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**A CASCADE DIFFUSION THEORY OF SINK CAPTURE FLUCTUATIONS
DURING IRRADIATION OF A SOLID**

L. K. Mansur, A. D. Brailsford, and W. A. Coghlan

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A CASCADE DIFFUSION THEORY OF SINK CAPTURE FLUCTUATIONS
DURING IRRADIATION OF A SOLID*

L. K. Mansur, A. D. Brailsford,[†] and W. A. Coghlan[§]

ABSTRACT

Fluctuations in the number of defects captured by sinks in an irradiated solid, that arise because of the stochastic nature of collision cascade events, are analyzed. Two types of sinks are considered, cavities (or voids) and dislocations. The importance of the physical size of the sink is emphasized, as also is the magnitude of the fluctuations in defect capture relative to the behavior of its statistical mean. In particular, it is shown that the ratio of the variance to the mean, for either a cavity or a dislocation segment, decreases rapidly as overall steady state is approached. Further analytical and computational aspects of a shell model that we introduced earlier are analyzed. The relationship of this model to a truly random system is established, and additional calculations are presented to exemplify some of the features predicted by the mathematical analysis. Importance functions describing the spatial origins of the point defects contributing to the average concentration and flux are described. The probabilities of special types of cascade coincidences are developed. The application of the present formalism to the problems of void nucleation, and dislocation climb over localized obstacles, in irradiated solids is indicated.

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1. INTRODUCTION

The point defects generated by the irradiation of a solid with energetic neutrons or fast charged particles are generally born in collision cascades. Each cascade consists of a certain number of interstitials and vacancies dependent upon the energy of the bombarding particle. Some fraction of these defects survive spontaneous or in-cascade recombination. Instead, they migrate towards the sinks such as voids and dislocations that are present in the material [1]. As a result of the preferential attraction of dislocations for interstitials, this migration tends to promote dislocation loop formation (and/or the dislocation climb rate), and to cause void growth [2-6], in the absence of competing recovery processes [7,8]. By such a sequence of events, irradiation can give rise to volume swelling, enhanced creep, solute segregation and/or phase instability and embrittlement in reactor components [9].

Although the cascade events are both discrete in time and localized spatially, many of the mechanisms underlying the above phenomena can be described quantitatively by macroscopic averaging procedures. In such an approach, the defect production is taken as uniform in both time and space at an appropriate mean value. In the same vein, the effects of the discrete sinks (voids and dislocations, for example) are described by the properties of a spatially homogeneous lossy continuum known as the Effective Medium [5,10,11]. Long-term intrinsic recombination (about which we shall say nothing further in this paper) may also be incorporated in this formalism. Thus the rudimentary picture that arises is the following: in effect, every point in the continuum gives rise to an infinitesimal number of point defects, and every point, likewise, makes an

infinitesimal contribution to the sink character of the system for each loss process. Effective Medium theory furnishes the loss rate parameters of the continuum in terms of the measurable physical parameters (such as the void density and radius, and the dislocation density, for example). The end result is a coarse-grained spatial and time dependent description of the defect production and loss processes. This is often referred to as Chemical Rate Theory.

By virtue of the nature of its construction, such a theory gives the correct value for temporal and spatial averages of the physical quantities of interest. This we shall also have occasion to confirm later. However, it clearly ignores any effects of fluctuations about the mean in both the random production of defects and in the spatial dispersion of sinks. These are quite distinct issues which may be investigated separately, and in fact one of us has already shown [10] that sink-sink correlation effects are reasonably well described by Effective Medium Theory. Thus there only remains the question of the effect of fluctuations in cascade production. It is their role in the context of void nucleation and growth, and dislocation climb, which constitutes the subject of this paper.

Specifically, we shall be concerned with the statistical aspects of the defect response arising in an Effective Medium wherein cascades occur randomly. We shall present derivations of the defect concentration at a general observation point, the flux to a void or dislocation, and the number of defects collected in a given time. Both their statistical means and variances will be investigated. The relevance of these for void nucleation and dislocation climb will also be made evident.

This investigation is a natural outgrowth of our earlier work on a cascade diffusion theory [11]. The latter provided the first evidence of the extremely sporadic nature of the point defect concentrations at an arbitrary reference point when nearby cascades are treated as discrete temporal events. For though we found mean values conforming to those prescribed by Chemical Rate Theory, it was equally clear that fluctuations in concentration could lead to the climb of dislocations held up at localized obstacles. Thus, the concept of cascade induced creep was born and later quantified [12].

Our original investigation [11] of cascade effects, being somewhat exploratory, contained several ingredients which were of concern to us. The first was that the Effective Medium was presumed to have the same characteristics (vis-a-vis defect loss rates) as in steady state theory. In order to ascertain the viability of this approach, therefore, we have since been led to generalize Effective Medium Theory to time-dependent production processes [13]. Corrections to prior theory on this score were found, but we have been able to demonstrate that these are small as long as the volume fraction of voids is also small. Hence, once having indicated below how our newer results [13] reduce to the old, we shall continue to use the simplified Effective Medium Theory employed earlier.

A further issue of doubt concerns the matter of the relation of the concentration at an arbitrary reference point to the flux of defects to a sink placed in its vicinity. One might guess (as we did) that the two are (approximately) linearly related. Rate theory lends some credence to this tack [5]; yet the point is far from obvious. Stated bluntly, this prescription amounts to computing the concentration at some point with

the sink absent and then presuming that when the sink is inserted it has no effect. Obviously, this cannot be correct precisely even for an average property such as the flux to the sink, while its use for non-near properties such as the variance is even more questionable.

Later extensions of our work by others [14,15], while making useful extensions in several directions, have ignored both the above aspects and yet a further point worthy of investigation. Namely, the extent to which fluctuations about some average state depend upon the nature of the average state itself. To be specific, suppose the production rate is, on average, independent of time. Then Chemical Rate Theory describes how the average state evolves in time from some assumed initial condition towards steady state. To us, it seems intuitively clear that fluctuations will have a greater significance initially than as time evolves, if the starting condition is other than the microscopic steady state itself. This point is particularly vital to understand when considering spatially and temporally localized events such as void nucleation or dislocation climb over discrete obstacles. For one must ask, in assessing the effect of fluctuations on either of these processes, whether or not they can arise prior to the establishment of steady state in the local environment for each point defect type. It is not our intent here to explore the physics of these situations in detail but rather to highlight the importance of the character of the average state, for interstitials and vacancies individually. For unless this is appreciated, the effect of fluctuations about the mean may be over-estimated.

The above serves to highlight some of the reasons for undertaking the present study. The system investigated here is an idealization of reality

in two aspects. Namely, we consider only cavities of fixed size and cylindrical sinks that do not move. These are accepted prescriptions for mimicking (growing) voids and (climbing) dislocations. Moving boundary effects are known to be small for the mean properties. But for fluctuations (non-linear effects) one has no known yardstick. Thus we can do no more than mention this limitation of our treatment and express the belief that moving sink boundary effects will be minimal. This should particularly be the case, we submit, for a time-integrated property such as the total number of defects collected by a sink over a given time interval. Such a quantity, in contradistinction to the current at a particular time, does not depend upon a gradient at a particular point in space. If our model is only subsequently augmented by defect conservation at the sink (causing growth or climb as the case may be), we believe the overall prescription will nevertheless furnish an accurate physical description.

The paper is structured as follows. In the next section we define and solve the basic mathematical problem. Namely that of determining the time evolution of the flux entering a spherical cavity or hollow cylinder after the initiation of a cascade in its vicinity. The presence of the sink does indeed modify the flux to it and in a manner which can be shown to be entirely consistent with the Effective Medium in which it resides. This is demonstrated in Sect. 3, where the statistical averages simulating spatially uniform (but potentially time-dependent) irradiation are derived. Section 4 contains an analysis of the accompanying fluctuations in the defect flows to different sink types, as measured by the variance of these quantities. The importance of the nature of the average defect

state is there established. Finally, in Sect. 5, we present the numerical results from some model calculations. These serve to highlight some additional statistical aspects of cascade generation. They indicate that parameters additional to rms fluctuations may be of significance in localized defect processes, although the matter is only superficially examined. The paper is concluded with a brief summary in Sect. 6.

2. DEFECT FLOWS TO SINKS

In our companion paper [13] we showed that the continuum defect loss rate, $L(\underline{r}, t)$, embodied in the relation

$$L(\underline{r}, t) = Dk^2 c(\underline{r}, t) + D \int_0^t \psi(t - t') \frac{dc(\underline{r}, t')}{dt} - S(t) , \quad (1)$$

led to a self-consistent description of defect losses to a random array of voids and dislocations for spatially uniform irradiation. In this equation D and $c(\underline{r}, t)$ are the defect diffusivity and concentration respectively, while k^2 is the total steady state sink strength pertaining to all sinks in the system [5,16].* The functions ψ and S are defined below.

When dislocations and cavities alone are present

$$k^2 = k_D^2 + k_C^2 , \quad (2)$$

where the respective contributions for each sink type are [16]

$$k_D^2 = Z\rho_D , \quad (3)$$

and

$$k_C^2 = k_0^2 (1 + kr_C) . \quad (4)$$

*We use k^2 and ρ_D here to denote sink strength and dislocation density for consistency with the companion paper Ref. [13]. Elsewhere as in Ref. [11] we often use the symbol S to denote sink strength and L to denote dislocation density.

Here r_c is the cavity radius and

$$k_0^2 = 4\pi r_c C, \quad (5)$$

with C the cavity volume concentration. In Eq. (3) ρ_D is the dislocation density (line length per unit volume) and Z is a parameter dependent upon the nature of the defect — i.e., whether interstitial or vacancy. Since we ignore intrinsic recombination, it is not necessary to make the latter distinction in much of what follows. Thus we shall omit the redundant subscript for defect species where possible. The approximation sign associated with the equation in question arises from the customary neglect of the modest dependence of the bias parameter of the dislocation, Z , upon the dislocation density. Further details on this point are given in Ref. [13].

The integral term describes the additional losses of point defects above those in steady state due to time changes in the concentration. The function $\psi(t)$ in Eq. (1) is given by [13]

$$\psi(t) = \beta k_0^2 r_c \left[\frac{e^{-\beta^2 t}}{\beta (\pi D t)^{1/2}} - \operatorname{erfc}(\beta (D t)^{1/2}) \right], \quad (6)$$

where

$$\beta = \{k_0^2 + Z\rho_D + (\frac{1}{2} k_0^2 r_c)^2\}^{1/2}, \quad (7)$$

(both in the constant Z approximation). As we have shown by the analysis of several examples [13], effects associated with the presence of the ψ integral are comparatively small when the volume fraction of cavities, δ , is small. For since $k_0 r_c = (3\delta)^{1/2}$, it follows that $\beta \approx k$, whence the integral term has a magnitude of the order of $k_0 r_c$ times that of the loss

terms that are proportional to $c(\underline{r}, t)$. It is possible to carry through much of the ensuing analysis retaining this integral term but it appears that nothing particularly different arises apart from a complexity of mathematical detail. Thus we shall immediately restrict ourselves to the small swelling regime. In that instance, the ψ -integral may legitimately be discarded to obtain a first approximation to physical quantities.

