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Inhomogeneous nucleation and growth in irradiated materials

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Abstract

The presence of planar sinks for mobile point defects in irradiated materials is shown to give rise to an unusual type of competition between the nucleation and growth of defect clusters and mesoscopic cavities. Numerical solutions of non-linear diffusion equations describing the binary field of mobile vacancies and interstitial atoms show the formation of a characteristic profile of inhomogeneous swelling that exhibits features similar to those observed experimentally.

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I. INTRODUCTION

The kinetics of phase transformations in materials driven far from equilibrium has recently attracted considerable attention stimulated by the need to develop better understanding of how materials behave in a hostile environment [1]. A typical example of an evolving non-equilibrium system is given by a material irradiated by a flux of energetic particles [2], and this is rapidly becoming one of the issues central to the design of a fusion power station [3,4].

The evolution of the microstructure of an irradiated material is characterized by the presence of dynamic quasi-equilibrium between the generation of mobile point defects by the incident energetic particles and the absorption of these defects by dislocations, grain

boundaries and cavities in the material. A chemical reaction type theory describing the temporal evolution of *spatially averaged* concentrations of mobile vacancies and interstitial atoms in the presence of randomly distributed mesoscopic lattice defects was formulated thirty years ago by Brailsford and Bullough [5]. Recent theoretical advances have been associated with the development of a more accurate treatment of effects of cascade damage that are described by either the molecular dynamics [6,7], the kinetic Monte-Carlo [8] or the continuum [9] models. One of the aspects that emerges from recent theoretical studies concerns the importance of taking into account spatial fluctuations of concentrations of point defects in the material, see e.g. [10,11].

Spatially inhomogeneous concentration profiles naturally appear in the treatment of kinetics of nucleation and growth where growing clusters act as sources or sinks for the diffusion fields [12,13]. In a binary system described by the $\mathbf{r}$- and t-dependent concentrations $c_v(\mathbf{r},t)$ and $c_i(\mathbf{r},t)$ of mobile vacancies and interstitial atoms an even more complex case is encountered. Here the extended lattice defects act as sinks for the diffusion fields $c_v(\mathbf{r},t)$ and $c_i(\mathbf{r},t)$ reducing concentrations of mobile point defects in the immediate vicinity of each sink. Furthermore, since the rate of absorption of mobile point defects by a sink depends on the type of a point defect (typically, mobile interstitial atoms are absorbed at a higher rate than vacancies [5]), the presence of sinks gives rise to vacancy supersaturation $S(\mathbf{r},t) = D_v c_v(\mathbf{r},t) - D_i c_i(\mathbf{r},t)$, which is the parameter that determines the rate of growth of vacancy clusters and mesoscopic cavities [14]. Averaging of diffusion fields over the position of randomly distributed sinks results in the positive mean value $\langle S(\mathbf{r},t)\rangle = V^{-1}\int_V S(\mathbf{r},t)d\mathbf{r}$ of vacancy supersaturation [5]. Therefore, the function $S(\mathbf{r},t)$, considered as a function of coordinate $\mathbf{r}$ for a *given* spatial configuration of sinks, has a local maximum in the vicinity of each sink. This gives rise to an unusual type of competition between the nucleation of vacancy clusters and cavities which is suppressed in the vicinity of sinks, and the growth of clusters and cavities which is favoured in the very same areas where their nucleation is suppressed.

In this paper we investigate a model describing the evolution of a binary diffusion field

$\{c_i(\mathbf{r},t), c_v(\mathbf{r},t)\}$ in the vicinity of a planar lattice defect acting as a sink for mobile vacancies and interstitial atoms. We consider the dynamics of nucleation and growth of vacancy clusters assuming that the sink absorbs interstitial atoms at a higher rate than it absorbs vacancies. We find that the competition between nucleation and growth leads to the formation of a zone of spatially inhomogeneous growth of cavities. The area where cavities grow at the highest rate is separated from the plane of the sink by a certain characteristic distance, which decreases monotonically as a function of time. The type of behaviour exhibited by the model is similar to that observed experimentally for the case of nucleation and growth of cavities in the vicinity of a grain boundary [11,15].

II. THE MODEL

The time-dependent distribution of concentrations of vacancies and interstitial atoms in the vicinity of a sink is given by the solution of a system of two equations describing the generation, diffusion, recombination and absorption of point defects

$$\frac{\partial}{\partial t}c_i(\mathbf{r},t) = D_i\frac{\partial^2}{\partial \mathbf{r}^2}c_i(\mathbf{r},t) + K - [\rho+\omega(\mathbf{r},t)]D_i c_i(\mathbf{r},t) - \alpha c_i(\mathbf{r},t)c_v(\mathbf{r},t) - \sigma_i(\mathbf{r},t),$$
$$\frac{\partial}{\partial t}c_v(\mathbf{r},t) = D_v\frac{\partial^2}{\partial \mathbf{r}^2}c_v(\mathbf{r},t) + K - [\rho+\omega(\mathbf{r},t)]D_v c_v(\mathbf{r},t) - \alpha c_i(\mathbf{r},t)c_v(\mathbf{r},t) - \sigma_v(\mathbf{r},t). \quad (1)$$

In these equations K is the rate of generation of vacancies and interstitial atoms in the material, D_i and D_v are the diffusion coefficients ($D_v \ll D_i$) and ρ is the density of randomly distributed dislocations forming the homogeneous absorbing background. The term $\omega(\mathbf{r},t)$ describes the absorption of point defects by growing cavities and α is the recombination constant. Here we are interested in tracing the evolution of the binary diffusion field $\{c_i(\mathbf{r},t), c_v(\mathbf{r},t)\}$ in the vicinity of an extended lattice defect, and functions $\sigma_v(\mathbf{r},t)$ and $\sigma_i(\mathbf{r},t)$ represent the rates of absorption of vacancies and interstitial atoms by this defect. In solving equations (1) we are going to concentrate on the effects associated with the difference between these absorption rates. We assume that the background absorption of diffusion fields remains unbiased, i.e. that the effective value of ρ is the same both in the

first and in the second equation (1).

