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Monte Carlo modelling of damage accumulation in metals under cascade irradiation

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Abstract

The Monte Carlo (MC) method is used to study cascade damage effects in damage accumulation in pure metals at temperatures below stage III, when vacancies and their clusters are immobile. The irradiation is modelled by sequential introduction of collections of defects representing the primary damage state of cascades placed randomly in the simulation volume. The cascades generated in molecular dynamics (MD) simulations for recoil energies from 2 to 10 keV are used. Concentrations of point defects as well as defect cluster densities are monitored as a function of dose up to 0.02 dpa. The results are compared with those obtained in the mean-field (MF) approximation. Factors responsible for the difference in damage accumulation under homogeneous and cascade irradiation conditions are revealed. Problems in using MC modelling to study damage accumulation when interstitial clusters move one-dimensionally are investigated and discussed.

1. Introduction

Point defect clusters formed during the cooling-down stage of cascades play an important role in damage accumulation in metals under neutron or heavy-ion irradiation. The mean-field (MF) approach is often used for the description of microstructure evolution [1]. This approach accounts for only part of the fluctuations that take place under cascade damage conditions, however, and does not include fluctuations in defect production in space and time associated with cascades. Earlier investigations of these effects have been performed for three-dimensional diffusing defects and have mainly used analytical methods (see review [2]). For typical cascade production conditions the standard deviations in the point defect concentrations were found to be comparable to or even larger than their mean values. No indication of any significant effects on void growth was found, however. Some effects of the fluctuations were found in the nucleation of the defect clusters. More extensive study of these and similar effects requires methods going beyond the MF approach and this accounts for the growing interest in applying the Monte Carlo (MC) method, which in some cases is less restrictive than analytical methods.

Recent work provides convincing evidence of the significant role clusters of self-interstitial atoms (SIAs) play in damage accumulation in metals under cascade irradiation conditions [1,3–6]. Molecular dynamics (MD) simulations show that SIA clusters undergo preferentially one-dimensional motion [7–10], but in the investigations of the effects of fluctuations in the defect accumulation reviewed in [2] this fact has not been taken into account. The kinetics of one-dimensional migrating defects exhibit some distinguishing features as compared with that for three-dimensional diffusion [1,3–6]. For this reason, we will pay particular attention in the present paper to SIA clusters and their contribution to the damage accumulation. Since little experience has been gained so far in studying one-dimensional migrating defects by MC, this work is partly concerned with methodological aspects of the problem.

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The main objectives of the present work are: (1) to study the effects in damage accumulation of fluctuations in defect generation associated with cascade irradiation and (2) to investigate the suitability of MC simulations for studying damage accumulation.

2. Calculations

We have used the MC method to study cascade damage effects in metals at temperatures below stage III, when vacancies and their clusters are immobile. We define the cascade effects as those resulting in deviation of the defect densities from predictions made in the framework of the MF approximation, which assumes homogeneous generation of the defects. To reveal these effects, the calculations were performed for two conditions, namely those for cascade irradiation and those appropriate to the MF approximation.

2.1. Cascade irradiation conditions

In this case the actual spatial positions of the defects as they appear in cascades were taken into account. The cascades generated in MD simulations for recoil energies from 2 to 10 keV in α-Fe [11] were used. The irradiation was modelled by sequential introduction of collections of defects representing the primary damage state of cascades placed randomly in the simulation volume with a time interval corresponding to the dose rate 0.003 dpa/s (NRT-standard). To reveal the effect of recoil energy, one cascade of a given PKA energy was used repeatedly in each calculation. The concentration of the point defects and the defect cluster densities were monitored as a function of dose up to 0.02 dpa.

