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1. Introduction

During the past two decades, rate theory has been applied to the interaction of point defects with microstructural features. In this approach, both vacancies and interstitials are assumed to be produced uniformly in time and homogeneously in space. Based upon this concept of point defect generation, rate equations have been developed for the description of diffusion, recombination and interaction of point defects with dislocations, grain boundaries, cavities, and precipitates.

Under neutron or ion irradiation conditions, point defects are produced in ensembles resulting from a sequence of collisions in cascades. As such, primary knock-on atoms (PKAs) generate a series of displacements that are closely situated. The generation of cascades is random in space and time. Therefore, a microstructural feature will see and interact with a fluctuating concentration of point defects. Rate theory fails to account for the fluctuations in point defect concentrations, since the theory is formulated for the average behavior of defects. In some non-linear material phenomena, such as irradiation creep and defect nucleation, it is expected that rate theory gives less accurate results. Mansur, Coghlan and Brailsford [1] formulated a cascade diffusion theory for the description of point defect concentrations in irradiated solids. They represented defect cascades as points (δ-functions) in space and time. They also applied the theory to void growth [1] and irradiation creep [2]. Gurol and Wolfer [3] also used the same approach in a Fokker–Planck formulation of the climb-glide creep model to analyze the effects of fluctuations in defect concentrations on irradiation creep. By essentially using the point model, Marwick [4] allowed the cascades to diffuse initially to a radius of 30 Å before starting long range diffusion of the cascade contents. He was able to analytically describe the root mean square (RMS) value of the fluctuation in point defect concentration at different damage rates. Also, he evaluated the temperature dependence of defect fluctuations. It is noted that the radius selected in his treatment is much smaller than the size of high energy cascades and the inter-sink distance (absorption mean free path) which is on the order of 1000 Å for his case. Also, he pointed out that other fluctuation contributions should be considered, such as a spectrum of cascade sizes. Recently Mansur, Brailsford and Coghlan [5] have treated the effects of sink capture distributions, and the location of different sink types on the fluctuation problem.

In the present analysis, we will relax the assumption of point cascades represented as δ-functions and address the effects of cascade properties, such as size, PKA energy and number of defects, upon the fluctuations in point defect concentrations.

2. Theory

Diffusion of point defects in irradiated materials is governed by the space–time continuity equations. These equations have the form [6]

$$\mathrm{d}C_v/\mathrm{d}t = P(\boldsymbol{r}, t)_v - \alpha C_v C_i - \operatorname{div} \boldsymbol{J}_v, \tag{1}$$

and

$$\mathrm{d}C_i/\mathrm{d}t = P(\boldsymbol{r}, t)_i - \alpha C_v C_i - \operatorname{div} \boldsymbol{J}_i, \tag{2}$$

where subscripts v and i stand for vacancy and interstitial respectively. C is the point defect concentration, $\boldsymbol{J}$ denotes the point defect flux, and α is the point defect thermal mutual recombination coefficient. The production rate of point defects by irradiation in eqs. (1) and (2) is represented by a time–space function $P(\boldsymbol{r}, t)$ where $\boldsymbol{r}$ is the vector position of defect generation, and t is the time of defect generation.

Production of point defects is random both in space and time. However, for ion and neutron irradiation, this "randomness" is not complete, since ensembles of defects are produced in close spatial proximity. Moreover, the time interval for the generation of such ensembles of defects is extremely short, on the order of 10^{-11} s. This is typically 5–6 orders of magnitude shorter than the diffusion time of the fastest moving species (self interstitials). During this time interval, a major fraction of the point defects generated in ensembles is lost due to defect quenching within the cascade (instantaneous recombination). This effect can be separated from the thermal mutual recombination terms in eqs. (1) and (2) because of the time scale involved. Therefore, it is possible to separate point defect generation from their subsequent diffusion and interaction, if one is only interested in the behavior of the contents of one cascade. Needless to say, it is quite formidable to solve eqs. (1) and (2) for an arbitrary random source of point defects $P(\boldsymbol{r}, t)$. In order to obtain an analytic solution, simplifications in eqs. (1) and (2) are needed. In this regard the non-linear point defect mutual recombination term $\alpha C_i C_v$ is neglected in both equations. Furthermore, it is assumed that the point defect diffusion coefficient is space independent and that the flux divergence (div $\boldsymbol{J}$) is considered as an effective absorption rate. By the application of Fick's Law in an effective lossy medium, the flux divergence can be written as [1,6]:

$$\operatorname{div} \boldsymbol{J}_{v,i} = -D_{v,i}\nabla^2 C_{v,i} + D_{v,i} S_{v,i} C_{v,i}, \tag{3}$$

where $S_{v,i}$ are effective homogenized sink strengths (cm^{-2}), and $D_{v,i}$ are spatially independent diffusion coefficients (cm^2/s), for vacancies and interstitials, respectively.