The one remaining unspecified function in $L(\underline{r}, t)$ is the source term $S(t)$. In general, the latter depends upon the thermal emission rate of defects (vacancies) from the sinks and upon the nature of the microscopic initial state around each sink at $t = 0$. With the neglect of ψ the latter dependence disappears. We shall further assume that the temperature is low enough for thermal emission effects to be negligible. In that case $S \rightarrow 0$ and Eq. (1) reduces to $L(\underline{r}, t) = Dk^2 c(\underline{r}, t)$, implying that the loss rate here used has the same functional form as that which prevails in steady state [5,16]. The approximate nature of this step is openly acknowledged.

The continuity equation for either defect type is therefore

$$\frac{\partial c(\underline{r}, t)}{\partial t} - (D\nabla^2 - Dk^2)c(\underline{r}, t) - G(\underline{r}, t) \approx 0, \quad (8)$$

where G is the defect production rate. The latter is synthesized from spatially and temporally discrete cascade events, the details of which we shall discuss later. Suffice it to note here that if we can solve

$$\left[\frac{\partial}{\partial t} - D(\nabla^2 - k^2) \right] g(\underline{r}, \underline{R}; t, t') = \delta(\underline{r} - \underline{R})\delta(t - t') \quad , \quad (9)$$

with the Green's function g satisfying the same boundary conditions as

those upon $c(\underline{r}, t)$, then

$$c(\underline{r}, t) = \int dt' \int d\underline{R} g(\underline{r}, \underline{R}; t, t') G(\underline{R}, t') \quad (10)$$

Clearly, the function g has the physical significance of being the concentration at $\underline{r}$ and time t arising from a Dirac delta function cascade at $\underline{R}$ and t' . If physical cascades are taken to have this spatial form, then Eq. (10) is tantamount to a sum over cascades. On the other hand, if cascades are presumed to have some other physical shape (e.g., a Gaussian centered upon $\underline{R}$ initially), then Eq. (10) entails an integration which transforms g from that appropriate to a delta function to that appropriate to the presumed shape (e.g., Gaussian) as well as the cascade sum. In either case, the basic quantity governing the response is g ,* and the nature of g will depend upon the boundary conditions associated with Eq. (9) (i.e., or the defect concentration). These are different for each of the three problems we now discuss.

2.1 THE CONCENTRATION AT A DISTANT REFERENCE POINT

By a distant reference point we mean a point far from any sink. (We shall be more specific in Subsect. 2.2 below.) The boundary conditions upon c (and hence g) are taken to be $c = 0$ for $t < t'$ and $c \rightarrow 0$ for $r \rightarrow \infty$ for all $t > t'$. Clearly the solution depends only upon $\underline{\rho} = \underline{r} - \underline{R}$, and is spherically symmetric about the origin of $\underline{\rho}$.

Using this observation, we let $g(\underline{r}, \underline{R}; t, t') = \bar{g}(\underline{\rho}; t, t')$ so that Eq. (9) becomes

*In the subsequent analysis, where the arguments of functions may be inferred without ambiguity, we shall omit them.

$$\left[\frac{\partial}{\partial t} - D \left(\frac{1}{\rho^2} \frac{\partial}{\partial \rho} \rho^2 \frac{\partial}{\partial \rho} - k^2 \right) \right] \bar{g}(\rho; t, t') = \delta(\rho) \delta(t - t') \quad (11)$$

As in our earlier work [13] we choose the origin of time as the point at which the irradiation commences. Then t' is necessarily positive and we solve the above by Laplace Transform methods. After multiplying Eq. (11) on the left by $\exp(-pt)$ and integrating over t from zero to infinity one finds

$$\left[\frac{1}{\rho^2} \frac{d}{d\rho} \rho^2 \frac{d}{d\rho} - k^2 + \frac{p}{D} \right] \bar{g}_p = -\frac{\delta(\rho)}{D} e^{-pt'} \quad (12)$$

where $\bar{g}_p$ is the Laplace Transform [17] of $\bar{g}$:

$$\bar{g}_p(\rho) = \int_0^\infty g(\rho; t, t') e^{-pt} dt \quad (13)$$

The appropriate solution of Eq. (12) is

$$\bar{g}_p = \frac{\exp[-(k^2 + p/D)^{1/2} \rho - pt']}{4\pi D \rho} \quad (14)$$

which may be inverted [17] to give

$$\bar{g}(\rho; t, t') = \frac{\exp[-\rho^2/4D\tau] \exp(-Dk^2\tau)}{(4\pi D\tau)^{3/2}} \quad (15)$$

where $\tau \equiv t - t'$. The result applies for $\tau > 0$; for $\tau < 0$, $\bar{g}$ is zero.

The form given in Eq. (15) is that quoted in our earlier analysis [11] apart from the change of notation noted after Eq. (1). It is the first of the three response functions we shall require for the subsequent discussion.

2.2 DEFECTS COLLECTED BY A CAVITY FROM ONE CASCADE

In order to calculate the quantities of interest for sink growth, it is not enough to know the defect concentration (or Green's function) appropriate to distances far from all sinks. For, since the medium is lossy, only cascades in the vicinity of a sink will yield any appreciable flux to it [11]. Moreover, sinks are not point objects. Rather, their surfaces constitute finite boundaries upon which the concentration must have some fixed value for all times. In our case, this fixed value is zero.* Thus the Green's function we now require, though still a solution of Eq. (9), must satisfy the constraint that g be zero on the sink surface.

For the cavity problem the geometry we consider is illustrated schematically in Fig. 1. The solution of Eq. (9) satisfying $g = 0$ on $r = r_c$ we decompose into two parts:

$$g(\underline{r}, \underline{R}; t, t') = v(\underline{r}, \underline{R}; t, t') + u(\underline{r}, \underline{R}; t, t') \quad . \quad (16)$$

Here the function v is identical to the former g of Eq. (15). We have simply changed the name given to the function. Thus, since v is a solution of the inhomogeneous Eq. (9), u must satisfy

$$\left[\frac{\partial}{\partial t} - D(\nabla^2 - k^2) \right] u(\underline{r}, \underline{R}; t, t') = 0 \quad , \quad (17)$$

and assure that $(u + v) = 0$ at $r = r_c$ for all t .

*It is assumed that local transport of defects across the sink-medium interface is always sufficiently rapid for equilibrium to be maintained at the surface. The approach we develop, however, could be generalized to any linear boundary condition.

Fig. 1. The coordinate systems for the calculation of the cavity Green's function.

Fortunately, for our later applications it is not necessary to explore all details of u . Equation (17) is linear, so that we can imagine its solution being expanded in spherical harmonics [18]. Whatever its detailed structure, only the totally spherically symmetric component will yield a non-zero contribution to the surface integral of the radial defect flux at the void surface. Using Laplace Transform techniques, as before, we can immediately write down what the Laplace Transform, u_p^0 must be. Namely,

$$u_p^0 = B r^{-1} \exp[-(k^2 + p/D)r - pt'] \quad , \quad (18)$$

where B is some constant of integration. [The r -independent factor

$\exp(-pt')$ is added for convenience.] The inverse of u_p^0 is the spherically symmetric part of $u(\underline{r}, \underline{R}; t, t')$ itself.

Like the equation for u , the boundary condition upon u at $r = r_c$ is also linear. Thus the form of Eq. (16) can also be made to satisfy these conditions. Further we can imagine v as being expanded in spherical harmonics (about the origin of $\underline{r}$, not the vector $\underline{\rho}$). The spherically symmetric component, v_p^0 , of v_p will be

$$v_p^0 = \frac{1}{4\pi} \int d\Omega_r v_p \quad , \quad (19)$$

where v_p is equal to the right-hand member of Eq. (14) and $d\Omega_r$ is the element of solid angle at $\underline{r}$. From the last relation and the boundary condition that $v_p^0 + u_p^0 = 0$, at $r = r_c$, we determine the constant B , thus completing the solution for the spherically symmetric part of g .

The result obtained for v_p^0 is

$$v_p^0 = (1/8\pi D R r q) \{ \exp[-q|\underline{r} - \underline{R}|] - \exp[-q(r + R)] \} \exp(-pt') \quad , \quad (20)$$

where $q \equiv (k^2 + p/D)^{1/2}$. From this we find B as indicated above and so arrive at the following for u_p^0 :

$$u_p^0 = -(1/8\pi D R r q) \{ \exp(qr_c) - \exp(-qr_c) \} \exp[-q(R + r - r_c) - pt'] \quad . \quad (21)$$

Hence we obtain the Laplace Transform, g_{cp}^0 say, of the spherically symmetric part, g_c^0 , of the desired Green's function by addition of Eqs. (20) and (21):

$$g_{cp}^0(r, R; t') = (1/8\pi D q R) \chi_p(r, R) \exp(-pt') \quad , \quad (22)$$

where

$$\left. \begin{aligned} \chi_p(r, R) &= [\exp(qr) - \exp(-qr + 2qr_c)] \exp(-qR); \quad r < R, \\ &= [\exp(qR) - \exp(-qR + 2qr_c)] \exp(-qr); \quad r > R. \end{aligned} \right\} \quad (23)$$

Two quantities of later interest are the defect current to the cavity due to the cascade at R , $I_c(t, t')$ and the total number of defects collected, $n_c(t, t')$, up to time t . These are defined respectively by

$$I_c(t, t') = 4\pi r_c^2 D \left(\frac{\partial g_c^0}{\partial r} \right)_{r_c}, \quad (24)$$

and

$$n_c(t, t') = \int_0^t I_c(t'', t') dt'' . \quad (25)$$

The Laplace Transform, I_{cp} , of $I_c(t)$ follows immediately from Eq. (23).

It is

$$I_{cp} = (r_c/R) \exp[-q(R - r_c) - pt'] . \quad (26)$$

Using the tables in Ref. (17), $I_c(t, t')$ is found to be

$$\left. \begin{aligned} I_c(t, t') &= \frac{r_c(R - r_c)}{2(\pi D \tau^3)^{1/2} R} \exp[-(R - r_c)^2/4D\tau] \exp(-Dk^2\tau); \quad \tau > 0 \\ &= 0; \quad \tau < 0 . \end{aligned} \right\} \quad (27)$$

Here $\tau = t - t'$ as before. An integration of Eq. (27) then gives $n_c(t, t')$. This will not be written down explicitly here. However, in order to provide a link to the more familiar, note that in the limit $k \rightarrow 0$

Eq. (27) yields

$$I_c(t, t') \xrightarrow{k \rightarrow 0} (r_c/R) \frac{d}{d\tau} [\operatorname{erfc}\{(R - r_c)/2(D\tau)^{1/2}\}] ; \quad \tau > 0 \quad (28)$$

In addition, the total number of defects collected by a cavity over all time from a cascade born at time t' (at $r = R$), $n_c(\infty, t')$, is given by the limit of Eq. (26) when $p \rightarrow 0$. Hence the two special cases are

$$\left. \begin{aligned} n_c(t, t') &\xrightarrow{k \rightarrow 0} (r_c/R) \operatorname{erfc}\{(R - r_c)/2(D\tau)^{1/2}\}; \quad \tau > 0, \\ \text{and} \\ n_c(\infty, t') &= (r_c/R) \exp\{-k(R - r_c)\}. \end{aligned} \right\} \quad (29)$$

The last is of interest because it substantiates one's physical intuition in the following manner. If the cavity is small, its overall effect on the diffusion field ought to be small also. The role of the cavity should be simply that of collecting all defects that impinge upon it. This being the case, if we integrate the concentration at an arbitrary reference point over all time subsequent to the cascade event [see Eq. (15)], we should mimic the cavity's effect. To transform to a number collected, Rate Theory suggests we multiply the result by the factor $4\pi r_c D$. Using this ruse produces the result for $n_c(r, t')$ given above multiplied by the factor $\exp(-kr_c)$, which is of order unity when $kr_c \ll 1$. This is in fact the approximation used in Ref. [11]. However, the reader should not infer from this that the more complicated analysis is unnecessary. The result given here is an asymptotic ($t \rightarrow \infty$) and linear property only. At arbitrary times we need the full mathematical framework in order to obtain the physical quantities we require for the later analysis of a sequence of cascades near a cavity.

