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Thermally activated transport of a dislocation loop within an elastic model

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Abstract

We report thermally activated transport of a dislocation loop in terms of a line tension model, where the dislocation line is assumed to be a flexible string. According to conventional rate theory, the features of thermal activation are determined by the saddle-point geometry in high dimensional configuration space. If the circumference of a dislocation loop L is longer than a critical length L_c, the selected saddle-point configuration is the well known double-kink type solution. On the other hand, the manner of the thermal activation of a dislocation loop shorter than L_c is rather point-defect-like. In the present work, we pay attention to the temperature dependence of transition rate which is represented such as $v_0^* \exp(-E/k_B T)$. The pre-exponential factor depends on temperature like $v_0^* \sim T^{-1/2}$ for sufficiently long dislocation loops on the basis of the analysis.

1. Introduction

Prismatic dislocation loops are nucleated in metals by high-energy particle irradiation. In particular, interstitial loops in BCC metals are quite mobile along a close-packed direction and considered to play an important role in the microstructural evolution in irradiated metals. In fact, such dislocation loops are assumed to be active sinks for point-defects in terms of the production bias model (PBM) [1,2]. Subsequently, a generalized PBM was proposed, where a part of the interstitial loops have high-mobility [3].

The interstitial loops are regarded as self-interstitial atom (SIA) clusters located in a habit plane. It was first revealed that the SIA clusters (interstitial loops) are nucleated within the cascade region of high-energy radiation damage by molecular dynamics (MD) simulations [4]. Subsequently, the thermally activated transport of a variety size of SIA clusters and single SIA (crowdion) along a close-packed direction has been investigated at finite temperatures by MD simulations to estimate their mobility [5,6]. The correlation between the jumps of an SIA cluster and individual crowdions contained in the cluster has been clarified in a kind of MD modeling [7]. Moreover, the motion of crowdions and SIA clusters has been so far studied in the Frenkel–Kontorova model [8] or a special random-walk model [9] as well.

As mentioned above, a variety of modeling methods have been extensively proposed to study the motion of dislocation loops in metals. However, the thermally activated transport of dislocations,

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in particular straight dislocations, has been so far investigated within the framework of conventional rate theory and elastic model. According to rate theory [10], every atomistic arrangement in the matrix corresponds to a point in high dimensional configuration space, and the transition path (minimum energy path) from a stable state to another must pass through at least one saddle-point. One of the typical elastic models is the line tension model (LTM) [11], where the dislocation is assumed to be a smooth flexible string under the influence of a potential barrier. In particular, Celli et al. [11] inspected the saddle-point geometry to estimate the pre-exponential factor of the Arrhenius' equation for dislocations. The present work follows this line of research history and applies these conventional methods to the studies of the thermal activation of dislocation loops. Needless to say, such modeling includes some approximations, and the obtained results do not always agree with those from MD simulations and other modeling. However, such research may suggest new perspectives to the studies of the thermal activation of defects. In fact, we proposed a substantial transition of the dislocation loops from point-defects to dislocations in our early work [12].

The present model cannot be applied to small-size dislocation loops, where the elasticity theory is not valid. In addition, we ignore the effect of the self-interaction between the dislocation segments, which sometimes comes into question, and we checked the validity of these approximations [12].

2. Line tension model and saddle-point energy

We introduce a modified LTM for the dislocation loop to investigate the one-dimensional transport along the closed-packed axes. The displacement of a dislocation line $z(r)$ is described by the equation of motion, such as

$$\rho_0 \frac{\partial^2 z}{\partial t^2} = \gamma_0 \frac{\partial^2 z}{\partial r^2} - \frac{\partial V}{\partial z}, \tag{1}$$

where ρ_0 and γ_0 are effective mass per unit length and strength of line tension, respectively. Because the circumference of the dislocation loop is assumed to be L, periodic boundary conditions are imposed such as $z(r) = z(r + L)$. We use a sinusoidal function as the potential barrier