Let the point defect source $P(\boldsymbol{r}, t)$ be a unit delta function $\delta(\boldsymbol{r} - \boldsymbol{r}_c, t' - t_c)$, where $\boldsymbol{r}_c$ and t_c are time and position of generation. The solution to eqs. (1) and (2) for $t' > t_c$ is Green's function $G(\boldsymbol{r} - \boldsymbol{r}_c, t' - t_c)$. This has the form

$$G(\boldsymbol{r} - \boldsymbol{r}_c, t' - t_c) = \exp[-DS(t' - t_c)] \times \exp\left[-(\boldsymbol{r} - \boldsymbol{r}_c)^2/4\pi D(t' - t_c)\right]^{3/2}, \tag{4}$$

where t' is the real time and $\boldsymbol{r}$ is the vector position to the point of observation.

Earlier attempts to describe point defect diffusion resulting from randomly produced cascades have treated cascades as points in space and time (δ-functions). In the work of Mansur et al. [1], the point defect concentration contributed by a cascade containing ν defects (a cascade strength of ν defects) for either interstitials or vacancies is given by

$$C(x, t) = \nu\, \mathrm{e}^{-DSt} \mathrm{e}^{-x^2/4Dt}/(4\pi Dt)^{3/2}, \tag{5}$$

where the notations $x = |\boldsymbol{r} - \boldsymbol{r}_c|$ and $t = t' - t_c$ are used. In eq. (4), t is the time elapsed after the generation of the cascade and x is the distance between the point of observation and the point of cascade generation. Marwick [4] allowed point cascades to diffuse for a time t_0 to an "effective" radius r_0, such that

$$t_0 = r_0^2/4D. \tag{6}$$

The cascade, therefore, has an initial Gaussian distribution of defects and the point defect concentration distribution is given by

$$C(x, t) = \nu\, \mathrm{e}^{-DSt} \mathrm{e}^{-x^2/4D(t+t_0)}/\left[4\pi D(t + t_0)\right]^{3/2}. \tag{7}$$

It is shown [3,4] that the relative RMS value of point defect fluctuation is quite large for both vacancies and interstitials. The point defect concentration fluctuations are analogous to noise analysis of electronic signals and can therefore be measured in a quantitative way by using the RMS value. This can be expressed as:

$$\mathrm{RMS} = (\sigma^2)^{1/2}, \tag{8a}$$

where σ^2 is the average of point defect concentration variance over a long time interval, t, at the point of interest. This has the form

$$\sigma^2 = \left[\int_0^t (C - \langle C\rangle)^2 \mathrm{d}t\right]\Big/ t = \left[\int_0^t C^2 \mathrm{d}t\right]\Big/ t - \langle C\rangle^2, \tag{8b}$$

and $\langle C\rangle$ is the average point defect concentration over the same time period. For a theoretical investigation of the concentration fluctuation, $\langle C\rangle$ is taken to be the theoretical point defect concentration in this analysis.

The relative RMS (RRMS) value is defined as

$$\mathrm{RRMS} = \sigma / \langle C \rangle. \tag{8c}$$

RRMS is a measure of the relative fluctuation of the point defect concentration. For vacancies under various irradiation conditions within typical temperature ranges, this value is 2–20; while for interstitials, it is around 10^4–2×10^5. It has also been discussed [2,3] that non-linear irradiation phenomena are very sensitive to this parameter. It is important, therefore, to assess the dependence of this value on cascade properties, such as cascade size, cascade strength (defect content) and PKA energy.

In order to take account of cascade size effects in the present analysis, we consider a cascade produced at time t_c and position $\boldsymbol{r}_c$ with an initial point defect distribution $P(\boldsymbol{r}_c, t_c)_{v,i}$ where v and i stand for vacancies and interstitials, respectively. The solution to eqs. (1) and (2) with defect source $P(\boldsymbol{r}_c, t_c)_{v,i}$ by using Green's function for $t' > t_c$ is given by

$$C_{v,i}(x, t) = \int_{V_c} G(x, t) P(\boldsymbol{r}_c, t_c)_{v,i} \mathrm{d}^3 \boldsymbol{r}_c. \tag{9}$$

The above integration is performed over the cascade volume V_c.

Experimental observations have concluded that depleted zones are mainly composed of vacancies, while the near outer cascade regions contain self-interstitials [8,9]. Therefore, vacancies and interstitials are assumed to separate into two distinct regions within the cascade volume, after initial instantaneous recombination. For further simplicity, we represent the vacancy cascade as a uniform distribution inside a sphere of radius r_s. The interstitial cascade is then represented as a uniform distribution inside a spherical shell of inner radius r_s and shell thickness Δr. Solution to eqs. (1) and (2) are then directly obtained by incorporation of eq. (4) into (9), with the appropriate form of $P(\boldsymbol{r}_c, t_c)$. For the vacancy cascade the concentration $C_v(x, t)$ is given by:

$$C_v(x, t) = \frac{3\nu\, \mathrm{e}^{-DSt}}{8\pi r_s^3} \left\{ \mathrm{erf}\left[\frac{x + r}{(4Dt)^{1/2}} \right] - \mathrm{erf}\left[\frac{x - r_s}{(4Dt)^{1/2}} \right] - \frac{4Dt}{x(\pi)^{1/2}} \times \left[\mathrm{e}^{-(x-r_s)^2/(4Dt)} - \mathrm{e}^{-(x+r_s)^2/(4Dt)} \right] \right\}, \tag{10}$$