2.2. MF conditions

Analysis of the damage accumulation in the framework of the MF approach assumes homogeneous production of the point defects and their clusters over the volume. In order to simulate the MF conditions in this paper, the MC calculations were performed for homogeneous generation of the point defects and clusters which survive 'short-term annealing' of cascades [12]. The purpose of this annealing calculation is to account for the correlation in the positions of the defects as they appear in cascades, which results in enhanced reaction rates between point defects and their clusters in the near cascade region, as compared with that calculated for homogeneous production of the defects. The resulting distribution of the surviving defects is more appropriate for use as input in subsequent calculations for homogeneous production of the defects. The application of the short-term annealing is suitable if the characteristic time of this process is much less than the mean time between the appearance of cascade in the simulation box. This condition is satisfied in this paper. Two sets of calculations were performed, one for temperature below stage I and the other one for temperature above stage I but less than stage III. In the former case, all defects are assumed to be immobile and hence no annealing of the cascades is required. In the latter case, the short-term annealing was performed for individual cascades for the time it takes all the mobile defects to escape from the simulation box. This was repeated for over 100 different runs for each cascade energy. The results were then averaged to give the distributions of defects used in the homogeneous generation modelling.

All the results on the concentration of the defects are plotted against the NRT dose to make the results obtained by different approaches comparable to each other. The calculation of the NRT dose has been performed using data on cascade efficiency (surviving fraction of the defects) from [13], that is an efficiency of 0.5 for $E_{PKA} = 2$ keV and 0.3 for $E_{PKA} = 10$ keV.

2.3. MC algorithm and boundary conditions

A computer code was written with an algorithm similar to that of the ALSOME code [12]. As a test, the results of the two codes were compared for some simulations. The simulation box was taken as a cube of edge equal to 150 lattice parameters. Boundary conditions of two different kinds, either periodic (PBC) or pseudo-PBC, were applied. In the pseudo-PBC a defect crossing a boundary appears at a random position on the other side of the simulation box [12,14]. Both types of boundary condition have advantages and disadvantages for simulations of this sort. The PBC introduces periodicity into the spatial positions of the defects in the system, which influences their evolution. Use of the pseudo-PBC eliminates this periodicity and is appropriate for three-dimensional diffusing defects in the system, since their mean-free path is on the order of the distance between nearest sinks (less than several tens of nm) and an appropriate size of the simulation box is achievable. The mean-free path of *one-dimensional* diffusing defects can be several μm, however, and this leads to important consequences in damage accumulation [1,3–6]. It will be demonstrated here that the use of the pseudo-PBC with a simulation box which is small in comparison with the mean-free path of the clusters destroys the one-dimensional character of cluster motion.

2.4. Model

In the calculations performed for the temperature above annealing stage I, SIAs were assumed to undergo three-dimensional random walk. The input parameters for the MC calculations are listed in Table 1. The SIA

Table 1
Input parameters for the Monte Carlo calculations (a is the lattice parameter)

Parameter	Value	Comments and Ref.
Simulation box	Cube of edge of $150a$	
Dose rate	0.003 dpa/s	NRT-standard
Cascade efficiency		
$E_{PKA} = 2$ keV	0.5	For MF irradiation
$E_{PKA} = 10$ keV	0.3	conditions [13]
Defect mobility		
Point defects		
vacancy	Immobile	
SIA	3-D[a], $\nu_{SIA} = 10^7$ s^{-1}	For $T >$ annealing stage I
Clusters		
$\leqslant 10$ SIAs	1-D[a], $\nu_{clus} = 10^7$ s^{-1}	
>10 SIAs	Sessile	
Reaction distances, d^* (see Eq. (1))		For iron, [15]
Vacancy–vacancy	0	
SIA–vacancy	$0.7a$	
SIA–SIA	$1.4a$	

[a] 3(1)-D – three (one)-dimensional random walk along $\langle 1\,1\,1\rangle$ direction with jump frequency ν.

clusters were considered to have one of two configurations, namely glissile (mobile) and sessile (immobile), both in the form of dislocation loops with Burgers vector $b = 1/2\langle 1\,1\,1\rangle$. The mobile SIA clusters were assumed to migrate one-dimensionally along the $\langle 1\,1\,1\rangle$ crowdion direction, as observed in MD simulations for α-Fe [7–10]. Clusters of less than 11 SIAs were considered to be mobile and, since MD modelling has shown a weak dependence of cluster mobility on cluster size [7], the jump frequency of all mobile clusters was assumed to be equal to that of the single SIA. Clusters of more than 10 SIAs were assumed to be immobile.