2.3 DEFECTS COLLECTED BY A DISLOCATION FROM ONE CASCADE

The calculation needed next is similar in principle to that just performed. Only the geometry differs; the sink is now a straight cylinder rather than a sphere. Accordingly we shall here simply highlight points along the derivation and leave some of the details for the reader to verify.

The geometrical aspects of the problem are illustrated in Fig. 2. The dislocation is modeled as a cylinder of radius r_1 which is centered upon the z -axis of a cylindrical coordinate system. An arbitrary point on this axis is taken as the origin. In this coordinate system the z component of $\underline{R}$ is denoted by z_R and the distance of the cascade from the z -axis by R' . In vector notation, $\underline{R} = \underline{R}' + \underline{z}_R$, where, by convention, the first written lies in the transverse plane and the second along the z -direction. In this system

$$\delta(\underline{r} - \underline{R}) \rightarrow \delta(z - z_R) \delta_2(\underline{r}' - \underline{R}') , \quad (30)$$

where the three-dimensional vector $\underline{r}$ is written similarly as $\underline{r} = \underline{r}' + \underline{z}$. (We shall now immediately drop the prime on $\underline{r}'$ and $\underline{R}'$ for notational simplicity, having made clear their two-dimensional character.) The suffix 2 on the second Dirac delta function is simply a means of indicating that it refers to two-dimensional integrations.

Using the prescription of Eq. (30), one must now solve Eq. (9) subject to the boundary condition that g vanish when the two-dimensional vector $\underline{r}$ (see above) has magnitude r_1 . The algebra is simplest if we work first with the Fourier Transform with respect to z as well as the Laplace Transform with respect to time. The former, for any function $f(z)$ is

Fig. 2. The geometry for the calculation of the dislocation Green's function.

defined via

$$f_{kz} = (2\pi)^{-1/2} \int_{-\infty}^{\infty} f(z) \exp[-ik_z z] dz \quad (31)$$

so that

$$f(z) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} f_{kz} \exp[ik_z z] dk_z \quad (32)$$

It follows then from Eq. (9) that the double transform, g_{pk_z} , of the function g must now satisfy

$$\nabla_2^2 g_{pk_z} - Q^2 g_{pk_z} = \frac{-\delta_2(\underline{r} - \underline{R})}{(2\pi)^{1/2} D} \exp[-(ik_z z_R + pt')] , \quad (33)$$

where

$$Q^2 = q^2 + k_z^2 \equiv k^2 + k_z^2 + p/D , \quad (34)$$

and ∇_2^2 is the two-dimensional Laplacian. A solution of the inhomogeneous Eq. (33) appropriate to infinite space (i.e., ignoring the presence of the cylinder) is $g_{pk_z} = v_{pk_z}$ where

$$v_{pk_z} = \frac{K_0(Q|\underline{r} - \underline{R}|)}{(2\pi)^{3/2} D} \exp[-(ik_z z_R + pt')] . \quad (35)$$

Here K_n is the Modified Bessel Function of the second kind of order n [18]. The preceding is the solution which is isotropic in angle about a coordinate system that is translated parallel to the dislocation axis so that it passes through the cascade point. It is not angle-independent about the z -axis of Fig. 2, but is, in fact, the transformed counterpart of the Green's function of Subsect. 2.1.

The Green's function sought here is again that discussed above plus a solution of the homogeneous equation, the latter being included to satisfy the boundary condition on $r = r_1$. In this two-dimensional case, the angular functions appropriate for an expansion are the cosine and sine functions $\cos n\theta$ and $\sin n\theta$, respectively (with n an integer or zero). Now only the $\cos n\theta$ term with $n = 0$ will contribute to the surface integral of the current into a length of the cylinder. In terms of the double

transforms used here this means that we need only consider augmenting v_{pk_z} by the angle-independent solution of the homogeneous equation. Such a solution is

$$u_{pk_z}^0 = -E \frac{K_0(Qr)}{K_0(Qr_1)} \exp\{-(ik_z z_R + pt')\} , \quad (36)$$

where E is a constant. (The remaining r -independent terms are added for later convenience). Thus it only remains to determine the angular average, $v_{pk_z}^0$ say, of v_{pk_z} to determine E from the condition that the sum $(v_{pk_z}^0 + u_{pk_z}^0)$ vanish on $r = r_1$.

We find, after some analysis, the following result for $v_{pk_z}^0$:

$$v_{pk_z}^0 = \frac{I_0(QR)K_0(Qr) \exp[-(ik_z z_R + pt')]}{(2\pi)^{3/2}D} ; \quad r > R , \quad (37)$$

and

$$v_{pk_z}^0 = \frac{K_0(QR)I_0(Qr) \exp[-(ik_z z_R + pt')]}{(2\pi)^{3/2}D} ; \quad r < R , \quad (38)$$

where I_n is the Modified Bessel Function of the first kind of order n . From Eqs. (36) and (38) the constant E may then be determined via the boundary condition at $r = r_1$. The end result is the following expression for the double transform, $g_{Dpk_z}^0$ say, of the angle-independent part, g_D^0 , of the required Green's function:

$$g_{Dpk_z}^0 = \frac{[K_0(Qr_1)I_0(Qr) - I_0(Qr_1)K_0(Qr)]K_0(QR)}{(2\pi)^{3/2}DK_0(Qr_1)} \times \exp[-(ik_z z_R + pt')] ; \quad r < R , \quad (39)$$

and

$$g_{Dpk_z}^0 = \frac{[K_0(Qr_1)I_0(QR) - I_0(Qr_1)K_0(QR)]K_0(Qr)}{(2\pi)^{3/2}DK_0(Qr_1)} \quad (40)$$

$$\times \exp[-(ik_z z_R + pt')] ; \quad r > R .$$

From the first of the above we can immediately evaluate the double transform of the current per unit length flowing into the cylinder due to the cascade. The current itself is

$$i_D(z, t, t') = 2\pi r_1 D \left(\frac{\partial g_D^0}{\partial r} \right)_{r_1} ; \quad (41)$$

hence its double transform is

$$i_{pk_z} = \frac{K_0(QR) \exp[-(ik_z z_R + pt')]}{(2\pi)^{1/2} K_0(Qr_1)} . \quad (42)$$

(A lower case symbol, i , is used here to emphasize that the quantity is a current density.) The current collected by a finite length, and the associated number of defects accumulated in a given time will be evaluated shortly (see Subsect. 3.2). It is convenient first, however, to discuss some of the statistical aspects of the defect generation process prior to developing this aspect.

We now have at hand all the three Green's functions needed for our later analysis.

3. STATISTICAL MEAN VALUES

3.1 GENERAL FEATURES

Defects arise from the cascade events initiated by primary knock-on atoms [19]. We shall ignore all details of the spread in energy of the

bombarding particle and of the structure of cascades themselves. Each cascade beyond the first is taken as the precise duplicate of its predecessor. The only variable element in the process that we shall consider is that cascades may occur in any point in space and time once the irradiation has commenced. The mean rate of cascade generation is taken to be the product of the flux of bombarding particles, ϕ , the atomic displacement cross section, A , and the volume density of lattice sites N_0 . Thus the mean generation rate of defects per unit volume per unit time, G_0 , is

$$G_0 = N_0 A \phi \nu , \quad (43)$$

where ν is the number of defects generated per cascade.

These production events are taken to be perfectly random; there is no correlation between events in the same volume element at different times or between events in different volume elements at any time. Thus they conform to the requirements for a Poisson Distribution [20]. It is convenient to divide space up into volume elements (labeled j) and time intervals of length Δt (labeled α). Within the volume element ΔV_j surrounding the point $\underline{R}_j$ we suppose there are N_j^α cascades in the interval of time Δt_α centered upon the time t_α .

The probability of the above situation is [20]

$$P(N_j^\alpha; \lambda \Delta t_\alpha) = \frac{(\lambda \Delta t_\alpha)^{N_j^\alpha}}{N_j^\alpha!} \exp(-\lambda \Delta t_\alpha) . \quad (44)$$

The mean value of N_j^α , $\overline{N_j^\alpha}$ say, is therefore

$$\overline{N_j^\alpha} = \sum_{n=0}^{\infty} n P(n; \lambda \Delta t_\alpha) = \lambda \Delta t_\alpha \equiv G_0 \Delta V_j \Delta t_\alpha / \nu . \quad (45)$$

The last step identifies λ as the mean cascade rate in the volume ΔV_j . Similarly, the statistical mean (or expectation) of any physical quantity $M_j(t, t_\alpha)$ that depends linearly upon the number of cascades within ΔV_j during Δt_α at t_α will have the mean value $\overline{M_j(t, t_\alpha)} = (G_0 \Delta V_j \Delta t_\alpha / v) m_j(t, t_\alpha)$, where $m_j(t, t_\alpha)$ is the contribution to M_j per cascade. Quantities which depend, in addition, upon contributions from cascades all arising at different points in space-time must be comprised of sums of the preceding over all j and α . The prescriptions

$$\left. \begin{aligned} \sum_j \{ \dots \} \Delta V_j &\longrightarrow \int \{ \dots \} dV_j \\ \sum_\alpha \{ \dots \} \Delta t_\alpha &\longrightarrow \int_0^t \{ \dots \} dt' \end{aligned} \right\} \quad (46)$$

then indicate how spatial sums and temporal sums, from the onset of the irradiation to the time of observation, t , are to be evaluated.

The number of defects at an observation point from all prior cascades, and the current collected by a sink as a function of time are both in this category. They also are proportional to the number of defects per cascade. (The appropriate m is proportional to v ; thus v drops out of the bookkeeping.) Hence, if we idealize cascades at their inception as delta functions in space at time, we may evaluate the physical quantities just mentioned by appropriate integration of the Green's functions we have already derived. This will be our next topic.

