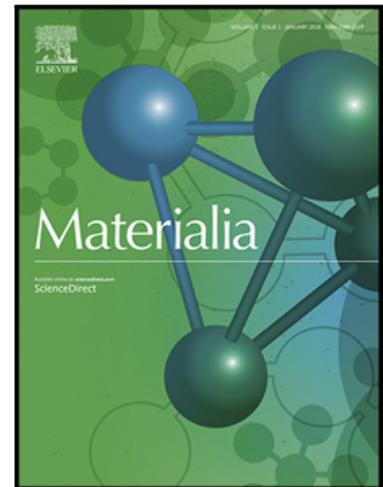


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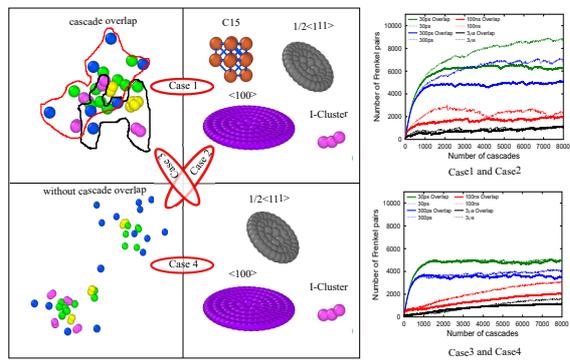
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Graphical Abstract



Effect of cascade overlap and C15 clusters on the damage evolution in Fe: An OKMC study

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Abstract

In order to investigate the long-term evolution of radiation-induced defects in the fission- and fusion-relevant material iron, we introduce cascade overlap effects into Object Kinetic Monte Carlo simulations. In addition to cascade overlap, we study the effect of introducing discrete C15 Laves phase clusters into the simulations. By applying either, none, or both of these effects we identify how they influence the evolution of the system. We find that both cascade overlap and C15 clusters affect the evolution of the radiation damage in different ways and on different time scales. Cascade overlap is found to reduce the number of Frenkel pairs. On the other hand, the explicit consideration of C15 Laves phase clusters increases the accumulation of defects at low dose. The results are compared to Molecular Dynamics simulation results under similar conditions.

Keywords: Cascade overlap, Object Kinetic Monte Carlo, Radiation damage, Iron, C15 clusters,

1. Introduction

Iron alloys are widely used in current nuclear power plants and are also proposed to be used in future ones as structural materials. The harsh environment in the form of elevated temperatures and continuous irradiation will degrade the material over time. This has led to extensive research focusing on radiation damage in Fe and Fe-based alloys [1–23]. Experimental studies of radiation damage in iron have shown that the accumulation of defects depends on dose, dose rate, and temperature [1, 2]. In these studies, transmission electron microscopy (TEM) and positron annihilation spectroscopy (PAS) techniques were used to detect the defect number and defect structure. It has been shown that by increasing dose, the defect density will saturate [1, 2]. TEM studies showed that the density of visible defects increases with an increasing dose rate. It should be noted that due to the detection limit of TEM techniques, there are some features of radiation damage that cannot be observed. Since TEM is a diffraction-based technique, it has a very weak

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21 sensitivity to vacancy-type defects, such as voids. The detection limit of TEM also causes dislocation loops
22 smaller than 1 nm to become invisible. Vacancy densities can be measured by PAS, and has for instance
23 been carried out on iron irradiated up to a few tenths of a dpa at room temperature [1]. These kinds of
24 experiments can directly be compared with both MD and OKMC simulations.

25 Additionally, Molecular Dynamics (MD) simulations have been used for characterising primary damage
26 caused by irradiation [3]. The defect production and defect evolution can be described up to nanosecond
27 timescales with MD simulations. This method has been used to study both the damage produced in single
28 cascades [4] as well as the effect of overlapping cascades [6, 24–26]. The latter has mainly been used to
29 obtain higher doses, closer to the ones in both experiments and in nuclear reactors. The main drawback
30 of MD simulations is the limited timescale reachable, which is due to the simulation of discrete atoms
31 and the simulation of the full trajectories of all atoms. Single impact simulations have revealed how the
32 primary damage created is dependent on PKA energy, alloy composition, choice of interatomic potential
33 and temperature [4, 24]. Additionally, the clustering and the spatial distribution of the created defects have
34 been studied [4]. The cumulative irradiation studies have revealed how the defect number, the defect cluster
35 size distribution and dislocation networks evolve as a function of dose [5–7].

