Transport, dissociation and rotation of small self-interstitial atom clusters in tungsten

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Abstract

Numerical calculations have been performed to study the thermal motion of self-interstitial atom (SIA) clusters in tungsten (W). Molecular dynamics simulations show that SIA clusters exhibit a fast one-dimensional (1D) motion along the close packed (111) direction accompanied by a significant mass transport in this direction. A low frequency vibration mode is identified and considered to assist the motion of SIAs. The migration energy of SIA clusters are weakly dependent on their size in the average value of 0.019 eV, which is due to the strong interaction between SIAs revealed by calculating the potential energy curve of artificially moving the SIAs along (111) direction as well as nudged elastic band (NEB) method. The rotation process of SIA cluster is studied by activation–relaxation technique and the results show that SIA cluster presents complex rotation process. Our results on the motion SIA cluster may provide updated understanding on the performance decay of materials related to SIA defects.

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1. Introduction

Divertor region in tokamak fusion facilities experiences high fluxes of 14.1 MeV fusion neutrons and ions (i.e. D, T and He ions) as well as high heat load [1]. Tungsten (W) and its alloys are presently considered as candidate materials for divertor because of their high temperature strength, good thermal conductivity, and low sputter rates [2,3]. Particle bombardment will produce large amount of defects mainly consisting of self-interstitial atoms (SIAs) and vacancies. SIA/vacancy clusters or dislocation loops are formed by aggregation of SIAs/vacancies [4] or directly from cascades [5]. Understanding the evolution of these defects needs the energetic and kinetic properties of SIAs and SIA loops [6–8]. Therefore, the knowledge of the structures and dynamics of SIAs is essential to recognize the performance decay of materials under irradiation.

The most stable configuration of single SIA in iron (Fe) is found to be the (110) dumbbell by ab initio calculations [9]. When the number of aggregated SIAs becomes more than 5, the SIA clusters prefer to align (111) direction [9]. These (111) oriented SIA clusters or dislocation loops can migrate fast one-dimensionally along the close packed direction with low activation energy, which has been predicted by molecular dynamics (MD) simulations [10–12] and then confirmed by experiments [13]. Heinisch and Singh show that the one-dimensional (1D) migration of SIAs plays a crucial role in void lattice formation by kinetic Monte Carlo (KMC) simulations [14]. This 1D migration of SIAs has also been taken into account in rate theory (RT) and the results show that it has significant effects on temporal evolution of defects [15,16].

For single SIA in W, the most stable configuration is (111) crowdion or dumbbell based on ab initio or empirical calculations [17,18]. The energy difference between two configurations is very small and it is believed that the (111) defect can move even at 27 K [19]. MD simulations carried out by Derlet et al. [18] and Dudarev [20] indicate that the diffusion coefficients of SIA clusters exhibit non-Arrhenius behavior, which has been explained by the multistring Frenkel–Kontorova model developed by Dudarev [20]. However, the loop size considered there is either too small (only one in Ref. [18]) or too large (19 and 31 in Ref. [20]). Actually the mesoscale SIA clusters (e.g. di-SIAs and tri-SIAs) play important roles in defect evolution and are regarded as possible sources of the long tail on the experimental annealing spectrum of W [21,22]. The rotation of small SIA clusters contributed to three dimensional (3D) motion of SIAs play an important role in the void lattice formation [23]. In this paper, we focus on the dynamics behavior of N-SIA clusters (2 < N < 7), where N is the number of atoms in a cluster.

By simulation, we have observed that all small SIA clusters have a fast 1D motion along the (111) direction and this 1D motion will produce a significant mass transport in (111) direction. Through vibration analysis, a low frequency vibration mode is identified and considered to assist the SIAs motion. The eigenvector of this
mode shows that the atoms compressed by SIAs (including SIAs) in (1 1 1) direction could move as a whole. The migration energy barriers corresponding to this 1D motion of SIAs are weakly dependent on their size with average value of 0.019 eV. Through inspecting the potential energy curve both by artificially dragging SIAs along (1 1 1) direction and nudge elastic band (NEB) calculations, we have confirmed that there exists a strong interaction between the SIAs and the motion style of SIA is a creeping motion [24].