where erf stands for error function, and the concentration contributed by an interstitial cascade is as follows:

$$C_i(x, t) = \frac{3\nu\, \mathrm{e}^{-DSt}}{8\pi \Delta r (r_s^2 + r_s \Delta r + \Delta r^2)} \left\{ \mathrm{erf}\left[\frac{x + r_s + \Delta r}{(4Dt)^{1/2}} \right] - \mathrm{erf}\left[\frac{x - r_s - \Delta r}{(4Dt)^{1/2}} \right] + \mathrm{erf}\left[\frac{x + r_s}{(4Dt)^{1/2}} \right] - \mathrm{erf}\left[\frac{x - r_s}{(4Dt)^{1/2}} \right] - \frac{4Dt}{x(\pi)^{1/2}} \left[\mathrm{e}^{-(x-r_s-\Delta r)^2/(4Dt)} - \mathrm{e}^{-(x+r_s+\Delta r)^2/(4Dt)} + \mathrm{e}^{-(x-r_s)^2/(4Dt)} - \mathrm{e}^{-(x+r_s)^2/(4Dt)} \right] \right\}. \tag{11}$$

The relationship between the PKA energy, cascade size and cascade strength are obtained from the code TRIPOS developed by Chou and Ghoniem [7] for the *TR*ansport of *I*ons in *PO*lyatomic *S*olids. The code uses the Monte Carlo method to simulate ion transport in amorphous polyatomic media, composed of multilayers. It is worth mentioning that a quenching survival efficiency (fraction) for instantaneous recombination is needed to correlate the cascade defect contents resulting from TRIPOS calculations to the cascade defect contents which are left to diffuse and interact with microstructural features.

3. Monte Carlo analysis

For point defect concentration calculations Mansur et al. [1] found that it is sufficiently accurate to consider all the cascades generated within a unit cell sphere of radius r_u around the point of interest (observation). The unit cell radius r_u is defined to be seven absorption mean free paths for a point defect. An absorption mean free path l is given by

$$l = S^{-1/2}, \tag{12}$$

where S is the sink strength for point defect absorption, and

$$r_u = 7l. \tag{13}$$

In table 1 it is shown that the calculated point defect concentrations by taking all the δ-function model

Table 1
Dependence of relative concentration and relative variance on sampling volume for δ-function cascade model

Sampling volume radius in absorption mean free path	C/C_{th} from inside of sampling volume	C/C_{th} from outside of sampling volume	Relative concentration [a] contribution outside of sampling volume	Relative variance contribution outside of sampling volume
0	0.0	1.0	1.359	∞
1	0.2642	0.7358	1.0	1.0
3	0.8009	0.1991	0.2707	8.247×10^{-3}
7	0.9927	0.07295	0.09915	1.667×10^{-6}
10	0.9995	4.994×10^{-4}	6.787×10^{-4}	3.372×10^{-9}
20	1.0000	4.328×10^{-8}	5.883×10^{-8}	4.766×10^{-18}
30	1.0000	2.901×10^{-12}	3.943×10^{-12}	7.935×10^{-27}
50	1.0000	9.837×10^{-21}	1.337×10^{-20}	2.588×10^{-44}
∞	1.0000	0.0	0.0	0.0

C_{th} is theoretical concentration from rate theory.
[a] Relative concentration and variance contributions are normalized to the case when sampling volume has a radius of one absorption mean free path.

cascades generated within radii of 1, 3, 7, 10, 30, and ∞ absorption mean free paths are 26.42%, 80.09%, 99.27%, 99.95%, 100.0%, and 100.0% of theoretical point defect concentration, respectively. In other words, the concentration contributions from the δ-function cascades generated outside of radii 1, 3, 7, 10, 30, and ∞ absorption mean free paths are 0.7358, 0.1992, 0.07295, 2.901 $\times 10^{-12}$, and 0.0, respectively, of theoretical concentration. Therefore, for the purpose of reducing computation time in evaluating point defect concentrations, it is justified to consider all the cascades generated within a radius of r_u from the point of observation. However, this is only true for defect concentration calculations for the δ-function cascade model.

For defect concentration fluctuations, Marwick's formulation [4] suggests that the average fluctuation is divergent for δ-function cascades. The formulation by Gurol et al. [3] also supports the divergence of concentration fluctuation for δ-function cascades. We have analytically evaluated the relative variance for the δ-function representation of point cascades. Table 1 gives the relative variance contribution from outside the sampling volume as a function of the sampling volume radius. Also shown is the relative concentration contribution from outside of the sampling volume as a function of the sampling volume radius. The variance contributions are weighted heavily by cascades generated close to the point of interest as compared to the concentration contribution. Furthermore, the variance contribution goes to infinity for point cascades generated at the point of interest, if the observation time is the same as cascade generation time. The fluctuation singularity can not be practically shown by the Monte Carlo method, since an infinitely large sample has to be studied for events to be generated exactly at the point of observation. Therefore, the calculated fluctuation will always be finite as compared to the infinite fluctuation evaluated analytically. Fortunately, when cascades are produced, they have a finite volume. Cascades are not generated instantaneously in time nor produced infinitesimally small in size. Cascade generation time is around the order of PKA slowing down time and cascade size corresponds roughly to the PKA range. Also point defect mutual recombination can mitigate this problem.

