(3.6), the form

$$\dot{C}_s(\mathbf{R}_s)=-\operatorname{div}_s\mathbf{j}_s+\frac{1}{\tau_{VS}}C(\mathbf{R}_s+\lambda\mathbf{n})-\frac{1}{\tau_{SV}}C_s(\mathbf{R}_s)+\frac{1}{\tau_T}[C_T(R_s)-C_s(\mathbf{R}_s)],\qquad(3.7)$$

where the quantities τ_{VS} and τ_{SV} are given by

$$\frac{1}{\tau_{VS}}=\int\limits_{R>R_s}\frac{d^3R}{\omega_v}W_{VS}(\mathbf{R}\to\mathbf{R}_s),\qquad\frac{1}{\tau_{SV}}=\int\limits_{R>R_s}\frac{d^3R}{\omega_v}W_{SV}(\mathbf{R}_s\to\mathbf{R});$$

is the effective radius of the functions W_{VS} and W_{SV} ($\lambda\approx a$, where a is the lattice period), and n is a unit vector directed along the outward normal to the pore surface.

Strictly speaking, the condensation and evaporation times τ_{VS} and τ_{SV} (as well as the time τ_T) depend on the radius of the pore. But for large pores in most cases this dependence can be neglected and one can the values of these parameters for a flat crystal surface [see the remark concerning formula (3.18) below].

In the region $R > R_S + \lambda$, the vacancy diffusion is described according to (3.2) by the equation

$$\dot{C}(\mathbf{R}) = D_v \Delta C - \gamma (C - C_0) + G. \tag{3.8}$$

Here

$$D_v = \frac{1}{6} \int \frac{d^3R}{\omega_v} R^2 W_v(R), \quad \gamma = \beta^2 D_v.$$

The equations (3.7) and (3.8) for the surface and volume diffusion of the vacancies must be supplemented by a boundary conditions, which we obtain by equating the vacancy flux from the surface of the pores to the volume flux at the point $\mathbf{R}_S + \lambda\mathbf{n}$:

$$\frac{\lambda}{\tau_{SV}} C_S(\mathbf{R}_s) - \frac{\lambda}{\tau_{VS}} C(\mathbf{R}_s + \lambda\mathbf{n}) = -D_v (\mathbf{n}\nabla) C(\mathbf{R}_s + \lambda\mathbf{n}). \tag{3.9}$$

Strictly speaking, the connection between $C_S(\mathbf{R}_s)$ and $C(\mathbf{R}_s + \lambda\mathbf{n})$ should be sought by solving Eq. (3.2) in the region $R_s < R < R_s + \lambda$. In the calculations that follow, however, we shall use Eq. (3.9), as is customary in the kinetics of weakly rarefied gases when boundary layers are considered.

The number m of vacancies in the pore changes substantially over a characteristic time τ_m on the order of [see (3.17) below]

$$1/\tau_m \approx \dot{m}/m \sim D_v C / R_m^2,$$

and the characteristic times of establishment of the quasistationary distribution of the vacancies in the surface layer (τ_{st}^s) and in the volume (τ_{st}^v) are, according to (3.7) and (3.8), of the order of

$$\frac{1}{\tau_{st}^s} \approx \max\left(\frac{D_s}{R_m^2}, \frac{1}{\tau_{SV}}, \frac{1}{\tau_T}\right), \quad \frac{1}{\tau_{st}^v} \approx \max\left(\beta^2 D_v, \frac{D_v}{R_m^2}\right).$$