The rotation process of 2-SIA cluster can be regarded as two SIAs rotate synchronously and parallel to each other in (1 1 0) planes with a 1.307 eV barrier. These results may help us understand the mechanisms of SIAs motion in W and also can be used as input data in mesoscale methods, such as KMC simulation or RT.

2. Computational details

All atomistic simulation results are obtained with MD++ code [25] using a Finnis–Sinclair (FS) [26] type potential modified by Ackland and Thetford [27]. The coordinate axes of the simulation box are oriented along \( x = [1 1 0] \), \( y = [1 1 2] \), and \( z = [1 1 1] \), comprising \( 6 \times 4 \times 12 \) unit cells. The SIA clusters are constructed as the same way in Fe by Osetsky et al. [10]. Specifically, the 7-SIA cluster has a hexagonal shape viewing from the [1 1 1] direction. The positions of SIAs are determined by Wigner–Seitz (WS) cell method [28]. The detailed MD simulation processes can be found elsewhere [29].

It is well known that NEB method [30,31] is effective to obtain the minimum energy path (MEP), saddle point state and migration energy when we know the initial and final state which can be obtained directly from MD simulations.

Vibration analysis is normally used to study the motion of SIAs and the normal vibration modes can be obtained by diagonalizing the Hessian matrix, which is evaluated by a finite difference method and the details are given in our previous paper [29]. In order to reduce the computation cost, we cut a cylinder region containing 1367 atoms, yielding 4101 normal modes. The cylinder radius of 1.2 nm is large enough to include the modes assisting SIA motion.

3. Results and discussion

3.1. 1D motion of SIA clusters along (1 1 1) direction

MD simulations of SIA clusters are performed at 300 K, 600 K and 900 K, respectively. Through visualizing the motion of SIA clusters, we do not find any rotation of SIA clusters even for the smallest cluster of 2 SIAs. This is different from the case in Fe which shows that the migration is three dimensional (3D) for 2-SIA cluster and a mixed 1D–3D motion for 3- to 5-SIAs clusters [32]. Squared displacement of all atoms (ASD) is used to analyze the motion of SIAs and the 1D characteristics can be seen clearly. Fig. 1 shows the ASD of a 7-SIA cluster at 300 K. The [1 1 0] and [1 1 2] components of ASD are both \( \sim 0.105 \) nm\(^2\), which is induced by thermal fluctuation. On the contrary, the large value of ASD in [1 1 1] direction means that the 7-SIA cluster produces a significant mass transport in this direction. This phenomenon also exists in other size of SIA clusters. Similar results have been found by Osetsky et al. when studying SIAs loop motion in Fe and Cu using MD simulation [10,11]. Inspecting the coordinates of atoms during MD simulations, it is found out that those atoms contributing to the [1 1 1] direction mass transport are those in the same row as the SIAs in [1 1 1] direction, which means that the [1 1 1] component of trajectory for mass center of the cluster (MCC) must be correlated with ASD as shown in Fig. 1.

This phenomenon suggests that some particular phonons should contribute to the SIA cluster motion in this direction. According to transition state theory (TST) [33,34], the vibration mode contributing to the jump of SIAs will disappear or significantly attenuate at the saddle point state. Hence the local density of states (LDOS) [35] which projects the phonon density of states on a given atom along a specific direction, can be used to reveal the modes assisting the motion of SIA clusters. The LDOS is defined as:

\[
g'_i(\omega) = \sum_{j=1}^{N} |e'_{ij}|^2 \delta(\omega - \omega_j)
\]

where \( \omega \) is frequency index, \( e' \) is the polarization vector associated to atom \( i \) and \( p' \) is the projected direction vector. Here we only plot the atoms belonging to the interstitial atoms identified by WS method.