Interaction between defects was assumed to be spherically isotropic and attractive for defects with separation d less than some critical value d^*:

$$d = R_{12} - r_1 - r_2 < d^*, \tag{1}$$

where r_1 and r_2 are the radii of the defects and R_{12} is the distance between their centres of gravity. For a loop $r = (N\Omega/\pi b)^{1/2}$, where N is the number of point defects, $\Omega = a^3/2$ is the atomic volume and a is the lattice parameter. The critical distances d^* for the different types of interaction are given in Table 1. They were found to be the best-fit values to the measurements of the resistivity recovery of the electron irradiated iron [15].

We do not ascribe this model to any particular metal except that the direction of motion of the glissile SIA clusters is appropriate for the bcc crystallography. However, it includes the main features of damage accumulation usually used in theoretical models [1,3–6].

3. Results

3.1. Temperature below stage I

In this regime, all the defects are immobile. The results obtained for $E_{PKA} = 10$ keV are shown in Fig. 1. For simplicity, only data for concentrations of single

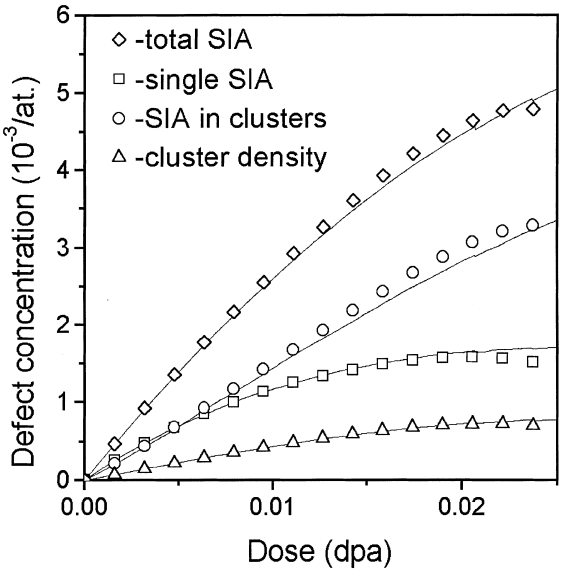

Fig. 1. Dose dependence of the defect concentration accumulated in different forms under irradiation with cascades of $E_{PKA} = 10$ keV (□) at a temperature below stage I, for which all defects are immobile, in comparison with that in the MF approach (–).

and clustered interstitials are presented. The majority of vacancies accumulated in the form of single defects. As can be seen, in this temperature regime the defect accumulation calculated in the MF approach is nearly the same as that under cascade irradiation conditions. Similar agreement was observed for the vacancy concentration and for recoil energies of 2, 5, and 20 keV (data not presented here).

3.2. Temperature above stage I but less than stage III

In this case, vacancies and their clusters are immobile and SIAs and some of their clusters are mobile. In this case the SIAs accumulate in clusters, while the majority of vacancies are in the form of single defects. The data on population of defects used as input for the MC calculations for either cascade conditions or MF conditions, i.e., after short-term annealing of the cascades, are collected in Table 2. As seen from the table, we use the simplest model for the distribution function of the defects after the short-term annealing of the cascade, namely, we distinguish sessile and glissile clusters according to their size and characterise each of them by the mean size and mean number of clusters averaged over all the anneals. Note that no sessile clusters are formed by short-term annealing for $E_{\mathrm{PKA}} = 2$ keV, and none are formed in the primary damage state obtained in MD modelling.

It should be noted that for the size of simulation box used ($150a$) the minimum irradiation dose (due to one cascade) is 2×10^{-6} for 2 keV and 6×10^{-6} dpa for 10 keV. The concentration of clusters created by these doses is very high. So, using the data from the Table 2 one can estimate that for $E_{\mathrm{PKA}} = 10$ keV the minimum cluster concentration C is 9×10^{-7} at.$^{-1}$ or 6.6×10^{22} m^{-3}. This is a limitation of the MC method in modelling damage accumulation.

The calculations have shown that the results obtained are not sensitive to the sink strength of the defects preexisting in the matrix before irradiation, because the defects created by irradiation quickly become the dominant sinks in the system. Some calculations performed for a sink strength of 10^{14} m^{-2} support this conclusion. In addition, in the temperature range considered the jump frequency of SIAs and their clusters is not an important parameter because, at high concentration of the defects, the absorption of a defect at a sink occurs very quickly, well before the next cascade event. An increase in the size of the simulation box provides a solution to this problem (of decreasing the minimum irradiation dose), but results in an increase in the computation time. We discuss this problem further below.

