FINALCOMPARISON OF VARIOUS SINK STRENGTHS FOR ANALYZING
RADIATION CREEP, GROWTH AND SWELLING*F. A. Nichols
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Abstract

The essential physics involved in the reaction-rate-theory analysis of radiation effects at temperatures where both vacancies and self interstitials are mobile is contained in the expressions used for the strengths of distributed point-defect sinks such as dislocations, cavities and grain boundaries. These sink strengths have been obtained by various authors in distinctly different ways, thus giving rise to some possible confusion in comparing the various results. This is even more true with respect to the effect of interaction fields on these sink strengths and the so-called bias factors or sink efficiencies have been defined in entirely different ways, thus rendering quantitative comparisons difficult. We present here a comparison of several procedures in the literature and attempt to make reasonable quantitative comparisons.

Key words: radiation, interstitial, vacancy, dislocations, cavities (voids), interaction fields, sink strengths, bias factor (sink efficiency), swelling, growth, creep

Introduction

During irradiation, producing only isolated, single point defects at a fixed rate, simple conservation requires

$$\frac{dc_i}{dt} = \dot{a}_i - \sum_{\alpha} r_{i\alpha} - R c_i c_v$$

and

(1)

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*Work supported by the U. S. Nuclear Regulatory Commission, Reactor Safety Research Branch.

$$\frac{dc_v}{dt} = \dot{a}_v - \sum_{\alpha} I_{v\alpha} - R c_i c_v$$

where $c_{i,v}$ = interstitial (vacancy) concentration, t = time, $\dot{a}_{i,v}$ = interstitial (vacancy) production rate $I_{i\alpha, v\alpha}$ = loss rates (currents) of interstitials (vacancies) absorbed at all sinks of type α and R = recombination rate constant. The rate of any particular kinetic process will be proportional to the difference in currents of vacancies and interstitials at a particular type of sink. For example, the rate of void (cavity) swelling is given by

$$\delta \equiv \frac{d\left(\frac{\Delta V}{V}\right)}{dt} = I_{vc} - I_{ic} \quad (2)$$

where $\frac{\Delta V}{V}$ = fractional volume increase due to cavities, and concentrations and currents are expressed in terms of atom fractions. Similarly, the average climb rate of a randomly distributed network of edge dislocations of Burgers vector b is given by

$$v_d = 2 \pi [J_{id}(b) - J_{vd}(b)] \quad (3)$$

where $J_{id, vd}$ = flux of interstitials (vacancies) into the core of a particular dislocation segment. On the other hand, the growth (no-load) or creep rate due to the differential climb of two types of dislocation sinks is proportional to

$$v'_d = 2 \pi \left\{ [J_{id(1)}(b) - J_{id(2)}(b)] - [J_{vd(2)}(b) - J_{vd(1)}(b)] \right\} \quad (4)$$

This is the origin of the so-called SIPA (stress-induced preferred absorption) model of radiation creep,⁽¹⁾ where the dislocations $d(1)$ and $d(2)$ have their Burgers vectors differently oriented with respect to the applied stress system. In addition, the number densities of the two types of dislocations may differ (say due to cold work) and produce a net (growth) strain even in the absence of applied stress. A completely analogous equation obtains for the differential normal motion of grain boundaries of different orientation⁽²⁾ and this is sometimes considered a significant contribution to the growth of polycrystalline materials with a non-equiaxed grain structure.

It should be clear from the above that all predictions of the various kinetic processes of interest rest heavily upon precisely how the various fluxes or currents to the different sinks are evaluated. The real situation is extremely complex in that local defect gradients exist around each of the multitudinous sinks in any real system. In addition, some sinks produce significant interaction-energy gradients with the point defects and these often have angular as well as radial variations. Such complexities have necessitated the introduction of various approximations in order to obtain a tractable problem. Before discussing these, let us consider, in schematic fashion, the physical situation which must exist in a real system in order to produce the kinetic effects of interest. As we have seen, net differences in currents must exist for at least two different types of sink. This means that the concentration profile between neighboring sinks of two different types must have the character of that shown in Fig. 1 along any given vector connecting the two sinks. The concentrations at the sink surfaces will in general be determined by the character of the sink, the interaction fields and any applied loads on the system. On the other hand the level of the profiles in between will be determined largely by the rate of production, the

interaction fields and the respective diffusivities. Fig. 1 is drawn assuming that the interstitial is more mobile than the vacancy, and that recombination is not dominant. For illustrative purposes, the levels for the point defects are shown to be similar whereas for typical choices of physical parameters, as seen below, the more mobile interstitial concentrations peak at levels many orders-of-magnitude lower than those for vacancies. The arrows on the profiles represent the point on that connecting vector at which the point-defect current is zero, such that to the left of the arrow there is a flow of defects toward sink #1 and to the right of the arrow there is a flow toward sink #2. (Note that when interaction energies differ for the two sinks the zero-current points do not coincide with the zero-concentration-gradient points.) If vectors are drawn out in all directions from the center of any one sink and the points of zero current are determined for all of them, these points will form a surface surrounding each sink over which there is zero flow of that particular point defect. If this is done for both types of point defect, two different sets of surfaces will result in general. If these two sets of surfaces enclose two different volumes, then there will be a net point-defect current into that sink of the type represented by the larger volume. It follows that the existence of different average volumes surrounding individual sinks for the two types of point defects is a necessary and sufficient condition to obtain non-zero rates for any of the kinetic processes discussed above, provided the production rates $\dot{a}_i$ and $\dot{a}_v$ are equal. Now if one type of sink is to receive on the average a net influx of one type of point defect, it follows (since recombination must always remove vacancies and interstitials at exactly equal rates) that there must exist at least one other different type of sink. The term "different" means either physically distinct (such as dislocations and cavities) or possessing

different interaction fields with one or both types of point defect (such as dislocations with Burgers vectors of different orientation with respect to an applied stress). If $\dot{a}_i \neq \dot{a}_v$ then a net influx of the type of point defect with the higher production rate can occur even with no significant difference between sinks. For example, for temperatures $\lesssim 0.3T_m$, a significant fraction of vacancies formed in a given cascade may be immobilized in the form of depleted zones such that $\dot{a}_i > \dot{a}_v$ in Equation (1). This can obtain of course only as long as the depleted-zone vacancy inventory does not saturate, beyond which such saturation $\dot{a}_i = \dot{a}_v$ must result. At any temperature, it is also possible that one type of defect is preferentially trapped, say by impurities, so that the effective production rate of the other type is larger, but again only until those traps become saturated.

Since our purpose here is to elucidate differences in the way various authors have estimated loss rates to various inexhaustible sinks, we shall henceforth assume $\dot{a}_i = \dot{a}_v = \dot{a}$, shall ignore thermal point-defect generation, recombination and trapping and shall also assume steady-state conditions in the point-defect concentrations. Under these assumptions, normally invoked by all authors, Eqs. (1) become simply

$$\dot{a} = \sum_{\alpha} I_{i\alpha} = \sum_{\alpha} I_{v\alpha} \quad (5)$$

Our task then is to explore the various ways in which the $I_{\beta\alpha}$'s have been estimated (β refers to the type of point defect).

Reaction-Rate-Theory Formalism

For some time now, the predominant method of analysis has employed the so-called reaction-rate-theory formalism.⁽³⁾ This had its origin in the

analysis of chemical rate processes where initial, uniform concentrations of reacting species were specified and where the rates were proportional to those concentrations and to the diffusion coefficients. Thus one usually sees the form

$$I_{\beta\alpha} = D_{\beta} c_{\beta} \Sigma_{\beta\alpha} \quad (6)$$

where D_{β} = diffusion coefficient of species β (assumed constant) and $\Sigma_{\beta\alpha}$ is the sink strength of sink-type α which it presents to defect species β . Though Eq. (6) is quite appropriate for the chemical reaction rates, it introduces a degree of artificiality into the problems of interest here since the I 's are directly proportional to the production rate and totally independent of the diffusivities.

