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Behavior of a self-interstitial-atom type dislocation loop in the periphery of an edge dislocation in BCC-Fe

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ABSTRACT

The behavior of the dislocation loop of a self-interstitial atom (SIA) near an edge dislocation and its conservative climb process were modeled in body-centered cubic Fe by incorporating loop rotation. The stable position of the loop and its rotational angle due to the interaction with an edge dislocation were evaluated through molecular dynamics simulations and calculations of the isotropic elasticity. The results were used as input variables in kinetic Monte Carlo simulations to model the absorption of the loop by the dislocation via a conservative climb. Loop rotation was found to affect the velocity of the conservative climb only at short-distances because the gradient in the interaction energy between the dislocation and an atom at the edge of the loop, which is a driving force of the conservative climb, could not be precisely evaluated without loop rotation. Depending on the distance between the dislocation and the loop, allowing the loop rotation resulted in either an increase or decrease in the velocity of the conservative climb.

1. Introduction

Ferritic/martensitic stainless steels are potential structural materials for fusion reactors. Although such materials are known to be more resistant to swelling than austenitic stainless steels [1], swelling still occurs. At sufficiently high neutron doses, the steady-state swelling rate is constant at approximately 0.2% per displacement per atom (or 0.2%/dpa) [2]. On the microscale, the swelling mechanism is known to be the preferential absorption of self-interstitial atoms (SIAs) by dislocations rather than vacancies. In the operating environment of a fusion reactor with highly energetic neutron irradiation and the corresponding high energies of primary knock-on atoms (E_{PKA}), atomistic simulations have revealed that collision cascades directly create SIA dislocation loops (hereinafter shortened as SIA loops), as well as mono-defects and vacancy loops [3–5]. These SIA loops can glide one-dimensionally because of their low migration energy [6], and they tend to move to stable positions in response to elastic interactions with a stress field, which mainly originates from a dislocation. However, in the case of parallel Burgers vectors, more than just the glide motion is needed for absorption of the loop attracted by the dislocation [7]. For the loop to be absorbed, either a change in the Burgers vector of the loop or a conservative climb is necessary. Previous studies have indicated that large loops containing more than five to seven SIAs hardly change the Burgers vector [8,9]. Based on the results of molecular dynamics (MD) simulations, which showed that the maximum loop size can be as large as 81–100 SIAs for $E_{PKA} = 50$ keV [3], ~25 SIAs for $E_{PKA} = 100$ keV [4], and 89 SIAs for $E_{PKA} = 200$ keV [5], SIA loops formed directly during a collision cascade under fusion reactor conditions have a higher probability of being absorbed via a conservative climb than those under fission reactor conditions. Therefore, a model for the conservative climb needs to be developed to precisely predict the material performance under fusion neutron irradiation.

In this study, we evaluated the absorption process of an SIA loop by an edge dislocation via the conservative climb, where pure body-centered cubic (BCC)-Fe was used as a model metal for

Abbreviations: kMC, kinetic Monte Carlo; MD, molecular dynamics; SIA, self-interstitial atom.

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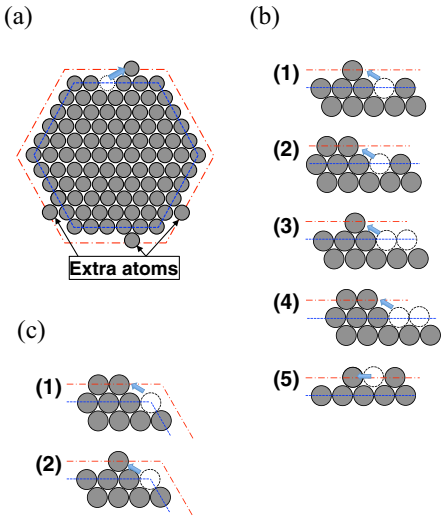

Fig. 1. (a) A hexagonal [111] SIA loop with several extra atoms. (b) Five possible configurations along a line or at a jog that involve ΔE_{tot}: (1) 1.74 eV; (2) 1.03 eV; (3) 0.91 eV; (4) 0.30 eV; (5) 0.72 eV (c) ΔE_{tot} at a corner: (1) 0.30 eV; (2) 0.91 eV

ferritic/martensitic stainless steels. We focused on the case with parallel Burgers vectors because the interaction is the strongest and the probability of the loops being trapped is the highest. We incorporated the detailed loop behavior near the edge dislocation, especially the trajectories and loop shape evaluated by MD and isotropic elasticity calculations. These were used as input variables of the kinetic Monte Carlo (kMC) simulations to quantify the conservative climb motion.