A realistic model for cascades requires a non-zero cascade size and a non-zero generation time spread. An equivalent time spread, τ_{eq}, due to both cascade generation time spread and size can be defined as

$$\tau_{eq} = \tau_1 + \tau_2 = \tau_1 + R_2^2/6D, \tag{14}$$

and an equivalent cascade size, R_{eq}, due to both effects can be defined as

$$R_{eq}^2 = R_1^2 + R_2^2 = 6D\tau_1 + R_2^2, \tag{15}$$

where τ_1 is the generation time spread, R_1 is the radius associated with τ_1, R_2 is the generation size, and τ_2 is time spread associated with R_2. In Marwick's work [4], diffusional spreading is assumed to dominate the determination of cascade size, as in eqs. (14) and (15). In the present work, the initial concentration of point defects within the cascade is not assumed to be determined by diffusional spreading, but rather by collisional events. We therefore can study the effects of the initial damage structure within the cascade on point defect fluctuations.

For spherical cascades with radii r_s there is a chance that cascades can be generated between radii r_u and $r_u + r_s$ from the observation point. Those cascades physically overlap with the unit cell. Therefore, they have to be considered in order to obtain the same degree of accuracy for the analysis. In other words, the actual sampling volume has a radius of $r_s + r_u$ for the case of spherical cascades. The position of generation for any defect cascade which can contribute to the point defect concentration at the point of observation is given as follows:

$$x = (7l + r_s)\xi^{1/3}, \tag{16}$$

where ξ is generated random number with value between 0 and 1. And r_s is the cascade radius.

The time of generation is determined by using a Poisson's distribution, which has the form

$$P(N, R) = e^{-R}R^N/N!, \tag{17}$$

where R is the average number of cascades generated per unit time within a sphere of radius r_u. N is the actual number of cascades generated within a given unit time. Let us define a cumulative distribution function $P_c(n)$ as

$$P_c(n) = \sum_{N=0}^{n} P(N, R). \tag{18}$$

First, a random number ξ_1 is generated. Then it is compared to $P_c(n)$. If $P_c(n) < \xi_1 < P_c(n+1)$, it is assumed that n cascades are generated in the time interval of interest. Then a series of n random numbers are generated in order to distribute cascades randomly within the time interval.

For the cases of very large cascades, a homogeneous distribution of defects within the cascade, as used here, may not be an adequate representation. Heinisch [10] has investigated the formation of lobes and subcascades within a large cascade by using Monte Carlo simulations. It is shown that high energy cascades have tree-like structures for point defect distribution. We will approximate such structures by considering two specific cases; a tree subcascade model and a uniform subcascade model. For the tree subcascade model we assume that all subcascades are generated along a given vector whose length is the diameter of the large cascade. For the uniform subcascade model, on the other hand, we assume that all subcascades are generated randomly within the volume of the large cascade. Fig. 1a is a schematic representation of the homogeneous subcascade model, while fig. 1b illustrates the tree subcascade model. Both models do not exactly duplicate the cascade structures produced by Monte Carlo simulations. Nevertheless, the two models bound the extremes of actual defect generation distributions; namely, highly anisotropic and homogeneous. Therefore, we expect the results for defect concentration fluctuations of subcascade structures to lie in between these two extreme cases.

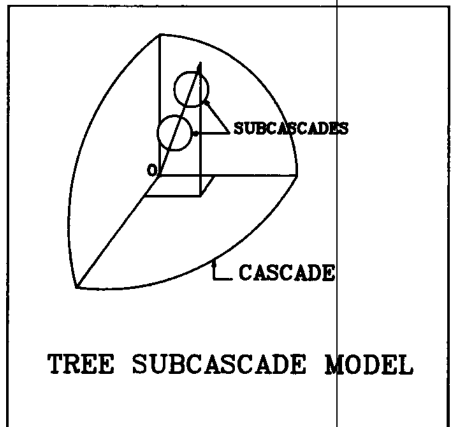

Fig. 1a. Schematic for tree subcascade within a high energy cascade.

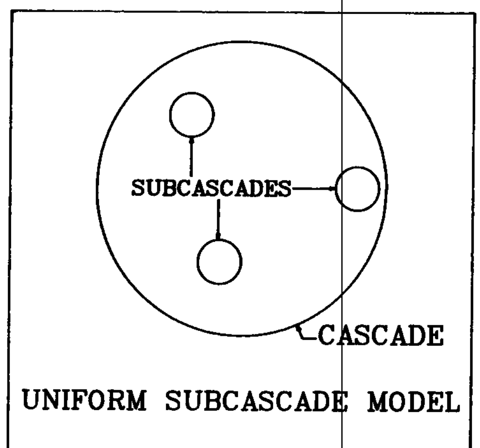

Fig. 1b. Schematic for uniform subcascade within a high energy cascade.

4. Results

In this analysis, the following parameters for either nickel or stainless steel are used [1,2]: $D_0^v = 0.014$ cm^2/s, $E_m^v = 1.4$ eV, $S_v = 10^{11}$ cm/cm^3, $D_0^i = 0.008$ cm^2/s, $E_m^i = 0.15$ eV and $S_i = 1.1 \times 10^{11}$ cm/cm^3. The defect generation rate is 10^{-6} dpa/s and the temperature is 500°C.

