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Properties and evolution of sessile interstitial clusters produced by displacement cascades in α-iron

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Abstract

Recent molecular dynamics (MD) studies of displacement cascades in α-iron have shown that although most self-interstitial atoms are created in the form of single defects or glissile clusters, sessile clusters are also formed during the quenching stage of a cascade. Statistics on the size and number of sessile interstitial clusters have been determined as a function of cascade energy and irradiation temperature. The thermal stability of three common forms of sessile cluster has been investigated by MD, and the lifetime and activation energy for transforming into glissile form have been estimated. Most sessile clusters transform within a few hundred ps at about 500 K with an activation energy of between 0.35 and 0.5 eV. This suggests a re-assessment of the interpretation of recovery stage II in iron. One type of cluster having a compact three-dimensional configuration of high symmetry is found to be stable for at least 500 ps at temperatures up to 1500 K. The interaction of sessile clusters with point defects and glissile clusters has been studied, and the possibility of their subsequent transformation into glissile clusters is discussed.

1. Introduction

Defect production in metals subjected to fast neutron irradiation from power reactor cores is initiated by displacement cascades. Molecular dynamics (MD) computer simulation provides a powerful means of investigating these events and the atomic mechanisms that lead to defect production and clustering in cascades have been reviewed elsewhere [1–3]. Two key features of cascade damage have been recognized. First, the number of Frenkel pairs, N_F, generated by displacement cascades is calculated to be smaller (~20–40%) than that predicted by the NRT standard formula [4]. This is consistent with experimental evidence [5,6]. Second, computer simulation has revealed that many of the self-interstitial atoms (SIAs) created in cascades are in clusters, and the probability of clustering and the size of the largest cluster tends to increase with increasing PKA energy and temperature [7,8]. It is also found that some of these clusters form as interstitial dislocation loops. In bcc α-iron they have a perfect Burgers vector, **b**, equal to $1/2\langle 111\rangle$, and can move conservatively on their glide prism. Such 'glissile' clusters have a high binding energy and can migrate away from their parent cascades to be absorbed preferentially at sinks such as dislocations and grain boundaries. This provides an explanation as to why some specific microstructure features which arise from cascades cannot be modelled using the conventional rate theory approach based on three-dimensional single defect reaction kinetics [9].

Not all interstitial clusters produced in MD simulations of cascades are glissile. In low stacking fault energy fcc metals, for example, interstitial loops can be formed with a partial Burgers vector of $\mathbf{b} = 1/3\langle 111\rangle$ and are intrinsically sessile. However, another form of sessile cluster can arise, which is metastable with respect to the glissile dislocation configuration. It often has a three-dimensional morphology and has been observed in MD-generated cascades in α-iron (see later), α-titanium (hcp) [10] and α-zirconium (hcp) [11]. In the case of zirconium, for example, the largest interstitial cluster found in all the MD simulations for energy up to 20 keV consisted of 25 defects and had a sessile form. The recognition that

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such metastable sessile clusters can be produced in the cascade process leads to the following questions. (i) Are these clusters stable for temperatures and times of interest for practical concern? (ii) Can they transform into glissile clusters due to interaction with point defects and their glissile counterparts?

This paper will address these aspects for sessile clusters produced by displacement cascades in α-Fe. Statistics on the size and number of sessile interstitial clusters at the end of the cascade process as a function of cascade energy and irradiation temperature are provided. The thermal stability of some typical clusters has been examined, and their lifetime and activation energy for conversion into glissile clusters have been determined. The interaction of these sessile clusters with point defects and glissile clusters has also been investigated.

2. MD model and simulation method

The interstitial clusters considered here were created in the simulations of cascades of energy from 2 to 40 keV in α-Fe at either 100 or 600 K [3,12]. In any cascade event, at a given energy, a range of point defect clusters is produced and their type and population varies from event to event. In this work an interstitial atom is defined to be part of a cluster if it has at least one nearest-neighbour at an interstitial position. Interstitial sessile clusters were identified in the debris of cascades by their morphology and inability to glide, as visualised using a graphics package on a workstation. A selection of those clusters most commonly identified was then chosen for further simulation.