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

where b is the Burgers vector. Therefore, two neighboring stable states in the present model are $z(r) \equiv \pm b/2$, i.e. the dislocation loop lying in the potential valley. Thus, the thermal activation of the dislocation loop means the transport from the stable state $z(r) \equiv -b/2$ to the next one $z(r) \equiv b/2$, and vice versa. Equilibrium conditions should be satisfied everywhere on the dislocation line at the stable state and saddle-point.

$$\gamma_0 \frac{\mathrm{d}^2 z}{\mathrm{d}r^2} = \frac{\mathrm{d}V}{\mathrm{d}z}. \tag{3}$$

According to our early work [12], one obtains two kinds of saddle-point configurations of the dislocation loop according to Eq. (3). One of them is the trivial solution

$$z(r) \equiv 0. \tag{4}$$

The other is a double-kink type solution. When the bow-out of the dislocation line is z_0 ($0 \leqslant z_0 < b/2$), the solution is represented as [13]:

$$z_{\mathrm{k}} = \frac{b}{\pi} \sin^{-1}(s_0 \cdot \mathrm{sn}(R, s_0)), \tag{5}$$

where $s_0 = \sin \pi z_0/b$, $R = 2\pi r/L_{\mathrm{c}}$, sn is an elliptic function and the subscript k means kink.

The critical length of the dislocation loop and characteristic energy unit are defined as:

$$L_{\mathrm{c}} = \sqrt{\frac{\gamma_0}{V_0}}b \quad \text{and} \quad E_0 = \sqrt{\gamma_0 V_0}b, \tag{6}$$

respectively.

We obtain the saddle-point energy E_{s} as a function of the loop length L, i.e. circumference of the dislocation loop, as shown in Fig. 1. The trivial solution in Eq. (4) is possible for arbitrary loop

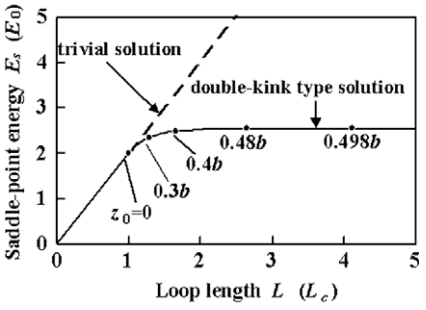

Fig. 1. Saddle-point energy E_{s} versus loop length L [12]. Saddle-point energy for the trivial and double-kink type solutions bifurcate at $L = L_{\mathrm{c}}$. The solid line represents the realized activation energy. The values of the bow-out of the dislocation line z_0 are exhibited at some points.

length. The saddle-point energy E_s for the trivial solution is merely proportional to the loop length $E_s = 2V_0L$ because the potential height is $2V_0$. The double-kink type solution as shown in Eq. (5) exists for the case of $L > L_c$. The saddle-point energy for the double-kink type solution is almost constant and lower than that for the trivial solution. Therefore, the former is selected as the saddle-point configuration in this range.

3. Transition rate of dislocation loop

3.1. Rate theory

According to the conventional rate theory, the transition rate Γ from one stable state to the next one, i.e. the jump frequency, is determined by the geometry of the configuration space, as schematically shown in Fig. 2. The transition rate for a minimum energy path from A to B through the isolated saddle-point P_0 is expressed as [10]:

$$\Gamma = \sqrt{\frac{k_B T}{2\pi}} \frac{\int_S e^{-\phi(P_0)/k_B T}\, dS}{\int_{\Omega_A} e^{-\phi(A)/k_B T}\, dV}, \tag{7}$$

where $\phi(A)$ and $\phi(P_0)$ are the potential energy around the stable state A and saddle-point P_0, respectively. Integration with respect to S is performed over the hyper-surface S which contains the isolated saddle-point P_0 and is perpendicular to the contours of constant ϕ everywhere. Similarly, integration with respect to V is performed over the portion of configuration space to the A-side of the hyper-surface S. Only the integrations in the vicinity of A and P_0 effectively contribute to Eq. (7) because of the Boltzmann factor. Therefore, we employ the theory of small vibrations to approximate Eq. (7) assuming that the potential energy ϕ around A and P_0 can be expanded in Taylor series truncated at the second order terms