The cascade rate used corresponds to a unit cell of a radius r_u, as defined earlier. As we discussed in the previous section, it is found that the δ-function cascade model is not valid for concentration fluctuation analysis based on the RMS value. We therefore assume that the size of the point model cascade corresponds to a radius of 50 Å.

Generally, it is observed that larger cascades result in less fluctuations in vacancy concentration as compared to point cascades. A statistical sampling on the order of a few thousand cascades is needed for vacancy cascades before agreement between rate theory and cascade diffusion theory is achieved. On the other hand, it is found that a smaller sample size of interstitial cascades is needed before rate theory and cascade diffusion theory reach agreement.

We will first discuss the results of analysis for a homogeneous distribution of defects within the cascade volume. Then, we will show the implications of sub-cascade formation. Fig. 2 shows the relative RMS value as a function of vacancy cascade radius. It is shown for large cascade sizes, the relative RMS value is small, and rate theory is expected to be a good approximation for vacancies. In fig. 3, the relative RMS value is shown as a function of the interstitial inner radius. The behavior for interstitial cascades is comparable to that of vacancy cascades with the exception that the value of the relative RMS value is four orders of magnitude higher than that for vacancy cascades. The interstitial cascade shell thickness, Δr, is assumed to be 15 Å.

In the preceeding analysis, a cascade strength of 100 defects is used. However, larger size cascades generally contain more point defects. Under a constant damage

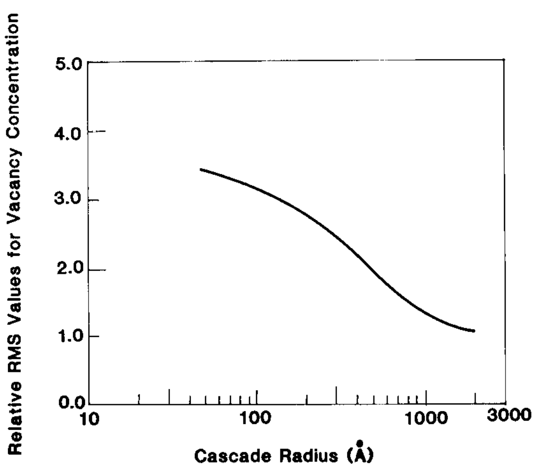

Fig. 2. Relative RMS value for vacancy concentration as a function of vacancy cascade radius.

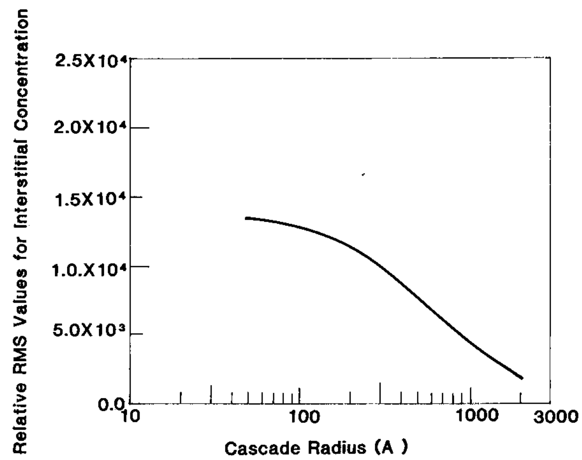

Fig. 3. Relative RMS value for interstitial concentration as a function of interstitual cascade inner radius.

rate, the arrival rate of larger size cascades will be lower. This increases the fluctuation in defect concentrations due to the lower frequency of occurance. In order to make a more realistic picture of the effects of cascades on fluctuations, an investigation of the effects of PKA energy, cascade size and cascade strength on fluctuations is necessary. For this purpose, PKA transport analysis using the TRIPOS code [6] is performed. Fig. 4 shows the average diameter of cascades generated as a function of PKA energy using the TRIPOS code. Fig. 5 shows cascade quenching survival efficiency (fraction) as a function of PKA energy, as determined by Heinisch [11]. The cascade strength is obtained by multiplying the number of freshly produced defects in each cascade by the quenching survival efficiency. The relationship between the cascade strength and cascade radius is finally shown in fig. 6. Fig. 7 shows the vacancy relative RMS value for both point cascades with radii fixed at 50 Å and spherical cascades as functions of the "actual" cascade radius. It shows that for a larger cascade radius and higher cascade strength, point cascade model tends to overestimate the magnitude of fluctuations in vacancy concentration. On the other hand, the spherical cascade model predicts that the fluctuations increase first, then level off, and eventually decrease as a function of the cascades size and cascade strength. This can be explained by the fact that a larger cascade size inherently causes less fluctuation due to the assumption that defects are homogeneously distributed within the cascade spherical volume. This effect dominates the increases in fluctuations due to the lower arrival frequency of large size cascades. Fig. 8 shows the interstitial relative RMS value for both point cascades with radii of 50 Å and