Fig. 2 presents LDOS of the initial and saddle point state of 7-SIA cluster jumping, which is defined as that the MCC moves about \( \sqrt{3}/2a_0 \) (\( a_0 \) is the lattice constant of W) along the [1 1 1] direction. The projected direction is [1 1 1] and the projected atom is the corner atom in 7-SIA cluster. A low frequency mode (\( \sim 3.44 \times 10^{11} \) Hz) disappears at the saddle point state as indicated by black arrow in Fig. 2. This mode is called as the (1 1 1) translation mode, and its eigenvector is shown in Fig. 3(a). The plane shown in Fig. 3(a) is a (1 1 0) plane which cuts the center of 7-SIA cluster. We only plot the atoms with large vibration amplitude. It is noticeable that those atoms are in the same row as the SIAs in [1 1 1] direction and are compressed by SIAs (red atoms in Fig. 3(a)). Vibration amplitude of the atoms which are not in the same row as the SIAs in [1 1 1] direction can be ignored, which is clearly seen in

Fig. 1. ASD and MCC of 7-SIA cluster at 300 K. ASD of [1 1 0] and [1 1 2] directions are near zero (\( \sim 0.105 \) nm\(^2\)) compared to that of [1 1 1] direction.

Fig. 2. LDOS of 7-SIA cluster at initial and saddle point state. The projected direction is [1 1 1] direction and the projected atom is the corner atom of 7-SIA cluster.
As pointed out in our previous work, the jump frequency of a SIA exists in phonon spectrum of single SIA[29]. This mode is induced by the compressed field of SIAs and therefore exists universally in phonon spectrum of SIAs. We could expect that the ASD has large value component in compressed direction compared with other directions for the case of SIAs motion in other metals using MD simulations.

3.2. Formalization of SIA clusters jump

To obtain a more detailed understanding of SIA cluster migration, we monitored the jump rate of SIA clusters. The jump frequencies and the migration energy of SIA clusters are also crucial input data for KMC simulations[6,7]. According to Osetsky et al.[11], the jump frequency of a SIA cluster could be described by Arrhenius equation:

\[ \nu_N = \nu_0^S \exp \left( -\frac{E_m^S}{k_B T} \right) \]  \hspace{1cm} (2)

where \( \nu_0^S \) is the attempt frequency, \( E_m^S \) is the migration energy, \( k_B \) is the Boltzmann constant and \( T \) is the absolute temperature.

Arrhenius plot of SIA cluster jump frequency is shown in Fig. 4. Our obtained attempt frequency and migration energy are listed in Table 1. The migration energy of all clusters we concerned here are nearly the same showing weak dependence on the cluster size. Therefore Eq. (2) can be rewritten as[11]

\[ \nu_N = \nu_0^N S^{-1} \exp \left( -\frac{E_m}{k_B T} \right) \]  \hspace{1cm} (3)

where the constant \( \nu_0^N \) is interpreted as the jump frequency prefactor for the single SIA[32] and \( S \) is theoretically explained to take values between 0.5 and 1[12], which are obtained by least-squares fitting to the data in Table 1 as shown in Fig. 5. \( (E_m)_{av} = 0.019 \text{ eV} \) takes the average migration energy of all clusters.

The fact that the migration energy of SIA clusters is nearly independent on their size is an unusual property and uneasy to understand, which also exists in Fe[11], Cu[11] and V[36]. Knowing the potential energy landscape and atomistic details of SIAs’
motion should help us to understand such weak dependence. In order to do this, we use two methods to explore the potential energy surface (PES) of SIA clusters along \((111)\). One is mapping the PES by moving SIAs. The other one is the NEB method. For the sake of clarity, we take 2-SIA cluster as an example.