36 To follow the evolution of defects induced by displacement cascade simulations on a longer time scale,
37 several different Kinetic Monte Carlo (KMC) methods have been developed [8, 27–29]. Object Kinetic
38 Monte Carlo (OKMC) is one of these methods and can simulate annealing of defects on extended time
39 scales [9, 29, 30]. In this method, each defect is considered as an object. In iron these objects include single
40 interstitials, single vacancies, interstitial clusters, vacancy clusters, voids, $1/2\langle 111 \rangle$ loops, $\langle 100 \rangle$ loops and
41 C15 Laves phase clusters. These objects can migrate, dissociate, and interact with each other. Several
42 OKMC simulations have been carried out on radiation damage in Fe and Fe-alloys [9–11, 29, 30]. These
43 studies show how parameters related to defect properties and their interactions affect the evolution of the
44 system. For example, formation of $\langle 100 \rangle$ loops during irradiation of Fe was the main topic of a recent
45 study [9]. The formation of $\langle 100 \rangle$ loops is possible via different mechanisms, 1) interaction of two $1/2\langle 111 \rangle$
46 loops [12] and 2) collapse of C15 clusters [7, 13]. Comparison of experimental results and OKMC simulation
47 results utilising both mechanisms suggested that the most probable mechanism is the latter one. However,
48 the effect of the presence of discrete C15 clusters in OKMC simulations and the effect of cascade overlap on
49 the defect evolution in iron have not yet been studied.

50 The migration and formation energies of each object are the two most important parameters in OKMC
51 simulations. DFT calculations can provide accurate data for point defects and small defect clusters, while
52 the calculation of migration energies of large defect clusters is not usually possible due to computational
53 limitations of this method. However, to calculate the formation energies of large clusters, recently ab initio
54 accurate models have been developed [14]. Molecular Dynamics and Molecular Statics simulations are other
55 sources used to obtain input parameters for OKMC simulations. These include defect structure, defect

56 morphology and spatial distribution of defects as a result of a collision cascade. Additionally, formation
 57 and migration energies of defect clusters, interactions between defects, and interaction between cascades
 58 and defects can be obtained from MD. The interaction between pre-existing debris and a nearby collision
 59 cascade is important when we want to investigate the evolution of materials under continuous irradiation.
 60 In iron and tungsten this interaction has been investigated in several studies [15, 16, 31]. It was found
 61 that the effect of a collision cascade in the vicinity of pre-existing defects and defect clusters will depend
 62 on the separation distance between them. For instance, the number of surviving point defects depends
 63 dramatically on this distance. It was observed that cascade overlap can completely change the defect
 64 morphology of interstitial clusters, e.g. change the Burgers vector of a dislocation loop [17]. In the same
 65 studies for iron, it was shown that the effect of interaction between cascades and pre-existing vacancy type
 66 clusters was not as significant [16].

67 In this study, we use OKMC simulations to study the evolution of radiation-induced defects in the fission-
 68 and fusion-relevant model material iron. To keep the atomistic accuracy of Molecular Dynamics, we have,
 69 in addition to what previous OKMC studies have incorporated, added the results of cascade overlap effects
 70 and effect of C15 Laves phase cluster formation. The former is based on MD results of cascades overlapping
 71 with pre-existing defects. We simulate different relaxation times between collision cascades, from very short
 72 times comparable with MD simulations, up to longer relaxation times more comparable to experiments.
 73 We investigate how both cascade overlap and C15 Laves phase clusters formation affect the evolution, by
 74 applying them individually and with both turned on and off.

75 2. Methods

76 OKMC simulations were carried out with the MMonCa code [30]. The migration and binding energies
 77 of each object larger than four defects are listed in Table 1. Formation and migration energies of interstitial
 78 type defects up to the size of 4 was extracted from DFT calculations [18]. Formation energy of dislocation
 79 loops and C15 clusters were the ones based on DFT in Ref. 14. For diffusion of $1/2\langle 111 \rangle$ loops, molecular
 80 dynamics data was used [19]. The binding energy of defect clusters with sizes larger than 4, was calculated
 81 as $E_b = E_f(n-1) + E_f(1) - E_f(n)$, where n is the number of defects in the cluster. Using recent DFT-
 82 based formation energies of interstitial clusters [14] and values from Ref. 20 for vacancies in the above-
 83 mentioned equation, the binding energies were obtained (also presented in Table 1). In OKMC simulations,
 84 objects interact with each other if they are located within a certain capture radius. The capture radius
 85 between interstitials was between the third and the fourth nearest neighbor and the capture radius between
 86 vacancies was between the second and the third nearest neighbor. The capture radius between vacancies
 87 and interstitials was $1.9a_0$, where a_0 is the lattice constant [21].

88 The new implementation of cascade overlap was extracted from Ref. 15. This paper describes the
 89 interaction between cascades and pre-existing interstitial-type clusters. The effect of cascade overlap with

vacancy-type defect clusters was not included in this study, as the effect was found to not be as considerable as for interstitial-type clusters [16]. The number of new Frenkel pairs (FPs) created in the close vicinity of a pre-existing cluster was presented by an analytical model [15]. This model shows that the number of new Frenkel pairs decreases as the distance between the center of the cascade and the pre-existing cluster is less than a critical value, given by the size of the cluster and the cascade core. When cascade overlap happens, the probability of forming various types of self-interstitial clusters with certain size depends primarily on the relative formation energies of the different cluster types predicted by the used interatomic potential. We have used the probabilities found in Figures 15 and 16 in Ref. 15, one set which correspond to the interaction in the AM04 interatomic potential [22] and the other set to the M07-B interatomic potential [5, 23].