$E_{PKA} = 2\ keV$: Figs. 2(a) and (b) show the results obtained for the SIA cluster density and the total number of defects accumulated, respectively, for $E_{\mathrm{PKA}} = 2$ keV. The results were obtained using the pseudo-PBC. As can be seen, there is little difference between accumulation kinetics under cascade irradiation conditions and those of the MF approach. In both cases the concentration of SIA clusters reaches the same steady-state value for the same dose, while the total concentration of defects accumulated steadily increases with dose. We attribute some of the difference observed in the defect accumulation to the coarseness of the model used for description of the defects remaining after short-term annealing of the cascades.

$E_{PKA} = 10\ keV$: Figs. 3(a) and (b) present the results obtained for the SIA cluster density and the total number of defects accumulated, respectively, for

Table 2
Cascade defects before and after 'short-term annealing' (notation: N_{v} – number of vacancies; N_{I} – number of SIAs; N_{Cl} – number of SIA-clusters; x – number of SIAs in a cluster)

E_{PKA} (keV)	N_{v}	N_{I}	N_{Cl}	$\langle x \rangle$	SIA-clusters: size (number)	
Cascade defects after thermal spike						
2	14	6	3	2.67	4(1), 2(2)	
5	27	14	4	3.25	6(1), 3(1), 2(2)	
10	40	23	6	2.83	4(2), 3(1), 2(3)	
20	66	38	11	2.55	5(1), 3(3), 2(6)	
E_{PKA} (keV)	N_{v}	N_{I}	Glissile ($x \leqslant 10$)		Sessile ($x > 10$)	
			N_{Cl}	$\langle x \rangle$	N_{Cl}	$\langle x \rangle$
Cascade defects after short-term annealing						
2	8.37	0.95	1.99	3.73	–	–
5	13.17	1.54	3.42	3.40	–	–
10	26.06	3.16	4.79	3.87	0.35	12.46
20	40.93	3.76	7.06	4.04	0.68	12.72

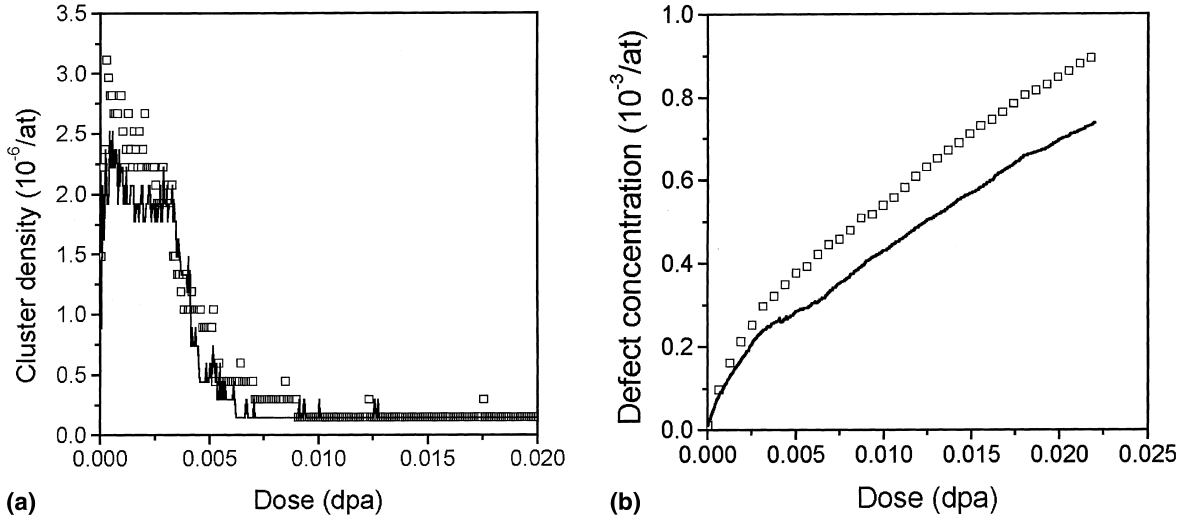

Fig. 2. Dose dependence of (a) SIA cluster density and (b) the total SIAs accumulated in clusters under irradiation with cascades of $E_{PKA} = 2$ keV (□) at a temperature above stage I but less than stage III, in comparison with that in the MF approach (–).