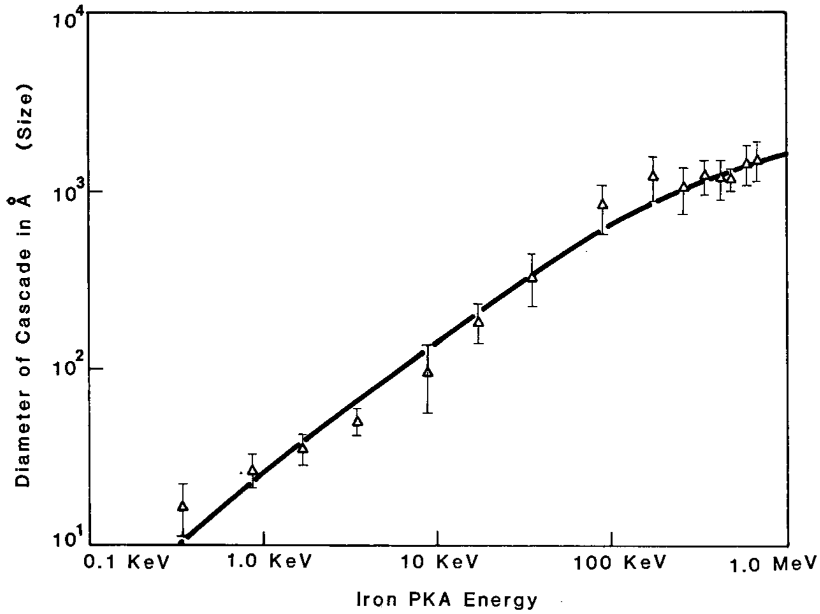

Fig. 4. Average cascade diameter (cascade size) as a function of PKA energy from TRIPOS simulation.

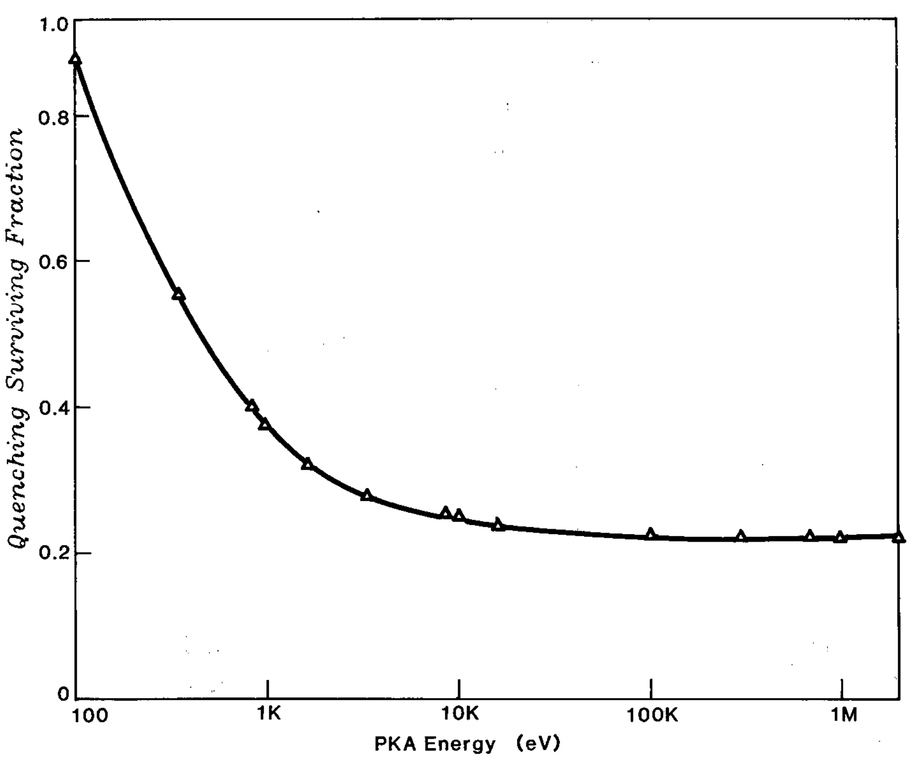

Fig. 5. Cascade quenching survival fraction (efficiency) as a function of PKA energy.

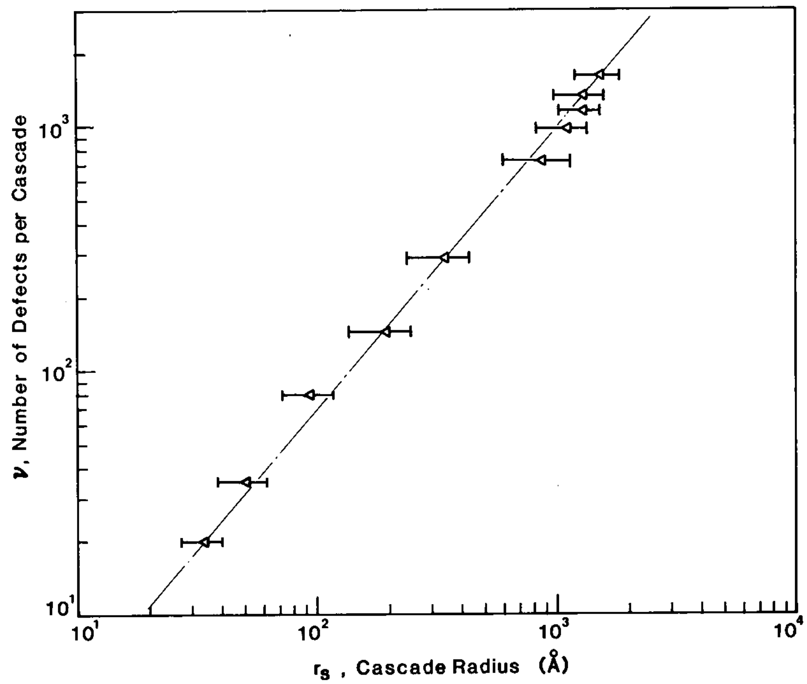

Fig. 6. Cascade strength (defects/cascade) as a function of cascade radius.