The concentration profiles like Fig. 1 must now be replaced by average concentrations (averaged over all space, including all sinks) and the discrete sinks must be imagined to be smeared out, i.e. distributed uniformly as point sinks of equivalent net strength. Furthermore D_{β} must also be averaged over all space with all sinks present since the interaction fields may affect it. Under these assumptions then the average concentrations are easily shown to be proportional to $\bar{a}/\langle D_{\beta} \rangle$, thus maintaining the physical requirement that all the I 's be proportional to $\bar{a}$ and independent of the D 's. The task of the analyst is then to estimate the sink strengths in a manner consistent with all these assumptions and we shall discuss below how various authors have approached that task.

Since the existence of a net kinetic rate process requires that for at least two types of sinks $I_{I\alpha} \neq I_{V\alpha}$, it is natural to split the Σ 's into two factors, one of which represents the physical sink structure and the other of

which contains a preference (bias) factor, or sink efficiency as some authors⁽⁴⁾ have called it. Thus, Eq. (6) is re-written

$$I_{\beta\alpha} = \langle D_{\beta} \rangle \langle c_{\beta} \rangle Z_{\beta\alpha} S_{\beta\alpha} \quad (7)$$

where $Z_{\beta\alpha}$ = sink efficiency of sink type α for point-defect type β , and $S_{\beta\alpha}$ is defined as $\Sigma_{\beta\alpha} / Z_{\beta\alpha}$. The precise manner in which the sink strength is split into these two (rather arbitrary) factors differs with the various authors. Further possibilities ensue from the recognition that the preference of one sink type for one point-defect type is generally assumed to arise from the presence of interaction fields. Thus, with the superscript o denoting the absence of all interaction fields, it is convenient to write (assuming, as is usual, that $S_{\beta\alpha}$ is chosen for convenience to be independent of interaction fields)

$$I_{\beta\alpha}^o = D_{\beta}^o \langle c_{\beta}^o \rangle Z_{\beta\alpha}^o S_{\beta\alpha} \quad (8)$$

where the complexity built into this model becomes strikingly apparent. Both D_{β} and c_{β} are spatial functions of the interaction fields and Z depends on the fields but may also contain other (geometric) effects. Since all authors employing this approach have ignored the effect of the interaction fields on the diffusivities, we shall here follow suit and assume from this point on that $\langle D_{\beta} \rangle = D_{\beta}^o = D_{\beta}$ and drop the superscript.

A common approach has been to select simple functional forms for the S 's related to what would obtain from simple models assuming only a dilute concentration of that one type of sink. (This leaves some geometrical effects in the Z 's and not simply in the S 's.) In this approach then

$$Z_{\beta\alpha}^{(1)} \equiv \frac{I_{\beta\alpha}}{D_{\beta} \langle c_{\beta} \rangle S_{\beta\alpha}} \text{ and } Z_{\beta\alpha}^{o(1)} \equiv \frac{I_{\beta\alpha}^o}{D_{\beta} \langle c_{\beta}^o \rangle S_{\beta\alpha}} \quad (9)$$

where the superscript of $Z_{\beta\alpha}$ in parenthesis denotes the type of approach.

Since the Z-factors are introduced solely to depict the effect of interaction fields, a more natural approach seems to be that proposed recently by Mansur et al.⁽⁵⁾ This second approach uses a particular choice of the S's, i.e. those which are appropriate with no interactions present, i.e. $S_{\beta\alpha} \equiv S_{\beta\alpha}^o$, thus normalizing their Z's to be unity for the no-interaction case. Thus they define

$$Z_{\beta\alpha}^{(2)} \equiv \frac{I_{\beta\alpha}}{D_{\beta} \langle c_{\beta} \rangle S_{\beta\alpha}^o}$$

and (10)

$$Z_{\beta\alpha}^{o(2)} \equiv 1$$

It should be noted that although in Eqs. (9) the S-values may be chosen in a totally arbitrary manner, the normalization invoked in the second of Eqs. (10) requires that $S_{\beta\alpha}^o$ be the physically appropriate value for the case of no interaction fields. Thus $S_{\beta\alpha}^o$ in general cannot be determined solely by that particular sink but must be affected by all the sinks in the system and thus it varies with the number density and physical dimensions of all sink types. That is, $S_{\beta\alpha}^o$ must include the "volume-fraction" and "multi-sink" effects sometimes addressed in the literature.^(4,6) On the other hand, $S_{\beta\alpha}$ in Eqs.

(9) need not contain any of these effects, which simply means the effects are relegated to the Z-factors, and the S's may be chosen as simple functions of the parameters of that one sink. Let us say at this point that since the defining of the Z's involves arbitrary definitions, there is no "right" or "wrong" procedure. However, the analyst must estimate the values of the parameters in a manner which is consistent with his choice of definitions.

An Alternative Formalism

Because of the somewhat unnatural introduction of the $D_3 c_3$ products in the reaction-rate-theory approach, and because of the difficulty of making internally consistent estimates of the ZS products, we introduced⁽⁷⁾ an alternative formulation which does not invoke rate theory at all. Since it is the currents which determine the rates of interest, we defined our Z-factors directly on them by writing

$$Z_{\beta\alpha}^{(3)} \equiv \frac{I_{\beta\alpha}}{I_{\beta\alpha}^o}$$

and (11)

$$Z_{\beta\alpha}^{o(3)} \equiv 1$$

where the implication is clear that the I's must be obtained with spatial variations and all sinks present. We shall discuss below the model we developed for doing this but here we wish to point out the relationships which exist between the three sets of Z's. From Eqs. (9)

$$Z_{\beta\alpha}^{(1)} = \frac{I_{\beta\alpha}}{D_{\beta} \langle c \rangle_{\beta} S_{\beta\alpha}} \cdot \frac{Z_{\beta\alpha}^{o(1)} \langle c_{\beta}^o \rangle}{Z_{\beta\alpha}^{o(1)} \langle c_{\beta}^o \rangle} = \frac{I_{\beta\alpha}}{I_{\beta\alpha}^o} Z_{\beta\alpha}^{o(1)} \frac{\langle c_{\beta}^o \rangle}{\langle c \rangle_{\beta}} \quad (12)$$

which yields the relation

$$Z_{\beta\alpha}^{(1)} = Z_{\beta\alpha}^{o(1)} Z_{\beta\alpha}^{(3)} \frac{\langle c_{\beta}^o \rangle}{\langle c_{\beta} \rangle} \quad (13)$$

Again from Eqs. (10),

$$Z_{\beta\alpha}^{(2)} = \frac{I_{\beta\alpha}}{D_{\beta} \langle c_{\beta} \rangle S_{\beta\alpha}^o} \cdot \frac{\langle c_{\beta}^o \rangle}{\langle c_{\beta}^o \rangle} = \frac{I_{\beta\alpha}}{I_{\beta\alpha}^c} \cdot \frac{\langle c_{\beta}^o \rangle}{\langle c_{\beta} \rangle} \quad (14)$$

which in turn gives

$$Z_{\beta\alpha}^{(2)} = Z_{\beta\alpha}^{(3)} \cdot \frac{\langle c_{\beta}^o \rangle}{\langle c_{\beta} \rangle} \quad (15)$$

Equation (15) was previously derived by Mansur et al.⁽⁵⁾ From this they concluded that $Z_{\beta\alpha}^{(2)}$ cannot be quantitatively equated with $Z_{\beta\alpha}^{(3)}$ and with this we totally agree. We regret that our use⁽⁷⁾ of the word "equivalent" misled them in this regard. We did, however, compare on a quantitative basis only a particular combination of $Z^{(3)}$'s (which we called the "bias factor" for swelling) with the analogous combination of $Z^{(1)}$'s employed by others in a rate-theory formalism, the value of which was backed out of experimental data. In fact, however, we erred in this comparison, as we shall show below.