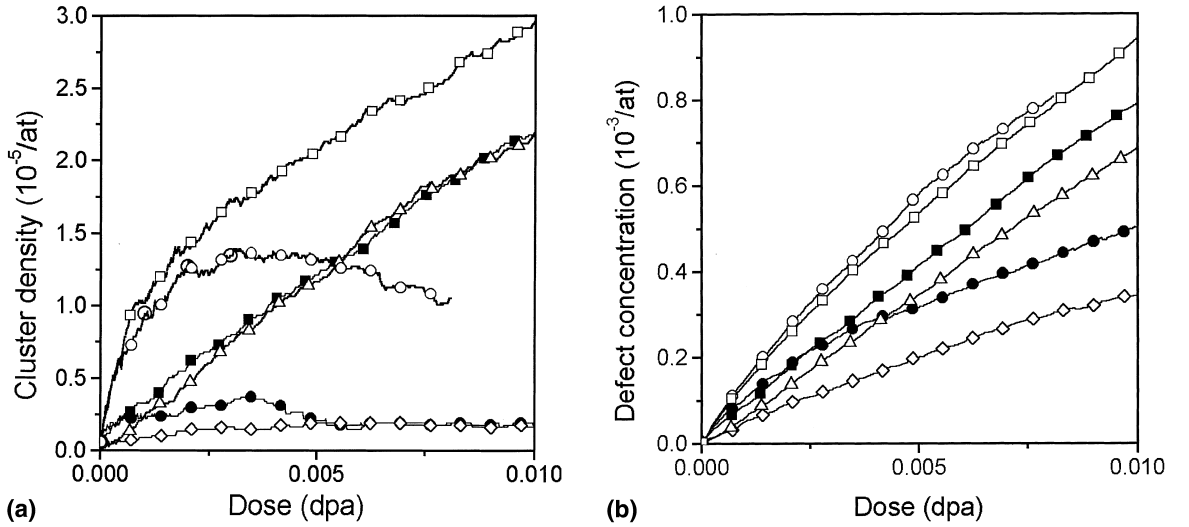

Fig. 3. Dose dependence of (a) the SIA-cluster density and (b) the concentration of SIAs accumulated in clusters under irradiation with cascades of $E_{PKA} = 10$ keV at a temperature above stage I but less than stage III, in comparison with the results of the MF approach. ●: cascade irradiation conditions (pseudo-PBC); ■: the MF approach (pseudo-PBC); ○ and □: same calculations for the PBC; ◇ and △: same calculations assuming three-dimensional migration of clusters (PBC).

$E_{PKA} = 10$ keV. Three different calculations are presented: (1) for the cascade irradiation (●) and for the MF approach (■) obtained using the pseudo-PBC; (2) the same as (1) but for the PBC (○ and □); and (3) for cascade conditions with the PBC assuming three-dimensional migration of clusters (◇ and △). As can be seen, significant difference exists between the kinetics of defect accumulation under cascade irradiation and in the MF approach when the pseudo-PBC is used. The main difference is in the concentration of SIA clusters (Fig. 3(a)), for over the dose range studied this function reaches steady state under cascade irradiation conditions, whereas it keeps increasing in the MF approximation.

The results obtained by the two different approaches agree with each other below 10^{-3} dpa, but above this, the difference in concentration of SIA clusters steadily increases. By this dose the concentrations of the clusters are high and the difference observed arises in the following way. In the case of cascade irradiation, a

mobile cluster has a higher probability of being captured by a pre-existing cluster than interacting with another cluster originating from the same cascade and forming a new sessile cluster. This explains the steady-state SIA cluster concentration reached in this case. In the MF approach, this process is not taken into account, since the prior short-term annealing of the cascades is performed for an otherwise perfect matrix. In this case the sessile clusters are generated directly by the irradiation and, as a result, the concentration of the clusters is proportional to the probability of their appearance in the volume, as observed in the figure. This effect does not occur at $E_{PKA} = 2$ keV due to the absence of sessile clusters after annealing of the cascade (see Table 2).