At large distances from the sink where $\omega(\mathbf{r},t) \ll \rho$ the stationary concentrations of interstitial atoms and vacancies are given by

$$c_i(\infty) = \frac{\rho D_v}{2\alpha}\left[-1+\sqrt{1+(4K\alpha/\rho^2 D_i D_v)}\right],$$
$$c_v(\infty) = \frac{\rho D_i}{2\alpha}\left[-1+\sqrt{1+(4K\alpha/\rho^2 D_i D_v)}\right]. \qquad (2)$$

From (2) it follows that at large distances from the sink the vacancy supersaturation $S(\mathbf{r},t)$ vanishes $S(\infty) = c_v(\infty)D_v - c_i(\infty)D_i = 0$.

Given that the characteristic scale of the spatial variation of concentrations equals $\tilde{z} \sim \rho^{-1/2}$ we obtain that the temporal variation of concentrations is characterized by the timescale $\tilde{t} \sim (D\rho)^{-1} \sim 10^{-3}$s for $D \sim 10^{-5}$ cm/s^2 and $\rho \sim 10^8$ cm^{-2}. Since the timescale characterising the rate of growth of cavities is of the order of 10^5 s, the time derivatives of concentrations entering the left-hand side of (1) may be neglected.

In what follows we consider the solution of (1) for the case of a one-dimensional sink (e.g. a grain boundary). Grain boundaries, as well as dislocations, interact with mobile point defects via long-range elastic forces [16] and this results in a rate of absorption for defects of one type that is higher than the absorption rate for the other type of defects [5]. An additional mechanism responsible for the difference in the absorption rates is associated with different probabilities of 'evaporation' of defects from the sinks. Experimental data show that in most cases the visible rate of absorption of interstitial atoms is higher than the rate of absorption of vacancies, and this gives rise to positive vacancy supersaturation. Positive vacancy supersaturation may also result from the formation of stable clusters of interstitial atoms in the cascades [11].

III. ANALYSIS OF THE MODEL

Consider a phenomenological model of a biased one-dimensional sink where the difference in the absorption rates is associated with the differences in the *local* kinetics of attachment

and detachment of mobile point defects to its surface

$$D_v\frac{d^2}{dz^2}c_v(z,t)+K-[\rho+\omega(z,t)]D_vc_v(z,t)-\alpha c_i(z,t)c_v(z,t)=\nu D_v[c_v(z,t)-\bar{c}_v]\delta(z).$$
$$D_i\frac{d^2}{dz^2}c_i(z,t)+K-[\rho+\omega(z,t)]D_ic_i(z,t)-\alpha c_i(z,t)c_v(z,t)=\nu D_ic_i(z,t)\delta(z). \qquad (3)$$

In this equation ν is a numerical factor characterizing the rate of absorption of diffusion fields by the sink and the term $\bar{c}_v$ describing thermally emitted vacancies in the right-hand side of the second equation accounts for the competition between absorption and evaporation of vacancies by vacancy clusters and void nuclei at the grain boundary [17,5]. Terms in the right-hand side of (3) are equivalent to a boundary condition on concentrations and fluxes of point defects at $z=0$. In the limiting case $\nu\to\infty$ and $\bar{c}_v\to 0$ this condition is equivalent to that used in Ref. [14].

In the absence of cavities (i.e. in the case $\omega(z,t)=0$) equations (3) may be solved analytically by linearizing them in the vicinity of values given by (2)

$$\begin{pmatrix}c_i(z)\\c_v(z)\end{pmatrix}=\begin{pmatrix}c_i(\infty)\\c_v(\infty)\end{pmatrix}+\frac{\nu}{2}\cdot\frac{D_v\bar{c}_v}{2\sqrt{\rho}+\nu}\begin{pmatrix}-D_i^{-1}\\D_v^{-1}\end{pmatrix}\exp(-\sqrt{\rho}|z|)$$
$$-\frac{\nu}{2}\cdot\frac{D_ic_i^{(\infty)}+D_v[c_v^{(\infty)}-\bar{c}_v]}{2[\rho^2+(4K\alpha/D_iD_v)]^{1/4}+\nu}\begin{pmatrix}D_i^{-1}\\D_v^{-1}\end{pmatrix}\exp(-[\rho^2+(4K\alpha/D_iD_v)]^{1/4}|z|). \qquad (4)$$

This solution shows two important features. First, it is characterized by two distinct scales, $z_1=1/\sqrt{\rho}$ and $z_2=1/[\rho^2+(4K\alpha/D_iD_v)]^{1/4}$, which determine how concentrations behave as functions of distance z from the grain boundary. Second, equation (4) shows that the system of equations (1) has two linearly independent solutions exhibiting two radically different types of behaviour near the origin, $z=0$. Figures 1 and 2 show that profiles of concentrations of both vacancies *and* interstitial atoms have deep minima in the vicinity of the sink while the supersaturation $S(z)$ is maximum at $z=0$. The latter fact can be easily verified by subtracting the first of the two equations (3) from the second and by solving the resulting *closed* equation on $S(z)$

$$S(z)=\nu\frac{D_v\bar{c}_v}{2\sqrt{\rho}+\nu}\exp(-\sqrt{\rho}|z|). \qquad (5)$$