To introduce a new cascade to our simulation cell, we used the resulting debris of 50 single cascades from MD simulations with a 5 keV PKA energy. Each cascade insertion to the OKMC simulation box was randomly chosen. Before each cascade insertion, the system was evolved up to a predefined evolution time. Here, we considered four evolution times: 30 ps, 300 ps, 100 ns, and 3 μ s at room temperature (300 K). The 30 ps evolution time is directly comparable with MD simulations of massively overlapping cascades [5–7]. When a new cascade was inserted, the distance between the cascade and the pre-existing interstitial clusters was calculated. If the separation distance was within the interaction range, the overlap effect was applied. The box size, 20 by 20 by 20 nm³, is comparable with previous MD simulations of overlapping cascades. Periodic boundary conditions were applied in all three dimensions. The evolution of the systems was followed for up to 8 000 inserted cascades, which represent a dose of about 0.37 dpa. Fifteen simulations for each different case were carried out to obtain statistically significant results. The dose was calculated based on deposited energy in the system by each cascade. The number of displacements (N_d) induced by each cascade can be calculated based on the NRT-dpa equation [32]:

$$N_d = 0.8T_d/2E_d,$$

where E_d is the threshold displacement energy and T_d is the damage energy which can be calculated as $T_d = E_{\text{PKA}} - E_{\text{ES}}$, where E_{ES} is the energy that is lost by electronic stopping. The number of displaced atoms induced by cascades divided by the number of total atoms (N_{atom}) can be considered as the dose. The relation between the number of cascades N_c and the dose can be calculated as follows:

$$\text{Dose} = 0.8N_c(E_{\text{PKA}} - E_{\text{ES}})/(2E_dN_{\text{atom}}).$$

The parameters T_d and E_{ES} were obtained from full MD simulations, E_d was 40 eV and N_{atom} the total number of atoms in the simulation cell.

To investigate the evolution of the system in OKMC, we consider two scenarios:

1. C15 laves phase clusters are directly included. Based on DFT calculations, C15 clusters are the most stable interstitial cluster up to sizes of around 50 interstitial atoms [14]. Larger than this size, the $1/2\langle 111 \rangle$ loop becomes the most stable interstitial cluster. Molecular dynamics studies have shown

that by growing C15 up to a critical size, it collapses into $1/2\langle 111 \rangle$ loops with a high probability and into $\langle 100 \rangle$ loops with a low probability [7]. Based on these studies, we have considered the following model for inserting C15 clusters in OKMC simulations. When the numbers of interstitials in clusters become five, they transform to C15 clusters with a 70% probability and to $1/2\langle 111 \rangle$ loops with a 30% probability. When the number of interstitials in a C15 cluster reaches 50, it will transform to a $\langle 100 \rangle$ loop with a 5% probability and with a 95% probability to a $1/2\langle 111 \rangle$ loop [7]. The shape of the C15 cluster was approximated by a sphere and the cluster was considered immobile. The atomic density of $3.5 \times 10^{22} \text{ cm}^{-3}$ was used for C15 clusters, which is similar to the density of them in MD simulations.

2. C15 was indirectly included in the simulations, similar to the nucleation model used in Ref. 9. In this scenario interstitial clusters with a size of 5 interstitials transform to $1/2\langle 111 \rangle$ loops with a 95% probability and to $\langle 100 \rangle$ loops with a 5% probability, skipping the intermediate step of C15 creation.

In both scenarios single interstitials and interstitial clusters of sizes up to 4 are mobile.

As the overlap effect depends on choice of interatomic potential, for the first scenario (with discrete C15) we employed the result from the M07-B potential, showing stable C15 clusters. For the second scenario (indirect C15 cluster effects) the result from the AM04 potential was used, where C15 is not stable. In order to investigate how cascade overlap affects the defect evolution in OKMC, we conducted two series of simulations. In the first series, cascade overlap effects are not imposed and in the other series the overlap effects are applied.

Defect Cluster	Binding energy (eV)	Migration barrier (eV)
C15 cluster ($I_{5 \leq n < 50}$)	$2.42 - 0.45(n^{2/3} - (n-1))^{2/3}$	immobile
$1/2\langle 111 \rangle$ loop ($I_{n \geq 5}$)	$3.77 - 1.60(\sqrt{n} \ln n - \sqrt{n-1} \ln(n-1)) - 5.35(\sqrt{n} - \sqrt{n-1})$	0.05
$\langle 100 \rangle$ loop ($I_{n \geq 5}$)	$3.77 - 1.78(\sqrt{n} \ln n - \sqrt{n-1} \ln(n-1)) - 7.16(\sqrt{n} - \sqrt{n-1})$	immobile
Vacancy cluster ($V_{n \geq 5}$)	$2.07 - 2.59(n^{2/3} - (n-1))^{2/3}$	immobile

Table 1: Binding energy (eV) and migration barrier (eV) of defect clusters with sizes larger than $n = 4$ interstitials (I) or vacancies (V).