3.2 CONCENTRATION AND CURRENT

From Eq. (15) we find that the concentration, $c_\infty(t)$ say, at a point far from sinks possesses the mean value (for uniform irradiation) of

$$\begin{aligned} \overline{c}_-(t) &= 4\pi G_0 \int_0^t dt' \int_0^\infty \rho^2 \frac{\exp[-\rho^2/4D\tau] \exp(-Dk^2\tau)}{(4\pi D\tau)^{3/2}} d\rho \\ &= (G_0/Dk^2)[1 - \exp(-Dk^2t)] \end{aligned} \quad (47)$$

This is a standard result of Chemical Rate Theory for time-independent irradiation. It is injected here simply as a first indication of how some familiar results may be gained from the present mathematics. Others follow equally simply if, unlike Eq. (47), we are content to derive only their limiting forms at large t (i.e., in steady state). Here a short-cut exists which may be understood as follows. The statistical mean of any quantity which is comprised of contributions from all prior cascades at all points in space is, as we have seen,

$$\overline{M}(t) = (G_0/\nu) \int_0^t dt' \int dV_j m_j(t, t') \quad (48)$$

Now causality ensures that $m_j(t, t')$ will be a function of $t - (t - t')$ only. [Equation (15) furnishes an explicit example of this, while the factor $\exp(-pt')$ in the Laplace Transforms of all the subsequently introduced quantities ensures the same behavior.] Hence, with an obvious abridgement in notation, and change of the variable of integration:

$$\overline{M}(t) = (G_0/\nu) \int_0^t d\tau \int dV_j m_j(\tau) \quad (49)$$

Thus the Laplace Transform, $\overline{M}_p$, of $\overline{M}(t)$ is

$$\overline{M}_p = (G_0/\nu p) \int dV_j m_{jp} \quad (50)$$

where m_{jp} is the transform of $m_j(t)$. But, from the fundamental integral

defining the Laplace Transform, if $\bar{M}(t) \rightarrow \bar{M}(\infty)$ as $t \rightarrow \infty$, then $\bar{M}_p \rightarrow \bar{M}(\infty)/p$ as $p \rightarrow 0$. Hence we see that the asymptotic value of $\bar{M}(t)$ is given by

$$\bar{M}(\infty) = (G_0/v) \int dV_j n_{j0} \quad (51)$$

We can use the above to regain other standard Chemical Rate Theory results. Recalling what has been said earlier about the v factor, the various Green's functions lead to the following. First, evaluate the integral in Eq. (51) using Eqs. (22) and (23) (the j suffix on dV_j is redundant once the volume element is identified with the cascade position R). In the limit $p \rightarrow 0$, $q \rightarrow k$. Hence the mean of the concentration around the cavity tends to

$$\bar{c}(r, \infty) = (G_0/Dk^2)[1 - (r_c/r) \exp\{-k(r - r_c)\}] \quad (52)$$

as a function of r . For $k(r - r_c) \gg 1$, $\bar{c}(r, \infty)$ tends to the finite limit $\bar{c}_\infty(\infty)$ obtained from Eq. (47). Equation (52), a familiar result [16], thus provides the specific meaning of the concentration derived via Subsect. 3.1. In the same vein, the asymptotic value $\bar{I}_c(\infty)$ of the mean current to the cavity is found from Eq. (26). It is

$$\bar{I}_c(\infty) = (4\pi r_c G_0/k^2)(1 + kr_c) \quad (53)$$

whence for C voids per unit volume, the asymptotic loss rate to them, L_c , is found to be

$$L_c = C \bar{I}_c(\infty) \bar{c}_\infty(\infty) \quad (54)$$

This much has to be true, since it is contained in our starting point implicitly. (We cannot seek more detail in the temporal behavior because of our discard of the ψ integral at the outset.) However, the point here is that one needs the correct Green's Function, one which reflects the presence of the cavity, to obtain the above form with the higher order sink correction [16] included.

Analogous results follow from the dislocation-associated Green's Function of Subsect. 2.3. The integration in Eq. (51) is now over z_R and over the transverse plane containing the two-dimensional vector $\underline{R}$ of Eq. (39), et. seq. Though we have only the Fourier Transforms, a first integration is relatively easy. Each transform depends upon z_R only through the phase term $\exp(-ik_z z_R)$. Thus the appropriate function itself (concentration or current density) is of the generic form

$$\phi(z) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} \phi_{k_z} \exp\{ik_z(z - z_R)\} dk_z . \quad (55)$$

Integrating this over z_R from $-\infty$ to $+\infty$ yields $(2\pi)^{1/2} [\phi_{k_z}]_{k_z=0}$; thereby yielding a simple prescription for performing the z_R integration without having to execute the inverse Fourier Transform to get $\phi(z)$ from ϕ_{k_z} . The remaining two-dimensional integrals can all be done analytically to obtain the following asymptotic mean values

$$\bar{c}(r, \infty) = (\omega_0/Dk^2) [1 - K_0(kr)/K_0(kr_1)] , \quad (56)$$

($r > r_1$), and

$$\bar{i}_D(\infty) = \frac{z_k G_0}{k^2} \equiv \frac{2\pi k r_1 K_1(kr_1) G_0}{k^2 K_0(kr_1)} . \quad (57)$$

These results also are identical to those of Chemical Rate Theory [16]. Again, we needed a Green's Function reflecting the presence of the sink to obtain them. Further, the loss rate per unit volume to a length ρ_D is $L_D = DZ_k \rho_D \overline{c_\infty}$, again consistent with the starting premise. (The limit $kr_1 \ll 1$ gives a slight dependence of Z_k upon k which, following customary practice, is neglected when permissible.) Hence all the above results substantiate the correctness of our mathematics and simultaneously provide a more detailed statistical picture of the origin of usual steady state theory.

3.3 THE SHELL MODEL

In seeking to ascertain certain specific effects associated with discrete temporal and spatial cascade production, it is sometimes convenient to investigate production sequences which do not fully conform to the Poisson distribution given earlier. Our former and present calculations (Sect. 5) constitute one such case. Our procedure is to construct spherical shells about a physical point of interest and to suppose the generation within each shell to be regular in time at an appropriate rate in each shell. Specifically, within each shell we consider a periodic sequence of delta functions in time. Thus events in each shell are correlated in time. Moreover, once the volume of each shell is specified, if the sequence in each is initiated exactly one-half period prior to the first event, there is also a correlation from shell to shell. Nevertheless, events at the observation point are still manifestly haphazard [11], though not random in the strict technical sense of the word. The point of the procedure is that it enables one to better track (numerically) the origin of coincidences of arrival of defects. We infer

from the comments in Ref. [15], where true Monte Carlo calculations are reported, and from our subsequent analysis, that our approach preserves the qualitative statistical aspects.

Suppose ΔV_j here represents the volume of the j^{th} shell around an observation point (or cavity, as the case may be). Within the shell, let the generation rate be spatially uniform but pulsed in time, with period τ_j . Specifically, let the generation rate in the j^{th} shell be $G_j(t)$:

$$G_j(t) = (\Delta V_j)^{-1} \sum_{n=0}^{\infty} \delta[t - (n + 1/2)\tau_j]; \quad t > 0. \quad (58)$$

Then the time average of $G_j(t)$ will be G_0 if we take $\tau_j = (G_0 \Delta V_j)^{-1}$ [11], here assuming unit cascades, $\nu = 1$. The ΔV_j relate to discrete regions of space, while $G_j(t)$ gives the value of $G(\underline{r}, t)$, [see Eq. (8)], when $\underline{r}$ lies within the j^{th} shell. With this $G(\underline{r}, t)$ we can evaluate the $\underline{R}$ integral of Eq. (10). If the shells are thin enough, we can ignore the variation of g with $\underline{R}$ in each shell, whence

$$c_{\omega}(\underline{r}, t) = \int_0^t dt' \left\{ \sum_j g(\underline{r}, \underline{R}_j; t, t') G_j(t') \Delta V_j \right\}. \quad (59)$$

(We have also explicitly inserted the fact that g vanishes for $t' > t$.)

The quantity $G_j(t') \Delta V_j$ is independent of the volume element, while the integral over t' is trivial. Whence the concentration obtained by this prescription (we attach a superscript s to denote its special significance) is

$$c_{\omega}^s(\underline{r}, t) = \sum_j \sum_{n=0}^{\infty} g(\underline{r}, \underline{R}_j; t, (n + 1/2)\tau_j). \quad (60)$$

(Note that it is the same for all points $\underline{r}$ because g depends only upon $|\underline{r} - \underline{R}_j|$.) This is the significance of the prescription of Ref. [11].

Equation (60) may be evaluated numerically. In addition one can obtain its asymptotic form at large t analytically. We begin by reverting to Eqs. (58) and (59). Since the value of the latter is unaffected if we change the range of the sum on n , from 0 to ∞ , to $-\infty$ to ∞ (because t is greater than zero) we consider this done. The resulting sum over the δ functions is then a periodic function of t which we Fourier analyze, viz.

$$\sum_{n=-\infty}^{\infty} \delta[t - (n + 1/2)\tau_j] = \sum_{l=-\infty}^{\infty} a_l \exp(2\pi i l t / \tau_j) , \quad (61)$$

where

$$a_l = \tau_j^{-1} \exp(-i\pi l) . \quad (62)$$

Accordingly, we can also write Eq. (59) as

$$c_{\infty}^g(\underline{r}, t) = G_0 \sum_{l=-\infty}^{\infty} (-1)^l \sum_j (\Delta V_j) \int_0^t g(\underline{r}, \underline{R}_j; t, t') \exp(2\pi i l t' / \tau_j) dt' . \quad (63)$$

Now g is given by Eq. (15), while the integral in Eq. (63) is, at large t , a phase factor ($\exp[2\pi i l t / \tau_j]$), times the Laplace Transform with respect to τ for the variable $p \rightarrow -2\pi i l / D\tau_j$. This transform is obtained from Eq. (14) by setting t' equal to zero and then making the last-named replacement for p . Hence we find

$$c_{\infty}^g(\underline{r}, t) \rightarrow$$

$$G_0 \sum_{l=-\infty}^{\infty} (-1)^l \sum_j \frac{(\Delta V_j)}{4\pi D\rho_j} \exp[-\{k^2 - 2\pi i l / D\tau_j\}^{1/2} \rho_j] \exp(2\pi i l t / \tau_j) , \quad (64)$$

where $\tau_j \equiv |r - R_j|$. The non-oscillatory component of the above expression is given by the $l = 0$ term in the sum. Hence the mean value of c_∞ has the asymptotic limit

$$\langle c_\infty^s \rangle = G_0 \sum_j \frac{\Delta V_j}{4\pi D \rho_j} \exp(-k \rho_j) , \quad (65)$$

which, upon using the transposition (46), is readily shown to lead to $\langle c_\infty^s \rangle = G_0/Dk^2$. Again, this is the Rate Theory result — as it has to be, granted the mathematics has been done correctly.* More significant to our further analysis will be the fact that the fluctuations inherent in c^s (for shells of finite thickness) are here obtained in closed form.

The manipulations which were performed with the first of our Green's functions can equally well be carried out with the remaining two. Or with their spatial derivatives with respect to r , for that matter, since the latter only involves an operation that is linear. To get at $I_c^s(t)$, for example, this being the current collected by the cavity with the present defect production model, one need simply replace g in Eq. (63) by I_c as defined in Eq. (27). After using the Laplace Transform result inherent in Eq. (26) this procedure is found to give (for large t)

$$I_c^s(t) \longrightarrow G_0 \sum_{l=-\infty}^{\infty} (-1)^l \sum_j \frac{(\Delta V_j) r_c}{R_j} \exp[-\{k^2 - 2\pi i l/D\tau_j\}^{1/2} (R_j - r_c)] \\ \times \exp(2\pi i l t/\tau_j) . \quad (66)$$

*Alternatively, one can say that the preceding constitutes a formal ab initio proof that numerical analysis based upon Eq. (60) must give an asymptotic mean value equal to the Rate Theory value. Our analysis [11] did indeed produce it.