2. Simulation method

2.1. Model of the conservative climb

Since details of the calculation method of the conservative climb process are described in our earlier work [10], they are presented in brief here. We begin with an irregularly shaped [111] SIA loop with some extra atoms on its edges (Fig. 1(a)), which significantly increase the velocity of the conservative climb.

The atoms on the outermost layer migrate along the edges of the loop with an activation energy of E_m. In the meantime, their migration is affected by two terms: (i) the change in the interaction energy of an atom on the outermost layer, with the stress field of the dislocation caused by a change in the distance from the dislocation due to one migrational displacement of the atom (ΔE_{int}); (ii) the change in total energy of the loop after one migrational displacement of an atom caused by a change in the shape of the loop (ΔE_{tot}). Here, we assume that these two contributions were decoupled. These values were evaluated by using the interatomic potential of BCC-Fe in MD or molecular statics simulations [11]. The simulation cell was set to [−2 1 1] 4.1 nm × [0 1 −1] 4.4 nm × [1 1 1] 3.6 nm for the *x*, *y*, and *z* directions, respectively, and periodic boundary conditions were employed in all directions. An extra *x*–*y* plane with a rectangular strip with approximate dimensions of 4.1 nm × 2.0 nm was inserted in the center of the cell to simulate the loop edge. The value of E_m was evaluated by placing a defect along the line of the extra plane and measuring the temperature dependence of the jump frequencies of the defect at 1100, 1200, 1350, and 1500 K; E_m was calculated to be 1.02 eV. For the evaluation of E_{int}, we also placed an atom along the line of the extra plane, and the change in the formation energy of the atom with respect to the local stress was measured:

$$E_{int} = 2.15 \times 10^{-30}\sigma_H + 1.51 \times 10^{-29}\sigma_{[111]}, \quad (1)$$

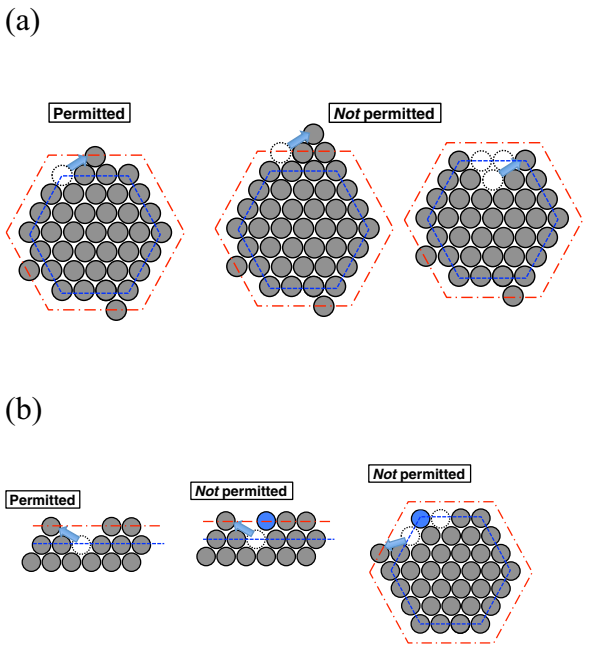

Fig. 2. Examples of the (a) first assumption and (b) second assumption of the migration of an atom.

where σ_H and $\sigma_{[111]}$ denote the hydrostatic and [111] uniaxial components of the stress, respectively. The value of ΔE_{int} was estimated by inserting the stress value at each position calculated by classical dislocation theory. There are five possible configurations that involve ΔE_{tot}, as shown in Fig. 1(b). The value of ΔE_{tot} at a corner was also evaluated by utilizing the results at a jog (Fig. 1(c)). Defining ΔE as the sum of ΔE_{tot} and ΔE_{int}, the activation energy for migration can be described as $E_m + \Delta E/2$.

