Activation energy and saddle point configuration of high-mobility dislocation loops: A line tension model

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We report an analytical study of thermally activated motion of perfect dislocation loops with high mobility in terms of an elastic model, where the dislocation loops are assumed to be smooth flexible strings under the influence of a potential barrier. The activation energy and saddle point configuration of the dislocation loops are analytically expressed within the present model. The activation energy monotonously increases with the loop length and converges to a finite value. However, the features of the thermally activated motion remarkably change depending on the loop length. If the dislocation loops are longer than a critical length L_c, the saddle point configuration is the well-known double-kink type. On the other hand, if the dislocation loops are shorter than L_c, the saddle point configuration is the so-called rigid type, that is, the dislocation loops overcome the potential barrier without changing their shapes except for thermal fluctuations. The former is regarded as dislocation-like transport, while the latter is point-defect-like migration. Therefore, as the dislocation loops grow, a transition from point defect to dislocation substantially occurs for the dislocation loops.

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I. INTRODUCTION

Theoretical studies of the thermally activated motion of dislocation loops have been so far performed by molecular dynamics (MD) simulations. However, we have never investigated the motion in the framework of a conventional elastic model. Although such model includes some approximations, it will give a new perspective to the studies. In the present paper, we present an elastic model corresponding to the thermally activated motion of dislocation loops and analytical solutions derived from it.

Prismatic dislocation loops are commonly observed in metals irradiated with high-energy particles.[1] The formation of interstitial-type dislocation loops around displacement cascades in the irradiated metals was first predicted by MD simulations.[2] In particular, one-dimensional (1D) motion of the interstitial-type dislocation loops in a matrix under irradiations plays an important role in the evolution of the damage structure. In fact, the 1D motion of such dislocation loops along a close-packed row of atoms is essential for the total understanding of the void swelling behavior in terms of the so-called production bias model.[3,4]

MD simulations have been extensively performed to study the thermally activated motion of the dislocation loops in the irradiated metals. In the simulations, the interstitial-type dislocation loops are described as clusters of self-interstitial atoms (SIAs) accumulated in a crystal plane, that is, the periphery of the planar SIA cluster corresponds to an edge dislocation loop. The motion of each atom in the simulation box containing the SIA clusters is computed using an empirical interatomic potential. The atomic configuration in finite temperatures and activation energy for the thermal diffusion of the SIA clusters have been calculated in pure metals, especially in α-Fe.[5–8] Special attention has been paid to SIA clusters composed of the so-called "magic number," 7, 19, 37, 61, 91,$\cdots$, SIAs because they are a stable subset of SIA clusters due to the symmetrical hexagonal shape.[5] These simulations show that the SIA clusters are quite mobile and migrate one-dimensionally along the close-packed directions in metals. Such 1D high mobility is intuitively attributed to the similar property of crowdions[9] because an SIA cluster is considered to be composed of the crowdions by taking into account the atomic structure.[5,6] Strictly speaking, $\langle 111 \rangle$ split dumbbells and crowdions are distinguished by Wirth *et al.*[5] but we merely call both of them crowdions in the present paper.

While the motion of the dislocation loops has been studied by MD simulations in advance, we have never investigated it in terms of an elastic model. On the other hand, many phenomena associated with lattice defects in solids have been studied in terms of appropriate elastic models. For example, interaction between moving dislocations and incoherent precipitates in a matrix was initially proposed as the well-known Orowan mechanism[10,11] within the framework of the elastic model, and it has been investigated by MD simulations lately[12] as a result of the increasing power of computational facilities. Needless to say, the results obtained from the original elastic model and those from the MD simulations are usually different. However, the comparison of their results is often very suggestive and fruitful to make progress of the studies. Thus, we undertake an analytical study of dislocation loops within the framework of the conventional elastic model.