$$\phi(A) = \phi_0(A) + 1/2 \sum_{n=0} (2\pi \nu_n q_n)^2, \tag{8}$$

$$\phi(P_0) = \phi_0(P_0) + 1/2 \sum_{n'=0} (2\pi \nu'_n q'_n)^2, \tag{9}$$

where q_n and q'_n are generalized coordinates; ν_n and ν'_n are normal modes. From the physical requirement of the saddle-point, it is necessary that there should be at least one imaginary mode in ν'_n. Inserting Eqs. (8) and (9) in Eq. (7), one obtains an explicit form of the transition rate:

$$\Gamma = \nu_0^* \exp\left[-\frac{\phi(P_0) - \phi(A)}{k_B T}\right], \tag{10}$$

where $\phi(P_0) - \phi(A)$ is the activation energy. The pre-exponential factor ν_0^* is expressed by the normal modes, as mentioned later.

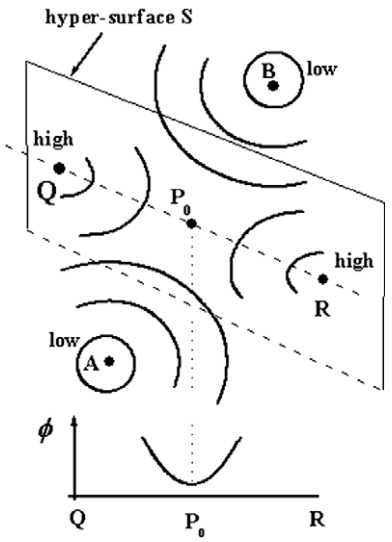

Fig. 2. Schematic view of contours of potential energy ϕ in high dimensional configuration space for a dislocation loop shorter than L_c. Points, A and B, are neighboring stable states and P_0 is isolated saddle-point corresponding to the trivial solution. Hyper-surface S separates the region around A from that around B and passes through P_0. The potential energy profile along the line QR is shown at the bottom of this figure.

3.2. Short dislocation loop, $L < L_c$

The saddle-point configuration of dislocation loops shorter than L_c is the trivial solution, as pointed out in the previous section. Therefore, normal modes about A and P_0 are analytically calculated from the equation of motion Eq. (1) as:

$$\nu_n^2 = \frac{V_0}{\rho_0 b^2}\left(\frac{L_c^2}{L^2} n^2 + 1\right) \quad \text{about } A, \tag{11}$$

$$\nu_n'^2 = \frac{V_0}{\rho_0 b^2}\left(\frac{L_c^2}{L^2} n^2 - 1\right) \quad \text{about } P_0, \tag{12}$$

where $n = 0, 1, 2, 3, \ldots$ and L_c is the critical length defined in Eq. (6). The frequency ν'_0 about the saddle-point P_0 is imaginary and called 'longitudinal transition mode'. By removing this unstable mode, the pre-exponential factor in Eq. (10) is expressed [10,11]

$$\nu_0^* = \prod_{n=0}^{\infty} \nu_n \left(\prod_{n=1}^{\infty} \nu'_n \right)^{-1}. \tag{13}$$

Inserting Eqs. (11) and (12) in Eq. (13), the pre-exponential factor is estimated as:

$$\nu_0^* = \sqrt{\frac{V_0}{\rho_0 b^2}} \sqrt{\frac{\sinh(\pi L/L_c)}{\sin(\pi L/L_c)}}. \tag{14}$$

The profile of ν_0^* is shown in Fig. 3.

