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Activation Energy for Double-Kink Formation on a Dislocation Line Estimated in a Finite Temperature 3D Crystal

Kazuhito Ohsawa and Eiichi Kuramoto
Research Institute for Applied Mechanics, Kyushu University
6-1 Kasuga-koen, Kasuga-shi, Fukuoka, 816-8580, Japan
Fax 81-(0)92-583-7767, e-mail:ohsawa@riam.kyushu-u.ac.jp

We report the results of molecular dynamics simulations of thermally activated motions of a screw dislocation under external stress. We investigate behaviors of the dislocation in a wide range temperature, especially the temperature dependence of frequency of the thermally activated motions. An obvious anomaly is found in Arrhenius' plot derived from the present simulations. In low temperature, the dislocation transfers to next Peierls trough through double-kink formation. On the other hand, in high temperature, whole of the dislocation moves toward the next trough all together, which is not expected by string model theory.

Key words: dislocation, Peierls potential, kink, thermal activation, Arrhenius' plot

1. INTRODUCTION

Nowadays, it enables to perform molecular dynamics (MD) simulations of crystal defects in a huge scale lattice model with massive computer. Behaviors of the defects and their migration energies are numerically calculated. For example, interstitial cluster migration processes were simulated at finite temperatures[1,2]. In the present work, we investigate thermally activated motions of dislocations.

Activation energies associated with dislocation transferences to next Peierls trough have been estimated as double-kink formation energies in a string model in which the dislocations have been regarded as a flexible string[3]. The formation energies for various kinds of Peierls potentials were obtained [4,5]. External stress dependences of the formation energies for the various potentials are expressed with simple power laws.

In the present calculations, we simulate thermally activated motions of a screw dislocation over a Peierls barrier under external stress at finite temperatures with MD. We obtain a lot of results about the thermally activated motions (e.g., dislocation line transitions during the activation processes, double-kink formations at low temperatures and activation energy, etc.). Some of the results in low temperature do not agree with the string model theory. In particular, we obtain an anomalous temperature dependence of frequency of the thermally activated motions.

2. COMPUTATIONAL MODEL

We simulate the behaviors of a screw dislocation in a cubic lattice, as shown in Fig. 1. In order to avoid boundary effects, it is desirable to prepare sufficiently large simulation box. In the present model, the length in the z direction parallel to the dislocation line is $201b$, where b is Burgers vector. Periodic boundary condition is imposed on the sides of the simulation box facing to the z direction. On the other hand, the length in the x and y direction is 40 atomic distances. Fixed boundary condition (i.e., the displacements of atoms located on the surface of the simulation box are determined from linear elastic solution) is imposed on the sides of the box facing to the x and y directions. An external shear stress, τ_{xz}, is applied to move the screw dislocation toward the positive y direction.

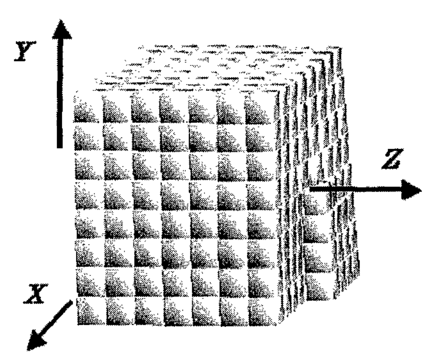

Fig. 1 Screw dislocation lying parallel to the z direction in a cubic lattice.