To study the thermal stability of a sessile cluster, its atomic coordinates were extracted from the MD cell containing all the residual defects at the end of the thermal spike phase of the cascade. These coordinates were then used to recreate the particular cluster in a much smaller MD block to enable its stability to be examined over much longer time period than would be possible with the large model crystal used for cascade simulations. For example, the model size employed for a di-interstitial sessile cluster was 8192 atoms, i.e. $(16a_0)^3$, where a_0 is the lattice parameter, and 54 000 atoms $(=(30a_0)^3)$ for a 13-SIA cluster, compared with 1 272 112 atoms for a 40 keV cascade. The crystal containing a sessile cluster was relaxed for about 5 ps at a temperature of 0 K to minimise the potential energy, following which a simulation was started by scaling the atomic velocities to a specified annealing temperature, $\langle T\rangle$ of between 300 and 900 K. The simulations were stopped either once the sessile cluster had become glissile, or after 1000 ps, whichever came soonest, and the corresponding time was reordered for future analysis. In order to generate meaningful statistics, many simulations were needed for each temperature. For example for a di-interstitial four simulations were run at each temperature with a different random number seed to scale the initial temperature of the block. Less comprehensive data was gained for other cluster sizes. To simulate interaction of another defect with a sessile cluster, a point defect or glissile cluster was recreated near the sessile cluster in the MD block, and then the whole configuration was relaxed for about 5 ps at a temperature of 0 K. Most simulations were performed for a few hundred ps at 300 K, a temperature at which sessile clusters are thermally stable, so that the dynamic process of interaction between the sessile and glissile clusters could be assessed.

The present work employed the MOLDY MD code, which is widely used for simulations of displacement cascades in metals, and the simulations were performed in a computational block at constant volume with periodic boundary conditions. The interatomic potential was the many-body form for α-Fe derived by Finnis and Sinclair [13], but modified as outlined in [14] to provide a better description of atomic interactions at high energy. The same potential has also been employed by Stoller [15] for modelling displacement cascades.

3. Sessile clusters produced by cascades

Although the configuration of the sessile clusters found in α-Fe can be complicated, most form from variants of three forms, typified by the following. The nature of some 2-, 8- and 13-SIA sessile clusters is illustrated in Fig. 1, where large spheres represent interstitial atoms and small ones indicate vacant sites. (An 'interstitial' is defined as an atom that does not lie within $0.3a_0$ of a lattice site and a 'vacancy' is a site which does not have an atom within $0.3a_0$ of it, as in [14].) The 2-SIA sessile cluster in Fig. 1(a) forms a two-dimensional configuration where three atoms effectively share one lattice site and are located between two $\{1\,1\,1\}$ planes. The 8-SIA sessile cluster in Fig. 1(b) has a three-dimensional form. It consists of $\langle 110\rangle$ dumbbells and is a highly symmetrical configuration where 28 atoms share 20 lattice sites. The 13-SIA sessile cluster in Fig. 1(c) is formed mainly by crowdions along a $\langle 111\rangle$ direction, but in addition there are two $\langle 110\rangle$ dumbbells which block the $\langle 111\rangle$ motion of the crowdions and result in a sessile cluster. It is convenient to identify these three forms of configuration as type A, B and C, respectively.

The interstitial clustering fraction, defined as the fraction of surviving interstitials found in clusters of size two or larger, is presented in [3] for energies up to 40 keV in α-Fe. The cluster fraction is found to increase with increasing energy and is probably consistent with the longer lifetime of thermal spikes at higher cascade energies. The cluster fraction includes the contribution from both glissile and sessile clusters, but the proportion

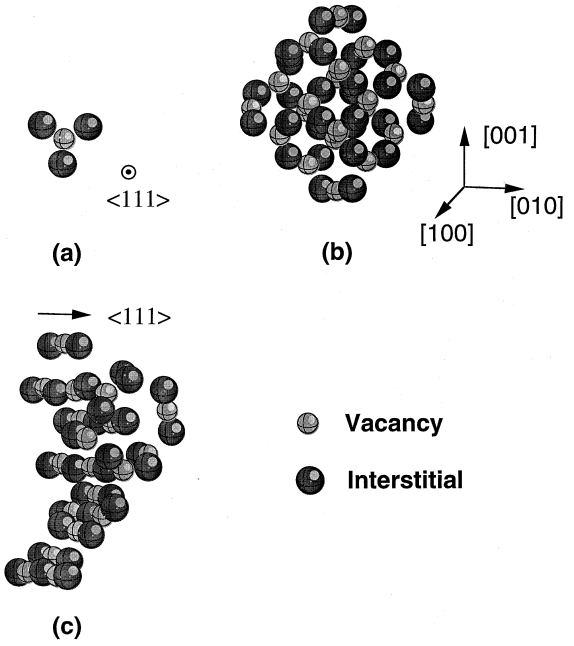

Fig. 1. Typical (a) di-, (b) 8- and (c) 13-SIA sessile clusters produced by displacement cascades in α-Fe. The large dark spheres represent atoms displaced to interstitial positions and the smaller, lighter spheres represent vacant lattice sites. The ⟨111⟩ axis is shown normal to the plane of projection in (a) and lying at approximately 39° to the plane in (c). In the latter case, this is the axis of the crowdions within the cluster. The three ⟨100⟩ axes are indicated in (b).