We now consider how the opposite trends exhibited by concentration and supersaturation profiles in the vicinity of a grain boundary influence the rate of nucleation and growth of mesoscopic cavities. A convenient measure of swelling of the material is given by the average volume of cavities

$$W(z,t) = \int da \left(\frac{4}{3}\pi a^3\right) F(z,a,t), \tag{6}$$

where $F(z,a,t)$ is the distribution of cavities over their radius a. Taking into account that [17]

$$4\pi a^2 \frac{da}{dt} = \frac{d}{dt}\left(\frac{4}{3}\pi a^3\right) = 4\pi a g(a) S(z,t), \tag{7}$$

we arrive at a simple relation between the local rate of swelling and the local rate of absorption of mobile point defects

$$\dot{W}(z,t) = \omega(z,t) S(z,t). \tag{8}$$

Using the expression for $\omega(z,t)$ derived in Appendix A, we arrive at a self-consistent nonlinear equation for the vacancy supersaturation

$$\frac{d^2}{dz^2} S(z,t) - \rho S(z,t) - 4\pi \left[\int a g(a) F(z,a,t) da\right] S(z,t) = \nu S(z,t)\delta(z) - \nu \bar{c}_v D_v \delta(z), \tag{9}$$

where the size distribution function $F(z,a,t)$ depends on $S(z,t)$ via the drift term in the Fokker-Planck equation [18]

$$\frac{\partial}{\partial t} F(z,a,t) + \frac{\partial}{\partial a}\left(\frac{g(a)}{a} S(z,t) F(z,a,t)\right) = 0. \tag{10}$$

Introducing a new function $H(z,a,t) = [g(a)/a]F(z,a,t)$ and two new variables $\theta = \int_0^t S(z,t')dt'$ and $\xi = \int_0^a da' a'/g(a')$, we arrive at a general solution of (10)

$$F(z,a,t) = \frac{a}{g(a)} H\left(\int_0^t dt' S(z,t') - \int_0^a \frac{a' da'}{g(a')}\right), \tag{11}$$

where the form of function H is determined by the boundary conditions. To find H we consider an auxiliary function

$$\tilde{F}(z,a,t) = N\frac{a}{g(a)}\delta\left(\int_0^t dt' S(z,t') - \int_0^a \frac{a'da'}{g(a')}\right). \tag{12}$$

This function satisfies the normalization condition

$$\int_0^\infty da\tilde{F}(z,a,t) = N, \tag{13}$$

which is independent of time t, and which describes the growth of a group of nuclei the concentration of which at $t = 0$ equals N. Using (13), we obtain the size distribution function of cavities nucleating homogeneously in the interval $\tau \in [0,t]$

$$F(z,a,t) = N(z)\int_0^t d\tau \frac{a}{g(a)}\delta\left(\int_\tau^t dt' S(z,t') - \int_0^a \frac{a'da'}{g(a')}\right). \tag{14}$$

According to the classical theory of nucleation [19–21], the rate $N(z)$ of nucleation of cavities of the critical size is proportional to the concentration of mobile vacancies $c_v(z)$, i.e. $N(z) \sim c_v(z)$. Substituting (14) into (25) we arrive at a closed non-linear integral-differential equation for the supersaturation of vacancies

$$\frac{\partial^2}{\partial z^2}S(z,t) - S(z,t)\left[\rho + 4\pi N(z)\int_0^t d\tau\sqrt{2\int_\tau^t dt' S(z,t')}\right] = \nu[S(z,t) - D_v\bar{c}_v]\delta(z). \tag{15}$$

The solution of (15) corresponding to $t = 0$ is given by (5). To solve (15) for $t > 0$ we represent the integral term in the form of a sum over a finite number of points $t_n = 0, \Delta t, 2\Delta t, ..., t$

$$\int_0^t \sqrt{2\int_\tau^t dt' S(z,t')} = \frac{\Delta t}{2}\sum_{n=0}^{t/\Delta t}\sqrt{\Delta t\sum_{n'=n}^{t/\Delta t} S(z,n'\Delta t)}, \tag{16}$$

and solve (15) iteratively taking $S(z,n\Delta t) = S(z,0)$ for $n = 0,1,2,...,t/\Delta t$ as a starting approximation.

The main difficulty associated with finding a numerically stable solution of equation (15) consists in eliminating the terms that grow exponentially in the limit $z \to \infty$. For example, the two linearly independent solutions of (15) corresponding to $t = 0$ are $S(z,0) \sim \exp(-\sqrt{\rho}|z|)$ and $S(z,0) \sim \exp(\sqrt{\rho}|z|)$, and to eliminate the exponentially growing solution

one needs to take into account the boundary condition $\lim_{z\to\infty} S(z,0) = 0$. Analysis of numerical solutions of (15) shows that conventional linear numerical approaches [22] do not make it possible to eliminate the exponentially growing terms and give rise to numerical instabilities. To obtain a numerically stable solution of (15) satisfying boundary conditions at $z = 0$ and $z = \infty$ we use the R-matrix algorithm described in Appendix B.