Note that for cascade irradiation conditions, the steady-state SIA cluster concentration is the same as that for three-dimensional diffusing clusters (cf. ● and ◇). For homogeneous defect generation, this agreement is observed over the whole dose range studied (cf. ■ and △). This indicates that in both cases the pseudo-PBC destroys the one-dimensional character of SIA cluster motion.

Calculations for the PBC (○ and □) show behaviour qualitatively similar to that for pseudo-PBC. For approximately the same dose range ($<10^{-3}$ dpa) the results for the cascade irradiation and MF conditions are close to those for homogeneous generation of the defects, but above this, the difference in concentration of SIA clusters steadily increases. By comparing the results obtained with different boundary conditions, it can be concluded that they are strongly sensitive to the boundary conditions applied.

Thus, the results show the existence of the effects due to fluctuations in damage accumulation when the concentration of the defects is high. In this case, the MF approach does not work well since it uses as input the results of the short-term annealing of cascades performed for a perfect matrix, and hence does not include the interaction of the cascade components with the pre-existing defects in the matrix. No firm conclusions can be made on the magnitude of, and difference between, the effects studied, since the results strongly depend on the type of boundary conditions applied.

3.3. Effect of box size and boundary condition on the kinetics of defect accumulation

To elucidate the peculiarities of modelling the kinetics of one-dimensional diffusing objects in small boxes, additional calculations were performed for the simpler problem of point defect accumulation under irradiation generating Frenkel pairs with a production rate $K = 10^{-3}$ dpa/s. Vacancies and SIAs were introduced randomly into the simulation box. SIAs were assumed to be in the crowdion configuration and migrate one-dimensionally along ⟨1 1 1⟩ directions with a jump frequency $\nu_{SIA} = 10^5$ s^{-1}. (It should be noted that the ratio K/ν_{SIA} is the parameter which governs the accumulation kinetics.) Only annihilation reactions between SIAs and vacancies were taken into account. The recombination distance r was taken to be equal to $0.7a$.

Fig. 4 shows the dose dependence of the defect concentration obtained by applying either the PBC or the pseudo-PBC for boxes of different size. In addition, MF results for the case of three-dimensional migration of SIAs are presented as obtained either by MC (–) or analytically (----). For the latter, the concentration is simply

$$C = \sqrt{K/D_{SIA}\mu_R}, \tag{2}$$

where $D_{SIA} = \nu_{SIA}a^2/8$ is the diffusion coefficient for three-dimensional migrating SIAs in a bcc lattice and $\mu_R = 4\pi r/\Omega$ is the recombination constant.

As can be seen from the figure, results for the pseudo-PBC are close to those obtained for three-dimensional diffusing SIAs, indicating that this boundary condition destroys the one-dimensional character of SIA migration and leads to underestimation of the defect concentration. The steady-state concentration of the defects increases quite slowly with increasing box size.

For the PBC the dose required to reach the steady state is higher than for pseudo-PBC and the steady-state defect concentration decreases with increasing box size, which indicates overestimation of the defect concentration. This is due to the introduction of periodicity in the sink positions when applying the PBC. As a consequence, the mean-free path L_1 of the crowdions is

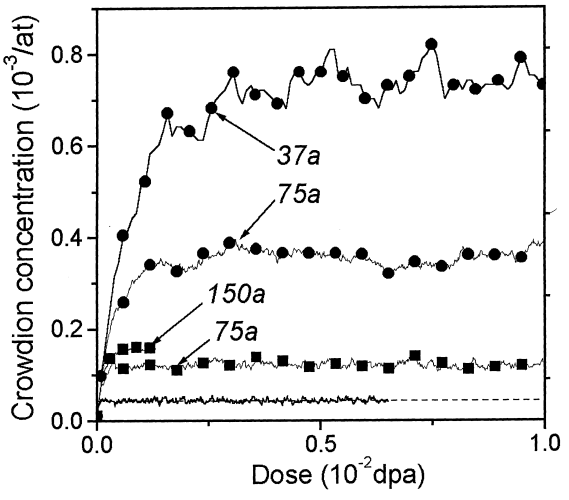

Fig. 4. Dose dependence of the point defect concentration in boxes of different size (shown by arrows), obtained by applying either the PBC (●) or the pseudo-PBC (■). The lower curves were obtained analytically (----) and by MC (–) in the MF approach for the case of three-dimensional migration of SIAs.