One of the plausible elastic models is the so-called line tension model (LTM), where the dislocation is described as a smooth flexible string with line tension under the influence of a potential barrier. This LTM has been so far applied to the investigations of the thermally activated motion of an infinitely long or pinned straight dislocation under the influence of a variety of Peierls potentials.[13–15] Then, the activation energy for thermal diffusion of the dislocation was estimated on the basis of a classical rate theory,[16] that is, the thermally activated process can be described as the so-called minimum energy path from a stable state to another in configurational

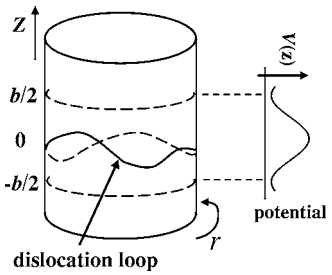

FIG. 1. Dislocation loop within the line tension model (LTM). A flexible edge dislocation with Burgers vector parallel to the z axis is on a circular cylinder. The potential barrier has maximum at $z=0$ and minimum at $z=\pm b/2$.

space; the state with the highest energy along the minimum energy path is the saddle point; the associated activation energy is defined as the energy difference between the saddle point and the initial stable state.

The present work stands on this line of the investigation history and extends this method to the studies of dislocation loops. For this purpose, we introduce a modified LTM, where an edge dislocation loop is bound on the lateral surface of a circular cylinder and its glide motion is restricted within the surface, as schematically shown in Fig. 1. The edge dislocation loop corresponds to the periphery of an SIA cluster in a plane normal to the z axis, and so the Burgers vector is parallel to the z axis in this case. The 1D motion of SIA clusters observed in actual metals and MD simulations is well taken into account in the present model.

We will discuss the validity, reliability, etc. of the present LTM later because this model includes some approximations. We had opportunities to discuss the problems of the present work with some researchers and obtained suggestions. For example, SIA clusters in α-Fe are usually located in the $\{110\}$ plane rather than $\{111\}$.[5] Thus, the direction where SIA clusters in actual metals move do not always correspond to the normal vector of the habit plane. However, such problems will be solved by improving the present LTM in the future. The most serious problem pointed out by them was the influence of the self-interaction between dislocation segments.[17,18] In particular, the motion of small-size dislocation loops had been expected to be crucially affected by the self-interaction. However, we originally ignored the self-interaction within the present LTM without justification to obtain analytical solutions. We will discuss the effect of the self-interaction on the dislocation motion in detail later. Fortunately, the effect is proved to be unexpectedly small.

From now on, we mainly mention interstitial-type dislocation loops in bcc metals, in particular α-Fe, as an example of actual metals. However, the results obtained from the present analysis can be applied to dislocation loops in other crystals, e.g., fcc metals,[19] by making a few modifications on the present model, if the dislocation loops are glissile and unfaulted type.

II. FUNDAMENTAL EQUATIONS

We derive analytical solutions for describing the saddle point configuration of a dislocation loop within the frame-

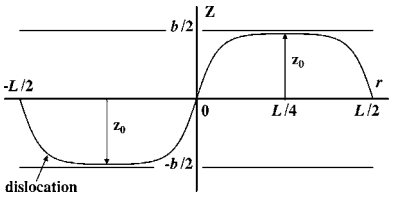

FIG. 2. Schematic view of the saddle-point configuration of the dislocation loop of double-kink type. Parameter z_0 indicates the magnitude of the bow-out of the dislocation.

work of the LTM. The dislocation loop is assumed to be on the lateral surface of the circular cylinder as shown in Fig. 1. The potential barrier $V(z)$ has minimum at $z=\pm b/2$ and maximum at $z=0$. From now on, we display the displacement of the dislocation line on a flat plane as shown in Fig. 2. Thus, the periodic boundary condition is imposed along the horizontal axis. In the case of a straight and infinitely long dislocation, the saddle point configuration is the well-known double-kink-type solution.[13–15] Therefore, we initially assume that the saddle point configuration of the dislocation loop is also the conventional double-kink type solution likely depicted in Fig. 2. The parameter z_0 in Fig. 2 indicates the magnitude of the bow-out of the dislocation. It is a quite important variable to obtain the analytical solutions for the saddle point configuration of the dislocation loop. Although a multiple-kink type solution[20] can also be the saddle point configuration, its total energy is most likely higher than that of the double-kink one.