spherical cascades as function of the cascade radius. Interstitial cascades show the same behavior as vacancy cascades, with the relative RMS value for interstitial cascades being about four orders of magnitude larger than that for vacancy cascades. However, it can be easily observed from figs. 7 and 8 that the results from the point cascade model with a radius of 50 Å give an agreement within a factor of 4 with those from the

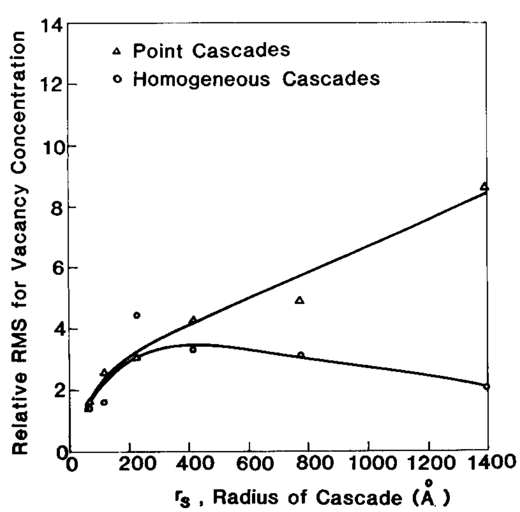

Fig. 7. Vacancy relative RMS values for both point cascades with radii fixed at 50 Å and homogeneous spherical cascades as functions of "actual" cascade radius.

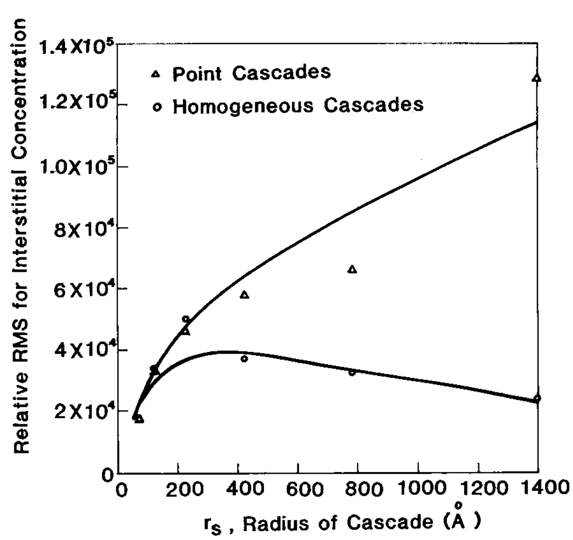

Fig. 8. Interstitial relative RMS values for both 50 Å point cascades and homogeneous spherical cascades as functions of "actual" cascade radius.

homogeneous cascade model. One point of caution is that the point cascade model results are very sensitive to the selection of the cascade radius. For instance, by taking a radius of zero, the results from the point cascade model diverge.

The decrease in the magnitude of fluctuation for larger-size cascades is in part due to the increase in the chances for large cascades to overlap with the point of observation in the homogenous model. In order to take account of this effect, simulations are performed for larger cascades breaking up into several subcascades. Such subcascades are considered to have an initially uniform point distribution. The number of subcascades within each high energy cascade can be approximated by using results from copper cascade computer simulation by Heinisch [10]. The relationship between the average number of subcascades per cascade and PKA energy is approximately linear from Heinisch's calculations. Since it is not possible to simulate a fraction of a subcascade by using the analog Monte Carlo method, we truncate the non-integer part of the number of subcascades in a cascade in this analysis. We further assume that the cascade energy is distributed equally among its subcascades and those subcascades have sizes corresponding to their energies. We can fit the figure of the number of subcascades per cascade from Heinisch's work by the following formula

$$N_{sub} = \text{Integer}[1 + E(\text{keV})/125.0], \quad (19)$$

where N_{sub} is the number of subcascades per cascade and E is the cascade energy content. Fig. 9 shows the dependence of the relative RMS on cascade size for the following cases: (1) Point Cascade Model, where the cascade radius is fixed at 20 Å; (2) Homogeneous Cascade Model, where point defects are initially homogeneous within the cascade spherical volume; (3) Uniform Subcascade Model, where subcascades are randomly distributed within the cascade sphere; (4) Tree Subcascade Model, where subcascades are produced along the diameter of the cascade sphere. It can be easily observed that results from the linear and homogeneous subcascade models fall between those of the point and homogeneous cascade models. Point defect concentration fluctuation for subcascade models increase first for smaller cascade size, then level off and remain relatively constant as the cascade size increases.