Therefore the following inequalities are always satisfied at $C \ll 1$:

$$\tau_{st}^s \ll \tau_m, \quad \tau_{st}^v \ll \tau_m.$$

This means that the distribution of the vacancies near the pore always adjusts itself adiabatically to the size of the pore. To determine the distribution of the vacancies near the pore and by the same token to find the kinetic coefficient (2.15), we can therefore use the stationary system of equations (3.7) and (3.8). In the vacancy-density gradient (if we neglect the internal stresses due to their gradient) the probability of vacancy hopping over the surface of the pore has a symmetrical form

$$W_{SS}(\mathbf{R} \to \mathbf{R}') = W_{SS}(\mathbf{R}' \to \mathbf{R}) \equiv W_{SS}^{(+)},$$

therefore the vacancy flux over the surface of the pore j_S does not contain a term with hydrodynamic drift ($V_S^\alpha = 0$) and the stationary system of equations, with (3.9) taken into account, takes the form

$$D_s \Delta_s C_S(\mathbf{R}_s) + \frac{D_v}{\lambda} (\mathbf{n}\nabla) C(\mathbf{R}_s + \lambda\mathbf{n}) + \frac{1}{\tau_T}[C_T(R_s) - C_S(\mathbf{R}_s)] = 0, \tag{3.10}$$

$$\Delta C(\mathbf{R}) - \beta^2 [C(\mathbf{R}) - C_0] + G/D_v = 0 \quad (R > R_s + \lambda). \tag{3.11}$$

Equations (3.10) and (3.11) with the boundary condition (3.9) determine completely the distribution of the vacancies near the pore. The solution of Eqs. (3.10), (3.11) with allowance for (3.9) is of the form

$$C_S(\mathbf{R}_s) = C_S^{(0)} + \mathbf{C}_S^{(1)} \mathbf{n}, \tag{3.12}$$

$$C(\mathbf{R}) = C_\infty + q/R - \mathbf{E}\mathbf{R} + \mathbf{d}\mathbf{R}/R^3. \tag{3.13}$$

Here C_∞ is the concentration of the vacancies far from the pore, the "external field" $\mathbf{E}$ is specified by the vacancy-density gradient, which is due to the overlap of the vacancion clouds surrounding the remaining pores (see below). The other parameters are

$$q = B_q R_s (C_m - C_\infty), \quad \mathbf{d} = B_d R_s^3 \mathbf{E},$$

$$B_q = \left(1 + \frac{\lambda}{R_s} \frac{\tau^*}{\tau_v}\right)^{-1}, \quad B_d = \left(1 - \frac{\lambda}{R_s} \frac{\tau^{**}}{\tau_v}\right) \Big/ \left(1 + 2\frac{\lambda}{R_s} \frac{\tau^{**}}{\tau_v}\right),$$

$$C_S^{(0)} = C_T(R_s) - \frac{\lambda}{R_s^2} \frac{\tau_T}{\tau_v} q, \quad \mathbf{C}_S^{(1)} = -\frac{\lambda \tau_T}{\varepsilon \tau_v}(1 + 2B_d)\mathbf{E}, \quad C_m = \frac{\tau_{VS}}{\tau_{SV}} C_T(R_s)$$

$$\tau^* = \tau_{VS}\left(1 + \frac{\tau_T}{\tau_{SV}}\right), \quad \tau^{**} = \tau_{VS}\left(1 + \frac{\tau_T}{\varepsilon \tau_{SV}}\right), \quad \varepsilon = 1 + 2\frac{D_s \tau_T}{R_s^2}, \quad D_v \approx \frac{\lambda^2}{\tau_v}. \tag{3.14}$$

In the case when the frequency of the surface processes is of the order of or higher than the frequency of the vacancy hops in the volume

$$1/\tau^* \approx 1/\tau^{**} \gtrsim 1/\tau_v, \tag{3.15}$$

the deviation of the coefficients B_q and B_d from unity can be neglected and we can write in place of (3.14)

$$q = R_s (C_m - C_\infty), \quad \mathbf{d} = R_s^3 \mathbf{E},$$

$$C_S^{(0)} = C_T(R_s) + \frac{\lambda}{R_s} \frac{\tau_T}{\tau_v} C_\infty, \quad \mathbf{C}_S^{(1)} = -3\frac{\lambda \tau_T}{\varepsilon \tau_v}\mathbf{E}.$$