According to the LTM,[13–15] the total energy E_t of the dislocation loop is written as

$$E_t = \int_{-L/2}^{L/2} \left[\frac{1}{2} \gamma_0 \left(\frac{dz}{dr} \right)^2 + V(z) \right] dr. \tag{1}$$

In Eq. (1), $z(r)$ is the displacement of the dislocation line at the point r, γ_0 is the energy per unit length of the dislocation, and L is the length of the dislocation loop. Strictly speaking, the parameter L indicates the circumference of the circular cylinder surrounded with the dislocation loop. However, we simply regard L as the loop length because it is almost constant during the thermally activated motion, as mentioned later. We here assume that the dislocation line is sufficiently smooth, i.e., the value of dz/dr is small everywhere along the dislocation line. In fact, the maximum value of dz/dr estimated from Eq. (4) is certainly proved to be small afterward.

One obtains the equilibrium condition satisfied at the stable state and saddle point (unstable equilibrium state) as follows;

$$\gamma_0 \frac{d^2 z}{dr^2} = \frac{dV}{dz} \tag{2}$$

One of the trivial solutions to Eq. (2) is

$$z(r) \equiv 0. \tag{3}$$

Then, we look for nontrivial solutions of the double-kink type likely depicted in Fig. 2. Integration of Eq. (2) yields

$$\frac{\gamma_0}{2}\left(\frac{dz}{dr}\right)^2 = V(z) - C_0, \tag{4}$$

where $C_0 = V(z_0)$. By separation of variables, one obtains

$$L = 2\sqrt{2\gamma_0}\int_0^{z_0} \frac{1}{\sqrt{V(z) - C_0}} dz. \tag{5}$$

Inserting Eq. (4) in Eq. (1), and using Eq. (4) again, the saddle point energy E_s is found to be

$$E_s = C_0 L + 4\gamma_0 \int_0^{L/4} \left(\frac{dz}{dr}\right)^2 dr$$

$$= C_0 L + 4\sqrt{2\gamma_0}\int_0^{z_0} \sqrt{V(z) - C_0}\, dz. \tag{6}$$

As a result, we obtain two fundamental equations, (5) and (6), on the basis of the LTM.

We take a sinusoidal function (sine-Gordon) as the potential barrier for the motion of the dislocation loop:

$$V(z) = V_0\left(1 + \cos\frac{2\pi z}{b}\right). \tag{7}$$

Inserting Eq. (7) to Eqs. (5) and (6), we obtain

$$L = \frac{2b}{\pi}\sqrt{\frac{\gamma_0}{V_0}} K(s_0), \tag{8}$$

$$E_s = \frac{4E_0}{\pi}\left(2E(s_0) - \cos^2\frac{\pi z_0}{b} K(s_0)\right), \tag{9}$$

$$E_0 = \sqrt{\gamma_0 V_0}\, b, \tag{10}$$

where $s_0 = \sin \pi z_0/b$, and K and E are complete elliptic integrals of the first and second kinds, respectively,[21]

$$K(k) = \int_0^1 \frac{1}{\sqrt{(1-t^2)(1-k^2t^2)}} dt.$$

$$E(k) = \int_0^1 \sqrt{\frac{1-k^2t^2}{1-t^2}}\, dt \tag{11}$$

In Eq. (10), E_0 means a characteristic energy unit. We add that periodic systems similar to ours have been already investigated, especially in the field of the solitons.[22] Inserting Eq. (7) in Eq. (4), we obtain saddle point configurations of the dislocation loop of the double-kink type, as shown in Fig. 3.

III. ACTIVATION ENERGY AND CRITICAL LENGTH

We mention here a remarkable feature of the thermally activated motion of the dislocation loop on the basis of the analytical solutions. The trivial solution in Eq. (3) can be the saddle point configuration of the dislocation loop of arbitrary length. On the other hand, the conventional double-kink-type solution is restricted with respect to the loop length L, according to Eq. (8). Let us define a critical length here:

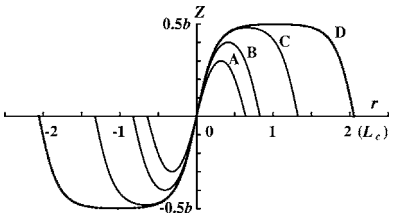

FIG. 3. Saddle point configurations of the dislocation loop of the double-kink type. Lines A, B, C, and D correspond to the analytical solutions for a variety of values of the bow-out of the dislocation, $z_0 = 0.3b$, $0.4b$, $0.48b$, and $0.498b$, respectively. The characteristic length L_c is defined in Eq. (12).

$$L_c = \sqrt{\frac{\gamma_0}{V_0}}\, b. \tag{12}$$

When and only when $L_c < L$, there exists a real solution to Eq. (8), because the complete elliptic integral of the first kind K is larger than $\pi/2$.[21] Therefore, both solutions (trivial and double kink) can be the saddle point configuration simultaneously in the range $L_c < L$. We will soon answer which the true saddle point is. On the other hand, the trivial solution in Eq. (3) is the unique saddle point configuration of the dislocation loop in the range $0 < L < L_c$.