Figure 2 shows the calculated profiles of vacancy supersaturation illustrating how this function evolves as a function of time t. The noticeable reduction in supersaturation seen in the region $z \geq 3\ \mu$ for $t \geq 2 \cdot 10^5$ s is due to the presence of the second term in square brackets in the left-hand side of equation (15). This term describes the absorption of mobile vacancies by growing cavities and it becomes significant only when the total surface area of cavities reaches some appreciable value.

Figure 3 shows how the total volume of growing cavities $W(z,t)$ (see equation (8)) varies as a function of t. Since the level of vacancy supersaturation decreases in the area $z > (\rho + \omega)^{-1/2}$ due to the absorption of vacancies by growing cavities, this suppresses further growth of cavities in this area. However, since the supersaturation remains high in the immediate vicinity of the plane of the sink, cavities continue to grow in this vicinity and the maximum of function $W(z,t)$ gradually drifts towards the grain boundary.

Experimental observations showing the presence of a time-dependent shift in the position of the peak of swelling in the vicinity of a planar sink were first reported by Green *et al* [15]. These observations have been recently reviewed by Singh [11]. It was found experimentally that the spatial distribution of growing cavities in the vicinity of a grain boundary is highly inhomogeneous. The volume concentration of cavities is maximum at a certain distance from the grain boundary, and the distance between the maximum and the boundary decreases as a function of time. The appearance of a maximum in the distribution of a quantity the evolution of which obeys the diffusion equation is anomalous, and early attempts to explain the experimentally observed effects on the basis of conventional rate theory proved to be unsuccessful [11]. Trinkaus *et al* [23] proposed a model explaining the nature of the observed phenomena. The model proposed in [23] is based on the assumption that the

motion of vacancy clusters near the grain boundary is one-dimensional and ballistic and is similar to the motion of particles colliding with a wall in a rarified plasma. However, more recent molecular dynamics studies [24] suggest that the motion of interstitial clusters, while remaining essentially one-dimensional, is diffusional rather than ballistic. The presence of random fluctuations of the direction of motion of clusters near grain boundaries alters the solution of the model proposed in [23] and this warrants further investigation of the role played by mobile interstitial clusters in the phenomenon of inhomogeneous swelling of irradiated materials.

To what extent are the results obtained above for the one-dimensional case of a planar one-dimensional sink applicable to the case of line (2D) and spherical (3D) sinks? Formally, the description of sinks as objects representable by delta-function terms encounters difficulties when applied to 2D and 3D cases, see e.g. a discussion of a similar issue in connection with the use of short-range potentials in the quantum-mechanical theory of scattering [25]. However, these difficulties can usually be circumvented by employing a suitable regularization procedure [25]. Following a line of argument similar to that given in [25] and taking into account the analysis of the one-dimensional case given above, we conclude that the formation of a pattern of spatially inhomogeneous swelling in an irradiated material containing biased sinks represents a general phenomenon which may manifest itself not only in the 1D case where it was already observed [15,11] but also in the 2D and 3D cases. This may also have important implications for the analysis of stability of materials used in fusion applications.

IV. SUMMARY

In this paper we showed how the absorption of binary diffusion field of mobile point defects by biased sinks in an irradiated material gives rise to an unusual type of competition between the nucleation and growth of vacancy clusters and cavities. This competition leads to the formation of a characteristic pattern of inhomogeneous swelling, and the temporal evolution of concentration and supersaturation profiles predicted by the model considered

above in this paper explains the origin of the anomalous behaviour observed experimentally.

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APPENDIX A

To evaluate the rate of absorption of point defects by randomly distributed cavities we consider an inhomogeneous diffusion equation

$$D\frac{\partial^2}{\partial \mathbf{r}^2}G(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}'), \tag{17}$$

the solution of which is

$$G(\mathbf{r},\mathbf{r}') = -\frac{1}{4\pi D|\mathbf{r}-\mathbf{r}'|}. \tag{18}$$

Now consider a spherical bubble of radius a growing by the attachment of diffusing particles to its surface. The concentration of diffusing particles around the bubble is given by [17]

$$c(\mathbf{r}) = c_\infty - \frac{a}{r}\frac{(av/D)}{1+(av/D)}[c_\infty - c^{(eq)}(a)], \tag{19}$$

where v is the effective velocity, which is a parameter entering the boundary condition for the rate of attachment of particles to the surface of the bubble

$$D\frac{\partial c}{\partial r}\Big|_{r=a} = v[c_\infty - c^{(eq)}(a)]. \tag{20}$$

Generalizing (19) to the case of a weakly inhomogeneous distribution of diffusing particles, we arrive at

$$c(\mathbf{r}) = c_0(\mathbf{r}) + 4\pi Da\frac{(av/D)}{1+(av/D)}\int d\mathbf{R}d\mathbf{r}'G(\mathbf{r}-\mathbf{R})\delta(\mathbf{R}-\mathbf{r}')[c_0(\mathbf{R}) - c^{(eq)}(a)], \tag{21}$$

where $\mathbf{r}'$ is the coordinate of the centre of the bubble and $c_0(\mathbf{r})$ is the diffusion field corresponding to the case where the perturbation associated with the bubble may be neglected. In what follows we assume that the average radius of the growing bubbles is greater than several interatomic distances. In this case the evaporation term in the right-hand side of (21) may be neglected and this equation becomes identical to the equation defining the T-matrix in the theory of scattering [26,27]

$$\psi(\mathbf{r}) = \psi_0(\mathbf{r}) + \int d\mathbf{R}d\mathbf{r}' G(\mathbf{r}-\mathbf{R})T(\mathbf{R},\mathbf{r}')\psi_0(\mathbf{r}'). \tag{22}$$