of each for a given cascade damage condition is also important in any realistic theoretical treatment of the microstructure evolution and defect accumulation [16]. To illustrate the extent of sessile cluster formation, we consider data for interstitials created by 40 keV cascades in α-Fe at the two temperatures 100 and 600 K. The mean values for the components of the interstitial cluster population are presented in Table 1. Here 57% of the SIAs were in clusters of size two or more at 100 K and each cascade generated 24 such clusters on average. Of these, 17 were glissile and 7 sessile, with sizes ranging from 2 up to 24 and 9, respectively, and average size 2.9 and 3.2. However, 70% of the SIAs formed clusters at 600 K, and of the 25 clusters created, 21 were glissile and 4 sessile. This reduction in the population of sessile clusters is presumably due to the higher probability of transformation from sessile to glissile form during the longer duration of a thermal spike at the higher temperature. We shall return to this point in the next section. The sessile fraction of all the SIA clusters found in cascades is plotted as a function of PKA energy and irradiation temperature in Fig. 2. The points denote the mean over all the cascades at each condition and the bars indicate the standard error.

The fraction of sessile clusters is weakly dependent on recoil energy. It is consistently larger at 100 K than that at 600 K, as noted above in Table 1 for 40 keV. About 35% of interstitial clusters produced by displacement cascades in α-Fe are sessile at 100 K and 25% at 600 K. The sessile clusters observed may not have sufficient time to either collapse or reorient during the period (20–30 ps) of the cascade simulations. In this connection, we note that although simulation of a cascade containing a 24-SIA sessile cluster in Zr was extended to 100 ps, no reconstruction was seen [11], indicating that an extension to such time periods would be of little value. It was decided to simulate the annealing of individual sessile clusters instead, as explained in Section 2.

4. The thermal stability of sessile clusters

The initial annealing temperature of a sessile cluster was 300 K, and if it did not transform within 500 ps, the temperature was increased. The simulations were stopped once the cluster became glissile, i.e. when it exhibited the form of clustered ⟨111⟩ crowdions and had high mobility. (The movement and the activation energy of migration of such clusters have been widely investigated and are described elsewhere [17,18].) The results revealed that small clusters containing two, three and four interstitials can become glissile after a few hundred ps at a temperature of about 500 K, and the 13-SIA sessile cluster also becomes mobile in this timescale at about 600 K. The lifetime of sessile clusters, τ, defined as the time to become glissile during the simulation, strongly depends on the annealing temperature, and decreases

Table 1
The number of Frenkel pairs, N_F, and the population and nature of interstitial clusters produced per 40 keV cascade in α-Fe at temperatures of 100 and 600 K. Each value is the average for four cascades

T	N_F	Number of SIA clusters	Percentage of SIA clusters	Number of glissile SIA clusters	Number of SIA in glissile clusters	Number of sessile SIA clusters	Number of SIA in sessile clusters	Percentage of clustered SIA in sessile clusters
100 K	129	24	57	17	50	7	23	32
600 K	121	25	70	21	69	4	17	20

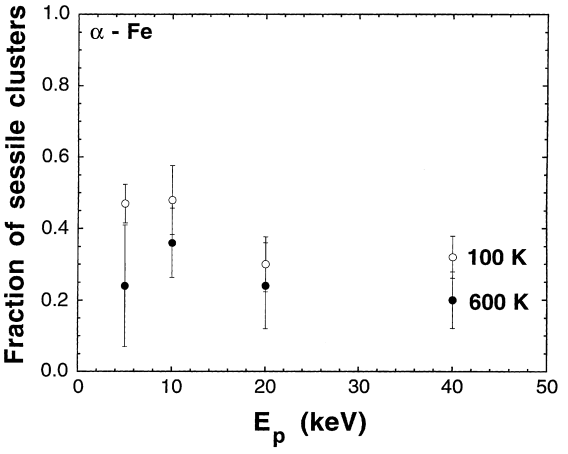

Fig. 2. The fraction of SIA clusters formed in a metastable sessile configuration by cascades in α-Fe as a function of PKA energy and irradiation temperature.

with increasing temperature. To show this qualitatively, we have studied the type A sessile di-interstitial in detail. The lifetime obtained for all the simulations is presented as a function of the reciprocal temperature in Fig. 3. For a 4-SIA cluster of type A and the 13-SIA cluster of type C, only one simulation was carried out for each temperature, but the results are included because they support the trend with temperature for the di-interstitial cluster.