All atoms in the cubic lattice are allowed to move only to the z direction, i.e., *on rail model* is assumed. If the deformation is small, every atom interacts with six neighboring atoms. The atomic bonds to the z direction are assumed to act as linear interaction. On the other hand, those to the x and y directions are assumed to act as non-linear interaction with cut-off length $b/2$. The non-linear potential used in the present simulations is described as follows

$$V(z) = -\frac{Gb^2}{4\pi^2(1+\lambda)}\left(\cos\frac{2\pi z}{b}+\frac{\lambda}{4}\cos\frac{4\pi z}{b}+1-\frac{\lambda}{4}\right), \quad (1)$$

where z is relative displacement between neighboring two atoms and G is shear modulus. We have still investigated Peierls stress, the least external stress to move a dislocation at 0K, for the non-linear potentials with parameter λ=0.0, 0.5, 1.0, as shown in Fig. 2 [6]. The Peierls stress is very sensitive to the potential shape, as listed on Table I. In the present work, we particularly investigate the case of the shallowest potential with parameter λ=1.0, because the Peierls stress is appropriate compared with experimental results for actual metals [7]. The stable core structure of the screw dislocation for the shallowest potential is shown in Fig. 3, which is 2-fold symmetry [6].

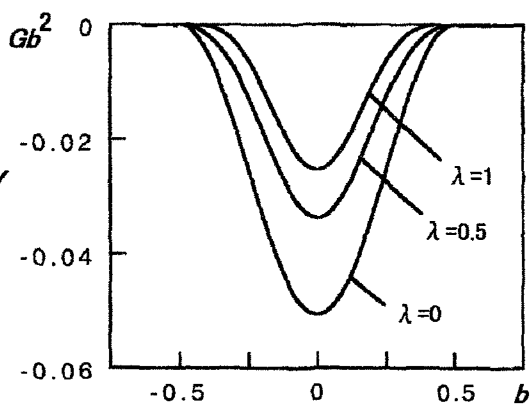

Fig. 2 Non-linear potentials expressed in eq.(1) with parameter λ=0.0, 0.5, 1.0.

Table I Peierls stresses for various depth potentials, where G is shear modulus.

λ	Peierls stress (G)
0.0	1.5955×10^{-2}
0.5	2.335×10^{-3}
1.0	7.20×10^{-4}

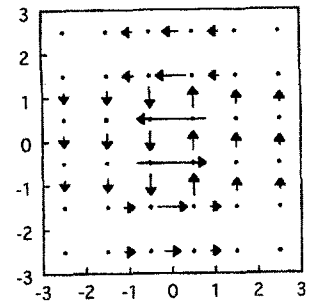

Fig 3 Stable core structure shown by Vitek's representation for non-linear potential with parameter λ=1.0 in Eq.(1).

We should consider correspondence of the present model to actual metals. For this purpose, we try normalization through Debye's frequency [8].

$$\omega_D = 2\pi(9rN/4\Omega)^{1/3}\left(1/c_l^{\,3}+2/c_t^{\,3}\right)^{-1/3}. \quad (2)$$

Since degree of freedom is restricted in the present *on rail model* (i.e., displacement only to the z direction is permitted), the Debye's frequency is estimated as 3.897. We compare this Debye's frequency to actual metals' ones. Approximately unit of time or temperature in the present model corresponds to 10^{-13} sec or 10^5K, respectively, as Table II.

In the present simulations, initial velocity of each atom is assigned from normalized Gaussian distribution. Since natural unit is assumed, the relation between mean velocity, $\langle v\rangle$, and temperature, T, is

$$\langle v\rangle^2 = T \quad . \quad (3)$$

The initial velocity of the i-th atom, v_i, is given as

$$v_i = \sqrt{T}R_i \quad , \quad (4)$$

where R_i is the i-th random variable derived from the Gaussian distribution.

Table II Debye's frequency of Fe, Cu, and the present *on rail model*. Unit of time or temperature of the present model corresponds to the actual metals' one as follows.