As shown in Fig. 4, the profile of the activation energy E_a drastically changes at the critical length, $L = L_c$. The activation energy E_a is merely proportional to the loop length L in the range $0 < L < L_c$, which is easily explained by considering that the saddle point configuration is the trivial solution. With increasing the loop length L, the two solutions (trivial and double kink) bifurcate at $L = L_c$, and both of them can be the saddle point configuration in the range $L_c < L$. Practically, the double-kink-type solution is realized in this range because the energetically lowest saddle point is chosen among plural saddle points,[16] which is frequently used logic in the field of chemical reactions.[23] In brief, the activation energy E_a is initially proportional to the loop length L as shown by the line A in Fig. 4, subsequently bifurcates at $L = L_c$, gradually increases along the line B, and finally converges to the finite value of $8E_0/\pi$. This value is, of course,

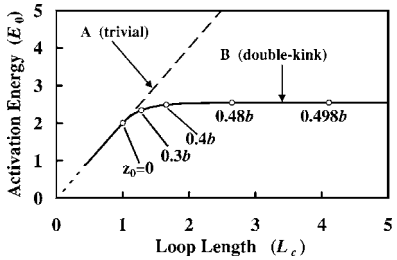

FIG. 4. Activation energy E_a versus dislocation loop length L. Lines A and B correspond to the saddle point energy of the trivial and double-kink-type solutions, respectively. The solid line represents activation energy realized within the present model. The magnitude of the bow-out of the dislocation z_0 is exhibited at some points.

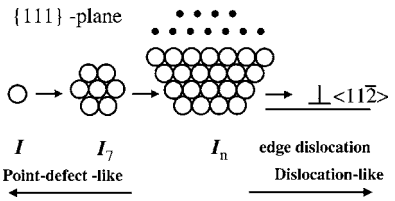

FIG. 5. Schematic view of formation of an edge dislocation in bcc by growth of SIA clusters in the {111} plane. Open circles represent SIAs (crowdions perpendicular to the plane).

equal to the double-kink formation energy on the infinitely long dislocation.[13]

Needless to say, the present analysis is inappropriate to apply to small-size loops where the elasticity theory is not valid. We will estimate the critical length L_c in actual metals later to determine the range in which the present analysis is reliable.

IV. TRANSITION BETWEEN POINT DEFECT AND DISLOCATION

We present a new concept of the thermally activated process of the dislocation loops (SIA clusters) on the basis of the present analysis. SIA clusters in bcc metals are composed of parallel crowdions by taking the atomic structure into consideration. Furthermore, an edge dislocation is also regarded as a large bundle of crowdions.[24] The reason is that the edge dislocation is made up by inserting an extra half-plane composed of an infinite number of SIAs into a perfect crystal. In brief, the single crowdion, SIA clusters of a variety of sizes (dislocation loops), and edge dislocation are essentially the same interstitial-type defects but different in size, as shown in Fig. 5. However, we infer that these SIA clusters should qualitatively change from point-defect-like to dislocation-like somewhere.

We propose that the critical length L_c defined in Eq. (12) would be an appropriate criterion to distinguish between point defect and dislocation. As mentioned before, dislocation loops shorter than L_c are expected to transfer to a next stable state without the double-kink formation, that is, the dislocation loops overcome the potential without changing their shapes except for thermal fluctuations. This so-called rigid motion can be regarded as point-defect-like migration. On the other hand, the dislocation loops longer than L_c transfer with the conventional double-kink formation, which is supposed to be dislocation-like transport. This result implies that a transition between point defect and dislocation substantially occurs for the dislocation loops depending on the loop length.