Prediction of Rates

Let us turn now to the prediction of rates of the various physical processes discussed above, in terms of the various types of Z-factors. Dividing the two terms on the RHS of Eq. (2) by $I_{vd} + I_{vc}$ and $I_{id} + I_{ic}$, respectively, while multiplying both by $\dot{a}$, we obtain

$$\delta = \left[\frac{I_{vc}}{I_{vd} + I_{vc}} - \frac{I_{ic}}{I_{id} + I_{ic}} \right] \dot{a} \quad (16)$$

which is legitimate (cf. Eq. (5)) providing we ignore recombination or consider $\dot{a}$ to be the fractional production rate of defects which do in fact arrive at sinks.⁽³⁾ This of course implies the capability of estimating this fraction by some analysis method. Using Eqs. (11), rearrangement yields easily

$$\delta = \dot{a} \frac{Z_{vc}^{(3)} I_{vc}^0 Z_{id}^{(3)} I_{id}^0 - Z_{ic}^{(3)} I_{ic}^0 Z_{vd}^{(3)} I_{vd}^0}{(I_{vd}^0 + I_{vc}^0) (I_{id}^0 + I_{ic}^0)} \quad (17)$$

Now if one makes the assumption that it is only the interaction fields which produce the biasing effect which leads to swelling, it is clear that this requires the assumptions $I_{id}^0 = I_{vd}^0 \equiv I_d^0$ and $I_{ic}^0 = I_{vc}^0 \equiv I_c^0$ in the absence of significant thermal effects. Now this has been the usual assumption of all investigators, but recently Bullough and co-workers^(8,9) have departed from this assumption for dislocations. That is to say, their approach would predict a bias effect in the total absence of interaction fields. We shall discuss this new approach with its implicit assumption of totally different physics for explaining bias effects later but for now we proceed with the usual assumption that, in the absence of interaction fields, sinks do not differentiate between vacancies and interstitials. With this assumption, Eq. (17) becomes

$$\delta = \dot{a} \left[z_{vc}^{(3)} z_{id}^{(3)} - z_{ic}^{(3)} z_{vd}^{(3)} \right] \cdot \frac{I_d^0 I_c^0}{(I_d^0 + I_c^0)^2} \quad (18)$$

It was this particular combination of $z^{(3)}$'s contained in the brackets of this highly symmetric relation which we previously assumed could be equated to an analogous combination of $z^{(1)}$'s, while recognizing the basic differences of the individual z 's.⁽⁷⁾ It is clear from the above analysis that this was an incorrect assumption. Inserting the correct interrelations between the different z 's given by Eqs. (13) and (15) yields

$$\delta = \dot{a} \left[\frac{z_{vc}^{(1)}}{z_{vc}^{o(1)}} \cdot \frac{z_{id}^{(1)}}{z_{id}^{o(1)}} - \frac{z_{ic}^{(1)}}{z_{ic}^{o(1)}} \cdot \frac{z_{vd}^{(1)}}{z_{vd}^{o(1)}} \right] \frac{\langle c_v \rangle \langle c_i \rangle}{\langle c_v^o \rangle \langle c_i^o \rangle} \cdot \frac{I_d^0 I_c^0}{(I_d^0 + I_c^0)^2} \quad (19)$$

and

$$\delta = \dot{a} \left[z_{vc}^{(2)} z_{id}^{(2)} - z_{ic}^{(2)} z_{vd}^{(2)} \right] \frac{\langle c_v \rangle \langle c_i \rangle}{\langle c_v^o \rangle \langle c_i^o \rangle} \cdot \frac{I_d^0 I_c^0}{(I_d^0 + I_c^0)^2} \quad (20)$$

If one relaxes the requirements that $I_{id}^0 = I_{vd}^0$ and $I_{ic}^0 = I_{vd}^0$, and returns to Eq. (17), the results can be written

$$\delta = \dot{a} \left[z_{vc}^{(1)} z_{id}^{(1)} - z_{ic}^{(1)} z_{vd}^{(1)} \right] \frac{s_c^{(1)} s_d^{(1)}}{\left[z_{vd}^{(1)} s_d^{(1)} + z_{vc}^{(1)} s_c^{(1)} \right] \left[z_{id}^{(1)} s_d^{(1)} + z_{ic}^{(1)} s_c^{(1)} \right]} \quad (19a)$$

and

$$\delta = \dot{a} \left[z_{vc}^{(2)} z_{id}^{(2)} - z_{ic}^{(2)} z_{vd}^{(2)} \right] \cdot \frac{s_c^{o(2)} s_d^{o(2)}}{\left[z_{vd}^{(2)} s_d^{o(2)} + z_{vc}^{(2)} s_c^{o(2)} \right] \left[z_{id}^{(2)} s_d^{o(2)} + z_{ic}^{(2)} s_c^{o(2)} \right]} \quad (20a)$$

Also, if we define a type of "sink strength" in our alternative approach by writing $I_d^o = \dot{a} s_d^{o(3)}$, $I_c^o = \dot{a} s_c^{o(3)}$, then Eq. (18) becomes

$$\delta = \dot{a} \left[z_{vc}^{(3)} z_{id}^{(3)} - z_{ic}^{(3)} z_{vd}^{(3)} \right] \cdot \frac{s_c^{o(3)} s_d^{o(3)}}{\left[s_d^{o(3)} + s_c^{o(3)} \right]^2} \quad (18a)$$

Also, we note that
$$\frac{I_d^o I_c^o}{\left(I_d^o + I_c^o \right)^2} = \frac{s_c^{o(3)} s_d^{o(3)}}{\left[s_d^{o(3)} + s_c^{o(3)} \right]^2} = \frac{s_c^{o(2)} s_d^{o(2)}}{\left[s_c^{o(2)} + s_c^{o(2)} \right]^2}$$

and so we can also write Eq. (20) as

$$\delta = \dot{a} \left[z_{vc}^{(2)} z_{id}^{(2)} - z_{ic}^{(2)} z_{vd}^{(2)} \right] \frac{\langle c_v \rangle \langle c_i \rangle}{\langle c_v^o \rangle \langle c_i^o \rangle} \frac{s_c^{o(2)} s_d^{o(2)}}{\left[s_d^{o(2)} + s_c^{o(2)} \right]^2} \quad (20b)$$

which serves to demonstrate the symmetry of the equations as we have written them, since the individual S's of approaches (2) and (3) are entirely different and even have different units. Finally, if we define the quantities

$$Q_{\beta} \equiv \frac{Z_{\beta d}^{(1)} S_d^{(1)}}{Z_{\beta c}^{(1)} S_c^{(1)}},$$

we can rewrite Eq. (19a) in the form

$$\delta = \dot{a} \frac{Z_{vc}^{(1)} Z_{id}^{(1)} - Z_{ic}^{(1)} Z_{vd}^{(1)}}{Z_{id}^{(1)} Z_{vd}^{(1)} S_d^{(1)}} \frac{S_c^{(1)}}{(1 + Q_i)(1 + Q_v)} \quad (19b)$$

The analogous equation given by Mansur⁽⁴⁾ (i.e., his Eq. 17), which does not contain the factor $Z_{id}^{(1)} Z_{vd}^{(1)}$ in the denominator, is incorrect.