Two assumptions are made for the simulation of the migration process. First, for the sake of simplicity, defects on the edges cannot be in a double-layered structure (Fig. 2(a)). Second, all atoms (except those at the corners) must have contact with two adjacent inner atoms. The atom at a corner, which, by nature, is surrounded by only one adjacent inner atom and two neighboring atoms on the edges must have contact with the adjacent inner atom and at least one of the two neighboring atoms (Fig. 2(b)). This assumption is necessary because an atom that does not meet the condition (e.g., blue atoms in Fig. 2(b)) would be unstable. Migrations that do not follow these two assumptions are not permitted.

KMC simulations were then conducted to simulate migration process of atoms on the outermost layer over time. The rate of migration of atoms is given as

$$\nu = \nu_0 exp\left(-\frac{E_m + \Delta E/2}{kT}\right), \quad (2)$$

where T and k represent the temperature and Boltzmann's constant, respectively. In our study, ν_0 was set to 10^{13} Hz. Initially, a climb distance (h_{climb} in Fig. 3) was set at approximately 10 nm, and several extra atoms were randomly placed on the edges.

After each migrational event of an atom on the outermost layer, we tentatively set the new center at one of the neighboring atoms of the original center that are nearer the dislocation; we then draw the edges with the new center. If this process reduces the number of defects on the edges, a conservative climb is considered to have occurred. Then, we restart the calculations by setting the new center and modifying the number and positions of defects; The value of h_{climb} was decreased by the projection of the distance between the original and new centers toward the h_{climb} direction (approx-

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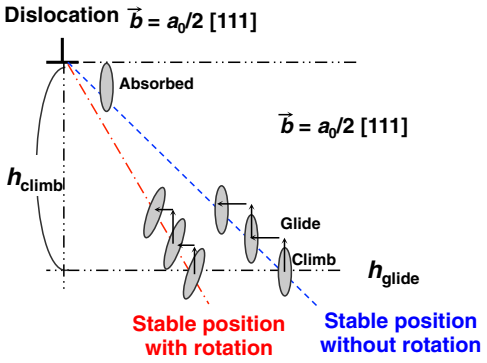

Fig. 3. Schematic illustration of trajectory of a loop.

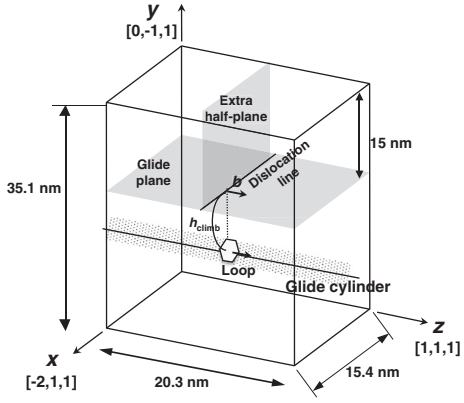

Fig. 4. MD simulation cell.

imately 0.2 nm for each step) in association with the change in h_{glide}. This process was continued until the loop was absorbed and $h_{climb} \approx$ loop radius.

Fig. 3 shows a schematic illustration of the trajectory of the loop near the dislocation [12]. Through a combination of glide and conservative climb, the loop moves in a zigzag motion along its stable positions. At a certain h_{climb}, a stable position of the loop along the glide cylinder (h_{glide}) can be derived by calculating the interaction energy between the dislocation and loop with a pure edge (without loop rotation). This calculation is conducted using classical elasticity theory. Since the glide of the loop to the stable position occurs immediately, we assume that the time required for the loop to be absorbed is equal to the total time required for the conservative climb motion only. When loop rotation is incorporated, the value of h_{glide} changes and it is located nearer the dislocation [12,13]. Consequently, the velocity of the conservative climb may change. In this study, h_{glide} and the associated rotational angle therein were derived through both MD simulations and elasticity calculations. Details of the method are described in the following subsections. The obtained results with loop rotation were used as input for the kMC simulations of the conservative climb.