If the processes that cause the vacancy change between the pore and the crystal and strongly hindered, so that

$$\frac{\lambda}{R_s} \frac{\tau^*}{\tau_v} > \frac{\lambda}{R_s} \frac{\tau^{**}}{\tau_v} \gg 1, \tag{3.16}$$

then we obtain a new result:

$$q = \frac{R_s^2 \tau_v}{\lambda \tau^*}(C_m - C_\infty), \quad \mathbf{d} = -\frac{R_s^3}{2}\left(1 - \frac{3}{2} \frac{R_s}{\lambda} \frac{\tau_v}{\tau^{**}}\right)\mathbf{E},$$

$$C_S^{(0)} = \frac{\tau_{VS}}{\tau^*} C_T + \frac{\lambda}{R_s} \frac{\tau_T}{\tau^*} C_\infty, \quad \mathbf{C}_S^{(1)} = -\frac{3}{2} \frac{R_s}{\varepsilon} \frac{\tau_T}{\tau^{**}} \mathbf{E}.$$

Satisfaction of the inequalities (3.16) can be expected in two cases. First, when the activation barrier that causes the adhesion of the vacancies to the surface of the pore is large compared with the activation barrier for the vacancy in the volume ($\tau_{VS} \gg \tau_v$). Second, when $\tau_{VS} \approx \tau_{SV} \approx \tau_v$, but the process of adhesion of the surface vacancy to the steps and to the breaks on the surface of the pore is strongly hindered ($\tau_T \gg \tau_v$).

The distribution of the vacancies near the pore and on the surface of the pore, (3.12) and (3.13), specifies directly the kinetic coefficients (2.15), which we now proceed to determine.

The rate of change of the number of vacancies in the pore, $\dot{m}$, equals according to (2.2), (2.6), and (2.15)

$$\dot{m} = -\frac{4\pi D_v}{\omega_v} q = -\frac{4\pi D_v}{\omega_v} B_q R_s (C_m - C_\infty). \tag{3.17}$$

From this expression and (3.14) it is seen that in the case (3.15) the pore growth rate is

$$\dot{R}_s=\frac{D_v}{R_s}(C_\infty-C_m). \tag{3.18}$$

This expression agrees with the previously known result,[6] but the role of the boundary condition on the surface of the pore is assumed in this case by the quantity

$$C_m=\frac{\tau_{VS}}{\tau_{SV}}C_T(R_s).$$

Since the time ratio τ_{VS}/τ_{SV} depends generally speaking on the radius of the pore, the known thermodynamic relation used in Ref. 6 as the boundary condition on the surface of the pore

$$C_m=C_{V0}\exp\{2\gamma\omega_v/RT\}$$

(γ is the coefficient of surface tension of the crystal) is determined in the present case by the joint action of the quantities $C_T(R_s)$ and τ_{VS}/τ_{SV}.

In the case (3.16), the growth of the pore is determined by the expression

$$\dot{R}_m=\frac{\lambda}{\tau^*}(C_\infty-C_m).$$

Inasmuch as here $\tau_v R_s/\tau^*\lambda \ll 1$, in the case when the vacancy exchange between the pore surface and the crystal is hindered the pore growth rate slows down considerably compared with the rate (3.18), and has a different dependence on the pore dimension.

We determine now the rate of displacement of the pore in the crystal. The processes of condensation and evaporation of the vacancies from the surface of the pore lead to displacement of the pore at a rate governed by volume diffusion processes and equal, according to (2.15), (2.9), and (1.12) to

$$\mathbf{v}_V=\mathbf{v}_P+\mathbf{v}_Q=-D_v(1+2B_d)\mathbf{E}. \tag{3.19}$$

Here and elsewhere we assume for simplicity $\omega_v/\lambda\omega_s \approx 1$.