In a similar fashion, the rates for dislocation climb, SIPA creep and growth due to grain-shape change can also be expressed in terms of the various Z's and S's using straightforward algebraic manipulations. We do not present these developments here.

Calculations of the Sink Strengths

Models based on reaction-rate theory

In the absence of interactions, the estimation of the sink strengths (Σ 's) has been the subject of many investigations in various fields of interest. In some of these fields, only one type of sink and one diffusing species are considered, greatly simplifying the problem, but even for this case the literature is extensive and somewhat conflicting. It is not our intent here to critically review all these approaches. We have made limited

attempts previously^(10,11) and Gösele⁽¹²⁾ has provided a useful comparison of various approaches, with special attention to the effect of large concentrations of sinks such that neighboring diffusion fields "overlap" significantly. He also clearly distinguishes between the continuous production of diffusing species of interest here and the "post-irradiation" case where an initial distribution (usually uniform) of defects is subjected to an anneal without further production. This is an excellent distinction which many authors have failed to make and the errors thereby introduced have received little attention.

The complexity of the problem can be appreciated when one recognizes that the Z's in approach (1) and the S's in approaches (2) and (3) are functions of the number densities and sizes of all the sinks in the system. In addition of course the Z's in all three approaches are affected by the interaction fields from all the sinks in the system. Thus, in principle, one needs to solve the real, physical problem of discrete sinks with surrounding diffusion fields all interconnected. But of course if one could do that in a reasonable manner (including production and recombination which adds even greater complexity) one would have no need for the reaction-rate-theory model in the first place. So, it is quite clear that approximations must be made. The first thing we shall do here is to ignore recombination. Once the Z's and S's are obtained, recombination can of course be included easily in the reaction-rate-theory model. The question of course arises as to what effect recombination has on the sink strengths themselves. Several authors have addressed this problem, analytically⁽¹³⁾ and numerically,⁽¹⁴⁾ and the general conclusion is that the neglect of recombination introduces relatively little error into the sink-strength estimates. Thus, we follow the usual procedure and neglect recombination, but one should bear in mind that doing so does no doubt

introduce some degree of error and so one should be very cautious in attributing too much "rigor" to the sink-strength estimates so obtained. We concur with Brailsford and Bullough⁽¹⁵⁾ that the neglect of recombination is probably necessary to obtain a tractable problem.

One approximation sometimes made is to neglect uniform defect production completely and simulate its effect by assuming a fixed concentration of defects is maintained at some surface surrounding a given sink. The surface is generally chosen to give a volume equal to the average volume per sink in the real system. All other sinks are totally neglected. The fixed concentration at the outer cell boundary is often assumed to correspond to $\langle c \rangle$ in the reaction-rate-theory model, though sometimes $\langle c \rangle$ has been equated to an intermediate value in the cell. The same cells are chosen for both vacancies and interstitials. Wolfer and Ashkin, e.g., used approach (1) above to define their Z's for spherical sinks⁽¹⁶⁾ (such as cavities) and edge dislocations⁽¹⁷⁾ and evaluated them by equating the current entering the sinks (which, of course, in their model is identically equal to the current entering their cell from their imaginary external source used to simulate defect production). They also assumed $S_{v\alpha} = S_{i\alpha} \equiv S_{\alpha}$ for both types of sinks. Specifically they took $S_c = 4\pi r_c N_c$, where r_c and N_c are the radius and number density of cavities, respectively, and $S_d = 2\pi\rho/\ln(R/r_0)$, where ρ is the dislocation density, R is the cell radius and r_0 is the dislocation core radius. These S's are of course the values one obtains⁽¹⁰⁾ from various analyses in the dilute concentration limit, i.e. they do not contain any multi-sink effects at all. That is to say, the Z-factor must contain not only interactive effects but also multi-sink effects if present. However, since Wolfer and Ashkin's model invokes only one type of sink, the effects of other types of sinks on each Z are totally absent. Also, as discussed by Gösele,⁽¹²⁾ the absence of

defect production within their calculational cell produces inaccuracies even in their predicted effects of the density of the same type of sink. The net effect of all this is the great difficulty of ascertaining the accuracy of the resulting Z 's.

Additional questions are raised by the evaluations in obtaining the Z 's. The interaction fields (based on continuum elasticity) of course have singularities at the center of the dislocation core and at the cavity surface. Wolfer and Ashkin follow the usual procedure for the dislocation and cut off the field at the core radius, thus avoiding the unrealistic infinite interaction energy at the center. However, with the cavity they do not do so and evaluate the field up to the cavity surface where it becomes infinite. Since the field is attractive, the authors considered that this had no significant effect, but Bullough and Quigley⁽⁸⁾ come to contrary conclusions and, as we shall see below, they state that cutting off the field at one atomic distance from the cavity surface changes the Z dramatically for very small cavities. Whereas the Wolfer-Ashkin procedure predicts $Z \rightarrow \infty$ as $r_c \rightarrow 0$, the Bullough et al. approach predicts finite values.

Another question arises in the Wolfer-Ashkin evaluation of Z_d . They employ a perturbation approach which predicts that the first-order size-effect interaction (due to its angular variation which produces an average value of zero) leads to no biasing at all and so their Z_d contains only second-order (and higher) effects. The net result of all their assumptions is that when they employ their Z_d 's and Z_c 's in a reaction-rate-theory model, they predict that small cavities will shrink rather than grow in the presence of edge dislocations. This led Wolfer and Mansur⁽¹⁸⁾ to propose that void swelling can occur only after cavities (initially stabilized by gas atoms) have become coated with impurity atoms (due to segregation during irradiation) such that

the different elastic properties of the coating strongly repel interstitials, thus strongly decreasing Z_{ic} relative for Z_{vc} , and thereby allowing void nucleation and growth in the presence of edge dislocations. We believe these concepts are invalid. We concur with Bullough and Quigley that cutting off the cavity interaction field at an atomic distance from the cavity surface to avoid the infinite value is physically much more satisfying and they claim this vastly changes the calculated Z_c 's for small r_c . This is exactly the cutoff procedure we previously used.⁽⁷⁾

A second cell model sometimes used allows for uniform defect production and thus eliminates the imaginary sources from outside the cell. The usual boundary condition at the cell surface is that of zero flux, the cell sizes are normally chosen to yield a volume equal to the average volume per sink (or average area per unit line length) and again the same cell sizes are used for vacancies and interstitials. As we discussed in connection with Fig. 1, this last assumption requires that in the steady state exactly equal currents of vacancies and interstitials enter the sink. This means of course that no biasing at all is possible in such a calculational cell. This approach was used by Bullough et al.⁽¹⁹⁾ and we previously expressed⁽¹¹⁾ our concerns. However, as Brailsford and Bullough subsequently pointed out,⁽¹⁵⁾ we also incorrectly stated that $D_i c_i - D_v c_v$ was identically zero throughout the cell. Though we agree this is not so, our concern that exactly equal currents of vacancies and interstitials enter the sinks remains valid. This paradox does not preclude the calculation of a net biasing effect in the reaction-rate-theory model, however, since different interaction fields in the cell model will produce different average concentrations and it is these average concentrations so calculated which are used, via Eqs. (9) or (10), to calculate the Z 's where in the cell model the I 's are each set equal to the

production rate in the cell. However, it should be noted that the appropriate average concentrations to be used in rate theory must correspond to those existing in the real system with all sinks present. There have been some attempts to minimize the effect of this inconsistency by somehow including effects of other sinks within the one cell, but the gross assumptions invoked⁽¹⁵⁾ make the results of dubious value. The simplest approach is to add smeared-out sinks to the cell to represent all other sinks in the system but analytical solutions are not available unless the interaction-field effects are approximated by invoking the capture-radius concept of Ham⁽²⁰⁾, where an attractive field is assumed equivalent to a larger sink with no field. Inaccuracies introduced by such mixtures of assumptions are difficult to assess.