To average (21) over the positions of centres of bubbles we now follow the procedure developed for equation (22) by Lax [28,29] and obtain

$$c(\mathbf{r}) = c_0(\mathbf{r}) + 4\pi Da\frac{(av/D)}{1+(av/D)}\int d\mathbf{r}' G(\mathbf{r}-\mathbf{r}')F(\mathbf{r}')c(\mathbf{r}'), \tag{23}$$

where $F(\mathbf{r}')$ is the volume density of cavities at point $\mathbf{r}'$. Representing this function in the form of the integral over the cavity size distribution function $F(\mathbf{r}',a)$ satsfying the condition $F(\mathbf{r}') = \int daF(\mathbf{r}',a)$, we arrive at

$$c(\mathbf{r}) = c_0(\mathbf{r}) + 4\pi D\int daa\frac{(av/D)}{1+(av/D)}\int d\mathbf{r}' G(\mathbf{r}-\mathbf{r}')F(\mathbf{r}',a)c(\mathbf{r}'). \tag{24}$$

Finally, acting on both sides of this equation by operator $D(\partial^2/\partial\mathbf{r}^2)$ and comparing the result with (1), we obtain

$$\omega(\mathbf{r},t) = 4\pi\int daag(a)F(\mathbf{r},a,t), \tag{25}$$

where $g(a) = (av/D)/[1+(av/D)]$.

V. APPENDIX B

The R-matrix method [30] is a convenient computational tool for eliminating the exponentially growing terms from solutions of systems of second order linear differential equations. To find a regular solution of (9) we re-write this equation in the form of a system of two linear equations

$$\frac{dP}{dz} = (\rho + \omega(z,t))S(z,t) + \nu[S(z,t) - \bar{c}_v D_v]\delta(z)$$
$$\frac{dS}{dz} = P. \tag{26}$$

Assuming that $z > 0$, we consider how the solution of (26) behaves on an (arbitrarily chosen) interval $[z_1, z_2]$, which we assume to be sufficiently small so that inside this interval function $\omega(z,t)$ can be approximated by a constant $\omega(z,t) \approx \omega(z^*,t) = \omega^*$, where $z^* \in [z_1, z_2]$. The matrix relating the solutions of (26) at both ends of the interval has the form

$$\begin{pmatrix} P(z_2) \\ S(z_2) \end{pmatrix} = \begin{pmatrix} M_D(z_2 - z_1), & M_T(z_2 - z_1) \\ M_B(z_2 - z_1), & M_D(z_2 - z_1) \end{pmatrix} \begin{pmatrix} P(z_1) \\ S(z_1) \end{pmatrix}, \tag{27}$$

where

$$M_D(z) = \cosh(\sqrt{\rho + \omega^*} z),$$
$$M_T(z) = \sqrt{\rho + \omega^*} \sinh(\sqrt{\rho + \omega^*} z),$$
$$M_B(z) = \frac{\sinh(\sqrt{\rho + \omega^*} z)}{\sqrt{\rho + \omega^*} z}, \tag{28}$$

and $\det \hat{M} = M_D^2 - M_T M_B = 1$. Introducing the R-matrix by the relation $P(z) = R(z)S(z)$, we obtain

$$R(z_1) = \frac{M_D(z_2 - z_1)R(z_2) - M_T(z_2 - z_1)}{M_D(z_2 - z_1) - M_B(z_2 - z_1)R(z_2)}. \tag{29}$$

This equation defines the rule according to which the R-matrix propagates from a distant point $z \to \infty$ to the origin $z = 0$. The value of supersaturation at $z = 0$ is given by

$$S(0) = \frac{\nu \bar{c}_v D_v}{\nu - 2R(0)}, \tag{30}$$

and the entire profile $S(z)$ can now be restored recurrently by using a relation similar to (29)

$$S(z_2) = [M_D(z_2 - z_1) - M_B(z_2 - z_1)R(z_2)]^{-1} S(z_1). \tag{31}$$

FIGURES

FIG. 1. Distribution of concentrations of mobile interstitial atoms and vacancies plotted as a function of distance z to the grain boundary. Profiles shown in this Figure were calculated using equations (2) and (3) and assuming that $\rho = 10^7$ cm^{-2}, $\nu = 10^6$ cm^{-1}, $D_v = 0.1 \times \exp(-0.8/k_BT)$ cm^2/s, $D_i = 0.01 \times \exp(-0.15/k_BT)$ cm^2/s, $T = 600$ K, $K = 10^{-7}$ s^{-1} and $\alpha = a(D_i + D_v)$, where $a = 10^{15}$ cm^{-2}.

FIG. 2. Profiles of the vacancy supersaturation $S(z,t)$ calculated for the same set of parameters as those used in Fig.1 assuming that the rate of formation of critical cavity nuclei $N(z)$ is given by $N(z) = \beta c_v(z)$, where $\beta = 5 \cdot 10^3$ μ^{-3} s^{-1}.

FIG. 3. Distributions of the relative volume of growing cavities $W(z,t)$ calculated by integrating equation (8) for the same set of parameters as those used in Figs.1 and 2. Arrows show the position of maxima of the curves. Note the shift in the position of peaks resulting from the accelerated growth of cavities in the vicinity of the sink.