The non-oscillatory component of this (for thin shells) is found to lead to

$$\langle I_c^s \rangle = 4\pi r_c (1 + kr_c) D \langle c_\infty^s \rangle ; \quad t \rightarrow \infty , \quad (67)$$

as Rate Theory dictates, for one cavity. In fact one can make a stronger statement than this. For, to lowest order in r_c (i.e., terms linear in r_c) the fact that the domain of R_j is the region exterior to $R_j = r_c$ may be ignored once r_c has been factored out of Eq. (66). To this extent, therefore

$$I_c^s(t) = 4\pi r_c D c_\infty^s(t) . \quad (68)$$

This is the relation we assumed in our earlier study [11].

For the dislocation problem one can conceive of a parallel numerical procedure in which the shells are defined by concentric cylinders centered upon the dislocation axis. The j^{th} shell has cross-sectional area ΔA_j and length Λ along the z -axis; $\Delta V_j = \Lambda \Delta A_j$. Consider the collected current density; the double transform of the appropriate Green's Function is Eq. (42). One proceeds along steps similar to those executed above, starting from the counterpart of Eq. (10). As before, we assume the shells are thin. Further assume that Λ is large enough so that in the integral over z_R , implied by the latter equation, the limits may be replaced by $z_R = \pm\infty$, [so that one may use Eq. (55)]. The end result, for discrete shells is

$$I_D^s(t) \rightarrow G \sum_{\ell=-\infty}^{\infty} (-1)^\ell \sum_j (\Delta A_j) \frac{K_0 \{ [k^2 - 2\pi i \ell / D \tau_j]^{1/2} R_j \}}{K_0 \{ [k^2 - 2\pi i \ell / D \tau_j]^{1/2} r_1 \}} \exp(2\pi i \ell t / \tau_j) . \quad (69)$$

(Recall that $\underline{R}_j$ is here a two-dimensional vector). The mean value of this expression then leads to

$$\langle i_D^S \rangle \rightarrow \sum_k G_0 / k^2 = \sum_k D \langle c_{\infty}^S \rangle , \quad (70)$$

the Rate Theory result [16]. (The total loss rate to dislocations per unit volume is ρ_D times the above.) Moreover, it is also possible to show that $i_D^S(t) \approx \sum_k D c_{\infty}^S(t)$. The steps in the proof entail re-evaluating Eq. (10) using cylindrical rather than spherical shells. One must also make use of (i) the slow variation of K_0 with respect to its argument when the latter is small, and (ii) the fact that the major contribution to $i_D^S(t)$ arises from terms of small l . The result then follows.

4. MEASURES OF FLUCTUATIONS

The irregularities in cascade formation in different regions of space or time are reflected in fluctuations of the defect current collected by sinks. In this section we derive some quantitative measures of these fluctuations for voids and for dislocation segments of finite length.

4.1 THE POISSON DISTRIBUTION

A fundamental measure of fluctuations in any random physical quantity (i.e., variable), M , is its variance [21], $\sigma(M)^2$:

$$\sigma(M)^2 = \overline{M^2} - (\overline{M})^2 , \quad (71)$$

where the bar signs represent weighted averages using Eq. (44).

For any given set $\{N_j^a\}$, M is a sum of contributions from cascades which were born in different spatial elements j at all prior times t_a :

$$M = \sum_a \sum_j N_j^a n_j(t, t_a) , \quad (72)$$

(M depends upon r and t, of course). To find the variance we must square M, multiply by the probability of the set $\{N_j^\alpha\}$ and sum over the N_j^α .

Because of the lack of correlations inherent in the Poisson distribution, the above process is not difficult to execute. Using the rule

$$\overline{N_j^\alpha N_k^\beta} = \overline{N_j^\alpha} \cdot \overline{N_k^\beta} \quad (73)$$

for $j \neq k$ and all α and β , or for $j = k$ as long as $\alpha \neq \beta$, it is found that

$$\sigma(M)^2 = \sum_j \sum_\alpha \sigma(N_j^\alpha)^2 m_j(t, t_\alpha)^2 \quad (74)$$

Since the variance of a Poisson distribution and its mean are equal [21] we find

$$\sigma(M)^2 = (G_0/v) \sum_j \sum_\alpha m_j(t, t_\alpha)^2 \Delta V_j \Delta t_\alpha \quad (75)$$

(Again, the v factor drops out if we use the Green's Functions derived earlier.)

Unfortunately, if one evaluates Eq. (75) with M identified as either the concentration at an observation point or as the current to a sink, the result is found to be infinite with the δ -function model of a cascade. The physical origin of this outcome is easy to establish once one recognizes that it persists even in the absence of other sinks in the system (i.e., as $k \rightarrow 0$). For example, the variance of the current to an isolated cavity becomes

$$\sigma(I_c)^2 = \lim_{r_0 \rightarrow 0} \left[\frac{G_0 r_c^2}{D} \int_{r_c + r_0}^{\infty} (R - r_c)^2 dR \int_0^t \frac{\exp[-(R - r_c)^2 / 2D(t - t')]}{(t - t')^3} dt' \right] \quad (76)$$

Here we have used Eqs. (27) and (46), and injected an arbitrary cut-off and limiting process to make a point [14]. Evaluating the above leads to

$$\sigma(I_c)^2 = \lim_{r_0 \rightarrow 0} \left[(4GD_c^2/r_0) \{ \exp(-y^2) - 1/2(\pi)^{1/2} y \operatorname{erfc}(y) \} \right], \quad (77)$$

where $y = r_0/(2Dt)^{1/2}$. Since the factor in braces tends to unity for $y \ll 1$, the limit is infinite. (Precisely the same limiting form arises if one retains finite k .) Of course one may obtain a finite result for the variance of the current (or the concentration) by attaching a physical significance to r_0 . This might be that cascades require a finite amount of space to form (or that they have a finite initial width [14]). This ruse, however, does not get at the heart of the issue. Namely, that cascades close to the cavity give comparatively enormous currents over very short time spans. If, in Eq. (75), M is identified with the concentration at a point, or the current to a sink, one is effectively attempting to integrate over time a function which, to all intents and purposes, is like the square of a delta function. The far more significant physical quantity is the *number* of defects collected by the sink, or its variance, because clearly both of these must be bounded. It is impossible to capture more defects than are in each cascade at its birth.

4.2 VARIANCE IN THE NUMBER COLLECTED BY CAVITIES

The calculation of $\sigma(n_c)^2$ is a fruitful but tedious exercise which is outlined in the Appendix. It is shown there that $\sigma(n_c)^2$ is of the form

$$\sigma(n_c)^2 = (4\pi G_0 r_c^2 / Dk^3) F(Dk^2 t), \quad (78)$$

where the general form of F is prescribed. Here we note only the limiting forms

$$\begin{aligned}
 &F(x) = \frac{1}{2} x \quad ; \quad x \gg 1 \\
 \text{and} \quad &F(x) = (8/3\pi^{1/2})(1 - 2^{-1/2})x^{3/2} \quad ; \quad x \ll 1 \quad .
 \end{aligned}
 \tag{79}$$

The general form for $\overline{n_c(t)}$ is also derived in the Appendix. We find that

$$\overline{n_c(t)} = (4\pi G_0 r_c / Dk^4) H(Dk^2 t) \quad , \tag{80}$$

where

$$H(x) = e^{-x} + x - 1 + kr_c \left[\left(x - \frac{1}{2}\right) \operatorname{erf}(x^{1/2}) + (x/\pi)^{1/2} e^{-x} \right] . \tag{81}$$

From the above, the two subsequent limiting cases follow:

$$\frac{\sigma(n_c)^2}{\overline{n_c}} = \frac{kr_c}{2(1 + kr_c)} \quad ; \quad Dk^2 t \gg 1 \quad , \tag{82}$$

and

$$\frac{\sigma(n_c)^2}{\overline{n_c}} = 2(1 - 2^{-1/2}) \quad ; \quad Dk^2 t \rightarrow 0 \quad . \tag{83}$$

The transition of $\sigma(n_c)^2/\overline{n_c}$ between one limit and the other is shown in Fig. 3 for selected values of kr_c .

It is seen that $\sigma(n_c)^2$ has the usual statistical feature that it is proportional to the mean. However, there is an additional highly significant fact. Namely, that for $kr_c \ll 1$, the variance is strongly diminished once the characteristic response time $(Dk^2)^{-1}$ is exceeded. This time is essentially that required for the mean defect concentration to attain steady state [6,13] and is far shorter for the interstitial than the vacancy in metals. It should be recalled here that the initial conditions we posited were far from that appropriate to steady state for the uniform

point defect generation rate G_0 . Thus Fig. 3 justifies our earlier remark that fluctuations diminish in importance as steady state is approached.

Fig. 3. The ratio of the variance in the number of defects captured by a cavity in time t to the mean, as a function of time. The cavities are maintained at a fixed size, the irradiation has, on average, a constant value after being turned on at $t = 0$. The initial state is one with no defects in solution.

The values of kr_c quoted in the figure were selected simply to indicate the parametric dependence. We remind the reader here of our initial approximation in the step from Eq. (1) to the use of the steady state form of the loss rate. We anticipate corrections arising on this score for $kr_c > 1$. These we have not addressed.

4.3 VARIANCE IN THE NUMBER COLLECTED BY DISLOCATIONS

In considering defect capture by dislocations we shall determine the number (mean and variance) collected by some finite length, Λ . This will

be independent of the location of the segment we choose because of the translational invariance in our model. We have in mind, of course, subsequent application to climb of the segment over a localized obstacle. This will also be influenced, possibly, by defect core diffusion and localized stress-induced effects arising from the inevitable dislocation bowing. Such factors are here ignored.

Our calculations will be based, mainly, upon an expression for the current to the dislocation that is the counterpart of the constant Z -approximation mentioned earlier. The prescription for synthesizing this starts from the observation that i_{pk_z} of Eq. (42) is the Laplace Transform of

$$i_{k_z}(t, t') = (2\pi)^{-1/2} J(\tau) \exp[-D(k^2 + k_z^2)\tau - ik_z z_R] , \quad (84)$$

where $\tau = t - t'$ and $J(\tau)$ is the function with Laplace Transform

$$J = K_0(R[p/D]^{1/2})/K_0(r_1[p/D]^{1/2}) \equiv \frac{Z_\xi}{2\pi} \cdot \frac{K_0(R[p/D]^{1/2})}{\xi K_1(\xi)} , \quad (85)$$

where $\xi = r_1[p/D]^{1/2}$. We propose now to replace Z_ξ by the constant Z and take the limit $\xi \rightarrow 0$ in the remainder. This leads to the approximate result

$$J(\tau) \approx (Z/4\pi\tau) \exp(-R^2/4D\tau); \quad \tau > 0, \quad (86)$$

and $J(\tau) = 0$ for $\tau < 0$. The inverse Fourier Transform involves only a tabulated integral, whence, to this approximation

$$i_D(t, t') = [DZ/(4\pi D\tau)^{3/2}] \exp\{-[Dk^2\tau + \{R^2 + (z - z_R)^2\}/4D\tau]\} , \quad (87)$$

($\tau > 0$). (The subscript D on i denotes "dislocation".)