V. VALUES OF E_0 AND L_c IN ACTUAL METALS

We here estimate the values of E_0 and L_c in actual metals from Eqs. (10) and (12) by evaluating γ_0 and V_0. Although this estimation is somewhat crude, it is available and inevitable to determine the range where the present model is valid. We estimate these values in α-Fe, as an example of actual metals.

To estimate V_0, we assume that the potential barrier of the dislocation loops is identical to the Peierls potential of an infinitely long dislocation, which is plausible for somewhat long dislocation loops. One obtains a relation to calculate V_0 from the Peierls stress τ_P, the minimum external stress to move a straight dislocation, assuming that the potential is the sinusoidal one in Eq. (7),[13]

$$V_0 = \frac{b^2}{2\pi}\tau_P. \tag{13}$$

However, many researchers have extensively investigated the Peierls stress of screw dislocations (τ_P^s) in bcc metals[25,26] but not so much of edge dislocations (τ_P^e) because plastic deformation of actual bcc metals is controlled by the motion of the screw dislocations. *Ab initio* calculations have so far been performed for the screw dislocations.[27] The magnitude of τ_P^s is roughly of order of $10^{-3}G$,[28] where G is shear modulus. On the other hand, there is only a little knowledge about the plastic deformation due to nonscrew dislocations, e.g., a series of microyielding experiment[29,30] and simulations.[31] Anyway, they inferred that the value of τ_P^e should be about an order of magnitude smaller than τ_P^s. Recently, we also estimated as $\tau_P^e = 4\times10^{-4}G$ in α-Fe (Ref. 32) using Finnis-Sinclair potential,[33] which is acceptable in comparison with the above discussion.

About the energy per unit length of the dislocation γ_0, some researchers recommended that it is of the same order as or smaller than core energy.[13,15,34] We made sure that the value of γ_0 is almost constant for long dislocation loops, $L>30b$ by simulations.[32] Accordingly, we here assume that $\gamma_0 = 0.2Gb^2$.

As a result, we obtain the critical length $L_c = 56b$ from Eqs. (12) and (13), and the characteristic energy unit $E_0 = 0.040$ eV from Eq. (10) as one example, where $G = 117$ GPa.[35] Therefore, the activation energies E_a for sufficiently long dislocation loops are estimated as about 0.10 eV. The critical length estimated here, $L_c = 56b$, gives the loop diameter of about $20b$. This size is considered to be large enough for the elasticity theory to be valid. In addition to it, we obtain from Eq. (4) that the absolute value of the gradient of the dislocation line dz/dr is less than 0.036.

VI. INFLUENCE OF SELF-INTERACTION

The influence of the self-interaction between dislocation segments was ignored in the present analysis, which was pointed out as a serious problem by some researchers. Therefore, we discuss the validity of this approximation in detail here. In order to investigate the influence of the self-interaction easily, we introduce two variables, E_1 and E_2, which indicate the magnitude of the self-energy of the dislocation loop at two states within the present model.

E_1: stable state, i.e., $z \equiv \pm b/2$.

E_2: saddle point, i.e., analytical solution derived from Eq. (4) using the sinusoidal potential in Eq. (7).

Strictly speaking, in order to estimate the exact magnitude of the self-energy of the dislocation loop at the saddle point, we should determine the exact saddle point configuration by

TABLE I. Bow-out of the dislocation z_0, loop length, and self-energy of dislocation loops in α-Fe. The self-energies at the stable state and saddle point are E_1 and E_2, respectively, where cutoff lengths ρ_c are $0.707b$, $2.0b$, and $4.0b$. Similarly, loop lengths of the stable state and saddle point are L_1 and L_2, respectively. Differences, L_2-L_1 and E_2-E_1, are written in the parentheses.