In the case when the activation barriers for exchange of vacancies between the surface of the pore and the crystal are close to the activation barriers of the vacancies in the volume [see (3.15)], the pore velocity is

$$\mathbf{v}_V=-3D_v\mathbf{E},$$

and agrees with the known result.[6] Under conditions of slowed-down exchange of vacancies between the surface of the pore and the crystal [see (3.16)], the expression for the pore velocity becomes

$$\mathbf{v}_V=-\frac{3}{2}\frac{\lambda R_s}{\tau^{**}}\mathbf{E}.$$

As expected, the velocity of the pores whose surface layers hinder the landing if the vacancies on the pore surface is much lower than the velocity of the pores that do not produce an additional barrier for the hopping of the vacancies to the surface of the pores. The ratio of these velocities is

$$\frac{\tau_v}{\tau^{**}}\frac{R_s}{\lambda}\ll 1.$$

In addition to the processes of condensation and evaporation of the vacancies, a definite contribution to the pore velocity can be made also by surface diffusion of the vacancies over the surface of the pore. This mechanism of pore displacement is due to the fact that the distribution of the vacancies on the surface of the pore depends on the direction of the "external field" **E**: on one side of the pore the vacancy density is higher than on the other side. This leads to the appearance of directional motion of the vacancies, as a result of which the center of the pore shifts when the vacancies flow over the surface of the pore from one side to the other. Using (2.11), (2.13), (3.6), and (3.14), we calculate the pore velocity due to the surface diffusion of the vacancies, and represent it with allowance for (3.19) in the form

$$\mathbf{v}_S=-\frac{D_s\tau_T/R_s^2}{1+2D_s\tau_T/R_s^2}\mathbf{v}_V.$$

It is seen from this expression that the velocity $\mathbf{v}_S$ is directed opposite to the velocity $\mathbf{v}_V$ and is comparable with it (if $D_s\tau_T/R_s^2 \gtrsim 1$) or is smaller (if $D_s\tau_T/R_s^2 \ll 1$). Consequently, allowance for the surface velocity $\mathbf{v}_S$ does not influence the estimate of the resultant pore velocity

$$\mathbf{v}=\mathbf{v}_V+\mathbf{v}_S=\frac{1+D_s\tau_T/R_s^2}{1+2D_s\tau_T/R_s^2}\mathbf{v}_V. \tag{3.20}$$

We calculate now the intrinsic diffusion coefficient $\mathscr{D}$ of the pores. Substituting in (2.5), (2.9), and (2.13) the obtained vacancy distribution near and on the surface of the pore (3.12) and (3.13), we obtain in the isotropic case

$$\mathscr{D}^{\alpha\beta}=\mathscr{D}\delta_{\alpha\beta},\quad \mathscr{D}=\mathscr{D}_P+\mathscr{D}_Q+\mathscr{D}_S,$$
$$\mathscr{D}_P=\frac{\Omega\bar{C}(R_s)}{\tau_{VS}R_s^2},\quad \mathscr{D}_Q=\frac{\Omega\bar{C}_S(R_s)}{\tau_{SV}R_s^2},\quad \mathscr{D}_S=\frac{D_s\Omega\bar{C}_S(R_s)}{R_s^4}, \tag{3.21}$$

where

$$\bar{C}(R_s)\approx\frac{C_m+\lambda\tau^*C_\infty/R_s\tau_v}{1+\lambda\tau^*/R_s\tau_v},\quad \bar{C}_S(R_s)\approx C_S^{(0)}(R_s),\quad \Omega=\frac{3}{8\pi}\frac{\omega_v^2}{\omega_s}.$$

According to (3.21), the diffusion mobility of the pores is determined by the rate of surface diffusion of the vacancies and also by the rates of the vacancy exchange between the surface of the pore and the crystal. In the case when the distortions of the surface layer are small and do not influence the volume diffusion processes in the surface layer [see (3.15)], the total diffusion coefficient of the pores as a function of the pore dimension is given by

$$\mathscr{D}=\begin{cases} D_sC_T\Omega/R_s^4, & R_s<\lambda C_\infty/C_T \\ D_sC_\infty\lambda\Omega/R_s^5, & \lambda C_\infty/C_T<R_s<(D_s\tau_v)^{1/2}. \\ \lambda C_\infty\Omega/\tau_vR_s^3, & (D_s\tau_v)^{1/2}<R_s \end{cases} \tag{3.22}$$

Finally, if the near-surface layer hinders the landing of the vacancies on the surface of the pore [see (3.16)], then the diffusion of the pore at $(D_s\tau_v)^{1/2}<R_s<\lambda\tau^*/\tau_v$ is estimated at

$$\mathscr{D}\approx\Omega C_\infty/\tau_{VS}R_s^2.$$

Thus, the diffusion coefficient of the pore, depending on the size of the pore and on the relations between the characteristic times, is determined by different mechanisms and behave differently as a function of R_s.