The loop was set to have 4, 5, or 6 atoms on each edge ($l = 4$, 5,or 6), and the temperature was varied from 673 to 973 K. For each set of conditions, 40 repeated kMC simulations were performed either with or without loop rotation.

2.2. MD simulations

MD simulations were performed by using the LAMMPS code [14] and the interatomic potential of BCC-Fe [11]. Fig. 4 shows a schematic diagram of the simulation cell. The axes of the cell were set to [−2 1 1], [0 −1 1], and [1 1 1], and the dimensions of the cell were approximately 15.4, 35.1, and 20.3 nm in the *x*, *y*, and *z* dir ections, respectively. Periodic boundary conditions were applied in the *x* and *z* directions, whereas a free boundary was applied in the *y* direction. We placed an edge dislocation with the Burgers vector of $\vec{b} = a_0/2[111]$ and a hexagonal SIA loop with the parallel Burgers vector. The diameter of the SIA loop was set at 1.64, 2.10, and 2.57 nm for $l = 4$, 5, and 6, respectively. Initially, the loop was positioned exactly beneath the extra half-plane at a temperature of 500 K, and h_{climb} was set to be very small (at approximately loop radius) such that the loop and the extra half-plane would not be in physical contact. The cell was relaxed through conjugate-gradient energy minimization, after which the simulation continued with a constant time step of 1.0×10^{-15} s.

The rotational angle was determined by fitting a plane to the atoms along the loop edges using the least-squares method. The stable position and rotational angle were calculated and evaluated by averaging the recorded values at 0.2-ps intervals from 12 to 52 ps. The longer simulation time did not strongly change either of the results, but values that significantly differed from the others were excluded.

These calculations were repeated by increasing h_{climb} by one atomic diameter at a time until h_{climb} became larger than the loop diameter; beyond this distance, the approximation of an infinitesimally small loop was applicable.

2.3. Elasticity calculations

In the elasticity calculations, the circular loop was assumed to change its habit plane under the stress field originating from the dislocation. The stable position and rotational angle of the loop were evaluated by minimizing the sum of the interaction energy and self-energy, both of which are affected by loop rotation. The methods of calculation are described in detail in the literature [12, 13].

3. Results and discussion

3.1. Stable position and rotational angle of the loop

Fig. 5 compares the results of the elasticity calculations and MD simulations. At large distances (i.e., $h_{climb} \geq d$, where d is the loop diameter), incorporating loop rotation (data shown in purple) causes a significant difference in the stable position when compared to that without loop rotation (data shown in black). The difference is as large as 1.0 nm at the farthest position from the dislocation. When $h_{climb} \approx d$, which is the limit for the applicability of the infinitesimally small loop approximation, the results of elasticity calculations incorporating loop rotation agree quite well with the MD results (data shown in red), with a variation of approximately one atomic diameter. When the loop further approaches the dislocation (i.e., $h_{climb} \leq d$), the MD simulations revealed that the rotational angle of the loop becomes small, with its stable position nearly beneath the extra half-plane. All of these results were used as input for the kMC simulation.

3.2. kMC simulations

Fig. 6 shows an example of the loop behavior during the conservative climb process. It begins with six extra atoms placed on the edges of the loop with $l = 5$ (Fig. 6(a)). The atoms start preferentially migrating along the edges to positions that are nearer the dislocation (Fig. 6(b-1)). Because the change in the center from *C* to *C′* reduces the number of defects, we define a conservative climb has occurred, with a new configuration as shown in Fig. 6(b-2). It should be noted that for a regular hexagonal loop, the velocity of the conservative climb is very low at 973 K; consequently, it requires several hundred seconds for the SIA loop to be absorbed