3.3. Long dislocation loop, $L > L_c$

The saddle-point configuration of dislocation loops longer than L_c is the double-kink type solution. A schematic view of the potential energy ϕ in the configuration space is shown in Fig. 4. Although the saddle-point P_0 still exists, the energetically lowest saddle-points appear in the configuration space, such as P_1 and P_2. They are continuously distributed because the kink pair can be nucleated anywhere on the dislocation loop. We denote the equivalent saddle-points by the contour F in Fig. 4

The normal modes ν'_n around the double-kink type solution in Eq. (5) are derived from Lamé's equation [13,14], as follows. We assume infinitesimal vibration

$$z(t) = z_k + \xi_n \exp(2\pi \nu'_n t i). \tag{15}$$

Inserting Eq. (15) in Eq. (1) and neglecting the higher order terms, one obtains

$$\tilde{\nu}'^2_n \xi_n = -\frac{d\xi_n}{dR^2} + \{2s_0^2 \,\mathrm{sn}^2(R, s_0) - 1\}\xi_n, \tag{16}$$

where $\tilde{\nu}'^2_n = \rho_0 b^2 \nu'^2_n / V_0$. This equation has an infinite number of eigenvalues, and first three of them are analytically expressed as $\tilde{\nu}'^2_0 = s_0^2 - 1$, $\tilde{\nu}'^2_1 = 0$ and

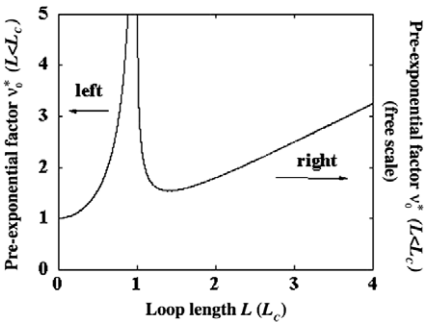

Fig. 3. Pre-exponential factor ν_0^* versus loop length L, and ν_0^* diverges at $L = L_c$. The value for $L < L_c$ (left) is analytically expressed but that for $L > L_c$ (right) is numerically calculated.

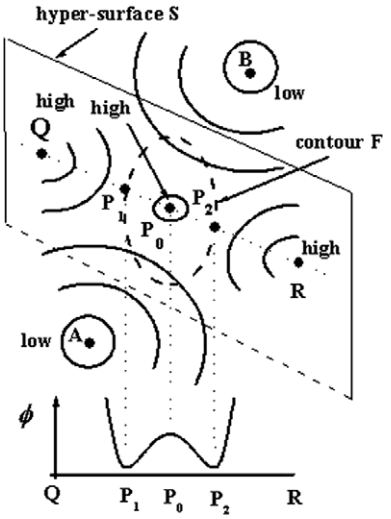

Fig. 4. Schematic view of contours of potential energy ϕ in the configuration space for a dislocation loop longer than L_c. Contour F is located in the hyper-surface S and indicates the continuous distribution of the energetically lowest saddle-points corresponding to the double-kink type solution. Points P_1 and P_2 are on the Contour F, and P_0 is isolated saddle-point corresponding to the trivial solution. Potential energy profile along the line QR is shown at the bottom of this figure.

$\tilde{\nu}'^2_2 = s_0^2$, where $s_0 = \sin \pi z_0/b$. The mode ν'_0 corresponds to the 'longitudinal translation mode' (imaginary frequency) and ν'_1 is called 'transverse translation mode' (zero frequency). In this zero frequency mode ν'_1, both sides of the kink pair move in the same direction, and their net separation is not changed during the vibration. The existence of the transverse transition mode means that Eq. (13) cannot be used directly for the calculation of the pre-exponential factor ν_0^*. In order to solve the problem, we introduce an appropriate cut-off length to perform the integration in Eq. (7), as follows

$$\sqrt{M_k} \int_{-L/2}^{L/2} dq'_1 = \sqrt{M_k} L, \tag{17}$$

where M_k is effective mass of the kink pair. Then, the pre-exponential factor is represented as [11]

$$\nu_0^* = L \sqrt{\frac{2\pi M_k}{k_B T}} \prod_{n=0}^{\infty} \nu_n \left(\prod_{n=2}^{\infty} \nu'_n \right)^{-1}. \tag{18}$$

In the present case of $L > L_c$, the pre-exponential factor ν_0^* depend on temperature as $T^{-1/2}$. Because one of the real modes ν'_2 approaches zero, ν_0^* diverges in the limit of $L \to L_c + \epsilon$ as well. The value of ν_0^* is approximately estimated only by a few

normal modes $\tilde{v}'_n$ obtained from numerical calculations, as shown in Fig. 3.