The data can be analysed further by assuming the temperature dependence of τ can be described by an Arrhenius expression

$$\tau = \tau_0 \exp(E_c/kT), \tag{1}$$

where τ_0 is a pre-exponential factor, E_c is the activation energy for the sessile–glissile transformation and k is the Boltzmann constant. The best fit of Eq. (1) to the di-interstitial data is shown in Fig. 3, where, despite the variability of data, the mean value of τ is described adequately by the Arrhenius relation. The parameters estimated from this fit are $E_c = 0.43$ eV and $\tau_0 = 0.018$ ps. The activation energy for transformation of sessile clusters of type A and C can be estimated to be between 0.35 and 0.50 eV.

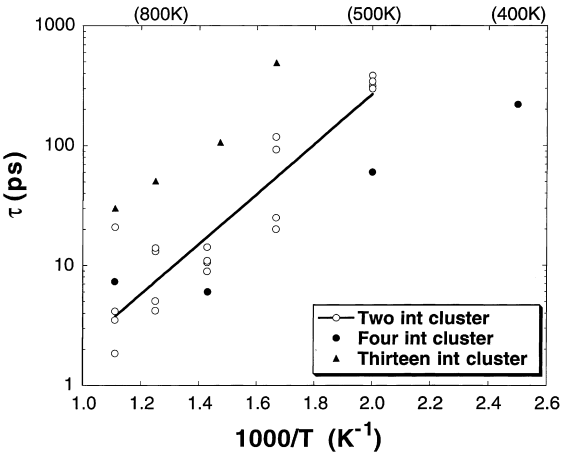

Fig. 3. The lifetime of several different metastable SIA sessile clusters in α-Fe as a function of annealing temperature.

In most of the MD simulations, sessile clusters of type A and C became mobile at temperature greater than 500 K, but the eight-interstitial cluster shown in Fig. 1(b) was an exception and demonstrated high thermal stability. Annealing simulations were carried out for ~500 ps at temperatures from 500 to 1500 K but no transformation occurred, even though the difference in formation energy between it and the stable, glissile form of ⟨111⟩ crowdions is small, i.e. 24.1 eV compared with 23.6 eV.

5. The interaction of sessile clusters with point defects and glissile clusters

As described in Section 1, the interaction of sessile clusters with point defects and glissile clusters is potentially an important issue for damage accumulation under cascade conditions. Thus, it is of interest to establish whether a sessile cluster can easily transform after absorbing either a point defect or another glissile cluster or remain in a sessile form. Since small sessile clusters of type A are the least stable during annealing (Section 4), we have considered only the 8- and 13-SIA sessile clusters shown in Fig. 1.

5.1. The interaction with point defects

A single interstitial was introduced at a distance of about $3a_0$ from the 13-SIA sessile cluster and the crystal was relaxed at an annealing temperature of 300 K as described in Section 2. This procedure was repeated for the 8-SIA cluster at 600 K. These temperatures correspond to those at which these clusters are thermally stable (Section 4). After a single interstitial was absorbed, the annealing was continued for at least 500 ps and if the new clusters remained sessile, the crystal was quenched to 0 K and the cluster energy calculated. Then another single interstitial was introduced and the simulation was repeated.

The single interstitial was absorbed preferentially into the 13-SIA clusters at the side where the ⟨111⟩ crowdions exist, as illustrated in Fig. 4. Similar behaviour occurred as further SIAs were absorbed until a 21-SIA cluster was formed, which became mobile after about 320 ps at 300 K. The formation energy, E_f, of clusters formed by growth from the 13-SIA cluster is plotted in Fig. 5 (open circles) as a function of the cluster