For the PES of SIA clusters, as we only observed 1D motion of SIA clusters, the actual change of potential energy due to the SIA motion is also 1D along \((111)\). Hence we move the displacement field of SIAs along \((111)\) artificially to map the potential energy change. The displacement vector is defined as \(\mathbf{r} = r_i - r_j\)\(^{60}\), where \(r_i\) is the position vector of atom \(j\) in perfect structure (without any SIAs) whose WS cell contains atom \(i\). The motion of single SIA can be viewed as the motion of displacement field along the close packed direction \([29]\). Consequently, we could move the displacement field of one SIA and fix the other one to explore the change of the potential energy with the relative distance between two SIAs. Fig. 6(a) and (b) show the potential energy change as moving one of SIAs forward and backward respectively. The moving distance of displacement field is about \(\sqrt{3}/2a_0\). The arrows in Fig. 6(a) and (b) indicate the direction of moving the displacement field and the atoms close to them have been displaced. It could be noticed from Fig. 6(a) and (b) that if we fix one of them and displace the other one as far as \(\sqrt{3}/2a_0\), the potential energy change reaches 0.481 eV (Fig. 6(a)) or 0.436 eV (Fig. 6(b)), which are both much larger than the average migration energy \((E_m) = 0.019\) eV, indicating evidently that one of two SIAs cannot jump individually as far as \(\sqrt{3}/2a_0\).

NEB method can give PES along the MEP and is effective to explore the details of atom motion during transition from initial state to final state. Subsequently, we use it to investigate the movement of 2-SIA cluster from one minimum state to the next minimum state along the \((111)\) direction. These two distinct states are minimized from the configurations saved during the MD simulations. Fig. 6(c) shows the potential energy change along the MEP, where the \(\nabla\) and \(\triangle\) indicate two fixed reference points and the arrow shows the motion direction. The left and right blue circles represent initial and final state of SIAs, respectively. The obtained migration energy of 0.025 eV is close to \((E_m)\) which is obtained from Arrhenius fitting of jump frequency. Through visualizing the atomistic configurations along the located MEP in Fig. 6(c), we find that the two SIAs move nearly simultaneously and before the 2-SIA cluster completes a jump, two SIAs drag each other forward in small displacements along \((111)\), which we call creeping motion and will discuss in details in a specific letter \([24]\). The creeping motion is resulted from the fact that the interaction energy between SIAs is sensitive to the relative distance between SIAs, which can be seen from Fig. 6(a) and (b). This strong interaction makes the 2-SIA cluster move like a single SIA, which is the reason that the migration energy of 2-SIA cluster is as low as that of a single SIA.

The inspection of PES for 7-SIA cluster along \((111)\) shows that the energies required to drag center atom (0.343 eV) and corner atom (0.115 eV) are both larger than 0.010 eV obtained from NEB calculation, which indicates that there also exists strong interaction between SIAs. We could safely infer that the 7-SIA cluster carries a creeping motion as well \([24]\). Under this motion picture, the SIAs in one cluster drag each other during the movement and the distance between them keeps being a small value to lower the interaction energy \([24]\).

### 3.3. Dissociation of SIA clusters

The creeping motion of SIA cluster means that the SIAs are tightly “bound”. Moving the displacement field artificially may cause the potential energy to rise abnormally because the atoms are not fully relaxed during the movement. The relative distance of two SIAs reaches \(\sqrt{3}/2a_0\) indicated in the above section at which the two SIAs still interact with each other strongly. In order to fully explore the PES of the SIAs at large range along \((111)\), we investigate the dissociation of SIA clusters using NEB method, which excludes the artificial effect. We still take the example of the simplest 2-SIA cluster.