REFERENCES

[1] E. Ma, M. Atzmon, P. Bellon and R. Trivedi, Eds., *Phase Transformations and Systems Driven Far from Equilibrium*, Materials Research Society Symposium Proceedings, vol. 481 (Materials Research Society, Warrendale, Pennsylvania, 1998)

[2] G. Martin, *Current Opinion in Solid State & Materials Science* **3**, 552 (1998)

[3] C. A. English and D. J. Mazey, *Nucl. Energy* **29**, 67 (1990)

[4] K. Ehrlich, *Phil. Trans. Roy. Soc. (London)* **A357**, 595 (1999)

[5] A. D. Brailsford and R. Bullough, *Phil. Trans. Roy. Soc. (London)* **A302**, 87 (1981)

[6] R. S. Averback and T. Diaz de la Rubia, *Displacement Damage in Irradiated Metals and Semiconductors*, in: Solid State Physics, vol. 51, eds. H. Ehrenreich and F. Spaepen (Academic Press, 1998) pp. 281-402

[7] D. J. Bacon, F. Gao, Y. N. Osetsky, *Journ. Nucl. Mater.* **276**, 1 (2000)

[8] N. Soneda and T. Diaz de la Rubia, *Philos. Mag. A* **78**, 995 (1998)

[9] C. H. Woo, B. N. Singh and A. A. Semenov, *Journ. Nucl. Mater.* **239**, 7 (1996)

[10] D. Walgraef, in: *Patterns, Defects and Materials Instabilities*, NATO Advanced Study Institute Series, Ser. E: Applied Sciences, vol. 183, eds. D. Walgraef and N. M. Ghoniem (Kluwer Academic Publishers, Netherlands, 1990) p. 73

[11] B. N. Singh, *Rad. Effects & Defects in Solids* **148**, 383 (1999)

[12] C. Sagui and M. Grant, *Phys. Rev.* **E59**, 4175 (1999)

[13] R. Burghaus, *Phys. Rev.* **E57**, 3234 (1998)

[14] B. N. Singh and A. J. E. Foreman, *Philos. Mag.* **29**, 847 (1974)

[15] W. V. Green, S. L. Green, B. N. Singh and T. Leffers, *Journ. Nucl. Mater.* **103/104**, 1221 (1981)

[16] A. P. Sutton and R. W. Baluffi, *Interfaces in Crystalline Materials* (Oxford University Press, 1996) p. 424

[17] E. M. Lifshitz and L. P. Pitaevskii, *Physical Kinetics* (Pergamon Press, Oxford, 1981), §100, p. 432

[18] V. A. Shneidman, *Phys. Rev. Lett.* **75**, 4634 (1995)

[19] R. Becker and W. Döring, *Ann. Phys. (Leipzig)* **24**, 719 (1935)

[20] Ja. B. Zeldovich, *Sov. Phys. JETP* **12**, 525 (1942)

[21] H. Vehkamäki and I. Ford, *Phys. Rev.* **E59**, 6483 (1999)

[22] W. H. Press, S. A. Teukolsky, W. T. Vetterling and B. P. Flannery, *Numerical Recipes in Fortran* (Cambridge University Press, 1994) §17

[23] H. Trinkaus, B. N. Singh and A. J. E. Foreman, *Journ. Nucl. Mater.* **206**, 200 (1993)

[24] D. Rodney and G. Martin, *Phys. Rev. Lett.* **82**, 3272 (1999)

[25] A. I. Bas, Ya. B. Zeldovich and A. M. Perelomov, *Scattering, Reactions and Decays in Non-relativistic Quantum Mechanics*, 2nd edition, (Nauka, Moscow, 1971) ch. IV, §11