Pore diffusion in the space of the dimensions m is determined by the cofficient J [see (2.15)], whose value is

$$J=(J_P+J_Q)/2,$$

$$J_P=\frac{4\pi R_s^2}{\omega_s}\frac{\overline{C}(R_s)}{\tau_{VS}},\quad J_Q=\frac{4\pi R_s^2}{\omega_s}\frac{\overline{C}_S(R_s)}{\tau_{SV}}.$$

We emphasize that the coefficient of pore diffusion in dimension space is proportional to the surface of the pore. The use of the law $J_P \propto R$, $J_Q \propto R$, which is frequently employed in the kinetics of nucleation of vacancion pores (see, e.g., Ref. 12), can therefore not be regarded as justified.

Thus, all the kinetic coefficients (2.15) in the kinetic equation (2.14) are determined and expressed in terms of parameters that characterize the external field for the given pore (the quantities C_∞ and $\mathbf{E}$) and the diffusion-process times τ_V, τ_{SV}, τ_{VS}, τ_s, and τ_T.

We now find the quantities C_∞, q, and $\mathbf{E}$ for a selected pore in an ensemble of pores. The diffusion of the vacancies in the space between the pores at $R > R_s + \lambda$ is described according to (3.2) by the equation

$$\Delta\psi-\beta^2\psi=0, \tag{3.23}$$

where

$$\psi(\mathbf{r})=C(\mathbf{r})-C_p,\quad C_p=C_0+G/\beta^2D_v.$$

We seek the solution of (3.23) in the form

$$\psi(\mathbf{r})=\sum_{i=1}^{N}\left\{\frac{q_i}{|\mathbf{r}-\mathbf{r}_i|}+\frac{\mathbf{d}_i(\mathbf{r}-\mathbf{r}_i)}{|\mathbf{r}-\mathbf{r}_i|^3}+\beta\frac{\mathbf{d}_i(\mathbf{r}-\mathbf{r}_i)}{|\mathbf{r}-\mathbf{r}_i|^2}\right\}\exp(-\beta|\mathbf{r}-\mathbf{r}_i|), \tag{3.24}$$

where $\mathbf{r}_i$ is a vector characterizing the absorption of the i-th pore; q_i and $\mathbf{d}_i$ are unknown quantities which will be determined later on.

We expand (3.24) near the selected pore $j(R_j \ll |\mathbf{r}_{ij}|$, $\beta R_j \ll 1)$ and represent the distribution of the vacancies near this pore in a form similar to (3.13), in which the coefficients $C_{j\infty}$ and $\mathbf{E}_j$ are given by

$$C_{j\infty}=C_p+\sum_i{}'\frac{q_i}{r_{ij}}\exp(-\beta r_{ij}), \tag{3.25}$$

$$\mathbf{E}_j=\sum_i{}'\frac{q_i}{r_{ij}^3}(1+\beta r_{ij})\exp(-\beta r_{ij})\mathbf{r}_{ij}, \tag{3.26}$$

where

$$\mathbf{r}_{ij}=\mathbf{r}_j-\mathbf{r}_i,\quad \sum_i{}'\equiv\sum_{i(i\neq j)}.$$

Thus, the external field E_j is expressed in terms of the unknown quantities $q_i(i=1, 2, 3, \ldots, N)$. We now obtain the quantity q_j. To this end we use the relation (3.14) and substitute in it the expression (3.25); as a result we obtain the following equation for q_j:

$$R_jB_q(R_j)[C_m(R_j)-C_p]=q_j+R_jB_q(R_j)\sum_i{}'\frac{q_i}{r_{ij}}\exp(-\beta r_{ij}). \tag{3.27}$$