3. Results

We categorize our simulations into four cases:

- *Case 1*: C15 is considered directly and overlap effects are turned on.
- *Case 2*: C15 is considered directly and overlap effects are turned off.
- *Case 3*: C15 effects are considered indirectly and overlap effects are turned on.
- *Case 4*: C15 effects are considered indirectly and overlap effects are turned off.

148 The results are shown in Figs. 1(a) and 1(b), for direct and indirect consideration of C15, respectively.
 149 In both figures the effect of overlap are visible in the number of Frenkel pairs. Fig. 1(a) compares *Case 1*
 150 and *Case 2* for four annealing times between each cascade and shows that the overlap effect decreases the
 151 number of surviving Frenkel pairs, especially at shorter relaxation times. We observe that the overlap effect
 152 is minimal when the relaxation time is $3 \mu\text{s}$. Fig. 1(b) compares *Case 3* and *Case 4* for four annealing times
 153 between each cascade and we notice that the effect is opposite to *Case 1* and *Case 2*. Without explicit
 154 C15 the overlap effect is minute at short relaxation times, but great at the longer relaxation times. As we
 155 observe an effect of cascade overlap, we looked at the number of overlap events (cascades close to previous
 156 debris) as a function of number of cascades, shown in Fig. 2. We clearly see that direct consideration of C15
 157 will increase the number of overlap events. Another trend seen is that a longer relaxation time will decrease
 158 the number of overlap events.

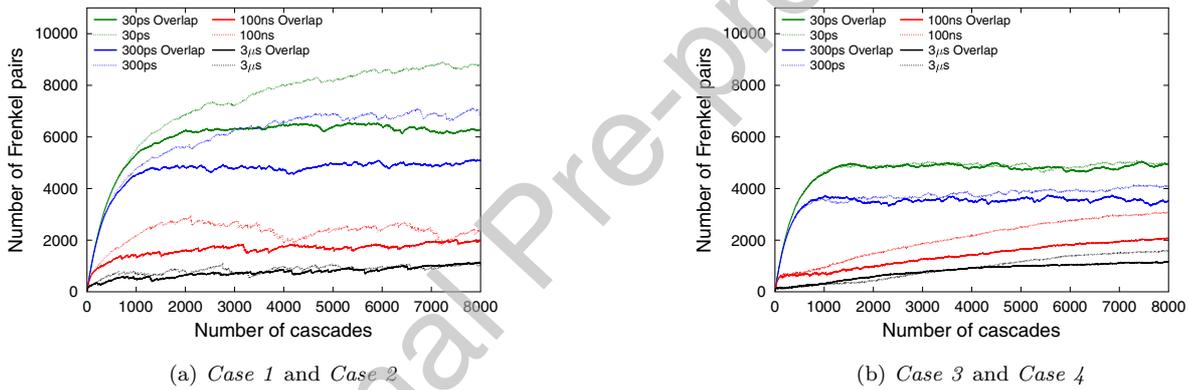


Figure 1: Number of Frenkel pairs as a function of number of cascades for (a) *Case 1* and *Case 2*, explicit C15 and with and without cascade overlap and (b) *Case 3* and *Case 4*, indirect C15 and with and without cascade overlap. The differences between different annealing times and cascade overlap effects are shown.

159 In Fig. 3 a comparison of the mean number of Frenkel pairs as a function of number of cascades for *Case*
 160 *1* and *Case 3* is shown. We observe that formation of discrete C15 during cascade overlap simulations affects
 161 the results. At low dose, considering C15 directly increases the number of Frenkel pairs for all relaxation
 162 times. For longer relaxation times, the effect of C15 on the number of surviving FPs is smaller. To interpret
 163 this behavior, we analyzed the number of interstitials in C15 clusters, $\langle 100 \rangle$, and $1/2\langle 111 \rangle$ loops for two
 164 different annealing times, shown in Fig. 4. Due to the low migration barrier of $1/2\langle 111 \rangle$ loops, they can
 165 easily be annealed through combination with vacancy clusters. C15 clusters and $\langle 100 \rangle$ loops are immobile
 166 and play important roles in the accumulation of defects. In *Case 3*, $\langle 100 \rangle$ loops are the only immobile
 167 interstitial-type cluster in the box, while for *Case 1* both C15 clusters and $\langle 100 \rangle$ loops are present and
 168 immobile. Fig. 4 shows that by increasing the number of cascades (dose) the concentration of immobile