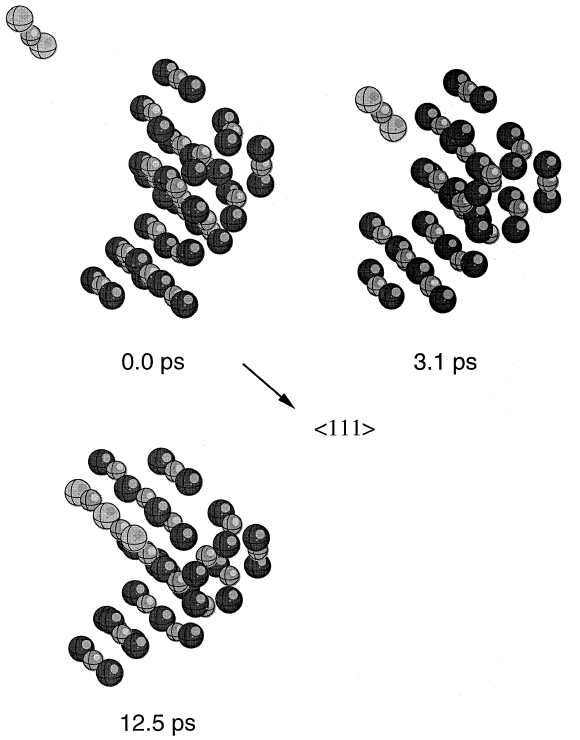

Fig. 4. Computer-generated images showing the interaction and absorption of a single interstitial with a 13-SIA sessile cluster for the three different times indicated. The single interstitial starts at the top left as a ⟨110⟩ dumbbell and the two displaced atoms that form it are plotted as light grey spheres. The projection of the ⟨111⟩ axis of the crowdions within the cluster is indicated.

size after defect absorption. Also calculated are energies for the corresponding stable glissile clusters consisting of ⟨111⟩ crowdions (open triangles) with centres in a {1 1 0} plane. (The formation energy of single interstitial in perfect crystal is 4.86 eV.)

The results for the 8-SIA sessile cluster reveal that the single interstitial moved to the periphery of the cluster along ⟨111⟩ directions, where it became trapped in the place corresponding to the minimum cluster energy. Similar behaviour was observed to occur in the further sets of simulations. This process is demonstrated in Fig. 6 when sequential absorption had created a 12-SIA cluster in a similar configuration to the original. The cluster grew to 19-SIAs in size and still retained the sessile form, even after a further anneal at 1500 K for 1000 ps. This highly stable, three-dimensional cluster is illustrated in Fig. 7, where its generic 8-SIA cluster is also plotted for comparison. The formation energy of the sessile clusters that grow from the 8-SIA defect is plotted in Fig. 5 (filled circles).

For the interaction with a single vacancy, we have considered the 8-SIA sessile cluster because the 13-SIA

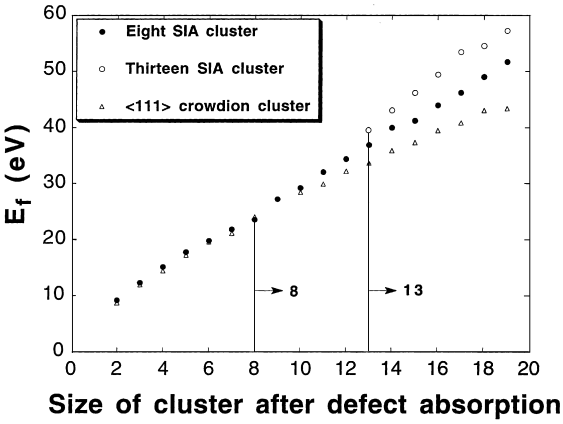

Fig. 5. The formation energy of metastable SIA sessile clusters formed when the 8-SIA and 13-SIA defects absorb point defects. The formation energy of glissile clusters consisting of the same number of ⟨111⟩ crowdions is also shown.

sessile cluster is less stable. A vacancy was put into the MD block of atoms near the 8-SIA sessile cluster and