This approach has been followed recently by Bullough and Quigley⁽⁸⁾ to develop Z's, using approach (1), for cavities after defining $S_c \equiv 4 \pi r_c N_c$. As noted above $\langle c \rangle$ is calculated for the cavity cell and Z's are then calculated from Eqs. (9). The omission of all other types of sinks introduces unquantified error, which the authors attempt to correct, thus introducing several new approximations. First they seek to include a smeared-out, reaction-rate-theory type of loss term into the cavity cell but comment that with the interaction field included they were unable to obtain an analytic solution. They therefore resort to the capture-radius concept of Ham. A capture radius, larger than r_c by the quantity δ , is specified as the inner surface of the diffusion cell and no interaction field is assumed present. This gives an analytic solution with δ as an adjustable parameter. This is then transformed to an alternative adjustable parameter, γ , by calculating the radius for which

$$\left| \frac{E_c(r)}{kT} \right|_{r = r_c + \delta} = \gamma \quad (21)$$

where $E_c(r)$ is an approximate cavity interaction energy and kT has its usual meaning. Normally in the capture-radius model, one takes $\gamma \equiv 1$, but Bullough and Quigley attempt a "calibration" of this model by "adjusting γ to fit to the accurate [sic] bias parameters." By "accurate" they presumably refer to their "embedding model" (which we shall discuss shortly) for the special case of no other types of sink and using the same approximate form of $E_c(r)$. With this calibration, they are led to select different values of γ depending on the point-defect type, namely

$$\gamma_i = 0.430, \gamma_v = 1.321 \quad (22)$$

It is not clear why different values should be obtained since the only differentiation in the model between the vacancy and interstitial is in their relaxation volumes (taken as -0.5 and 1.2 atomic volumes, respectively) which are quadratically related to $E_c(r)$. There is a discrepancy introduced in the model in that no accounting is made for the defects generated within the region $r_c < r < r_c + \delta$ and this region would be much larger for the interstitial if γ were taken as unity for both species. The actual values selected make these regions even more different and although the errors introduced may well be small considering the short-range nature of E_c , the existence of such inconsistencies is bothersome. The problem is more pronounced for dislocations with the longer range of E_d .

At any rate, with the above calibration to obtain a field-free cavity cell, Bullough and Quigley then obtain an analytic solution with defect production and "smeared-out" sinks of a second type, e.g. dislocations.

For dislocations, Bullough and co-workers have presented many different models and we have discussed several of these previously.⁽¹¹⁾ More recently, they presented⁽²¹⁾ a cell model, each cell containing one dislocation with no other sinks present. Here they included the full angular dependence of E_d and of necessity employed a numerical procedure. They applied their results to a calculation of SIPA creep and we previously compared⁽²²⁾ those results with results of our approach to be discussed below. Since we are concentrating here on void swelling we shall not repeat that discussion here.

Brailsford and Bullough recently concluded⁽¹⁵⁾ that "it is best to forget the entire matter and regard the Z 's as empirical parameters to be obtained from the analysis of experiments." Nevertheless, Bullough and Quigley⁽⁸⁾ subsequently presented yet another model for calculating the sink strength for long, straight, edge dislocations, employing their "embedding" approach. In this work the authors state that since the magnitude of the swelling rate depends on the preferential bias between the dislocations and interstitials compared with that between dislocations and vacancies, these sink strengths for the dislocations "must therefore be calculated with care if a quantitative theory of void swelling is required."

Bullough and Quigley state that, from the work of Brailsford and Bullough⁽¹⁵⁾ on a cell model containing smeared-out sinks of another type, they can justify the dropping of the angular variation of E_d . They then use a purely radial form in an "embedding model" to give what they call a "rigorous" dislocation sink strength. With the several approximations involved, it is not clear what the term rigorous is meant to imply.

In the embedding procedure, the dislocation is surrounded by an inner, sink-free region containing the radial interaction field and an outer surrounding region (with $r \rightarrow \infty$), called the "lossy medium," with no field but

with all sinks present in a smeared-out fashion. The idea is to calculate the current into the discrete sink in such a model, then equate it to the loss-rate to that same type of sink (far from the discrete sink) in the "lossy" medium of the model, and in turn equate this to the reaction-rate-theory loss term assuming the same average concentrations as exist far from the discrete sink in the "lossy medium." Though still subject to a number of approximations, this approach eliminates some of the inconsistencies of the other approaches discussed above.

The choice of the size of the sink-free region has gone through a number of revisions through the years, sometimes being omitted completely. In the Bullough-Quigley model, it is selected as the radius, R , at which the coefficient of the concentration c in the equation for the sink-free region

$$\frac{d^2 c}{dr^2} + \left(\frac{1}{r} + \frac{d\phi}{dr} \right) \frac{dc}{dr} + \left(\frac{d^2 \phi}{dr^2} + \frac{1}{r} \frac{d\phi}{dr} \right) c + \frac{\dot{a}}{D} = 0 \quad (23)$$

is equal to the coefficient of c in the equation describing the surrounding "lossy medium"

$$\frac{d^2 c}{dr^2} + \frac{1}{r} \frac{dc}{dr} - c \Sigma + \frac{\dot{a}}{D} = 0 \quad (24)$$

where $\phi(r) = E_c(r)/kT = -L/r$ and

$$L = \frac{(1 + \nu) \mu b |\Delta V|}{3 \pi (1 - \nu) kT} \quad (25)$$

where ν = Poisson ratio, μ = shear modulus, ΔV = relaxation volume of point defect. Thus, they have assumed the magnitude of their radial field to be $\sim 2/3$ of the maximum attractive value in its full angular form, which is roughly equivalent to averaging over the attractive region. We shall discuss this later.

The equating of coefficients of c appears to be an attempt to obtain the radius at which the interaction field has equal importance as the distributed sinks in the "lossy medium," but it is not clear why, in this rationale, the $\frac{d\phi}{dr} \cdot \frac{dc}{dr}$ term would be neglected. However, the authors compared the results for Z obtained by this approach using the so-derived

$$R = (L/\Sigma)^{1/3} \quad (26)$$

with numerical results employing smeared-out sinks throughout and no truncation of the interaction field. They found the two approaches to be essentially equivalent if the radius of the sink-free region was adjusted to 1.093 R . Why the model with the sink-free region should correspond accurately to one containing no sink-free region is not clear to us.

With the above calibration on R , the authors then select a core boundary condition by writing the flux of defects into the core

$$D \frac{dc}{dr} + \frac{d\phi}{dr} c = (n_j b) f \bar{K} c \quad (27)$$

where

$$\bar{K} = \frac{D}{b} \exp \left\{ (E_m - E'_m)/kT \right\} , \quad (28)$$

where E_m = normal (perfect crystal) defect migration energy and E'_m allows for the possibility of a modified final jump barrier. In this form, the boundary condition has three disposable parameters, E'_m , $n_j b$ (= jog concentration per atom plane along the dislocation) and the quantity f which is in turn related to the core radius r_0 by

$$f = \eta b / 2 \pi r_0 \quad (29)$$

which transforms f into another disposable parameter, η , which is the number of available sites from which capture is possible. The authors argue that atomistic calculations lead them to select $f_v = 1$ and $f_i < 1$ though otherwise fully "disposable."