It is easy to solve this equation for a narrow distribution of the pores in dimensions $R_j=\overline{R}+\delta R_j$, $\delta R_j/\overline{R} \ll 1$ (where $\overline{R}$ is the average radius of the pores in the ensemble),[13] and it takes the form

$$q_j=q(\overline{R})+A(\overline{R})\delta R_j-\overline{R}B_q(\overline{R})A(\overline{R})\sum_i{}'\frac{\delta R_i}{r_{ij}}\exp(-\varkappa r_{ij}), \tag{3.28}$$

where

$$\begin{gathered}q(\overline{R})=\frac{\beta^2}{\varkappa^2}\overline{R}B_q(\overline{R})[C_m(\overline{R})-C_p],\\ A(\overline{R})=\frac{\varkappa^2}{\beta^2}\frac{dq}{d\overline{R}},\quad \varkappa^2=\beta^2\left(1+\frac{4\pi\overline{R}B_q(\overline{R})}{\omega_L\beta^2}\right),\end{gathered} \tag{3.29}$$

ω_L is the volume per pore ($\omega_L \approx L^3$). With the aid of (3.28) we obtain the rate growth of the selected pore with account taken of the diffusion-induced influence on this pore by the remaining pores in the ensemble. Using (3.17) and (3.28) we obtain

$$\dot{R}_j=-\frac{D_v}{R_j^2}\left\{q(\overline{R})+A(\overline{R})\delta R_j-\overline{R}B_q(\overline{R})A(\overline{R})\sum_i{}'\frac{\delta R_i}{r_{ij}}\exp(-\varkappa r_{ij})\right\}. \tag{3.30}$$

It is seen from this expression that the diffusion interaction of the pores, which determines the growth rate of the individual pore, has a screening radius $\sim\varkappa^{-1}(\varkappa > \beta)$.

The rate of change of the average pore dimension in the ensemble, neglecting small local inhomogeneous fluctuations in the pore-size distribution, is, according to (3.29) and (3.30)

$$\dot{\overline{R}}=\frac{D_v}{\overline{R}}\frac{B_q(\overline{R})[C_p-C_m(\overline{R})]}{1+4\pi\overline{R}B_q(\overline{R})/\omega_L\beta^2}. \tag{3.31}$$

We now find the rate of motion of an individual pore with allowance for the diffusion interaction with the remaining pores. To this end we substitute in (3.19) and (3.20) the expressions (3.26) and (3.28), and obtain as a result the following expression for the velocity of the j-th pore:

$$\mathbf{v}_j=Q_j\sum_i{}'\frac{R_i^2}{r_{ij}^3}\dot{R}_i(1+\beta r_{ij})\exp(-\beta r_{ij})\mathbf{r}_{ij}, \tag{3.32}$$

where

$$Q_j=\frac{1+\varepsilon(R_j)}{2\varepsilon(R_j)}[1+2B_d(R_j)].$$

It is seen from this expression that the growing pores in the ensemble ($\dot{R}_i > 0$) are effectively repelled and move in opposite directions, while the evaporating pores ($\dot{R}_i < 0$) are attracted and move towards one another with definite velocity. We note that the pore velocity in the ensemble, as a result of the diffusion interaction with one another, in contrast to the velocity of two diffusely interacting pores[7] has a screening radius $\approx\beta^{-1}$, while the screening radius $\varkappa^{-1}$ of the pore growth rate is smaller than the screening radius β^{-1} of the pore velocity:

$$\varkappa^2/\beta^2=1+4\pi\overline{R}B_q(\overline{R})/\omega_L\beta^2>1.$$

4. STABILITY OF LATTICE OF VACANCION PORES

As first shown by Evans,[4] an ordered structure of vacancion pores is produced in a metal under certain conditions. The pore lattice is of interest because it had a macroscopic ordering period $L \approx 10^2a$ (where a is the period of the initial crystal lattice). The pore dimension distribution in the pore lattice is sufficiently narrow, and the average pore radius is $\overline{R} \approx 10a$. The ratio of the average pore dimension to the pore-lattice period is always small: $\overline{R}/L \approx 10^{-1}$. The symmetry of the pore lattice coincides with the symmetry of the initial crystal lattice.