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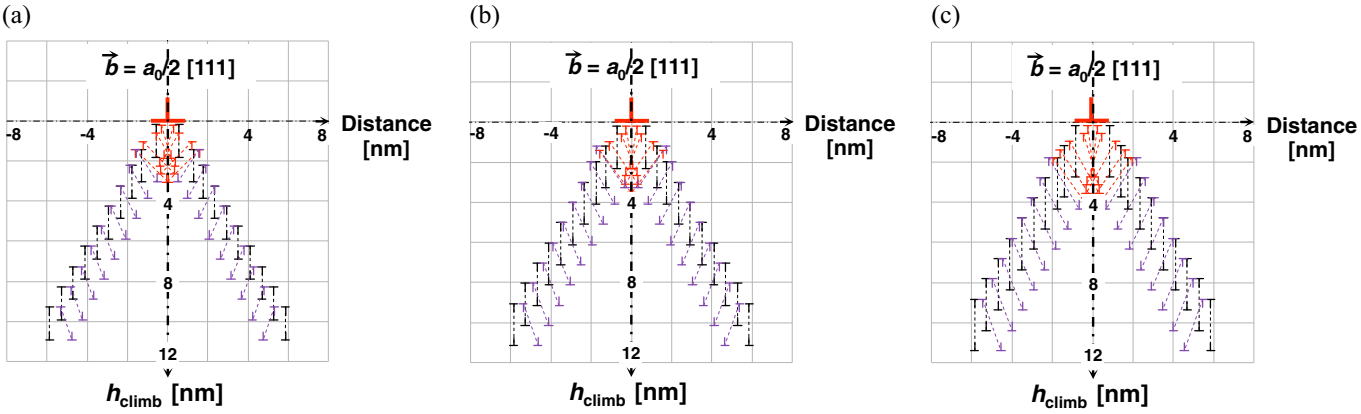

Fig. 5. Stable position and rotational angle of the loop calculated by MD simulations (red), elasticity with loop rotation (purple), and elasticity without loop rotation (black): (a) loop diameter = 1.64 nm ($l = 4$); (b) loop diameter = 2.10 nm ($l = 5$); (c) loop diameter = 2.57 nm ($l = 6$). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

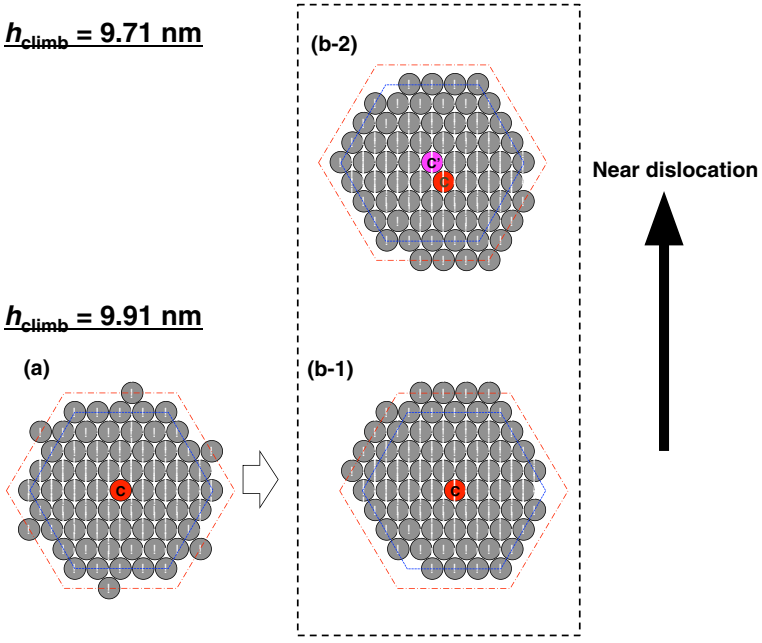

Fig. 6. Changes in the shape of the loop shape during a conservative climb at 773 K for a loop of $l = 5$ with six extra atoms: (a) initial shape; (b-1) after migrations of several atoms; (b-2) loop with the same shape as that in (b-1), with a new center and modified number and positions of defects.

from its initial position at ~10 nm. At lower temperatures, the velocity becomes much lower, which is beyond the limit of our calculation. Because the velocities of regular hexagonal loops or irregular loops with few extra atoms are very low, extra SIAs will have time to reach the loop from the bulk under irradiation, making the loop grow and also increasing its conservative climb velocity. In this study, the initial number of extra atoms was set to four, six, and eight for loops of $l = 4$, 5, and 6, respectively. For these numbers, the conservative climb is observed either with or without loop rotation.