The authors then reduce their number of disposable parameters to two by selecting $E'_m = E_m$ for simplicity. They state that the precise values of f (or η) and $n_j b$ are difficult to estimate and with this we certainly concur. In fact this is almost always the central problem with most any "rate limitation" or "surface-control" model. The equations, though having the appearance of elegance, introduce parameters which we are usually ill-equipped to estimate and they then become adjustable parameters. We also note that they have set up their model to specifically exclude the effect of core diffusion in greatly extending the effect of each jog. Even in the equilibrium thermal case, several authors have concluded by analysis and experiment that this effect typically makes a dislocation act as a perfect sink (at least for vacancies). In our opinion, during irradiation, jog concentrations far in excess of thermal-equilibrium values must be expected, so making the perfect-sink action even more likely. Because of all this, we have preferred to assume perfect sink action until quantitative comparisons are sufficiently

advanced to render this definitely incorrect. We do not believe such a situation is at hand.

Finally, these authors select their core radius as that value for which the potential varies by more than kT over one atomic distance, i.e.,

$$r_o = (Lb)^{1/2} \quad (30)$$

They then equate the currents into the cores to those in the effective medium far from the dislocation using approach (1) above, thereby obtaining their Z_d values (after selecting $S_d = \rho$, the dislocation density). This means they have neglected the defects generated within $r < r_o$, thus introducing errors which are different for the two types of point defects, though presumably these errors are small.

Though Bullough and Quigley made no attempt to choose the disposable parameters f and $n_j b$ which they feel are physically realistic, they do state that assuming dislocation sinks to be ideal or perfect sinks leads, in their model, to predictions of "ridiculous void growth phenomena." Unfortunately, they do not elaborate. We have shown previously that our model, assuming all sinks to be ideal and using no disposable parameters, leads to quite reasonable values of predicted void growth rates. Specifically, using parameters appropriate for austenitic steel, we predicted (for equal dislocation and void sink strengths) maximum swelling rates of $\sim 10\%$ per dpa. Considering that only a fraction of defects survive recombination in the cascade and are able to participate in long-range diffusion processes, this is in very reasonable accord with observed experimental values of $\sim 1\%$ per dpa when cascade effects are not considered.⁽²³⁾ Specifically, we previously estimated that the fraction of defects surviving cascade recombination is

~ 0.16 giving us a predicted value of $\sim 1.6\%$ per (calculated) dpa for experimental comparison. This accords well with experimental reports of steady-state swelling rates of $\sim 1\%$ per (calculated) dpa, when one considers the many uncertainties involved in choosing the appropriate parameters. We emphasize that our analysis contains no disposable parameters.

Bullough et al.⁽⁹⁾ employ the embedding model to estimate sink strengths for cavities. After noting that a model with an interaction field and smeared-out sinks throughout produces an equation with no available analytic solution, they adopt the concept of a sink-free region (with interaction field) surrounded by a lossy medium with smeared-out sinks but no interaction field. Assuming the cavities to act as ideal sinks, they obtain a solution and select the sink-free radius in a manner analogous to that of Bullough and Quigley.⁽⁸⁾ Finally, they define $S_c = 4 \pi r_c N_c$ to obtain their Z's by approach (1) above.

Model for alternative approach

Because of all the uncertainties introduced by the various models discussed above via such artifices as external sources to simulate defect production, "capture radii" to simulate interaction fields, as well as smeared-out sinks and sink-free regions in place of discrete sinks only, we developed a model⁽⁷⁾ which essentially eliminates all of these approximations. All sinks are treated in discrete manner with their spatially varying (radial) interaction fields and concentration gradients surrounding them. As in all other models, we select idealized diffusion-field symmetry around each sink but contrary to the embedding model we do not continue such symmetry to $r \rightarrow \infty$ for each type of sink. Instead, we assume that at a sufficiently large distance from each type of sink the precise symmetry of the

diffusion field becomes of little importance due to the fact that the gradients in both c and E become very small. This is completely analogous to the cell models discussed above and the roots of such an approach go back to the classic Wigner-Seitz analysis of electron distributions in metals. Hence the term Wigner-Seitz cell is often employed. However, our model differs from all other cell models in that we treat several types of cells simultaneously but still permit the diffusion fields to have different symmetry for the different types of sinks. Fig. 2 shows schematically how such cells are established for dislocations, cavities and grain boundaries, respectively. The choice of the cell sizes is somewhat arbitrary except that one should ascertain, ipso facto, that the gradients are truly small near the peripheries and that different choices of R 's meeting this condition do not yield significantly different results. So far we have not explored the effect of different R 's for different types of cells but have used only a single value, ignoring results which turn out to show significant gradients at any of the cell peripheries.

Having selected a cell to represent each type of sink, the cells are then "connected" by ensuring continuity in flow of defects across their peripheries, i.e. the total current leaving all cell boundaries of a given type of sink must equal the algebraic sum of currents entering all cell boundaries of all other types of sinks. It is also ensured that there is no significant difference in concentration at the cell peripheries of all types of sink. The continuity in currents is guaranteed precisely. The equality of concentrations is very closely approximated with sufficiently large cells and not meeting this condition yields a further reason for rejecting the calculated results. In practice, this is not a problem for the sink densities and interaction fields of interest. Fig. 3 shows actual concentration

profiles for rather large sink densities for vacancies and interstitials, respectively, both with and without the interaction fields. Magnitudes or gradients in both c and E at the cell boundaries are never more than a few % of their magnitudes at the sink surfaces, and only for interstitials in the presence of interaction fields is there even a noticeable mismatch in concentration (in this extreme case amounting to only $\sim 1\%$). The effect of the fields in attracting defects and thereby lowering their concentration levels is clear. In the reaction-rate theory this produces the lower average values which lead to the higher bias factors via Eqs. (9) and (10).

In our model depicted in Fig. 2, each cell may have a radial (but otherwise arbitrary) interaction field and in the calculations to date such fields are assumed to equal those for an infinite body. This assumption introduces slight errors in the matching of concentrations on the cell peripheries but for the fields of interest this has not been a serious problem. (The mismatches of Fig. 3 produce essentially no errors in the calculated results.) We have also performed calculations on SIPA creep using this approach⁽²⁴⁾ and also using "additive" fields from neighboring cells so as to form continuous fields which were identically equal and which had zero gradients in E and c at the cell peripheries, thus approximating the physical case of field "overlap" and leading to no mismatches in concentrations or gradients at the cell peripheries. The calculated rates were essentially unaffected for dislocation densities which are physically plausible.

We have been able to obtain solutions for the fluxes in each type of cell (ignoring, with all other authors, recombination effects) and thereby the kinetic rates expressed in relations like Eqs. (2)-(4). We also include the effect of the interaction fields on the diffusivities and show, in agreement with other authors,^(25,26) that the entire biasing effect is due to interactions in the saddle-points for diffusion of the point defects and

totally independent of interactions in the ground-states. No such distinction has been made in any of the previous models. We also find that the thermal fluxes are additive to those due to irradiation and are differently affected by the interaction fields. That is to say, the Z 's for thermal fluxes are different from those for radiation-induced fluxes. This result is supported by independent analytical results of Scattergood et al.⁽²⁶⁾ and contradicts the characteristic of all other models, that the same Z 's apply to both components.