We investigate now the stability of a lattice of vacancion pores using the kinetic equation (2.14) and the kinetic coefficients (2.15) obtained in the preceding sections. The stability of the pore lattice is influenced mainly by two processes: the growth of the pores and their displacement from the site positions. It is known that the spreading of the pore size distribution causes the pores whose size is less than critical, while the pores with size larger than critical grow at the expense of the disolving minute pores. A coalescence stage sets in.[14] In order for the pore lattice to be stable, it is necessary that its pore size distribution contain no pores smaller than critical. That is to say, the pore distribution must satisfy the condition

$$\bar{R}-R_c>(\overline{\delta R^2})^{1/2}. \qquad (4.1)$$

In the opposite case, the pores smaller than critical evaporate rapidly and the lattice of the pores vanishes with time.

As already noted, in the experimentally observed pore lattices the pore size distribution is very narrow. We shall show that under irradiation conditions the pore size distribution satisfying the condition (4.1) at the initial instant of time will satisfy this condition also subsequently, if the rate of vacancy generation exceeds a certain critical value.

Let us determine the time variation of the relative variance of the pore distribution in size $\xi(\xi^2=\overline{\delta R^2}/\bar{R}^2)$. With the aid of the obtained diffusion interaction of the pores (3.30), we write down an equation for the rate of change of the quantity ξ, which takes the form

$$\frac{d\ln\xi}{dt}=\frac{D_v}{\bar{R}^2}\left(3\frac{q(\bar{R})}{\bar{R}}-\frac{\varkappa^2}{\beta^2}\frac{dq}{d\bar{R}}\right).$$

It is clear that the pore size distribution is stable if $\xi<0$.

Substituting (3.29) in (4.1) we obtain

$$d\ln\xi/dt\approx-(G-G_{min}), \qquad (4.2)$$

where

$$G_{min}=\beta^2D_v[(C_m-C_0)+b\bar{R}|dC_m/d\bar{R}|].$$

Here $b=1/2$ if the distortions of the near-surface layer are small—(3.15), and $b=1$ in the opposite case—(3.16).

We can similarly rewrite expression (3.31) for the growth rate of the average pore dimension

$$\dot{\bar{R}}\sim[G-G_{min}+\beta^2D_vb\bar{R}|dC_m/d\bar{R}|].$$

Thus, if at the initial instant of time the vacancy generation due to the irradiation exceeds $G_{\min}$ in (4.2), then the pore lattice is stable with respect to smearing of the pore-size distribution. It is easily seen that in the course of time the pore lattice will remain stable, since the quantity $G_{\min}(R)$ decreases with increasing average pore dimension.

The second process that determines the stability of the pore lattice is the displacement of the pores from the sites of the pore lattice. According to the obtained kinetic equation for the vacancion pairs (2.14), the pores located at the sites of the lattice can irreversibly be displayed from their position, owing to the diffusion mobility, and smear out the ordered distribution of the pores in space. The pore lattice must therefore have a mechanism that returns the displaced pores to their sites. The diffusion interaction of the pores, from our point of view, is the principal mechanism that stabilizes the ordered position of the pores in the lattice.

Let us investigate the stability of the pore lattice to displacements of the pores from the site with the aid of the diffusion interaction (3.32). To this end we shift some selected pore (j) away from the pore-lattice site by a small quantity $\delta\mathbf{r}_j$ and determine the magnitude and direction of the velocity of the displaced pores. Expanding (3.32) in terms of the small parameter $|\delta\mathbf{r}_j|/L\ll1$ for a sufficiently narrow pore-size distribution in the pore lattice, and neglecting small local inhomogeneities in the pore size distribution, we obtain the following pore velocity

$$\mathbf{v}_j=-k_j\delta\mathbf{r}_j, \qquad (4.3)$$

$$k_j=\frac{1}{3}\beta^2\bar{Q}\bar{R}^2\dot{\bar{R}}\sum_i{}'\frac{\exp(-\beta r_{ij}^{(0)})}{r_{ij}^{(0)}}. \qquad (4.4)$$

It is seen from (4.3) and (4.4) that in the case of growing pores in the lattice ($\dot{\bar{R}}>0, k>0$) a pore displaced from the site moves in a direction opposite to the displacement vector $\delta\mathbf{r}$, and after a characteristic time $\sim k^{-1}$ the pore will return at this velocity to its initial state of the pore lattice. Therefore in the case of growing pores ($\dot{\bar{R}}>0$) the pore lattice can be stable to displacement from the site positions. On the other hand if the pores in the lattice evaporate ($\dot{\bar{R}}<0$), the displaced pore moves farther away from the site in the lattice and cannot return to the initial equilibrium position. In this case the pore lattice is not stable.