The leveling off can be further attributed to the fact that the fluctuation reduction due to the high spatial incoherence for subcascade generation is offset by an increase in fluctuation due to a high time coherence for subcascade generation.

An important question arises in conjunction with the analysis of pulsed or transient irradiation; and that is, how is point defect concentration influenced by fluctuations in this case? A number of Monte Carlo computer runs were performed for an irradiation pulse with an on-time of 10 s. In fig. 10, the Monte Carlo results are represented by the vertical bars to indicate the statistics due to cascades, while the solid line is the average rate theory solution. It is interesting to note that while the magnitude of fluctuation is significant during the on-time, it is less so during the off-time. This is primarily due to diffusional spreading of cascades retained during the on-time. It is therefore suggested that whenever the on-time is less than the average time between cascades (inter-cascade time), transient fluctuations may play an

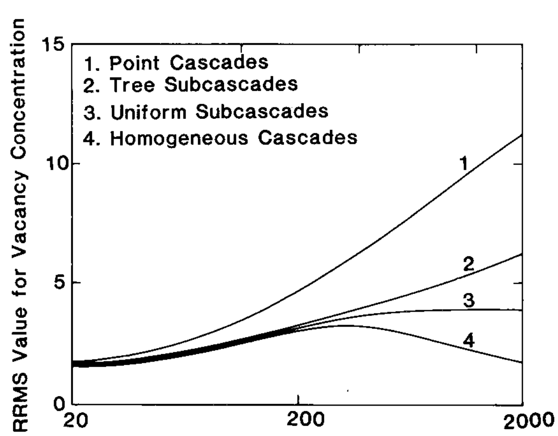

Fig. 9. Vacancy relative RMS values for 20 Å point cascades, tree subcascades, homogeneous subcascades are and homogeneous spherical cascades as function of cascade strength.

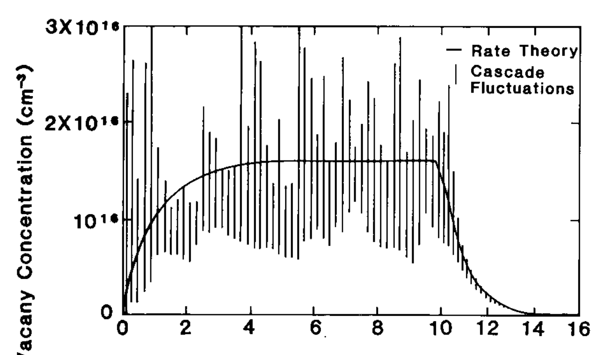

Fig. 10. Transient vacancy relative RMS value as a function of time for pulsed irradiation which is turned on at $t = 0.0$ and turned off at $t = 10.0$ s.

important role. Also, for off-times greater than several intercascade diffusion times, the role of fluctuations is diminished.

5. Conclusions

It is concluded here that the δ-function cascade model is only accurate for the analysis of point defect concentrations. For the evaluation of point defect concentration fluctuations, time singularities cause the fluctuation magnitude to become infinite. Therefore, a cascade with a non-zero equivalent size as defined by eq. (14) is required for this type of calculation, as was suggested by Marwick [4].

However, our results show that fluctuations in point defect concentrations are sharply reduced as compared to the point cascade model if the cascade size effect is taken into account. For larger size cascades, the spherical cascade model predicts a lower magnitude of fluctuation in point defect concentration. However, for cases where the damage rate is fixed and cascade strength and size are increasing, the decrease in point defect concentration fluctuations is partly due to an increase in the probability of cascade overlap with the point of observation and partly due to the homogeneous distribution of point defects within the cascade. Tree-like point defect distributions in large cascades can be approximated either by a linear subcascade model or by a homogeneous subcascade model. These two models depict extreme configurations observed in Monte Carlo simulations of defect structures in large cascades. Defect concentration fluctuations based on these two subcascade models fall in between those based on the point and homogeneous cascade models. For the same conditions, the point defect model gives a sharp increase in the magnitude of the defect concentration fluctuation, while the homogeneous cascade model actually predicts a decrease in the magnitude of this fluctuation. The actual concentration fluctuation behavior is expected to fall in between the results from the two subcascade models. For an anticipated fusion reactor neutron spectrum, cascades tend to have sizes that correspond to defect concentration fluctuations around the plateau region for the subcascade models.

A major conclusion of the present work is that cascade size and shape have important effects on point defect fluctuations. The work indicates that a more realistic representation of cascades will tend to reduce the magnitude of the fluctuation by a factor of 2–4 at high PKA energies.

A number of effects which can potentially contribute to the magnitude of fluctuations are undoubtedly left out. For instance, thermal recombination of vacancies and interstitials, distributions of cascade size and strength in a real irradiation environment, the heterogeneous distribution of local sink strength, and the local variation in point defect diffusion coefficients have to be considered. The present work indicates that there is a natural limit to the magnitude of concentration fluctuations, and that rate theory may be adequate for treating vacancies. It appears, though, that the great mobility of interstitials leads to a large degree of coherence and hence substantial fluctuations. Interstitial loop nucleation may be particularly sensitive to this behavior.

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