	loop length (b)		self-energy (Gb^3)					
			$\rho_c=0.707b$		$\rho_c=2.0b$		$\rho_c=4.0b$	
z_0 (b)	L_1	L_2 (L_2-L_1)	E_1	E_2 (E_2-E_1)	E_1	E_2 (E_2-E_1)	E_1	E_2 (E_2-E_1)
0	<56	…	…	…	…	…	…	…
		(0.0)						
0.3	71.838	71.851	26.262 01	26.263 35	17.660 48	17.661 20	11.965 46	11.965 79
		(0.013)		(0.001 34)		(0.000 72)		(0.000 33)
0.4	92.768	92.787	36.647 81	36.650 09	25.533 08	25.534 42	18.154 08	18.154 84
		(0.019)		(0.002 28)		(0.001 34)		(0.000 76)
0.48	148.345	148.367	66.633 20	66.636 68	48.849 29	48.851 57	37.013 61	37.015 18
		(0.022)		(0.003 48)		(0.002 28)		(0.001 57)
0.498	230.374	230.397	115.173 03	115.177 64	87.548 94	87.552 13	69.147 60	69.150 05
		(0.023)		(0.004 61)		(0.003 19)		(0.002 45)

taking into account the influence of the self-interaction, but it would be difficult. Instead of it, we use here the analytical solution as a substitute for the exact saddle point configuration. Although it is an approximation, we can estimate an upper limit of the activation energy increased due to the influence of the self-interaction, as mentioned later.

It should be emphasized that the contribution of the self-energy to the activation energy is not the absolute value itself but the energy difference between the saddle point and the initial stable state.[16] In addition to it, the self-energy depends only on the dislocation shape.[17] Therefore, as a special case, there is no contribution of the self-energy to the activation energy in the case of dislocation loops shorter than the critical length L_c within the present model, because the saddle point configuration is the trivial solution, that is, the dislocation loops are not deformed at all during the thermally activated motion. On the other hand, we have to actually calculate the self-energy at the saddle point for dislocation loops longer than L_c because they are transformed in the thermally activated motion.

The interaction energy between two dislocations is analytically expressed by a double integral along the dislocation lines.[17] The self-energy is similarly given by the double integral, but a cutoff length (dislocation core size) ρ_c has to be introduced to avoid the energy divergence. We are provided a computer code to calculate the interaction energy of dislocations with arbitrary shapes.[36] Table I shows the magnitude of the self-energies of dislocation loops at the stable state (E_1) and saddle point (E_2) in α-Fe estimated with the computer code. Then, we take a variety of cutoff lengths $\rho_c=0.707b$, $2.0b$, and $4.0b$, and calculate E_2, where $G=117$ GPa, $\nu=0.31$, and $b=0.248$ nm.[35] With increasing the cutoff length ρ_c, the self-energy and its difference E_2-E_1 decrease. As an example, Witrh *et al.* recommended it to be $\rho_c=2.9b$ in α-Fe.[5]

The lines S_i ($i=1,2,3$) in Fig. 6 shows the sum of the original activation energy calculated within the LTM and difference of the self-energies, E_2-E_1, where Gb^3 is estimated as 11 eV in α-Fe. The sum is not necessarily the exact activation energy taking into account the influence of the self-interaction but gives its upper limit. The reason is that the dislocation loops are intuitively most distorted at the saddle point in the thermally activated motion, and so the largest self-energy is achieved at that point. Therefore, the simple sum of the original activation energy and self-energy difference indicates sufficiently large energy for dislocation loops to overcome the potential barrier. Presumably, the exact activation energy taking into account the self-energy is lower than the magnitude of the simple sum by energy relaxation.

In conclusion, if the self-interaction is introduced in the present model, the activation energy most likely increases. However, the values of E_1 and E_2 are very close, as shown in Table I. Thus, the increment is so small that the self-interaction would not greatly affect the motion of the dislocation loops.

VII. DISCUSSION

The thermally activated transport of dislocation loops from a stable state to the next one is investigated within the

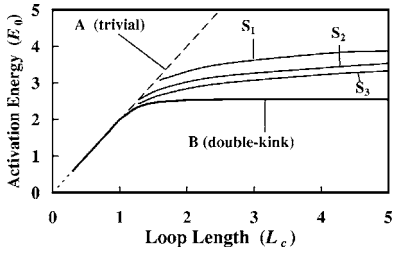

FIG. 6. Upper limits of the activation energy increased due to the influence of the self-interaction. Lines S_1, S_2, and S_3 correspond to the cutoff lengths $\rho_c=0.707b$, $2.0b$, and $4.0b$, respectively. Lines *A* and *B* mean the same saddle point energy in Fig. 4 derived from the LTM.

framework of the conventional LTM. As a result, we find that the saddle point configuration of the dislocation loops changes from the trivial solution to the double-kink one with increasing the loop length, and so the transition between point defect and dislocation is expected. Although the sinusoidal potential is used in the present work, such transition is not related to the specific potential but most likely occurs for many other potentials generally.