The MEP of 2-SIA cluster dissociation obtained by NEB method is shown in Fig. 7, where the marked replicas are presented in Fig. 8. The final state of replica 21 in Fig. 8(f) is constructed by moving the displacement field of one SIA and then minimizing the configuration until two SIAs are separated. The MEP of 2-SIA cluster dissociation process shown in Fig. 7 can be divided into three segments I, II and III. In the following, we will give a detailed analysis about the three segments.
In the segment-I in Fig. 7, the potential energy shows a nearly periodic change. The energy change is nearly the same when the system goes from replica 1 to 4, 4 to 6 and 6 to 8. From the atomic configurations shown in Fig. 10(a) and (b), we could find that replica 1 and 4 have similar atom arrangement except that the replica 4 moves in a nearest neighbor distance (\(\sqrt{3}/2a_0\) in BCC structure) in the \((111)\) direction. Thus the potential energy of two replicas are nearly the same. The transition between replica 4 to 6 and 6 to 8 is similar to replica 1 to 4.

In the segment-II, the potential energy shows a significant increase. We present the atomic configurations of replica 10, 13 and 18 in Fig. 10(e) respectively. A remarkable characteristic of these configurations is that the relative distance between the two SIAs becomes large comparing to that of the segment-I. This confirms the results that moving the displacement of SIAs will indeed cause the potential energy increase rapidly as we see in the previous section.

The fact that the potential energy change is small in segment-III means that there is only a weak interaction between the two SIAs. The replica 20 is the saddle point state having the highest potential energy along the MEP. The energy barrier of 2-SIA cluster dissociation is 2.460 eV, which is shown as energy barrier forward (\(E_{bf}\)) in Fig. 7. This large energy barrier indicates that the 2-SIA cluster is very stable. In contrast, there is only a small energy barrier of 0.016 eV for that two individual SIA reacts with each other forming a 2-SIA cluster (\(E_{bd}\) in Fig. 7). This low energy barrier indicates that the SIAs can aggregate along the \((111)\) direction following to the reverse process of dissociation (replica 21 to 1 shown in Fig. 8) even at very low temperature.

Up to now, we could get a full energy landscape of 2-SIA cluster motion in the \((111)\) direction. The large barrier \(E_{bf}\) indicates that the 2-SIA cluster is in a deep basin. Hence it is hard to dissociate two SIAs. But the bottom of basin is flat, which is shown as segment-I of MEP. Consequently the 2-SIA cluster can move easily in the bottom of basin, corresponding to the creeping motion of 2-SIA cluster which requires two SIAs move nearly simultaneously. The energy barrier of falling into the basin \(E_{bd}\) is low, indicating that two individual SIA can react each other along the \((111)\) direction and form a 2-SIA cluster easily.

The calculation process of 2-SIA cluster dissociation and the energy landscape of 2-SIA cluster motion can be easily generalized to other size clusters. Though the absolute value of \(E_{bf}\) and \(E_{bd}\) are different in other size clusters, the motion process is consistent with the 2-SIA cluster. In addition to the further confirmation the results of artificially moving the displacement field of SIAs in the previous section, the discussion of dissociation process also helps us to form an energy landscape of SIAs motion and presents the atomic details of dissociation process which provides a possible growth mechanism of SIA clusters. The results of SIA clusters growth and migration at low temperature indicate that the SIA clusters should be carefully considered in the annealing experiments related to W, which might be required by long time tail on the experimental annealing spectrum [22].

### 3.4. Rotation of SIA clusters

During the total simulation time (3 ns), we do not find any rotations of any SIA cluster. In the object kinetic Monte Carlo (OKMC) simulations [38], the movement of 2-SIA or other SIA clusters is considered to move along \((111)\) direction and cannot change their directions. The key issue is to what extent this assumption is correct. The knowledge about the barriers and attempt frequencies of SIA cluster rotation are essential. It was anticipated that the rotation barriers are much larger than that of 1D motion. However, it is difficult to calculate the rotation barriers because we do not know the processes of SIA cluster rotation. However, the activation–relaxation technique (ART) [39–42] has provided a way to explore the rotation processes of SIA cluster, which needs only the initial state and can find saddle point and final state automatically. In order to make sure the obtained results are independent to the atomic potential we use, all the rotation processes are checked by a new tungsten potential (EAM2 in Ref. [43]).