For simplicity, the same diffusional distance has been selected for each type of cell. This seems intuitively reasonable since it is the diffusional distance which determines how much the gradients have "flattened out" as we go out from a sink surface. Also in the same vein, we choose the same cells for vacancies and interstitials. This does not cause the inconsistency discussed above concerning other models since the peripheries of our cells are not forced to coincide with a zero-flux condition; the position of no flux will be determined by the interplay of the interaction fields and will produce the differences for vacancies and interstitials displayed schematically in Fig. 1, so that in fact the volume from which each type of point defect is drained to a given sink will precisely determine the current into the sink in the steady state. In fact this provides another check on the internal consistency of our model. The positions of zero flux are also shown in the calculated results of Fig. 3 by the vertical arrows which are identical for no interaction fields and which show, in the presence of interaction fields, the biasing of interstitial flow to dislocations and of vacancy flow to cavities.

Returning to Fig. 2, the basic equations and boundary conditions are presented below. A more detailed account is available elsewhere.⁽²²⁾ The

diffusional distance, R , is determined by ensuring that the total volume fraction occupied by all cells is equal to unity; thus

$$\frac{4}{3} \pi \left[(R + r_c)^3 - r_c^3 \right] N_c + \pi (R + r_o)^2 \rho + \frac{r_g^3 - (r_g - R)^3}{r_g^3} = 1 \quad (31)$$

where r_c = cavity radius, N_c = number of cavities per unit volume, r_o = dislocation core radius, ρ = dislocation line length per unit volume and r_g = grain radius (obtained by equating $3/(4\pi r_g^3)$ to the number of grains per unit volume). Note that the unit volume selected for all densities is solid volume, excluding void volume. It is easily shown that the point-defect flux can be written⁽⁷⁾

$$J = - D \exp(-E^S/kT) \frac{d}{dr} \left[c \exp(E^G/kT) \right] \quad (32)$$

where D = point-defect diffusivity in absence of interaction fields and E^S and E^G are interaction energies in the saddle-point and ground-state, respectively.

The general solution to Poisson's equation (with defect production) is

$$J = \frac{\dot{a}r}{2} + \frac{b_1}{r} \quad (33)$$

for cylindrical symmetry (dislocation cell) and

$$J = \frac{\dot{a}r}{3} + \frac{b_2}{r^2} \quad (34)$$

for spherical symmetry (cavity and grain-boundary cells). Boundary conditions are

$$c \exp (E_d^G/kT) \Big|_{r_o + R} = c \exp (E_c^G/kT) \Big|_{r_c + R} = c \Big|_{r_g - R} \quad (35)$$

and

$$2 \pi (r_o + R) \rho J_d \Big|_{r_o + R} + 4 \pi (r_c + R)^2 N_c J_c \Big|_{r_c + R} = \frac{3(r_g - R)^2}{r_g^3} J_g \Big|_{r_g - R} \quad (36)$$

where subscripts d, c and g refer to dislocation, cavity and grain boundaries respectively, the J's are point-defect fluxes (note that positive flux here means flux in the direction of increasing r) and the b's are constants determined by the boundary conditions.

Boundary condition (35) is equivalent to equating concentrations at the cell peripheries provided the E^G 's are ~ 0 there, a situation always obtaining in calculations to date. This is also checked, ipso facto, by ensuring that the peripheral c's are essentially equal, as discussed above in conjunction with Fig. 3. Eq. (36) expresses conservation since, in the steady state, all defects generated within the cells must enter the sinks. The relation holds for thermal fluxes as well which must originate at some sinks and terminate at others, i.e. no net overall production must exist.

We quote only the resulting equation for the flux in the dislocation cell when the grain size is large enough to make boundaries unimportant as sinks.

For a full discussion for all three cells and various grain sizes, previous publications may be consulted.^(7,22,24) The result for the case cited is

$$\begin{aligned}
 J_d = & \frac{\dot{a}r}{2} + \frac{1}{r} \left\{ \frac{2N_c}{\rho} D \left[c \exp(E_d^G/kT) \Big|_{r_o} - c \exp(E_c^G/kT) \Big|_{r_c} \right] \right. \\
 & - \dot{a} \frac{2N_c}{\rho} \left[\frac{1}{2} \int_{r_o}^{r_o+R} r \exp(E_d^S/kT) dr - \frac{1}{3} \int_{r_c}^{r_c+R} r \exp(E_c^S/kT) dr \right] \\
 & - \dot{a} \left[\frac{2N_c(r_c+R)^3}{3\rho} + \frac{(r_o+R)^2}{2} \right] \int_{r_c}^{r_c+R} \frac{\exp(E_c^S/kT)}{r^2} dr \Bigg\} \\
 & + \left\{ \frac{2N_c}{\rho} \int_{r_o}^{r_o+R} \frac{\exp(E_d^S/kT)}{r} dr + \int_{r_c}^{r_c+R} \frac{\exp(E_c^S/kT)}{r^2} dr \right\} \quad (37)
 \end{aligned}$$

There are several general characteristics of all the fluxes displayed by Eq. (37). First, the thermal fluxes are additive to the radiation-induced fluxes and are proportional to D and the difference in products of concentrations and exponentials on the ground-state interactions at the different types of sink. They are also affected by the interactions in the saddle-point. On the other hand, the radiation-induced fluxes are totally independent of the D 's. Also, when the radiation-induced fluxes for vacancies and interstitials are subtracted (as they always are to obtain net kinetic rates) the result depends solely upon the differences in various integrals involving interactions in the saddle-point and are independent of ground-state interactions. None of these physically required characteristics were found in

any of the other models we discussed above. In particular our Z's for thermal fluxes are totally different from those for radiation-induced fluxes, contrary to all other models. This will affect predicted temperature dependencies at higher temperatures. Since our interest here is primarily in radiation effects, henceforth we consider only temperatures for which the thermal rates are negligible.

Although the formulation in principle allows a distinction between E^G and E^S , our relative ignorance of this area and present purpose to keep things relatively simple cause us to ignore this distinction (whence D's become independent of the fields as assumed in all other models). We take then the interactions in both ground-state and saddle-point to be given by⁽¹⁶⁾

$$E_d = \frac{\mu V_\beta r_o e_\beta^o \sin \theta}{\pi r} \quad (38)$$

and

$$E_c = - \frac{\Omega^2 (e_\beta^o)^2 \mu (1 + \nu)^2}{36\pi (1 - \nu) r_c^3} \frac{2}{\zeta^4 (\zeta + 1)} \left[\frac{\zeta^3}{(\zeta - 1)^3} - \frac{\zeta^2 + 1}{\zeta^2 - 1} \right] \quad (39)$$

where V_β = point-defect volume, e_β^o = point-defect relaxation strain, Ω = atomic volume, θ = polar angle and $\zeta = r/r_c$. To avoid the unphysical singularity at r_c , we cut off E_c at $r_c + b$. The cavity field is radial but the dislocation field is not. Since our approach can accept only radial fields, we must address the question of an effective radial field, a common problem in dislocation theory.