We are concerned about the influence of the self-interaction neglected in the present analysis but the effect is small. The reason why the self-energies, E_1 and E_2, are very close is intuitively explained, as follows. According to Table I, the dislocation loops elongate only a little in the thermally activated transport. In addition to it, the critical length is approximately estimated as $L_c=56b$. Therefore, the loop length is sufficiently long compared with the elongation. This result implies that the dislocation loops are deformed only slightly during the thermally activated transport, and so the associated fluctuation of the self-energy is quite small. Even if the effect of the self-interaction is taken into account, the activation energy would increase only a little, and the value of the critical length introduced to distinguish between point defect and dislocation would also increase only slightly. Anyway, the self-interaction does not greatly affect the qualitative analysis such as the present work.

We have mainly mentioned dislocation loops in α-Fe as an example of actual metals because we have much knowledge about α-Fe by experimental results and simulations. However, the present analysis is generally applicable to dislocation loops in other bcc and fcc metals, if they are glissile perfect dislocations. Furthermore, it is possible to apply this to vacancy loops as well as interstitial loops. However, the present analysis gives the same results for both loop types because the parameters, V_0 and γ_0, of the vacancy loops are the same as those of the interstitial loops. This is a contradiction compared with other works. We have to improve the present work but it has not yet been considered.

We often see that SIAs or SIA clusters make continuous jumps over a few lattice sites in MD simulations. This fact means that the phenomena investigated in the MD simulations are affected by the so-called inertia effect, i.e., dynamical process. On the other hand, the present work is a kind of static method, i.e., the analysis on the basis of finding the saddle point along the minimum energy path in configurational space. The comparison of these results obtained from both methods would be useful for understanding of the thermally activated process. The studies on the basis of the minimum energy path have been performed in some fields lately, since an excellent algorithm (nudged elastic band method) was established to find the saddle points in systems with large degrees of freedom.[37] It has been applied to the research on the thermally activated motion of a straight dislocation[38] and crack tip[39] in crystal lattices.

The mechanism for the thermally activated transport of the dislocation loops (or SIA clusters) in metals has still been controversial. Osetsky *et al.*[6] showed the activation energies of SIA clusters in α-Fe do not depend on the cluster size (0.021–0.024 eV) and suggested that crowdions composing the SIA clusters independently migrate. This energy dependence is similar to our result for sufficiently long dislocation loops. However, we rather assume a kind of collective motion of each dislocation loop from a stable state to the next one. Soneda *et al.*[7] and Marian *et al.*[8] obtained similar results: the migration energies are calculated for SIA clusters composed of up to about 20 SIAs; the single and small SIA clusters, I_2 and I_3, have somewhat larger migration energies than others. Wirth *et al.*[5] investigated SIA clusters composed of "magic number" SIAs; the activation energies for I_{19} and I_{37} are 0.023 eV and 0.052 eV, respectively. The main reason why these results are different is that they used different interatomic potentials.

VIII. SUMMARY AND CONCLUSIONS

We study the thermally activated motion of the perfect dislocation loops within the framework of the conventional line tension model (LTM). The dislocation loops correspond to the periphery of self-interstitial atom (SIA) clusters. The associated activation energy is calculated from the saddle point configuration of the dislocation loops. We obtain analytical solutions for the saddle point configurations of the dislocation loops and the critical length L_c. The saddle point configurations are classified into two types, i.e., trivial solution and double-kink-type one. According to the classification, dislocation loops shorter than L_c are regarded as point defect. On the other hand, longer ones are the conventional dislocation. As a result, we propose the transition of the dislocation loops between point defect and dislocation. We estimate the critical length as $L_c=56b$ and characteristic energy unit as $E_0=0.040$ eV in α-Fe, as an example of the actual metals. The influence of the self-interaction of the dislocation loops is not initially considered in the present work. However, the influence is proved to be small, and we conclude that it does not seriously affect the motion of the dislocation loops.

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