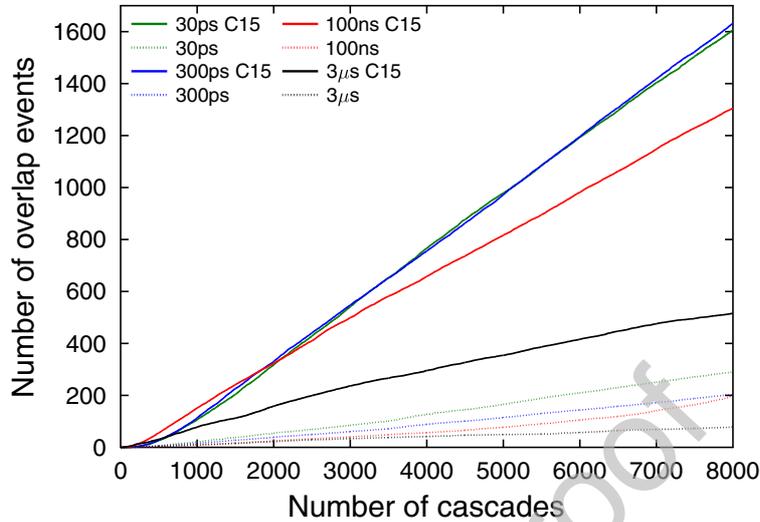


Figure 2: Number of overlap events as a function of number of cascades for different annealing times, when C15 is explicitly and indirectly considered.

169 clusters approach each other.

170 Looking at Figs. 1 and 3, we observe two general trends 1) Saturation in number of FPs is happening in
 171 all cases and setups; 2) By decreasing the evolution time between cascades (equivalent to increasing the dose
 172 rate) the number of residual defects increases. Results from MD simulations with the same time and size
 173 scale exist and the data from Figure 9 in Ref. 5 is plotted in Fig. 5. The MD simulation was carried out with
 174 the M07-B potential, which shows stable small C15 clusters. The relaxation time in the MD simulations
 175 was 30 ps. The OKMC results from this study, *Case 1*, with a relaxation time of 100 ns is shown in the
 176 same graph.

177 Fig. 6 shows the evolution of the microstructure in the OKMC simulations at various doses. In this
 178 figure we see the formation of point defects at low doses, and the defect accumulation and loop formation
 179 at higher doses. By increasing the dose, the number and the size of C15 clusters increase and the increase
 180 in size continues until C15 reaches its unstable size (50 interstitials) and collapse into $\langle 100 \rangle$ and $1/2\langle 111 \rangle$
 181 loops. The $1/2\langle 111 \rangle$ loops recombine with vacancies very quickly, while $\langle 100 \rangle$ loops continue to grow.

182 Fig. 7 shows the mean density of vacancies for all cases at various doses in log-log scale. Saturation of
 183 vacancies can be seen for most cases at high dose, previously seen for the same data in Fig. 1. However, this
 184 figure highlights the intermediate steps not clearly visible in Fig. 1.

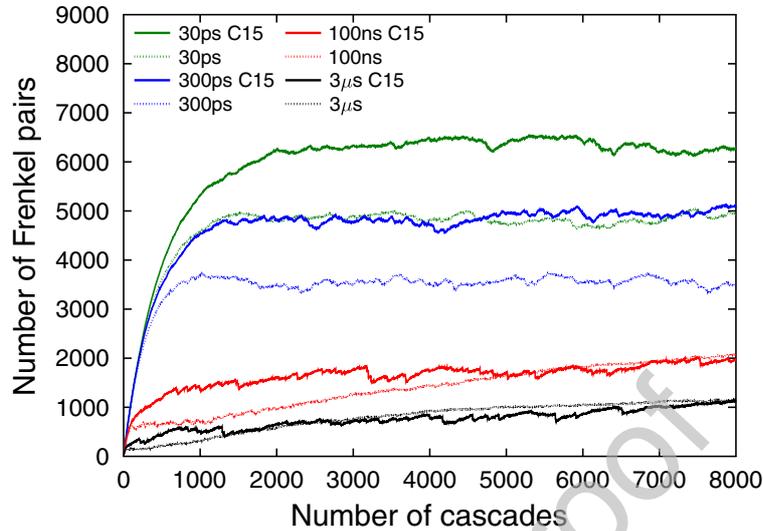


Figure 3: Comparison of number of Frenkel pairs as a function of number of cascades between the cases where C15 is explicitly and indirectly considered. Overlap effects are taken into account.

185 4. Discussion

186 In order to interpret the result of the overlap effect (Fig. 1(a) and Fig. 1(b)) we need to return to the
 187 analytical model for the interaction between single cascades and pre-existing clusters [15]. In this model,
 188 if the distance between the center of the cascade and the pre-existing cluster is below a certain value, the
 189 number of new Frenkel pairs produced is decreased. The type of the pre-existing cluster can also change,
 190 depending mainly on the relative formation energies of the different cluster types. In addition, to be able to
 191 investigate the overlap effect on defect morphology evolution, the number of surviving Frenkel pairs when
 192 overlap effects are turned on and off can be determined. Fig. 1(a) and Fig. 1(b) show that the overlap effect
 193 decreases the number of surviving Frenkel pairs. The reason for this decrease can be discussed as follows.