The algorithm introduced above may be checked by calculating the statistical mean of the number collected by a length Λ ; $\overline{n_D(t)}$. This turns out to be

$$\overline{n_D(t)} = (ZG_0\Lambda/k^2)[t - \{1 - \exp(-Dk^2t)\}/Dk^2] \quad (88)$$

For $Dk^2t \gg 1$, this is clearly equivalent to Eq. (57) for $Z_k \rightarrow Z$. For $Dk^2t \ll 1$, $n_D(t) \rightarrow 1/2 \Lambda Z G_0 t^2$. We think this will be accurate as long as $r_1/(Dt)^{1/2} < 1$. This is a very modest requirement. However the use of the constant Z approximation, entailing as it does the neglect of the r_1 dependence, inevitably leads to a modest loss of algebraic rigor.

We have succeeded in calculating the variance $\sigma(n_D)^2$ only in certain limiting cases. The details are furnished in the Appendix. The crux of the problem lies in the dependence of i_D upon z (a point on the finite segment that we are considering). Involved therein is the ultimate dependence of $\sigma(n_D)^2$ upon $k\Lambda$, which one can expect to arise if only because it is a possible counterpart to kr_c of the cavity problem. In fact what we find is the following:

4.3.1 $k\Lambda \ll 1$

$$\sigma(n_D)^2 \approx [Z^2 G_0 \Lambda^2 / \{4\pi(2)^{1/2} Dk^3\}] F(Dk^2t) \quad (89)$$

where F is the same function that arises in the cavity case. The result here is not substantially different from the earlier one if $4\pi r_c$ is replaced by $Z\Lambda$. Combining the above with Eq. (88) we find that

$$\frac{\sigma(n_D)^2}{\overline{n_D}} \sim [2Z(2^{1/2} - 1)/3(\pi)^{3/2}] \Lambda (Dt)^{-1/2}; \quad Dk^2t \ll 1, \quad (90)$$

and

$$\frac{\sigma(n_D)^2}{n_D} = \frac{Zk\Lambda}{8\pi 2^{1/2}} ; \quad Dk^2t \gg 1 . \quad (91)$$

The limit given by Eq. (90) is unquestionably wrong. It is included for completeness sake only. The limit as $t \rightarrow 0$ must be finite. Unfortunately the omission of the finite sink size (i.e., $r_1 \rightarrow 0$) destroys it. In fact we can show that in this one special limit, which corresponds to $k \rightarrow 0$ and $r_1/(Dt)^{1/2} > 1$ in the real problem, Eq. (90) should be replaced by

$$\frac{\sigma(n_D)^2}{n_D} = \frac{Z^2(2^{1/2} - 1)}{8\pi^{5/2}} \frac{\Lambda}{r_1} . \quad (92)$$

The origin of this new result (see Appendix) lies in abandoning the use of the constant Z approximation to find $\overline{n_D(t)}$. Unfortunately we have only succeeded in this one case. Yet it is sufficient to establish the essential fact that the ratio of the variance to the mean is always finite.

Of equal significance is the result in Eq. (91). This exemplifies the reduction in the variance, for short segment lengths, as steady state is attained.

4.3.2 $k\Lambda \gg 1$

Here we find that

$$\left. \begin{aligned} \sigma(n_D)^2 &= Z^2 G_0 \Lambda \left(\frac{1}{2} - 1 \right) Dt^2 / 8\pi ; \quad Dk^2t \ll 1 , \\ &= Z^2 G_0 \Lambda t / 32k^2 ; \quad Dk^2t \gg 1 . \end{aligned} \right\} \quad (93)$$

These lead to

$$\left. \begin{aligned} \frac{\sigma(n_D)^2}{n_D} &= Z\left(\frac{1}{2} - 1\right)/4\pi \quad ; \quad Dk^2t \ll 1 \quad , \\ &= Z/32 \quad ; \quad Dk^2t \gg 1 \quad . \end{aligned} \right\} \quad (94)$$

The two expressions immediately above are virtually the same. Overall, the qualitative behavior for the segment length is thus the same as that for the cavity, as shown in Fig. 3, with Λ replacing r_c . The paramount conclusion we reach is that whereas fluctuations maintain the same relative importance as a function of time for large sinks, for small ones these fluctuations diminish in importance as steady state is approached in their vicinity.

4.4 SHELL MODEL FLUCTUATIONS

The physical quantities in this model fluctuate in time because cascades from different shells take different amounts of time to reach a given point. Also, cascade births within a given shell are discrete events in time. However, they differ from a Poisson distribution in that, within each, they are periodic. Here we seek to determine to what extent the model gives, nevertheless, a reasonable portrayal of complete randomness. The quantity we will derive is

$$\lambda (n^s)^2 = \langle \{n - \langle n^s \rangle\}^2 \rangle \quad (95)$$

or, more specifically, its limit at large t . (Here λ denotes the analog of the variance for the shell model.) As before, angular brackets denote time average values, while n may be the number collected by either void or dislocation. We shall only evaluate the former.

If we wish to calculate the current to the void we must replace g in Eq. (63) by the quantity I_c of Eq. (27). This will yield $I_c^s(t)$ from which n_c^s follows by integration. Each (l, j) component of the double sum is then found to be

$$(-1)^l [Y_l \exp(2\pi i l t / \tau_j) - \{1 - \exp(2\pi i l t / \tau_j)\} \tilde{Y}] / 2\pi i l, \quad (96)$$

for $l \neq 0$. Here

$$Y_l^j = \int_0^t I_c(\underline{R}_j, \xi) [\exp(2\pi i l \xi / \tau_j) - 1] d\xi, \quad l \neq 0 \quad (97)$$

and

$$\tilde{Y} = \int_0^t I_c(\underline{R}_j, \xi) d\xi. \quad (98)$$

Equation (96) is obtained following an integration by parts. (We have also used the relation $G_0 \Delta V_j \tau_j = 1$.) The reason for introducing the particular functions Y_l becomes apparent when one next writes down the value of $n_c^s - \langle n_c^s \rangle$. This is

$$n_c^s - \langle n_c^s \rangle = \sum_j \sum_{l=-\infty}^{\infty} \frac{(-1)^l}{2\pi i l} Y_l^j \exp(2\pi i l t / \tau_j) - S, \quad (99)$$

where

$$S = \sum_j \tilde{Y} \sum_{l=-\infty}^{\infty} \frac{(-1)^{l-1}}{2\pi i l} \{ \exp(2\pi i l t / \tau_j) - 1 \}, \quad (100)$$

the prime on the summation denoting that the term $l = 0$ (which yields $\langle n_c^s \rangle$) is to be omitted. Now the sum over l in S may be performed [22] to yield

$$S = \sum_j \tilde{Y} \phi_j(t) \quad (101)$$

where ϕ_j is the periodic function of t which has the value

$$\phi_j(t) = t/\tau_j \quad (102)$$

in the fundamental interval $-\frac{1}{2}\tau_j < t < \frac{1}{2}\tau_j$. Thus ϕ_j is like a sawtooth fluctuating periodically (and linearly) between $-1/2$ and $+1/2$, shell-by-shell. For time scales large compared to any τ_j the mean for each shell is zero, and the sum on j is for arbitrary t , a sum of contributions with random phase. These fluctuations, we emphasize, have nothing to do with the physics of the problem, but are linked with the use of singular functions in the mathematics. The real fluctuations are contained in Eq. (99) with $S \rightarrow 0$, and henceforth we shall adopt this algorithm. It will correspond, in a numerical scheme, to computing the fluctuations in n_c^s over a time interval large enough so that there are many cascades in every shell that makes a significant contribution to this quantity. In the analytical scheme we have used earlier, and here further develop, for thin shells ($\tau_j \rightarrow 0$), it implies that the associated limit $t \rightarrow \infty$ is performed first.

With these prescriptions, upon squaring Eq. (99) one produces a four-fold sum of terms of the form

$$\frac{(-1)^{l+l'+1}}{4\pi^2 ll'} Y_l^j Y_{l'}^{j'} \exp[2\pi i(\frac{l}{\tau_j} + \frac{l'}{\tau_{j'}})t] \quad (103)$$

At large t , the Y_l^j become independent of t . (They are synthesized from Laplace Transforms of the current to the cavity.) Thus terms in

expression (103) will fluctuate in time according to the phase factor it contains. Hence, provided the shells have unequal volumes (i.e., $\tau_j \neq \tau_{j'}$), the only time-independent terms will arise from the joint coincidences $j' = j$ and $l' = -l$. In that case it follows that

$$\langle (n_c^s)^2 \rangle_{t \rightarrow \infty} \rightarrow \sum_j \sum_{l=-\infty}^{\infty} (|Y_l^j|/2\pi l)^2 \quad (104)$$

Furthermore, since the continuous limit $l \rightarrow 0$ shows that Y_l tends to a quantity proportional to $(\Delta V_j)^2$, while the sum itself is proportional to ΔV_j , we may now replace the sum over l by the integral and perform the latter. The result is that

$$\langle (n_c^s)^2 \rangle_{t \rightarrow \infty} \rightarrow 2G_0 \sum_j \Delta V_j \int_0^t I_c(\underline{R}_j, \xi) \int_0^\xi I_c(\underline{R}_j, \xi') \xi' d\xi' d\xi \quad (105)$$

One may next substitute for I_c from Eq. (27) and perform the sum (integral) over j followed by the remaining integrations. After some analysis one obtains

$$\langle (n_c^s)^2 \rangle_{t \rightarrow \infty} \rightarrow (2\pi G_0 r_c^2 / Dk^3) \chi(Dk^2 t), \quad (106)$$

where $\chi(x)$ is the complicated function defined by

$$\begin{aligned} \chi(x) = & \frac{1}{2} [\{2x^2 + 2x - 3/8\} \operatorname{erf}[(2x)^{1/2}] + (2x/\pi)^{1/2}(x + 3/4) \exp(-2x) \\ & - \{x^2 + x - 1/4\} \operatorname{erf}[x^{1/2}] + (x/\pi)^{1/2}(x + \frac{1}{2}) \exp(-x)] \quad (107) \end{aligned}$$

Although only valid at large t , it may be used to find $\langle (n_c^s)^2 \rangle$ as $k \rightarrow 0$.

In this limit one finds that

$$\langle (n_c^s)^2 \rangle = \frac{1}{4}(2^{1/2} - 1)\sigma(n_c)^2; \quad k = 0, \quad (108)$$

where σ is to be evaluated from Eqs. (78) and (79). On the other hand, when $Dk^2t \gg 1$ we find that

$$\frac{\langle n_c^2 \rangle}{\langle n_c \rangle^2} \longrightarrow \frac{kr_c}{32(1 + kr_c)} \frac{1}{Dk^2t} \quad (109)$$

Overall, therefore, fluctuations in the shell model (with periodic pulsing in each shell) will be smaller than with truly random generation. At very low sink density, $\langle n_c^2 \rangle \sim \sigma^2/10$, at large times, while with significant sink strengths fluctuations ultimately have no profound significance at all. This is because, unlike the Poisson distribution, the probability of a fluctuation, with many simultaneous cascades in a given volume element, is precisely zero in the shell model. Despite the quantitative differences, however, the trend in $\langle n_c^2 \rangle$ is qualitatively the same as that depicted in Fig. 3 as long as $kr_c \ll 1$.