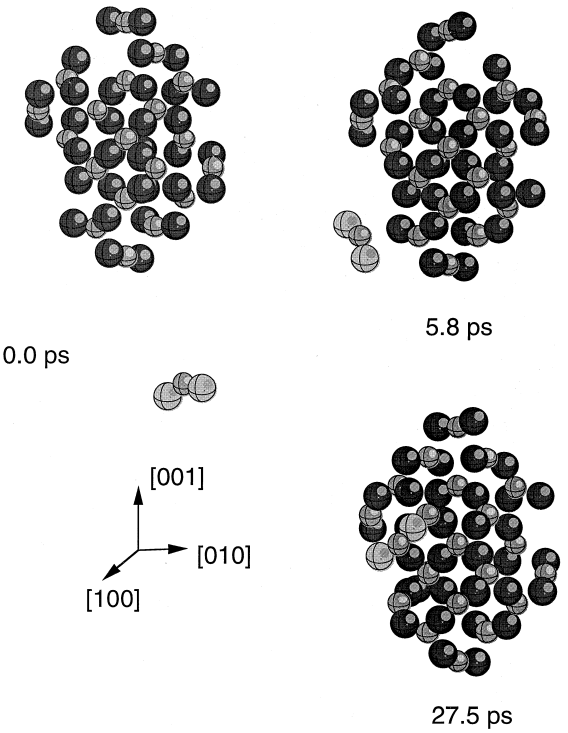

Fig. 6. Computer-generated images showing different stages in the process of absorption of a single interstitial by a 13-SIA sessile cluster, where the projection of the three ⟨100⟩ axes is indicated. The single interstitial starts at the bottom right as a ⟨110⟩ dumbbell and the two displaced atoms that form it are plotted as light grey spheres.

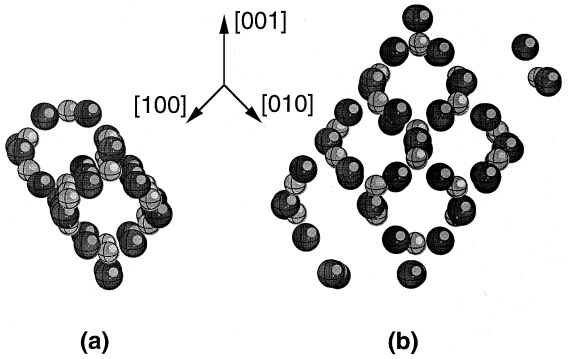

Fig. 7. Comparison of (a) 8-SIA and (b) 19-SIA sessile clusters, where the projection of the three ⟨100⟩ axes is shown.

the crystal was relaxed at 0 K for about 5 ps to minimise the potential energy. The temperature was raised to 1000 K, at which the vacancy became mobile and migrated to the cluster, presumably because of the elastic interaction. The crystal was then annealed for about 1000 ps, and, if the smaller cluster remained sessile, it was quenched to 0 K, and another vacancy was introduced and the cycle repeated. The 8-SIA sessile defect only became mobile when reduced to a single interstitial, showing that the clusters derived from the three-dimensional form (Fig. 1(b)) face a relatively high energy barrier for the sessile–glissile transformation. The formation energy of this series of clusters of decreasing size is plotted in Fig. 5 (filled circles).

5.2. The interaction with clusters

A di-interstitial glissile cluster was introduced at a distance of about $6a_0$ from the sessile cluster, and the crystal was then relaxed and annealed for 1000 ps at 300 K. At this temperature, the glissile cluster is mobile and the sessile cluster is stable (see above). If the glissile cluster was absorbed to form a larger sessile cluster, the simulation was continued for another 1000 ps to establish whether it transformed into a glissile state. If it remained sessile, the simulation procedure was repeated with a larger glissile cluster. The biggest glissile cluster considered contained six interstitials.

It was found that all the glissile clusters considered were repelled from the 8-SIA sessile cluster, independently of their initial position. This may be due to the rather symmetric three-dimensional nature of the 8-SIA sessile configuration (Fig. 1(b)). The same phenomenon occurred for some positions around the 13-SIA sessile cluster (Fig. 1(c)), but absorption was observed for most of the positions at which a glissile cluster was located. Small glissile clusters with two and three interstitials were absorbed by the 13-SIA sessile cluster within a time of about 30 ps, but a longer simulation time was required for the larger glissile clusters. The 13-SIA sessile cluster only converted into a glissile one when it captured a 6-SIA glissile cluster. This is illustrated by the computer-generated defect plots in Fig. 8, which show three stages of the absorption and transformation of a glissile cluster. The glissile defect is initially located $6a_0$ away from the larger cluster in Fig. 8(a) and its Burgers vector is along a ⟨111⟩ direction at an angle of 70° to the principal ⟨111⟩ axis of the sessile cluster. The structure at 6.2 ps in Fig. 8(b) is at the point of absorption of the glissile defect: here the cluster has moved along the direction of its Burgers vector towards the centre of the original sessile cluster to start to create a 19-SIA cluster. The interstitial atoms in this cluster then reorganize due to thermal vibration, and by about 21 ps (Fig. 8(c)) this reorganization is complete. The new defect is a glissile loop of 19 ⟨111⟩ crowdions with Burgers vector along a different ⟨111⟩ direction from that of the original 6-SIA defect. This is the first reported demonstration of a mechanism for a glissile interstitial cluster of such a large size to change its glide direction.