194 When C15 clusters are considered directly, a decreasing number of surviving Frenkel pairs is observed
 195 (Fig. 1(a)). The main reason of this decreasing trend is the lower number of new produced Frenkel pairs.
 196 In this case, the C15 clusters are immobile and cascade overlap will happen with a higher probability.
 197 By increasing the number of inserted cascades, the density of C15 in the box will increase and thus the
 198 probability of overlap will further increase. Fig. 2 shows the overlap events as a function of number of
 199 inserted cascades, which in this case increases dramatically.

200 When C15 clusters are not considered directly, the number of overlap events are fewer than in the case
 201 when C15 clusters are considered directly (Fig. 2). We see from Fig. 1(b), that after a certain dose, depending
 202 on annealing time, the overlap effect dominates. In this case, the density of immobile clusters (read $\langle 100 \rangle$)

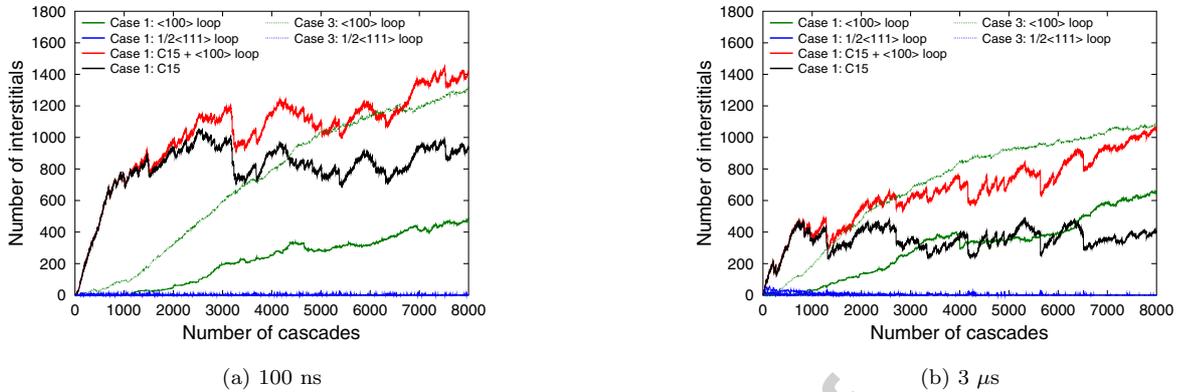


Figure 4: Comparison of the mean number of interstitials in mobile and immobile clusters as a function of number of cascades between the cases where C15 is explicitly and indirectly considered. The annealing time between each cascade is 100 nanoseconds (a) and 3 μs (b).

203 loops) determines the behavior, as the $\langle 100 \rangle$ loops behave as defect sinks. In addition to the decline in
 204 number of new Frenkel pairs produced due to overlap effects, change of Burgers vector of $\langle 100 \rangle$ loops by
 205 cascade overlap is the main source to the different behaviour between the cases with overlap effects turned
 206 on and off (Fig. 1(b)). Figure 15a in Ref. 15 shows that there is a high probability of changing Burgers
 207 vector of pre-existing $\langle 100 \rangle$ loops up to sizes of 30 SIAs during cascade overlap. Hence, overlap effects
 208 decrease the concentration of surviving $\langle 100 \rangle$ loops and thus reduce the number of accumulated Frenkel
 209 pairs, as the mobile $1/2\langle 111 \rangle$ loops can recombine with vacancies.

210 Up to a certain number of cascades (Fig. 3), the number of Frenkel pairs in the case where C15 was not
 211 considered directly is lower than when it was considered directly, when overlap effects are considered. The
 212 reason for this difference goes back to the mobility of clusters that form during the cascade simulations.
 213 In the case where the intermediate stage of C15 formation is neglected (*Case 3*), $1/2\langle 111 \rangle$ loops with low
 214 migration barrier are formed instead of immobile C15. Thus, the recombination rate of interstitials with
 215 vacancies increases and the number of Frenkel pairs in the box decreases. The immobile interstitial defects
 216 such as $\langle 100 \rangle$ loops and C15 clusters are the source of defect accumulation. Fig. 4 describes how the number
 217 of interstitials in immobile clusters in *Case 3* approaches the ones in *Case 1*.

218 For a similar setup, both MD and OKMC (*Case 1*), show a very similar trend in terms of number of
 219 Frenkel pairs (Fig. 5). In MD simulations, the M07-B interatomic potential had been used, which shows
 220 stable C15 clusters corresponding to *Case 1*. However, to obtain comparable results, the annealing time
 221 between each cascade is different between MD simulations (30 ps) and OKMC simulations (100 ns). The
 222 attempt frequency is on the order of 10^{13} s^{-1} , based on the Bortz-Kalos-Liebowitz (BKL) algorithm used
 223 for calculating evolution time in OKMC, which results in not many reactions occurring on the timescale of