Fig. 7 shows the velocity of the conservative climb. When $h_{climb} \geq 3$ nm, the velocity at 973 K is so high that one motion by the conservative climb takes microseconds. In contrast, the velocity at 673 K is so low that one motion takes several hundred seconds to several tens of kiloseconds. At this temperature, while some of the loops may be absorbed through this slow process, some of them that have been temporarily trapped at relatively high values of h_{climb} may be detrapped owing to thermal fluctuations or interaction with the stress field from other sources. Other loops may acquire more SIAs or SIA loops from the bulk to grow into larger loops that would take much longer to be absorbed.

The velocity of the conservative climb in the region of $h_{climb} \geq 3$ nm is found to be inversely proportional to the square of the distance between the dislocation and the loop, which agrees with a prediction according to the Einstein equation [10]. This dependency is found for all loop sizes and temperatures employed in this study. In this region, the loop rotation does not significantly change the results because the difference between E_{int} at the position closest to and that farthest from the dislocation does not change significantly with loop rotation, even though the loop rotation changes E_{int} to a certain extent. Allowing loop rotation changes h_{glide} by up to 1 nm at the farthest position. However, it does not alter the velocity of the conservative climb motion, even though the motion is induced by a change in the interaction energy due to only one migrational displacement of an atom (~0.23 nm) on the outermost layer.

On the contrary, when the loop approaches the dislocation ($h_{climb} \leq 3$ nm), the velocity of the conservative climb with loop

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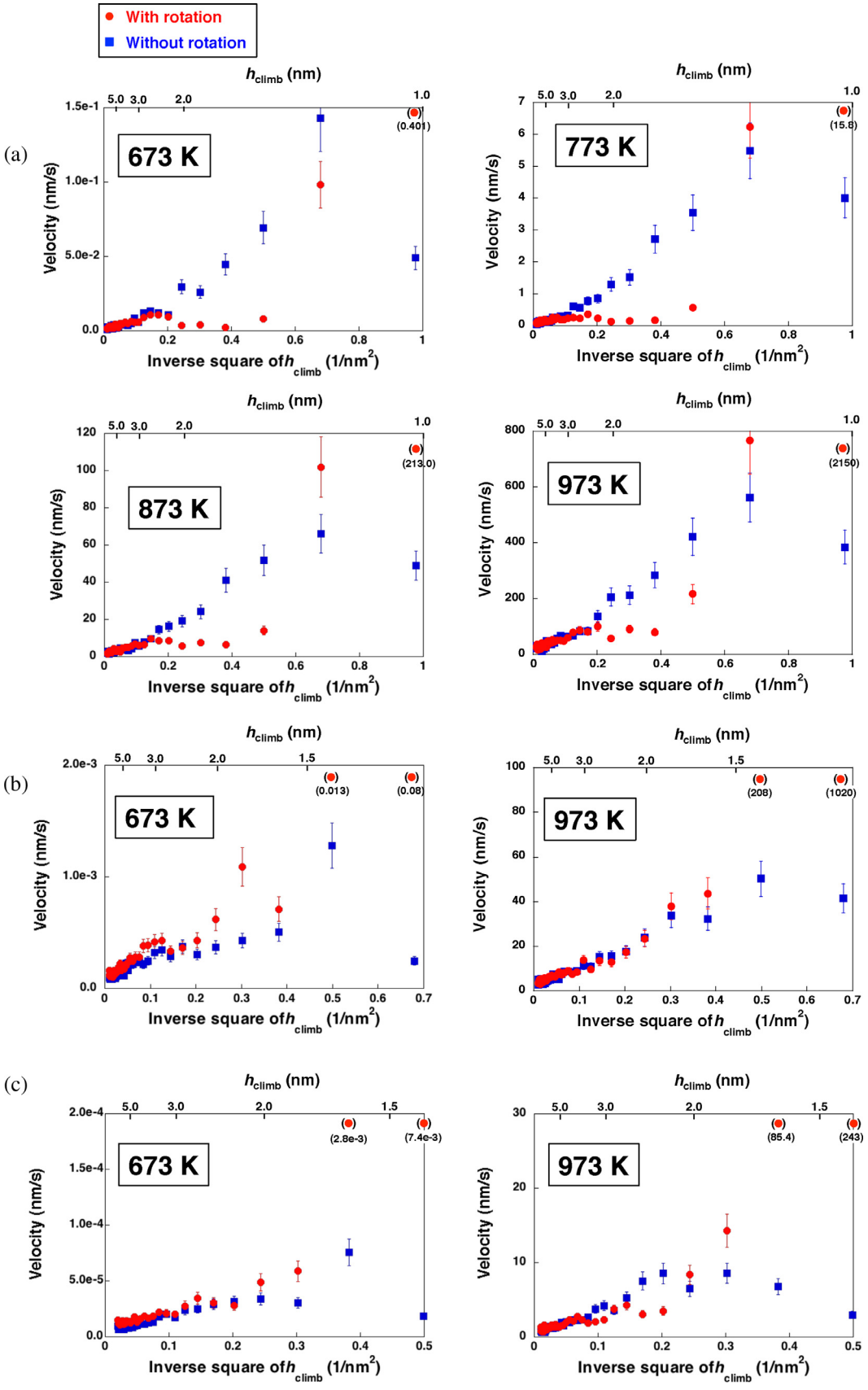