First, we summarize the characteristics of single SIA rotation: the saddle point state is \((110)\) dumbbell and the rotation happens in \((110)\) plane [18,29]. For bcc structure, the crystal can be represented as an ensemble of atomic strings parallel to the \((111)\) direction. If we observe the crystal from \((111)\) direction, we can see a hexagonal lattice as shown in Fig. 9.

Then, we analyze the possible rotation mechanisms of 2-SIA cluster. Due to the rotation of single SIA only occurring in \((110)\) plane, there are only 3 possible rotation modes of 2-SIA cluster: coplanar, non-coplanar and cross. The coplanar mode is that two SIAs rotate in the same plane in which they locate as P1 shown in Fig. 9(a). The non-coplanar mode is that two SIAs rotate in two parallel planes as shown P2 in Fig. 9(a). If we rotate P2 around the SIA 60° anticlockwise, we will get a case equivalent to P2 which we do not show. The cross mode is that one SIA keeps fixed and the other one rotates in P2 in Fig. 9(a). By performing the ART, we have obtained these three rotation modes of 2-SIA cluster successfully. Fig. 10 shows the atomic configuration and MEP corresponding to 3 different rotation mechanisms. Among the 3 cases, the non-coplanar rotation has minimum energy barrier of 1.307 eV. During the rotation, two SIAs move simultaneously. The saddle point state contains two parallel \((110)\) dumbbells as shown in Fig. 10(d)) obtained. The rotation barrier of coplanar rotation is 1.515 eV with the saddle point state like three parallel \((111)\) dumbbells located in \((110)\) plane as shown in Fig. 10(b). The cross rotation has 1.767 eV barrier and the final state is not stable, which can rotate back into initial state with a small barrier.

The results by using the recent published EAM2 potential [43] have exhibited similar rotation processes and barriers as listed in Table 2. The main difference of two potentials exists in the non-coplanar rotation. The saddle point state (two parallel \((110)\) dumbbells as shown Fig. 10(d)) obtained by AT potential is now a metastable state in EAM2, i.e. the 2-SIA cluster overcomes a 1.257 eV barrier and then a 0.094 eV barrier before finishing rotation. Certainly such a little difference does not change the rotation process.

The rotation mechanism of 3-SIA cluster is analyzed following 2-SIA cluster. Any two of the three atoms determine a plane such as plane P1 determined by 1 and 2 as shown in Fig. 9(b). The third
Fig. 8. Atomic configuration change along the MEP of 2-SIA cluster dissociation. The replicas shown here are those ones marked in Fig. 7. The atoms are colored by its potential energy between $-8.750$ and $-7.435$ eV and visualized by Atomeye [37]. The average potential energy for each atom in the perfect lattice is $-8.900$ eV. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Fig. 9. Hexagonal lattice of bcc structure seen from [111] direction. Each sphere represents an atomic string along [111] direction and the red spheres mean the atomic strings contain one SIA. (a) and (b) have two and three SIAs respectively. The dashed lines across the red spheres show the possible rotation planes of SIA cluster. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)
SIA (labeled 3 in Fig. 9(b)) can only rotate in the plane P1. The rotation barrier is 1.730 eV (using AT potential) or 1.718 eV (using EAM2 potential).