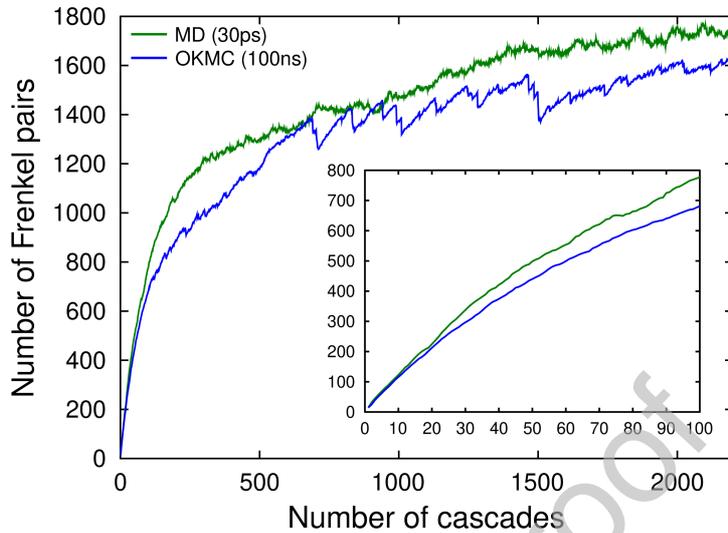


Figure 5: Comparison of Frenkel pairs as a function of number of cascades in MD [6] and OKMC simulations. In the MD simulations the annealing time between each cascade is 30 ps, while in OKMC simulation the annealing time is 100 ns. In the OKMC simulation both C15 and cascade overlap were considered. The inset is a zoom-in at the evolution up to 100 cascades.

224 picoseconds. This leads to accumulation of higher defect numbers in OKMC simulations when the annealing
 225 time between cascade is only on the order of tens of picoseconds. Another factor is the effects of elastic
 226 interactions, inherently accounted for in MD simulations, but not included in the current OKMC simulation.
 227 The elastic strain fields induced by the various defect clusters can change the migration barriers for nearby
 228 defects [33].

229 Generally, looking at the defect evolution in all simulations, we observe that there will be a build-
 230 up under all circumstances. Contrary to electron irradiation, where only point defects are produced, there
 231 would be almost no defect build-up at room temperature, as all defects would annihilate without any generic
 232 traps [34]. This shows that utilizing realistic cascade debris, not just the correct number of Frenkel pairs, is
 233 crucial for understanding the microstructure evolution.

234 Looking more closely at Fig. 7, we observe that for the longer relaxation times, the vacancy density
 235 seems to saturate at quite low doses, but starts to increase again at a bit higher doses. This is especially
 236 clear in the cases without discrete C15 clusters (*Case 3* and *Case 4*). The first saturation is due to the
 237 formation of mobile $1/2\langle 111 \rangle$ loops that easily can annihilate other defects. This is not as clearly seen in
 238 the cases where we have a quite high amount of immobile C15 clusters. However, as the dose increases, we
 239 form immobile $\langle 100 \rangle$ loops which do not recombine as easily with vacancies (which are also immobile). This
 240 formation of the immobile interstitial type defect clusters will dramatically increase the number of defects
 241 in the system (almost an order of magnitude). This shows the importance of the immobile C15 clusters on