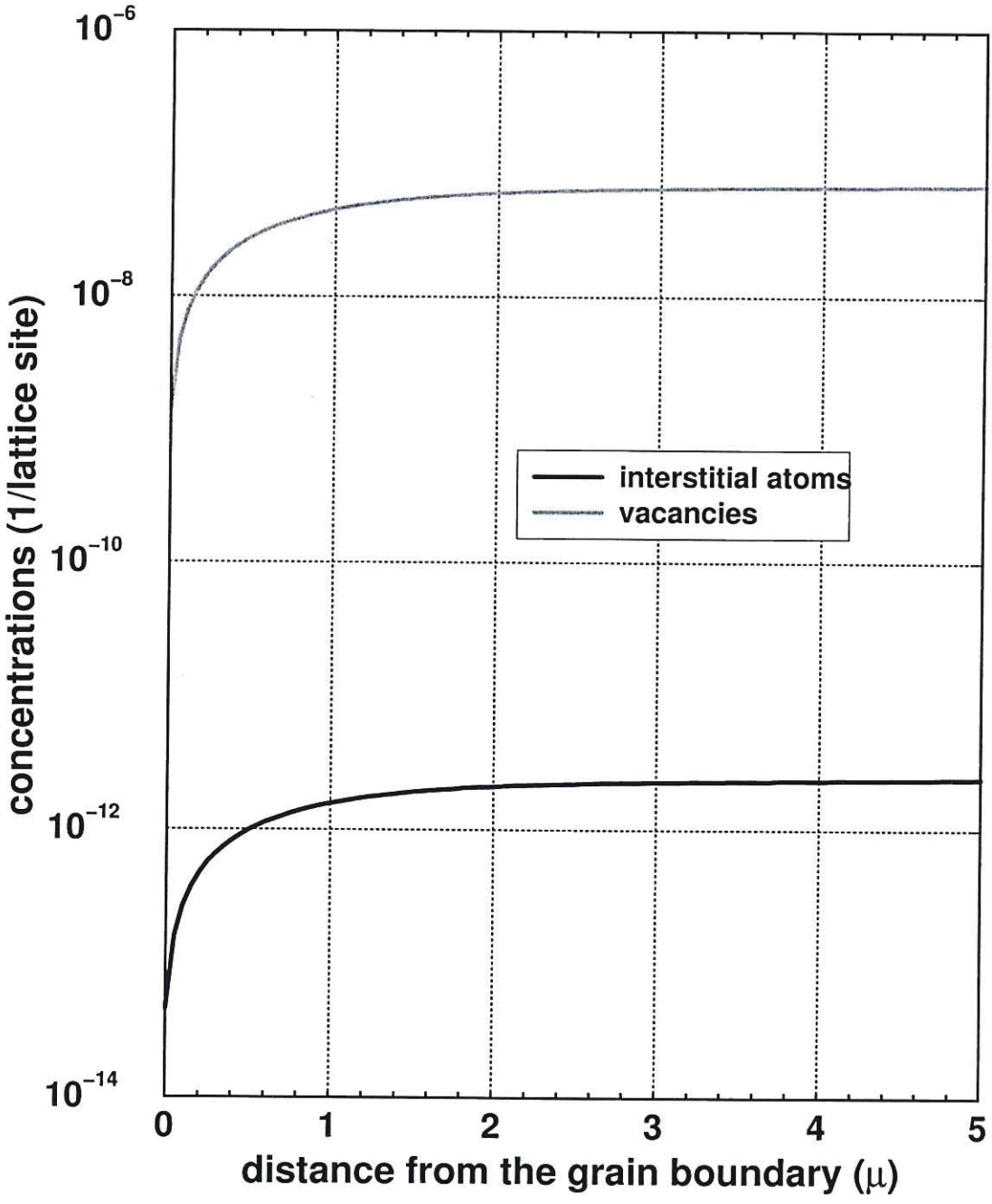
[26] M. L. Goldberger and K. M. Watson, *Collision Theory* (Wiley, New York, 1964)

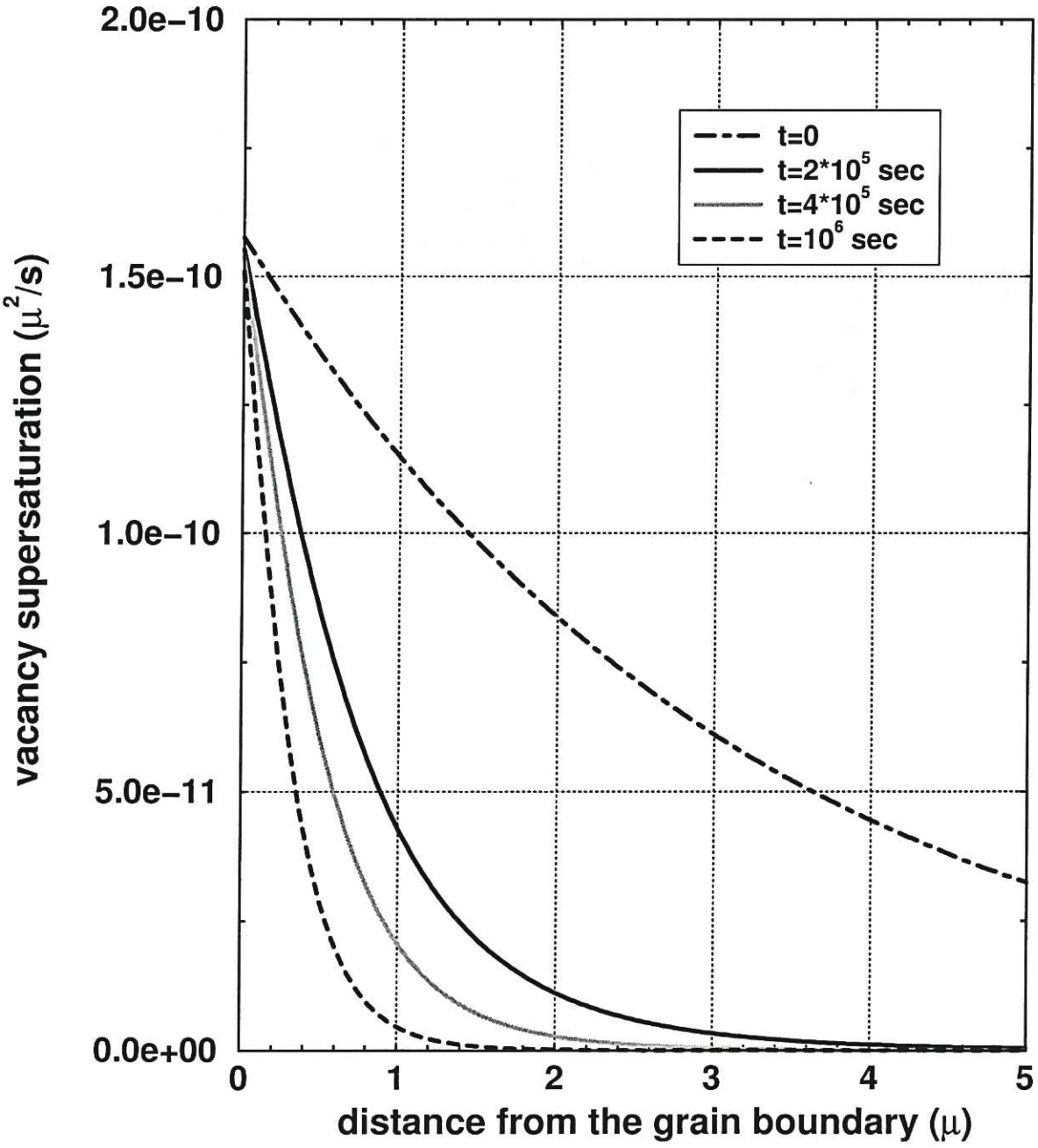
[27] J. M. Ziman, *Models of Disorder* (Cambridge University Press, 1979) §10