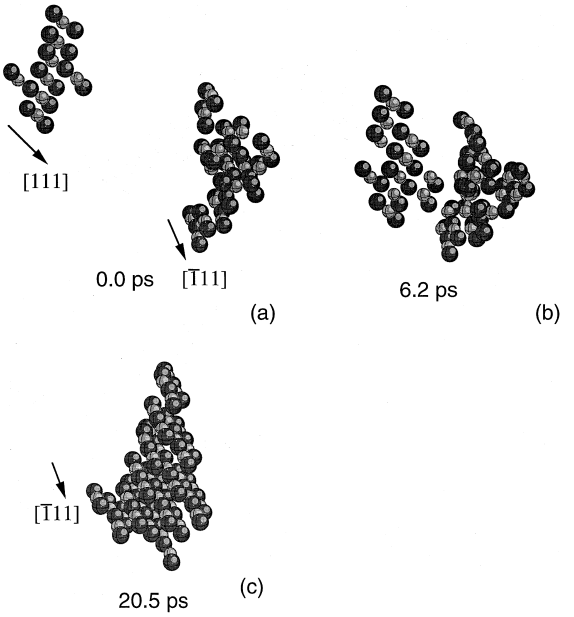

Fig. 8. Computer plots showing three stages of the interaction of a 6-SIA glissile cluster with 13-SIA sessile cluster and the direction change of the Burgers vector of the former. The projection of the ⟨111⟩ axis of the crowdions in each cluster is as indicated. Three stages are (a) the initial condition, (b) the point of interaction and (c) the developed glissile cluster.

6. Discussion

The modelling described here is the first detailed treatment of sessile interstitial clusters and the fundamental issues concerning their population, structure and

stability. The statistics presented on production of such clusters by displacement cascades in α-Fe were obtained from over a hundred cascades simulated in the energy range from 2 to 40 keV [3,12]. In this section, we summarize the main findings and discuss aspects not dealt with earlier.

The first point to note is that the proportion of sessile clusters formed within a cascade at a given temperature is almost constant within the range of PKA energy considered. However, about 10% more of the SIA clusters generated by displacement cascades at 100 K are sessile compared with 600 K. The decrease in the fraction with increasing temperature is consistent with the longer lifetime of the thermal spike at higher temperature, which allows more sessile clusters to transform either directly or by interaction with other SIAs. It is important to note that size distribution of the sessile clusters is comparable with that of the glissile ones. The statistics represent the primary state of damage, in which simulations are stopped when the cascade zone has cooled to the ambient temperature (after less than about 30 ps). As noted in Section 3, the overall trends are unlikely to be affected by extending simulations to a few hundred ps. This is supported by cascade modelling undertaken by Stoller [20] using the same interatomic potential, where annealing a 10 keV cascade to 100 ps at 100 K revealed very little restructuring.

The thermal stability of sessile clusters is an important issue because they have the potential to provide a continuous source of mobile clusters during neutron irradiation by either transformation into glissile clusters or acting as sinks for mobile defects if they are stable over long periods of time. The present modelling shows that provided the temperature is sufficiently high (>600 K) small clusters of type A containing two, three and four interstitials and clusters of type C, illustrated by the 13-SIA, defect can become glissile after a few hundred ps. This would be the case at temperatures of technological interest, ~600 K, where such defects should mainly affect the annealing of individual cascade debris. It is not surprising that the large type C defect has a similar activation energy to the small ones of type A since only a few SIAs are required to re-orientate in both cases. However, the sessile defect of type B, represented by the 8-SIA cluster, which has the high symmetry shown in Fig. 1, has been shown to be very stable, and no transformation to glissile form occurred over a time of 1000 ps at any of the temperatures simulated. This suggests that the energy barrier for transformation is high. The interatomic potential used in the present study is a short-range, many-body function in which the cohesive term is isotropic in character and does not include the angular nature of bonding that may be significant for bcc transition metals. It is not clear at present how sensitive some of the properties of these clusters are to the form of the interatomic potential. It will be of interest, therefore, to simulate sessile clusters in α-Fe using different potentials and this is now underway in this laboratory.