changed. In an infinite volume for random spatial distribution of spherical sinks,

$$L_1 \sim \Omega/\pi r^2 C_S, \tag{3}$$

where C_S is the sink concentration [3–6]. In the case considered here, vacancies are sinks for the SIAs. For the vacancy concentration of 4×10^{-4} (see results in Fig. 4 for the box size of $75a$ using the PBC), $L_1 \sim 800a$, which is much more than the box size. As a result, the trajectories of the majority of the crowdions do not intersect a vacancy. The lifetime of such a crowdion is determined by the mean time for a new defect to appear in its path due to irradiation, rather than by Eq. (3) which corresponds to the random walk of a defect between fixed sinks.

It should be noted that the problem arises only for one-dimensional diffusing defects. As seen from Fig. 4, for three-dimensional diffusing defects, the results obtained by the MC method and analytically in the framework of the MF approach are in agreement. This is because the mean-free path of the SIAs, which is equal to

$$L_3 \sim 1/\sqrt{4\pi r C_S/\Omega}, \tag{4}$$

is about $30a$ in this case and is smaller that the box size used.

One question that remains is what size of simulation box is required for proper simulation of the damage accumulation in relation with the mean-free path of the defects? An answer has been provided by Mansur et al. for three-dimensional migrating defects [16]. They found that the cascades appearing within a distance of $\sim 7L_3$ around a reference point contribute ~99% to the exact concentration of the defects at this point, whereas those within the distances $\sim 3L_3$ and $\sim L_3$ give ~80% and ~30% of the exact concentration, respectively. The mean-free path of the one-dimensional migrating defects is of order of 10 μm for typical irradiation conditions (see also estimates in [17]). Taking this into account, one can conclude that for proper simulation of the kinetics of one-dimensional diffusing defects, the size of the simulation box should be of the order of the grain size, which is unacceptable computationally. Depending on the calculation scheme, the calculation time of an MC code is proportional to the total number of defects to either power 1 or 2 [18] and hence to power 3–6 of the length of the simulation box edge. Therefore, an increase of the edge of the simulation box from 100 nm to 1 μm would result in an 10^3–10^6 increase in the calculation time. This indicates that incorporation of one-dimensional diffusing defects in a MC computer code in the way this is done for three-dimensional defects, is not possible. This restricts the applicability of MC modelling for studying damage accumulation to the case when one-dimensional diffusing SIA clusters have no significant influence on the microstructure evolution.

4. Conclusions

At temperatures below stage I the defect accumulation calculated in the MF approach is in agreement with that for cascade irradiation. At temperatures between stage I and stage III the fluctuations in defect generation associated with cascade irradiation lead to a decreasing total defect concentration and SIA cluster density compared with the predictions of the MF approach, and a decreasing dose for reaching a steady-state level of SIA cluster concentration. These effects appear at doses when high concentrations of the defects are accumulated in the matrix. The MF approach does not work well in this case since it uses as input the results for short-term annealing of the cascades in a perfect matrix. Since these effects arise only at high concentrations of accumulated sinks, they depend on the condition adopted in the model for the glissile-to-sessile cluster transformation. We ascribe the increasing difference between the cascade and MF calculations with increasing PKA energy to this condition. One of the most important conclusions made is that the results strongly depend on the type of boundary condition applied.

Calculations for Frenkel pair accumulation with one-dimensional migration of SIAs show that in a box smaller than the mean-free path of the SIA, the results depend on the box size and on the boundary condition applied. Pseudo-periodic boundary conditions destroy the one-dimensional character of SIA migration and lead to underestimation of defect density, whereas periodic boundary conditions introduce periodicity in sink positions and lead to overestimation of the defect density.

The mean-free path of SIA clusters could be up to several μm for typical irradiation conditions [1,3–6]. This implies that it may not be possible to apply MC modelling in a similar way to that used for three-dimensional defects for cases when one-dimensional diffusing SIA clusters have significant influence on damage accumulation.

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