5. DISTRIBUTIONS IN TIME AND SPACE

In this section we first report the results of a numerical investigation of the cascade generation and diffusion process using the shell model. This serves to highlight certain additional physical features beyond simply the mean or variance. Such features are addressed subsequently.

5.1 NUMERICAL RESULTS

The computational aspects of the shell model have been outlined earlier. Further details are given in Ref. [11]. It should be noted the computer program differs in one respect from that developed in the preceding section in that above the time between pulses corresponds to that

for unit cascades. The program utilizes $\tau_j' = (N_0 A \phi \Delta V_j)^{-1} \equiv v \tau_j$. These variables are defined in connection with Eq. (43). Otherwise they are equivalent.

Figure 4 shows the point defect concentration profiles at a reference point in the medium, $c_{\infty}^s(t)$. For $kr_c \ll 1$ these are also the current profiles (normalized to $4\pi r_c D$) for a void placed at the same point. The temperature assumed is 500°C and the mean dose rate is 10^{-6} dpa/s, (displacements per atom per second). Table 1 contains the other parameter values which were employed. Each cascade is taken to produce 100 free defects of which 20% survive in-cascade recombination, so that $G_0 = 2 \times 10^{-7} \text{ s}^{-1}$. This corresponds to an initial energy of the primary knock-on atom of 10 keV. Figures 4(a) and 4(b) illustrate the vacancy and interstitial profiles respectively. They show extremely large fluctuations. Those for the vacancy are tempered by the relatively slow diffusion of this defect. At any instant it is found that $\sim 10^3$ cascades make a non-negligible contribution to c_{∞}^s (or sink current, approximately). The interstitial

Table 1. Values of parameters used in calculations

Quantity	Symbol	Units	Value
Vacancy diffusion coefficient	D_v	m^2/s	1×10^{-15}
Interstitial diffusion coefficient	D_i	m^2/s	8.42×10^{-9}
Sink strength	k^2	m^{-2}	1×10^{15}
Defect generation rate	G_0	defects/atom/s	2×10^{-7}
Free defects per cascade	v	defects	20

Fig. 4. Shell model results for the time profile of the vacancy concentration at a point in the Effective Medium; (a) vacancy (b) interstitial.

contribution is more "spiky" because of the rapid interstitial diffusion. For most of the time the interstitial contribution is essentially zero. It is comprised of very large spikes of short duration, corresponding to the occurrence of a single cascade anywhere within the volume about the reference point making non-negligible contributions.

The characteristics of the fluctuations depend, of course, upon the dose rate, the temperature and the number of defects in each cascade. Figure 5 shows the effect of cascade size, ν , on c_{∞} , or current (kr_c small), for fixed dose rate. As ν increases (event frequency decreases) the profiles become rougher. The cases in Figs. 5(a) and 5(b) correspond to nominal cascade energies of 50 and 250 keV. The 10 keV result is given in Fig. 4(a).

A key issue in the present work is the effect of the sink size on the point defect current it collects. Figures 6 and 7 show the vacancy-associated temporal profiles for a cavity using the accurate expression, Eq. (27) and for comparative purposes, the $4\pi r_c D$ times Eq. (15) as described after Eq. (29), [Figs. 6(a) and 7(a), and Figs. 6(b) and 7(b), respectively]. In the results illustrated in Fig. 6, the cavity radius is 5 nm, in Fig. 7 it is 20 nm. The dislocation density for both cases is 10^{15} m^{-2} , leading to an absorption length, k^{-1} , of 32 nm. It can be seen that the profiles in Figs. 6(a) and 6(b) are quite similar. However, the profiles of Figs. 7(a) and 7(b) are quite different, indicating that the improvement incorporated in the finite size correction can be significant. It is a reflection, in the current, of the correction factor, $\exp(kr_c)$, appearing in Eq. (29). As we have remarked earlier, further differences might arise if one were to base the entire study upon the loss rate given

Fig. 5. Shell model results for the time profile of the vacancy concentration at a point in the Effective Medium for nominal cascade energies of 50 keV (a) and 250 keV (b).

Fig. 6. Shell model results for (a) the time profile of the vacancy current to the cavity, (b) the vacancy concentration at a reference point (multiplied by $4\pi Dr_c$) and (c) the difference between these two quantities. The cavity radius is 5 nm.

Fig. 7. The same quantities as in Fig. 6 but with an increase of the cavity radius to 20 nm.

in Eq. (1). However, our suspicion is that the latter will be of minor importance once steady state (of the mean) has been attained.

5.2 SPATIAL IMPORTANCE FUNCTION

For irradiation times t such that $Dk^2t \gg 1$ it is readily shown from Eq. (27) that the mean current to a cavity (for defects of one type) approaches I_∞ , where

$$I_\infty = 4\pi r_c G_0 \int_{r_c}^{\infty} R dR \exp[-k(R - r_c)] \quad (110)$$

The integrand has a maximum when $kR = 1$. Thus the largest contribution to I_∞ arises from (radial) shells one absorption length from the center of the cavity. (It is presumed that $kr_c < 1$, otherwise the contributions from successive shells would be monotonic decreasing). The maximum arises, of course, because although nearby cascades give the largest contribution per event, the volume element makes them, on average, less frequent.

The above discussion does introduce one additional limitation on the present analysis. Basically it relates to our use of the lossy continuum concept right up to the surface of the cavity. For example, suppose we calculate the number of cavities, N_c , within the volume enclosed by $R = r_c$ and $R = r_c + k^{-1}$ presuming $kr_c \ll 1$. Then $N_c \approx 4\pi C/3k^3$, which is consistent with a continuum approximation only if large compared to unity. Hence the number density of voids must be large to satisfy this requirement. At low sink densities it appears that one ought to incorporate around each cavity a sink-free region [16] separating the cavity and continuum. This ingredient may cause the transition in Fig. 3 to be

broadened somewhat as a function of Dk^2t . The issue is simply too complicated to resolve without detailed analysis. However, we believe that decreasing importance of fluctuations as steady state is approached will persist, although (perhaps) in not quite so dramatic a fashion as we have derived for the high sink density case.

The above issue aside, one may proceed in the same vein to find the contribution to the mean concentration at an arbitrary reference point in the medium from all prior cascades. For $Dk^2t \gg 1$ this is

$$c_{\infty} = (G_0/D) \int_0^{\infty} R dR \exp(-kR) , \quad (111)$$

as may be verified from Eq. (15). The above integral also derives its major contribution from $R = k^{-1}$. Of course, it may be performed in closed form to yield $c_{\infty} = (G_0/Dk^2)$. Nevertheless it is of interest to indicate how individual regions contribute. The contribution from cascades within radii X_1 and X_2 is

$$\frac{G_0}{Dk^2} \{ [\exp(-X_1) - \exp(-X_2)] + [X_1 \exp(-X_1) - X_2 \exp(-X_2)] \} . \quad (112)$$

In Fig. 8 we present plots of dC/dX and C as function of $X = kR$ where C is here the contribution to c_{∞} from the domain within R . Specifically,

$$C = (G_0/Dk^2)[1 - (1 + X) \exp(-X)] , \quad (113)$$

which is the lower of the two plots in Fig. 8.

Analogous quantities may clearly be defined for the current to the cavity. The only significant difference is that the lower limit of integration is r_c rather than zero. Integrating Eq. (27) from $\tau = 0$ to ∞ and integrating this result from X_1 to X_2 gives

Fig. 8. The dependence of the spatial importance function (a) and its integral (b) as a function of the argument of each.

$$I = 4\pi r_c \frac{G_0}{k^2} \exp(X_c) [(1 + X_1) \exp(-X_1) - (1 + X_2) \exp(-X_2)] \quad (114)$$

The contribution from the region enclosed within the radius R , and its derivative with respect to R , are shown in the lower and upper plots of Fig. 9 respectively.

5.3 SPECIAL COINCIDENCES

Quantities like the variance, or χ^2 , give only a coarse-grained measure of the magnitude of fluctuations. Physical phenomena such as the nucleation of voids or dislocation climb over small obstacles are clearly dependent upon the fluctuations in impinging flux instant by instant. This directs one's attention towards the maximum extent of fluctuations, not simply their mean.

We shall not address this fully, but merely point to two types of coincidences that must be of particular significance. The first concerns the reinforcement in the flux to a sink resulting from an *arrival* coincidence of two current bursts emanating from cascades born at different times and at different locations. Many of the high peaks in the vacancy profiles of Fig. 4(a) have this cause.

From Eq. (28) it is found that the current to the void from a cascade at $r = R$ attains a maximum at a time τ_m after the cascade event given by [11]

$$\tau_m = 3 \left[\left\{ 1 + \frac{1}{9} (k\rho)^2 \right\}^{1/2} - 1 \right] / 2Dk^2 \quad (115)$$

where $\rho \equiv (R - r_c)$. Hence the cascade born at R_1 at time t_1 gives the maximum current at $t = t_1 + \tau_{m1}$. Accordingly, a second cascade born at R_2 at time t_2 will maximally reinforce the first if $t_2 + \tau_{m2} = t_1 + \tau_{m1}$.

Fig. 9. The dependence of the spatial importance functions for the defect current to a cavity (a) and its integral (b) as a function of the argument of each.

The argument can clearly be extended to multiple coincidences, and these are clearly important in deciding whether a void embryo can survive (or be annihilated) or whether a dislocation can surmount a small obstacle.

In fact, the limiting factor in this regard may not be contingent upon such precise coincidences at the above. For, bearing in mind the great disparity between the interstitial and vacancy mobility, the occurrence of an adequate number of cascades in the vicinity may in itself be sufficient to govern the process under consideration. (We have in mind here a multiplicity of cascades over some time interval which is short enough for the vacancy distribution to be considered frozen at its birth form, but long enough for interstitial diffusion to occur.) On a time scale short compared to the vacancy life-time these might be called regional "coincidences."

Now it is the nature of the Poisson distribution that if the probability of n_j events in time t_j is $P(n_j; \lambda t_j)$, then the probability of $n = (n_1 + n_j)$ events in time $(t_1 + t_j)$ is

$$\sum_{n_j=0}^n P(n_j; \lambda t_j) P(n - n_j; \lambda t_1) = P[n; \lambda(t_1 + t_j)] \quad (116)$$

Applications of this rule show, therefore, that the probability of N cascades anywhere in a volume V in time t is $P(N; G_0 V t / v)$. Hence the probability of n or more events is

$$p_n(t) = \sum_{m=n}^{\infty} P(m; G_0 V t / v) \quad (117)$$

where P is given by Eq. (44). Figure 10 gives a plot of $p_n(t)$, for $n = 1$ to 20, as a function of t , for a spherical volume of radius k^{-1} . Part (a)

Fig. 10. The probability of n or more events in time t within a sphere of radius k^{-1} , as a function of time, (a) short times and (b) longer times.

shows a log-log plot down to 10^{-6} s, while part (b) shows the behavior down to 0.1 s on a linear-log plot. It can be seen that although p_n is small at small t , it is nevertheless finite. Very often within intervals of the order of the vacancy lifetime ($>10^{-3}$ s, for typical irradiation conditions and materials), and even within intervals of the order of the interstitial lifetime ($<10^{-6}$ s), several cascades may be expected to occur in a volume whose radius is of the order of the point defect absorption length. This leads to a significant number of defects when it is realized that typically $10^{21} - 10^{24}$ cascades occur per second per m^3 . Such potentially strong overlap effects would appear to have a profound role in nucleation processes of voids and interstitial loops or the climb of dislocation segments over localized obstacles.