We note that at small β the pore screening radius is large enough and it is possible to change over in (4.4) from summation to integration over the volume, as a result of which (4.4) takes the much simpler form

$$k=4\pi Q\bar{R}^2\dot{\bar{R}}/\omega_L. \qquad (4.5)$$

We see thus that the diffusion mechanism of stabilization of the pore lattice leads to a pore-interaction law L^{-3}. As shown by Krivoglaz,[6] the elastic interaction of two pores leads to a displacement velocity proportional to L^{-4}, which leads for a pore lattice to an L^{-5} law. Therefore diffusion pore interaction is the decisive mechanism, at least under conditions of strong vacancy generation.

We proceed now to estimate the stability of the pore lattice to smearing of the ordered arrangement of the pores, a smearing that can result from diffusion of the pores in coordinate space. To this end it is necessary to compare the terms $\mathscr{D}\Delta f$ and $\nabla(\mathbf{v}f)$ in the kinetic equation (2.14). The term with the mixed derivative

$$\frac{\partial}{\partial m}(\mathbf{v}_P-\mathbf{v}_Q)\nabla f$$

can be disregarded in this estimate, since it does not exceed the term $\nabla(\mathbf{v}f)$.

Since the ordered distribution of the pores in space smears out as a result of pore diffusion over a characteristic distance $\sim\delta r$, we can write for the terms $\mathscr{D}\Delta f$ and $\nabla(\mathrm{v}f)$ the following estimates:

$$\mathscr{D}\Delta f\approx\mathscr{D}f/(\delta r)^2, \quad \nabla(\mathrm{v}f)\approx vf/\delta r. \tag{4.6}$$

The diffusion mobility of the pores from the site positions in the pore lattice and the directional displacement of the pores into the lattice site with velocity (4.3) cancel each other according to (4.6) when

$$(\delta r/L)^2=\mathscr{D}/kL^2. \tag{4.7}$$

To estimate the pore-lattice spatial dispersion (4.7) we assume $G\gg G_{\min}$ and $R_s>(D_s\tau_V)^{1/2}$. According to (3.22), (3.31), and (4.5) we have in this case

$$\mathscr{D}\approx\left(\frac{\lambda}{R}\right)^3\frac{G}{\beta^2}, \quad k\approx\frac{R}{L}\frac{G}{(\beta L)^2}.$$

Then Eq. (4.7) takes the form

$$\left(\frac{\delta r}{L}\right)^2\approx\left(\frac{\lambda}{R}\right)^3\frac{L}{R}.$$

In the experiments of Evans and others $\lambda/R\approx R/L\sim10^{-1}$, and as a result $(\delta r/L)^2\ll1$. Thus, in this case the pore lattice is unstable to smearing of the pore distribution both in dimension space and in ordinary space.

Let now $G\gg G_{\min}$, but

$$R_s\ll(D_s\tau_v)^{1/2}, \quad R_s\ll\lambda G/\beta^2C_TD_v$$

[see (3.22)]. In this case

$$\left(\frac{\delta r}{L}\right)^2\approx\left(\frac{\lambda}{R}\right)^4\frac{L}{R}\frac{G_{\min}}{G}\frac{D_s}{D_v}.$$

If we assume $D_s/D_v\sim10^4$, then the lattice is stable in this case to spatial smearing only if $G_{\min}/G\ll10$.

Thus, the pore lattice is stable at a reasonable ratio of the parameters and at sufficiently strong vacancy generation under the irradiation conditions.

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