Another important issue related to SIA cluster rotation is the attempt frequency of rotation. The Vineyard formula\(^3\) provides us a method to calculate the attempt frequency \(C\) of SIA rotation, where \(m_{\text{init}}\) and \(m_{\text{saddle}}\) are vibration spectrum of initial and saddle point state respectively. Our calculated attempt frequency of 2-SIA cluster is \(0.3 \times 10^{12}\) Hz, which is close to the typical range \(10^{12} \sim 10^{13}\) Hz being used in KMC simulations\(^4\). Consequently, we take the \(10^{12}\) Hz to be a reasonable estimation of attempt frequency for all SIA clusters. Under the above considerations, the obtained rotation frequency of 2-SIA at 900 K is \(10^{12} \exp(-1.307/0.076) \approx 3.4 \times 10^4\) Hz. This indicates that in our MD simulation time of 3 ns, the 2-SIA cluster only rotates \(1.0 \times 10^{-4}\) times, which is too small to be observed. However, the

\begin{equation}
\Gamma = \frac{\prod_{i=1}^{3} m_{\text{init}}}{\prod_{i=1}^{3} m_{\text{saddle}}}
\end{equation}

Fig. 10. Atomic configuration change and MEP correspond to 3 different rotation modes of 2-SIA cluster. The potential we use is AT potential\(^2\). (a), (b) and (c) are the initial, saddle point and final states of coplanar rotation; (d) and (e) are the saddle point and final states of non-coplanar rotation; (f) and (g) are the saddle point and final states of cross rotation; (h) is the MEP of 3 different rotation modes and the red points are saddle points. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

<table>
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<th>AT</th>
<th>EAM2</th>
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<tr>
<td>Coplanar</td>
<td>1.515</td>
<td>1.572</td>
</tr>
<tr>
<td>Non-coplanar</td>
<td>1.307</td>
<td>1.257</td>
</tr>
<tr>
<td>Cross</td>
<td>1.767</td>
<td>1.957</td>
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Table 2 Rotation barriers (eV) of 2-SIA cluster obtained using AT\(^2\) and EAM2\(^3\) potential.

time of KMC can reach orders of seconds and the temperature varies from several K to about 1000 K [38,45]. Hence the 2-SIA and 3-SIA cluster can rotate during the KMC simulations though the rotation frequency is not very high.

When the size increases to 4 or larger cluster, the rotations of SIA clusters explicit complex processes like the unfulfilling mechanism of trapped SIA clusters in bcc Fe [46]. To describe the complex process, we needs an another long article which will be published in the near future.

4. Conclusion

The motion of \(N\)-SIA clusters \((2 \leq N \leq 7)\) in W and their corresponding mechanisms are studied by numerical methods. The following conclusions are obtained:

(i) SIA clusters undergo a fast diffusion along \((111)\) direction and do not show any rotation during our simulation time (3 ns) even for the smallest 2-SIA cluster, which is different from the case for the SIA clusters in Fe. This fast motion of SIA clusters also results in a significant mass transport in \((111)\) direction, induced by collective motion of SIAs and the atoms compressed by SIAs in \((111)\) direction. A low frequency vibration mode plays a role to assist the collective motion of SIA clusters.

(ii) The migration barriers of SIA clusters are nearly independent on their size. The jump frequency of SIA clusters can be fitted well by Arrhenius formula in an average migration energy \((E_{\text{m}})\) of 0.019 eV.

(iii) The SIAs of all size clusters are tightly bound together and move in a creeping style along \((111)\) resulted from the MEP analysis by NEB calculation. This creeping motion style of SIA cluster makes the migration barrier of SIA cluster is independent on their size. The energy barrier for individual SIA recombination along \((111)\) direction is very low, implying a possible growth mechanism of SIA clusters even at very low temperature.

(iv) The 2-SIA cluster can rotate simultaneously and parallel to \((110)\) plane with a barrier 1.307 eV. The saddle point state presents the atomic configuration in two parallel \((110)\) dumbbells. The rotation of 3-SIA cluster is that one SIA rotates parallel to the plane determined by the other two SIAs with a 1.730 eV barrier. The attempt frequency of SIA cluster rotation is in the order of \(10^{12}\) Hz. These results indicate that we need to consider the rotation of SIA cluster in the KMC or any other long-time/high temperature simulations.

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