4. Discussion

The critical length L_c defined in Eq. (6) would be an appropriate criterion to classify the dislocation loops into point-defects and dislocations. If the circumference of the dislocation loops is longer than L_c, the associated saddle-point configuration is the double-kink type solution and activation energy almost independent of the loop length L. These properties indicate dislocation-like transport. On the other hand, the trivial solution is realized as the saddle-point configuration in the case of $L < L_c$, which is regarded as point-defect-like migration. Although the analysis within the framework of the present LTM would be crude, such a transition is intuitively obvious. Small-size SIA clusters should be regarded as point-defects. Furthermore, an edge dislocation is also regarded as an extremely large SIA cluster because it is made up by an infinite number of SIAs filling up an extra half-plane. Thus, the SIA clusters should qualitatively change from point-defects to dislocations somewhere with increasing cluster size.

We calculate the pre-exponential factor v_0^* of the Arrhenius' equation on the basis of the rate theory [10], and it diverges at the critical length $L = L_c$, as shown in Fig. 3. The cause of the divergence is that the small vibration approximation used in Eq. (9) becomes inappropriate at $L = L_c$. If $L < L_c$, the potential energy ϕ is approximately represented by a parabolic shape around the isolated saddle-point P_0, as shown in Fig. 2. However, the bottom of the potential ϕ is supposed to be almost flat at the critical length $L = L_c$. Therefore, it is not appropriate that the potential energy ϕ is expanded in a Taylor series truncated at the second order terms. In order to avoid the divergence, we have to take into account the higher order terms in the expansion of the potential energy ϕ.

In the present work, we find the temperature dependence of the pre-exponential factor of Arrhenius' equation, such as $v_0^* \sim T^{-1/2}$, for sufficiently long dislocation loops. However, the manner of the temperature dependence of v_0^* has been still controversial. The reason is that we have not properly solved the problem of the divergence of v_0^* at $L = L_c$. Anyway, it is one of the typical properties of straight dislocations that v_0^* usually depends on temperature [15]. The present result reflects the dislocation-like transport as well. Finally, we would like to add that Marian et al. [6] also estimated the pre-exponential factor v_0^* on the basis of the normal modes about the stable state and saddle-point.

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References

[1] C.H. Woo, B.N. Singh, Philos. Mag. A 65 (1992) 889.
[2] B.N. Singh, A.J.E. Foreman, Philos. Mag. A 66 (1992) 975.
[3] S.I. Golubov, B.N. Singh, H. Trinkaus, J. Nucl. Mater. 276 (2000) 78.
[4] T. Diaz de la Rubia, M.W. Guinan, Phys. Rev. Lett. 66 (1991) 2766.
[5] B.D. Wirth, G.R. Odette, D. Maroudas, G.E. Lucas, J. Nucl. Mater. 276 (2000) 33.
[6] J. Marian, B.D. Wirth, A. Caro, B. Sadigh, G.R. Odette, J.M. Perlado, T. Diaz de la Rubia, Phys. Rev. B 65 (2002) 144102.
[7] A.V. Barashev, Yu. N. Osetsky, D.J. Bacon, Philos. Mag. A 80 (2000) 2709.
[8] S.L. Dudarev, Philos. Mag. 83 (2003) 3577.
[9] V.A. Ryabov, Philos. Mag. A 82 (2002) 751.
[10] G.H. Vineyard, J. Phys. Chem. Solids 3 (1957) 121.
[11] V. Celli, M. Kabler, T. Ninomiya, R. Thomson, Phys. Rev. 131 (1963) 58.
[12] K. Ohsawa, E. Kuramoto, Phys. Rev. B 72 (2005) 054105.
[13] I. Bakas, C. Sourdis, Fortschr. Phys. 50 (2002) 815.
[14] F.M. Arscott, Periodic Differential Equations, Pergamon Press, Oxford, 1964, p. 191.
[15] J.P. Hirth, J. Lothe, Theory of Dislocations, McGraw-Hill, New York, 1968, p. 484.