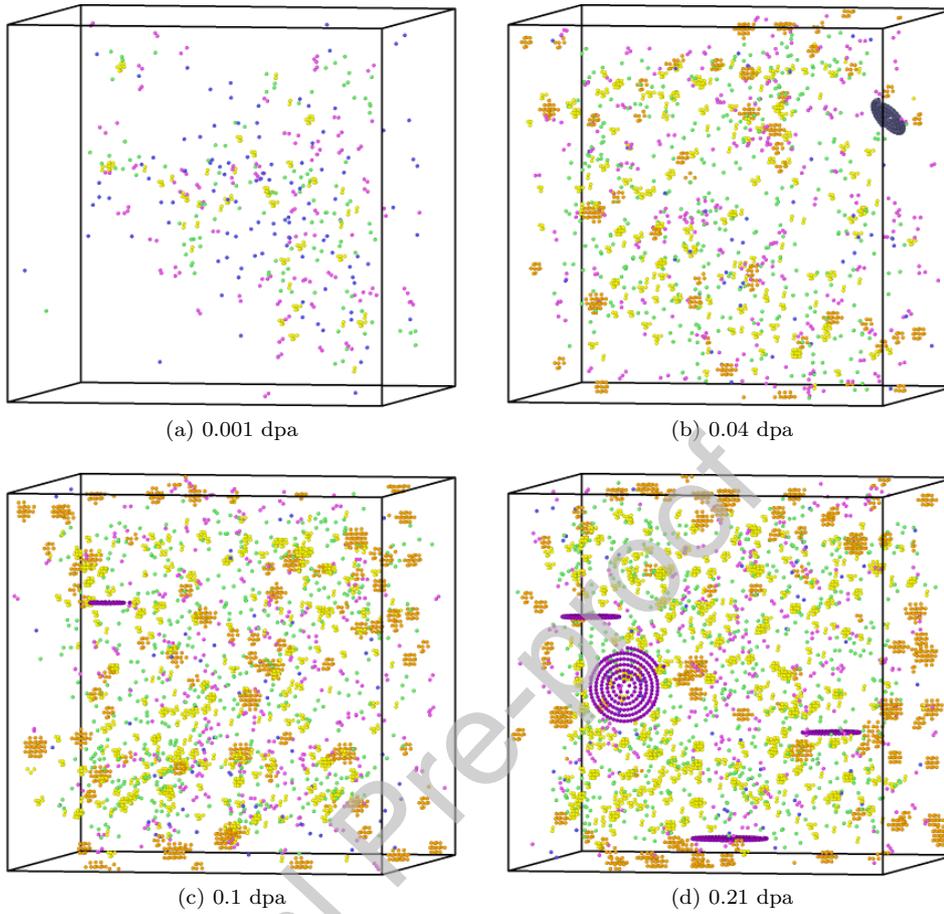


Figure 6: Snapshots of the OKMC simulation cell at various doses. In this figure both C15 and cascade overlap were considered and the relaxation time between cascades is 100ns. Green, blue, yellow, pink, orange, black and purple represent vacancies, interstitials, vacancy clusters, interstitial clusters (with size 2-4), C15 clusters, $1/2\langle 111 \rangle$ loops and $\langle 100 \rangle$ loops, respectively. The side length of the box is 20 nm.

242 the evolution, a similar trend was also seen in MD simulations [7].

243 5. Conclusions

244 Cascade simulations with four different annealing times have been performed by OKMC in this study.
 245 We implemented the effects of cascades overlapping with interstitial-type defect clusters in OKMC and
 246 studied the results with this implementation turned on and off. Additionally, we studied the evolution of
 247 defects during cascade simulations utilizing two different considerations of C15 Laves phase clusters. We
 248 have shown that both of these factors will affect the evolution of the system, both in terms of number of
 249 defects and defect morphology. Our summarized results and conclusions are the following:

- 250 1. Cascade overlap effects reduce the number of surviving Frenkel pairs.
- 251 2. The method of C15 Laves phase cluster consideration (direct or indirect) affects the results.

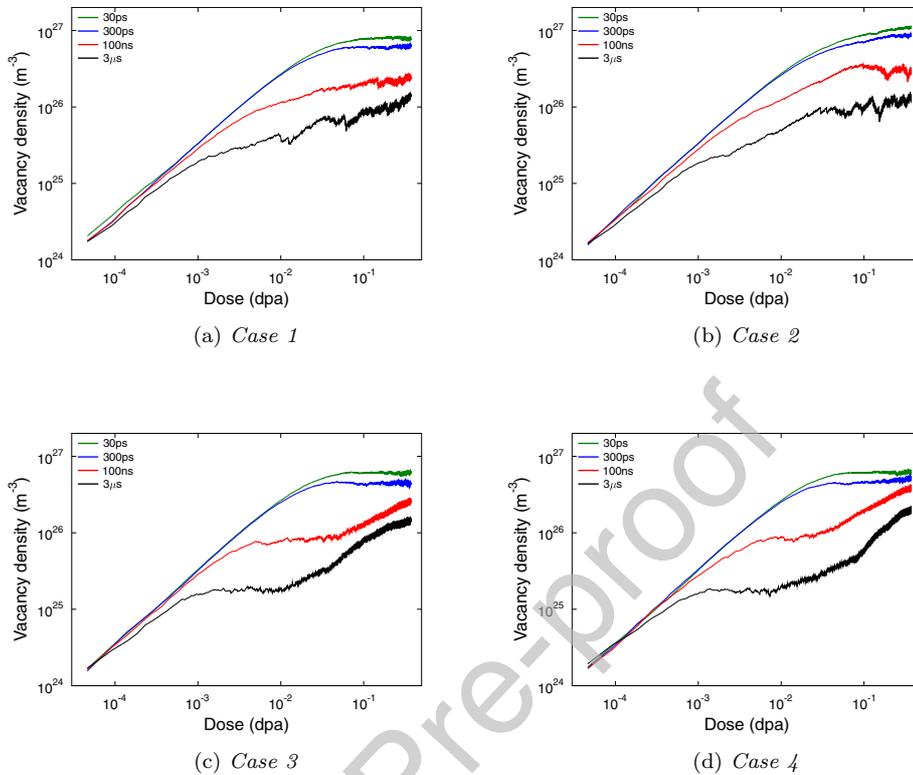


Figure 7: Vacancy density as a function of dose for all four cases at different annealing times in log–log scale.

- 252
- When considered directly, more defect accumulation is observed up to a certain dose and this
 - 253 dose depends on annealing time.
 - The different considerations also changed the defect build-up mechanisms.
- 254
3. Saturation of the number of Frenkel pairs happens in all setups investigated.
 - 255
 4. By decreasing the evolution time between cascades (equivalent to increasing the dose rate) the number
 - 256 of residual defects increases.
 - 257
 5. When the same setup is considered in both MD and OKMC, the Frenkel pair evolution is qualitatively
 - 258 the same. The annealing time, however, needs to be different in the different methods to obtain
 - 259 quantitative agreement.
 - 260

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Declaration of interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests:

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