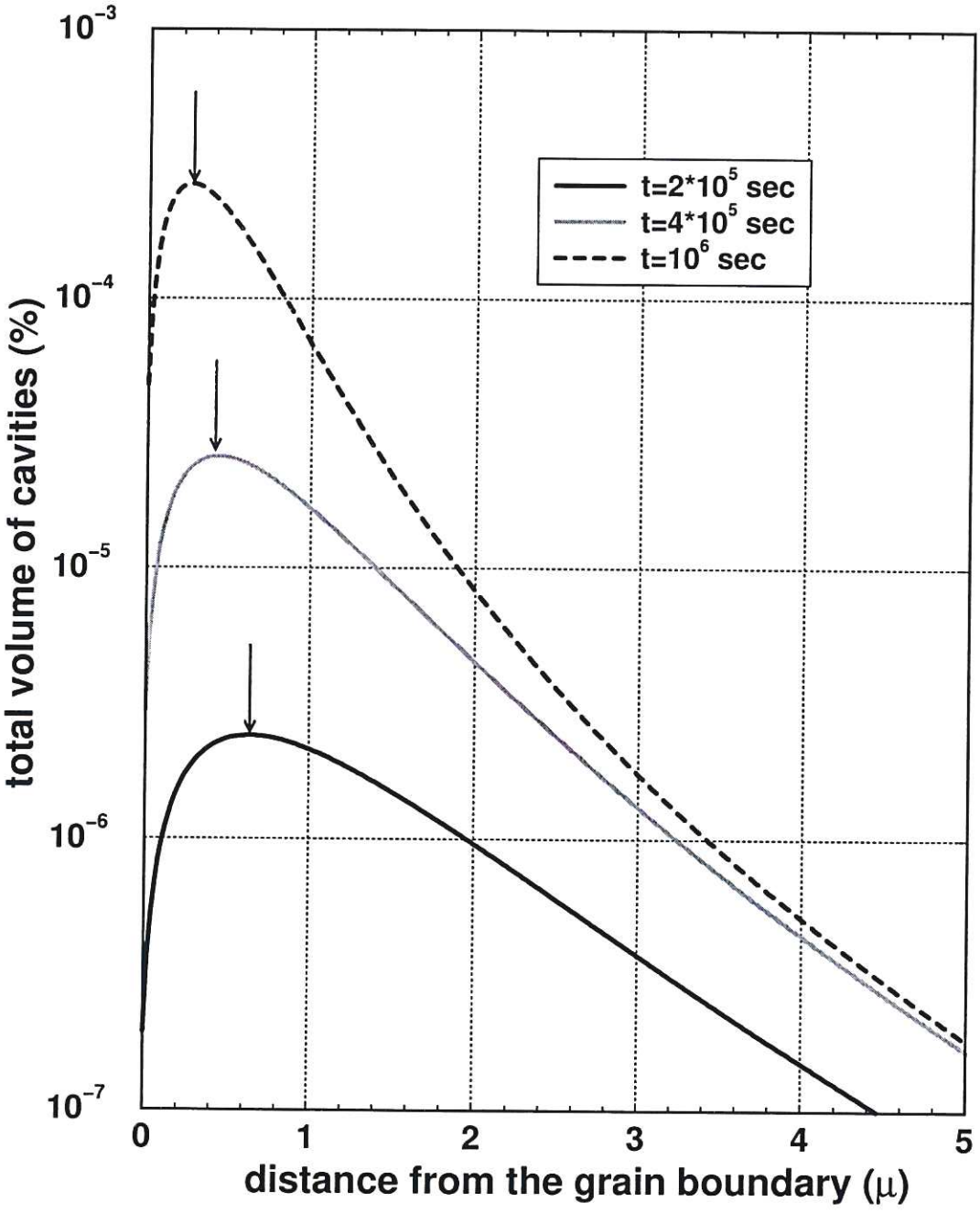
[28] M. Lax, *Phys. Rev.* **85**, 621 (1952)

[29] A. Ishimaru, *Wave Propagation and Scattering in Random Media* (Academic Press, New York, 1978)

[30] T. C. Zhao and S. Y. Tong, *Phys. Rev.* **B47**, 3923 (1993)


10^{-6}
10^{-8}
10^{-10}
10^{-12}
10^{-14}
concentrations (1/lattice site)
interstitial atoms
vacancies
0
1
2
3
4
5
distance from the grain boundary (μ)


2.0e−10
1.5e−10
1.0e−10
5.0e−11
0.0e+00
vacancy supersaturation (μ²/s)
0
1
2
3
4
5
distance from the grain boundary (μ)
t=0
t=2*10⁵ sec
t=4*10⁵ sec
t=10⁶ sec


10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
total volume of cavities (%)
t=2*10^5 sec
t=4*10^5 sec
t=10^6 sec
0
1
2
3
4
5
distance from the grain boundary (μ)