As mentioned above, Bullough and co-workers have assumed the field may be replaced by its average attractive value, and we have previously used that same assumption.⁽⁷⁾ However, numerical analyses by Scattergood employing the full angular field⁽²⁷⁾ have shown that this can lead to considerable error. As discussed elsewhere,⁽²²⁾ we have shown that the appropriate choice of the normalized radial field is $-1/4\langle(E_d/kT)^2$ to give excellent and quantitative agreement with Scattergood's numerical results. There exists analytical support also for such a form.⁽²⁸⁾ Since the $\sin^2\theta$ factor averages to $1/2$, this means that the maximum amplitude is normalized by kT , then squared and then divided by 8. We have shown before⁽²⁹⁾ that this produces quantitatively much different $Z^{(3)}$ -values than simply using the average attractive field. Figure 4 illustrates this effect. These calculations were run for the parameters below:

<u>Constant</u>	<u>Value</u>
μ	8.6×10^4 MPa
ν	$1/3$
r_o	0.126 nm
V_1, V_v, Ω	1.2×10^{-2} nm ³
e_i^o	1.4
e_v^o	-0.23
γ	1.5 Jm ⁻²
r_c	$10-100r_o$
N_c	$10^{19}-10^{21}$ m ⁻³
r_g	10 μ m
ρ	$10^{12}-6 \times 10^{14}$ m/m ³
T	600 K

$$D_i c_i = 1.58 \times 10^{-8} \exp(-51000/T) \text{ m}^2 \text{ s}^{-1}$$

$$D_v c_v = 10^{-5} \exp(-33950/T) \text{ m}^2 \text{ s}^{-1}$$

Although the individual $Z^{(3)}$'s are strongly affected by the choice of radial field, it is especially intriguing that the predicted swelling is not changed nearly so much, as displayed in Fig. 5 where the combination of $Z^{(3)}$'s given in Eq. (18) and defined as B , to which swelling rate is proportional, is plotted. With the improved effective radial field, the predicted bias is seen to be very nearly independent of the relative sink strengths of cavities and dislocations, indicating that very little geometry dependence remains in our bias factor as we have defined it. It is this value of $B \sim 0.5$ which we previously compared with the analogous combination of $Z^{(1)}$'s and which our analysis above showed to be inappropriate.

Comparisons between Different Approaches

Bullough et al.⁽⁹⁾ have presented comparisons between their Z -values for cavities and those due to Wolfer. Since both used approach (1), the Z 's should be directly comparable, but Fig. 6 shows how vastly different values can result from using different types of approximations in the actual evaluations. Wolfer employed the single-sink cell model with surface sources on its periphery to simulate production. Bullough et al. used the embedding model, with production, but with a sink-free zone surrounded by an effective medium containing smeared-out sinks. All calculations used the same cavity interaction field, Eq. (39), but Wolfer retained the functional form all the way to the cavity surface where $|E_c| \rightarrow \infty$. Bullough et al. "cut off" the field at its value for $r = r_c + b$ and used that value between that radius and r_c . They attribute the extreme divergence of values at small r_c to this difference. We believe the Bullough et al. approach is physically more plausible and used just that procedure here and in our previously published results.⁽⁷⁾ The differences at large values of r_c arise due to the multi-sink

interaction effects built into the embedding and cellular models but not accounted for in Wolfer's approach. This is because Wolfer considered only the case of an infinite sink-free region surrounding one cavity, the infinite-dilution case. However, with no interaction field and a finite cell size the strength using Laplace's equation (no production) contains, as we discussed previously,⁽¹⁰⁾ a factor of $1/(1-r_c/R)$ where R is the cell radius ($\equiv (3/4\pi N_c)^{1/3}$). The Wolfer case with the interaction field, if solved for such a cell, should contain a similar factor. If we apply this factor to the Wolfer results we see (as shown in Fig. 6) that a significant upswing at large r_c (the figure is drawn for an $N_c = 10^{22} \text{m}^{-3}$, hence $R = 28.7 \text{ nm}$) does result and its magnitude is in fact similar to, even somewhat larger than that of the embedding model. Thus, with this correction to Wolfer's calculations, the differences between the two approaches are not extreme for the sizes of most practical interest, i.e. $r_c \gtrsim 1 \text{ nm}$, though we believe the Bullough et al. values are more reasonable for smaller values of r_c . It should also be remembered that the embedding model allows for other types of sink and the Wolfer approach does not.

To make direct comparisons with our approach, we must use Eq. (13). Thus, we plot in Fig. 7 results of $Z_{\beta c}^{(1)}$ for which $Z_{\beta c}^{o(1)}$ is given by $I_{\beta c}^o / (D_\beta \langle c_\beta^o \rangle 4\pi r_c N_c)$, $Z_{\beta c}^{(3)}$, $I_{\beta c}^{o(3)}$, and $\langle c_\beta^o \rangle$ are calculated from our model, with all other physical parameters (e.g., D_β , r_c , N_c , etc.) identical to those of Bullough et al. Except for differences at large r_c (where multi-sink effects become prominent) we see an approximate agreement between our model and those of Bullough and co-workers, seemingly so different in their approach. In fact, the agreement is almost exact between our results and the results of Bullough and co-worker's "cell" model, also shown in Fig. 7.

Bullough et al. consider that cell models are more appropriate for an ordered array of sinks than for a "random" distribution. We do not believe this is necessarily true. In an ordered array, there must be asymmetries in the diffusion field surrounding any given sink and these asymmetries must display the periodicity of the lattice of the ordered array. Since our cell model (and essentially all others) assume totally symmetric fields around all sinks, it cannot represent an ordered array. Another way to phrase the argument is first to assume the model represents an ordered array. If so, the specific sink arrangement pattern of that array must be reflected in the model. But the model reflects no pattern of sink arrangement. Therefore, the model cannot represent an ordered array.

One could consider that in our cell model the sinks neighboring a particular sink are in effect "randomized" as far as their angular position from that sink. This "randomizing" is produced by assuming the fields around all sinks to be radially symmetric. It is true that our model assumes only an "average" neighborhood of each sink and specifically excludes the presence of other sinks closer than $\sim 2R$. However, as discussed above, the embedding model also randomizes the location of all surrounding sinks by using symmetric fields (in addition to "smearing out" those sinks) and it also introduces "sink-free" regions with no straightforward or standard method of establishing the size of such regions. In our model the cell size is selected in a straightforward manner, including the size and density of all sinks in a self-consistent manner such that, on the average, a region of equivalent size in the physical case would in fact contain no other sinks. Bullough and co-workers, on the other hand, select the size of a sink-free region based solely on the density or interaction field of that particular sink (meaning that the region of that size in the physical case may (on the average) contain many

sinks of another type). Neither model is exact. Which better describes the case of "randomly" distributed sinks (or, rather, the case of actual sink distributions) is, in our opinion, moot.

A quantitative comparison of the various models with respect to dislocations is much more complicated due to the introduction by Bullough and co-workers of "rate limitation" and its attendant set of disposable parameters. Hence we leave that comparison for a subsequent publication.⁽³⁰⁾

Summary

We have presented a comparison of various analyses employed to describe the sink strengths and/or bias factors of various types of point-defect sinks. These are of crucial importance in understanding the various kinetic processes occurring during displacement-producing irradiation, such as growth, creep and swelling.

The use of reaction-rate theory typically entails the splitting of each sink strength into the product of two factors, one describing geometrical effects and the other biasing effects (due to interaction fields around sinks). However, there is no unique way of doing this and usually some geometrical effects remain in the so-called bias factors.

We have also described an approach using Wigner-Seitz cells in which reaction-rate theory is not invoked and this arbitrary splitting-up of the sink strengths is not required.

Previous comparisons between the various approaches are sparse and have not always been done in a consistent manner. We have developed a consistent method for making such comparisons and have obtained quantitative comparisons for the case of spherical voids. The case of dislocation sinks is more complex and will be discussed elsewhere.

We conclude that, although significant quantitative differences exist between some estimates, there is little quantitative difference between the predictions of the Wigner-Seitz-cell approach and the so-called "effective medium" approach, for the case of voids. A quantitative comparison of predictions of kinetic rates awaits detailed comparisons of the sink strength and bias factor for dislocations.

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List of Illustrations

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Fig. 1

(a) DISLOCATION CELL

(b) CAVITY CELL

(c) GRAIN-BOUNDARY CELL

Fig. 3a

Fig. 3b

Fig. 5

Fig. 6

Fig. 7