By generating sufficient statistics, it is possible to estimate the activation energy for a sessile cluster to convert into a glissile one (Section 4). Despite the variability of data, the mean value of the lifetime is well described by the Arrhenius relation, and the estimated activation energy for the sessile-to-glissile transformation for clusters of types A and C is between 0.35 and 0.5 eV. It is of interest to note that this range overlaps the experimental value of activation energy associated with motion of small interstitial clusters in stage II (150–200 K) of resistivity recovery in α-Fe irradiated with electrons at low temperature in [21]. In this experiment a substage at 185 K was observed, which becomes more pronounced at higher irradiation dose and shifts to lower temperature, suggesting that it is related to the migration of small interstitial clusters formed by the interaction of single SIAs during annealing stage I. Recent MD simulations [22] have shown that the activation energy for migration of small glissile clusters is within the range of 0.024–0.030 eV, one order of magnitude less than the values suggested by the experiments. The present simulations suggest that the interpretation of stage II recovery in α-Fe should be reassessed to incorporate the thermally assisted transformation of small sessile clusters to the glissile form.

The interactions between sessile clusters and other defects simulated here were chosen for illustrative purposes. No attempt has been made to analyse the long-range interactions by elasticity theory: that would be a major task. However, a clear result to have emerged is that small mobile SIA clusters can be attracted to, and easily absorbed by, some sessile clusters (types A and C), and repelled by the 8-SIA sessile cluster (type B) due to its symmetric three-dimensional nature (Fig. 1(b)). Interestingly, the 8-SIA defect grows by capturing single interstitial atoms because a single interstitial can change its direction of migration due to the interaction and can be easily absorbed. A small cluster, however, migrates one-dimensionally along the ⟨111⟩ axis of its crowdions, and is repelled by the 8-SIA sessile cluster if its axis lies on the line through the centre of this defect.

It has also been seen that the larger SIA cluster formed by capture of a mobile SIA can convert into the glissile state within a few tens of ps. For example, the 13-SIA sessile defect transformed into a glissile one after capturing a 6-SIA glissile cluster. Moreover, the Burgers vector of the mobile cluster was changed due to this interaction. Previous MD simulation studies of isolated clusters in bcc α-iron have shown that only small ones (of size <4) can change their direction of thermally assisted motion: larger clusters migrate one-dimensionally along the ⟨111⟩ axis of their crowdions, even at high temperature [17–19]. The potential importance of the

example in Section 5.2 is that it demonstrates a mechanism by which a glissile cluster can change glide direction and thus change the kinetics associated with pure one-dimensional transport. By considering the consequences of allowing changes in the direction of the one-dimensional diffusion of SIA clusters, Golubov et al. [16] have recently explained the difference in the damage accumulation between bcc iron and fcc copper, and the development of a random distribution of vacancy clusters into a void lattice. The present investigation provides one example of how a glissile cluster can change its Burgers vector. There are probably other mechanisms, such as interaction with impurity atoms and the internal stress field of other extended defects in the crystal. These mechanisms also warrant further investigation.

7. Conclusions

1. Although most SIAs are created in the form of single defects and glissile clusters in displacement cascades in α-Fe, sessile clusters are also formed and can exist with size range comparable to that of the glissile component. These clusters may be important in subsequent evolution of the microstructure at low temperature.
2. The fraction of sessile clusters has little sensitivity to PKA energy, and is on average 35% of the total cluster population at 100 K and 25% at 600 K. This difference is consistent with the longer lifetime of the thermal spike at the higher temperature.
3. The clusters identified as type A and C can convert into glissile form in less than 500 ps at about 500 K, with an activation energy for the transformation of between 0.35 and 0.50 eV. This suggests that this process should be considered in the interpretation of stage II recovery in α-iron.
4. The sessile cluster of type B, which has a three-dimensional form of high symmetry, is stable for at least 1000 ps at temperatures from 500 and 1500 K.
5. Both single interstitial and vacancy defects are attracted to, and absorbed by, the 8-SIA and 13-SIA sessile clusters. The latter grows up to a 21-SIA cluster, and was then found to convert to glissile form after 320 ps at 300 K. The 8-SIA sessile cluster, on the other hand, can grow to a 19-SIA cluster and remain stable for at least for 1000 ps at 600 K. This is due to the retention of the symmetrical three-dimensional structure.
6. Small glissile clusters such as di- and tri-interstitials can be absorbed easily by the 13-SIA sessile cluster, and it has been observed to convert into a glissile form after 20 ps at 300 K on capturing a 6-SIA glissile cluster. The Burgers vector of the 6-SIA glissile cluster was changed by this interaction, providing a clear example of a way for SIA clusters which glide one-dimensionally to change the direction of their motion.

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