Fig. 7. Velocity of the conservative climb: (a) $l = 4$; (b) $l = 5$; (c) $l = 6$.

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rotation does not follow the Einstein equation. The velocity with loop rotation is lower in most of the loop positions, but it becomes much higher when the loop moves further toward the dislocation at the first and second closest positions. The velocity decreases with loop rotation because the interaction at the closest position to the dislocation is not the strongest with loop rotation. The reduction in the velocity is apparent for the smaller loop of $l = 4$; it becomes less significant with increasing loop size. Meanwhile, at the first and second closest positions, where the increase in the velocity of the conservative climb is observed with loop rotation, the loop is nearly beneath the extra half-plane, i.e., $h_{\mathrm{glide}} \sim 0$. At these positions, the velocity is underestimated without loop rotation. The difference becomes more significant with increasing loop size: several times at $l = 4$, and a factor of several hundred at $l = 6$. Hence, the loop rotation must be incorporated for a more precise quantitative investigation of the absorption process via the conservative climb, especially at short-distance to evaluate the stable position of a loop at any size.

4. Conclusions

MD simulations and isotropic elasticity calculations were conducted to evaluate the interaction without physical intersections between an edge dislocation and an SIA loop with $l = 4$–6 in BCC-Fe. The stable position of the loop and rotational angle were obtained by using both methods. The results of the two methods showed good agreement at the limit of applicability of the approximation of an infinitesimally small loop. These results were used as input in kMC simulations of the conservative climb process to evaluate the effect of loop rotation.

Loop rotation did not affect the calculated velocity of the conservative climb for loops at any size when $h_{\mathrm{climb}} \geq 3$ nm. However, when $h_{\mathrm{climb}} \leq 3$ nm, allowing the loop rotation decreased the velocity of the conservative climb because the gradient of the interaction energy was modified. The reduction of the velocity with loop rotation was more apparent for a smaller loop. In contrast, the velocity with loop rotation increased significantly in the region very close to the glide plane of the dislocation, where the loop tended to move beneath the extra half-plane. Therefore, loop rotation must be incorporated for a model that describes the absorption process by a dislocation through the conservative climb of loops at any size.

Acknowledgments

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