6. SUMMARY

In the study reported here we have augmented our earlier work on the cascade diffusion theory in several important aspects. We have, first of all, derived the effect of the finite size of a sink upon the current it collects from a cascade. The derivations have given the instantaneous currents to a dislocation and cavity as well as the total number collected by these sinks over time from a single cascade. These results are integrated over the cascade distribution to find the average current to a sink. The point defect current to cavities and dislocations may be estimated by using Eq. (15) integrated over the sink surface. This approximation is adequate for dislocations. However, for cavities the exact result is given by Eq. (27). These results have been shown to yield a value for the mean loss rates to sinks of different types that is completely consistent with steady state theory when the formalism is adapted

to uniform irradiation. The appropriate higher order sink corrections are included.

Fluctuations due to the statistical nature of cascade production have been investigated. Three main facts have been demonstrated. First that the quantity which gives the most accurate portrayal of physical events is the number of defects collected by a sink in a given time (and the variance of this number). Second, that such a variance depends upon the ratio of the sink size to the point defect absorption length. And third, that fluctuations are of much greater importance away from steady state than when that state has been attained.

We have shown also how the shell model that we have used in our numerical simulations is related to the results that would be obtained with truly random spatial and temporal generation. Differences in detail do arise in these two cases. Nevertheless it has been shown that the trends predicted by each, as far as the temporal dependence is concerned, are in qualitative accord. Further numerical analysis supplementing our earlier work has been presented. This has provided additional indications of the extremely sporadic nature of the point defect current that impinges upon any sink.

In the context of possible further numerical simulations, it has been shown that most of the defects contributing to the current to a sink arise from cascades born within a distance of the order of an absorption length of its center. More specifically, in terms of the concentration at an arbitrary reference point, more than 80% of the total value comes from within three absorption lengths, and more than 99% from within seven.

However, statistical means such as the variance may not be at all relevant for specific physical processes that require only relatively small numbers of defects. These processes include dislocation climb over small obstacles, or the formation and annihilation of small void embryos. The matter has not been investigated in detail. Yet it appears that special types of coincidence events may be significant in this context. Two such possibilities have been given attention here.

The Chemical Rate Theory that is in widespread use in Irradiation Effects Theory is a limiting case of our analysis, which follows when fluctuations about the mean are neglected entirely. Our results thus show that it is a remarkably good approximation as far as our estimates of the variance of the number of defects collected by a sink is concerned and, the longer the time for a particular physical process, the better it becomes. It is only in highly localized events, where special coincidences become of paramount importance, that we believe its application is open to serious question. Each such event then presents its own context where further analysis must be carried out on a topic by topic basis. Direct cluster nucleation by cascade coincidence, modified cluster nucleation in the presence of cascade-induced point defect current fluctuations, solute segregation and precipitation, and cascade-induced irradiation creep are but a few of these.

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APPENDIX

This section furnishes additional algebraic details related to the calculation of various physical quantities defined in the main text.

1. $\overline{n_c}(t)$

By virtue of Eq. (28), the number of defects collected up to time t from the cascade born at t_α at the point R is

$$n_c(t, t_\alpha) = (r_c/R) \int_{t_\alpha}^t dt'' \exp[-Dk^2 t''] \frac{d}{dt''} \operatorname{erfc} \left[\frac{R - r_c}{2(Dt'')^{1/2}} \right], \quad (A1)$$

where $t'' \equiv t - t_\alpha$. The statistical mean of this quantity after time t is

$$\overline{n_c}(t) = 4\pi r_c G_0 \int_{r_c}^{\infty} R dR \int_0^t dt_\alpha n_c(t, t_\alpha). \quad (A2)$$

[In line with what was said earlier, n_c is seen to depend only upon $(t - t_\alpha)$.] The spatial integration in Eq. (A2) may be performed first. An integration by parts is necessary to fully execute the remaining integrals. The final result is Eq. (81).

2. $\sigma(n_c)^2$

Equation (75) shows that, in terms of $n_c(t, t_\alpha)$,

$$\sigma(n_c)^2 = 4\pi r_c^2 G_0 \int_{r_c}^{\infty} dR \int_0^t [n_c(t, t_\alpha)]^2 dt_\alpha, \quad (A3)$$

with n_c given by Eq. (A1). It proves convenient again to perform the spatial integration first. This is of the type

$$\int_{r_c}^{\infty} dR \left[\frac{d}{dt''} \operatorname{erfc} \left\{ \frac{R - r_c}{2(Dt'')^{1/2}} \right\} \right] \left[\frac{d}{dt'} \operatorname{erfc} \left\{ \frac{R - r_c}{2(Dt')^{1/2}} \right\} \right] . \quad (\text{A4})$$

The differential operators may be taken out of the integrand. One further needs the result that

$$\int_0^{\infty} \operatorname{erfc}(\alpha z) \operatorname{erfc}(\beta z) dz = \pi^{-1/2} [\alpha^{-1} + \beta^{-1} - (\alpha\beta)^{-1} \{\alpha^2 + \beta^2\}^{1/2}] , \quad (\text{A5})$$

which follows from integration by parts. The result is that $\sigma(n_c)^2$ may be expressed in the form

$$\frac{\sigma(n_c)^2}{2(\pi D)^{1/2} G_0 r_c^2} = \int_0^t d\tau \int_0^{\tau} dy' \exp(-\lambda y') \int_0^{\tau} dy'' \frac{\exp(-\lambda y'')}{(y' + y'')^{3/2}} , \quad (\text{A6})$$

where $\lambda \equiv Dk^2$. The lengthy evaluation of this triple integral ultimately produces Eq. (78) of the text. The form of $F(x)$ so obtained is

$$F(x) = x[2f_1(x) - f_1(2x) + x\{f_2(x) - f_2(2x)\}] , \quad (\text{A7})$$

where

$$f_1(x) = (1 - 1/2x) \operatorname{erf}(x^{1/2}) + (\pi x)^{-1/2} \exp(-x) , \quad (\text{A8})$$

and

$$f_2(x) = (1 - x^{-1} + 3/4x^2) \operatorname{erf}(x^{1/2}) + (1 - 3/2x)(\pi x)^{-1/2} \exp(-x) . \quad (\text{A9})$$

3. $\overline{n_D}(t)$ and $\sigma(n_D)^2$

In the constant Z approximation,

$$\overline{n_D}(t) = G_0 \int_0^t dt_{\alpha} \int_{r_1}^{\infty} R dR \int_{-\infty}^{\infty} dz_R n_D(t, t_{\alpha}) , \quad (\text{A10})$$

where

$$n_D(t, t_\alpha) = \int_{-\Lambda/2}^{\Lambda/2} dz \int_0^t i_D(t', t_\alpha) dt' . \quad (A11)$$

This represents the number collected by a segment of length Λ spanning the origin in z . The evaluation of Eq. (A10) leads to Eq. (88).

When we seek to evaluate $\sigma(n_D)^2$ in this approximation we encounter an integral of the type

$$\int_{-\infty}^{\infty} dz_R \int_{-\Lambda/2}^{\Lambda/2} dz \int_{-\Lambda/2}^{\Lambda/2} dz' \exp[-\gamma \{2(z - z_R)^2 + \frac{1}{2}(z' - z_R)^2\}/4] , \quad (A12)$$

where $D\gamma \equiv (t' - t_\alpha)^{-1} + (t'' - t_\alpha)^{-1}$. The above integral is $(2\pi/\gamma)^{1/2}$ times the double integral

$$\int_{-\Lambda/2}^{\Lambda/2} dz \int_{-\Lambda/2}^{\Lambda/2} dz' \exp[-\gamma(z' - z)^2/8] . \quad (A13)$$

The integral over R in $\sigma(n_D)^2$ is easily performed. Thus, after some changes of variable we ultimately arrive at the following:

$$\begin{aligned} \sigma(n_D)^2 &= \frac{(Z\Lambda)^2 G_0}{8\pi(2\pi)^{1/2}k} \int_{-1/2}^{1/2} du \int_{-1/2}^{1/2} du' \int_0^t d\xi \\ &\times \int_0^{Dk^2\xi} dy \int_0^{Dk^2\xi} dy' \frac{\exp[-(y + y')]}{(y + y')^{3/2}} \exp\left[\frac{-k^2\Lambda^2}{8}(u - u')^2 \frac{1}{y} + \frac{1}{y'}\right] . \quad (A14) \end{aligned}$$

It is in handling the above that we have resorted to approximations. In the limit $k\Lambda \rightarrow 0$ the double integral over u and u' yields unity. The remaining integrations are then the same as those encountered in Eq. (A6),

and lead to Eq. (89) of the text. In the opposite limit of $k\lambda \rightarrow \infty$ we replace the limits $\pm 1/2$ by $\pm \infty$ in the u' integration, with the result that

$$\sigma(n_D)^2 \longrightarrow \frac{Z^2 \Lambda G_0}{4\pi k^2} \int_0^t d\xi \int_0^{Dk^2\xi} dy \int_0^{Dk^2\xi} dy' \frac{(yy')^{1/2}}{(y+y')^2} \exp[-(y+y')] \quad . \quad (A15)$$

When $Dk^2 t \ll 1$ we evaluate the above by setting the exponential equal to unity. When $Dk^2 t \gg 1$ we replace the upper limits in the y and y' integrations by infinity. These steps yield Eq. (93).

4. $\overline{n_D}(t)$ for $k = 0$

We have mentioned earlier that the constant Z approximation can lead to erroneous results at very short times. Here we provide an example.

Without any approximation, via Eq. (84) we can deduce that

$$\overline{n_D}(t) = 2\pi \Lambda G_0 \int_0^t d\tau \int_0^\tau d\tau' \int_{r_1}^\infty R J(\tau) dR \quad . \quad (A16)$$

Now at small times, a function of t is given by the inverse of its Laplace Transform at large p . Also, the Laplace Transform of the integral over R is

$$\int_{r_1}^\infty \frac{R K_0(R[p/D]^{1/2}) dR}{K_0(r_1[p/D]^{1/2})} = \frac{r_1 [D/p]^{1/2} K_1(r_1[p/D]^{1/2})}{K_0(r_1[p/D]^{1/2})} \quad . \quad (A17)$$

The right hand member tends to $r_1 [D/p]^{1/2}$ as $p \rightarrow \infty$. Thus the integral over R tends to $r_1 (D/\pi\tau)^{1/2}$ as $\tau \rightarrow 0$. The remaining integrations are now trivial. We find

$$n_D(t) \xrightarrow[t \rightarrow 0]{} (8\pi/3) G_0 \Lambda r_1 D^{1/2} t^{3/2} \quad . \quad (A18)$$

This is the origin of Eq. (92) of the text.

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