	ω_D(rad/sec)	Time (sec)	Temperature(K)
Model	3.897	1	1
Fe	6.205×10^{13}	6.280×10^{-14}	105000
Cu	4.386×10^{13}	8.879×10^{-14}	63500

3. RESULTS OF SIMULATIONS

We calculate the thermally activated motions of the screw dislocation under various external stresses. However, we mention here the results for external stress, $\tau=6.9\times10^{-4}G$, which is about 96% of the Peierls stress, $\tau_P=7.2\times10^{-4}G$. Let's consider the temperature dependence of frequency of the thermally activated motions. The vertical axis, ν, in Fig. 4 represents inverse time span in which a part of the dislocation line becomes a bow-out configuration and starts to transfer to the next Peierls trough. We make lots of pictures and, if necessary, movies like Figs. 5 to determine the time span in a wide range temperature. An obvious bending point appears in the Arrhenius' plot, as shown in Fig. 4. These simulations are performed with four different initial velocity distributions, however the bending point appears in all cases. The temperature range divides into two regions by this bending point. Higher or lower temperature side is named "Region H" or "Region L", respectively. In Region H, the value of ν moderately decreases as temperature decreases. On the other hand, the reduction of ν is quite rapid in Region L.

Figures 5 show transitions of the slip plane in chronological order. The shear strain field on the slip plane (i.e., the relative displacements between two atoms facing across the slip plane) is expressed with colored squares. A red square expresses the relative displacement is larger than $0.5b$ and blue one is less than $0.4b$. Middle displacement between these two extremes is represented by color graduation. The attachments below these figures are time span from the beginning of the simulation. In both figures 5(a) and 5(b), we recognize forward noses and the following surmounting motions over the Peierls barrier. However, the features of thermally activated motions of dislocations in Region H and L are qualitatively different. As shown in Fig. 5 (a), three forward noses simultaneously appear at t=44. Of course, it might be difficult to distinguish true forward nose from thermal fluctuation. However, at least, we suppose that quite wide dislocation segment transfer to the next Peierls trough all together. The following side motion is also very fast and rest of the segment moves to the next Peierls though rapidly. On the other hand, as shown in Fig. 5(b), only one forward nose late appears at t=1788 in low temperature. Before then, nothing happens on the slip plane but thermal fluctuation. The following side motion also slowly propagates.

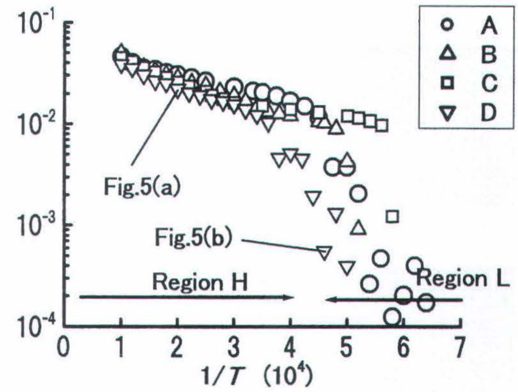

Fig. 4 Temperature dependence of frequency of thermally activated motions simulated from four different initial velocity distributions from A to D. The points marked by Fig.5(a) and (b) are detailed in Figs. 5.

4. DISCUSSIONS

The remarkable result of the present simulation is that the bending point appears in Arrhenius' plot, as shown in Fig. 4. Besides, smooth double-kink does not appear in the higher temperature side, Region H. We suppose that dislocation runs up the Peierls barrier at a dash by thermal support without double-kink formation. On the other hand, clear double-kink formation is observed in Region L. We therefore conclude that the behaviors of dislocations in Region L correspond to the traditional thermally activated process expected by the string model. So, activation energy should be estimated from the results obtained in Region L. According to Fig. 4, we obtain

$$\nu \approx 3.2\times10^{3}\exp\left(-2.9\times10^{-4}/T\right). \quad (5)$$

Though we describe only the case of the external stress, $\tau=6.9\times10^{-4}G$, the bending point always appears in Arrhenius' plot for other external stress, provided that more ambiguous bending point is observed in the case of lower external stress applied.

However, the dislocation behaviors in Region H are still controversial, we suggest a hypothesis. The bending point in the Arrhenius' plot appears around T=0.22$\times10^{-4}$. On the other hand, the deficiency of the applied stress to the Peierls stress is $\tau_P-\tau=0.3\times10^{-4}\,G$. We suppose, when the temperature is close or over the deficiency, dislocation can transfer to the next Peierls valley without double-kink formation.

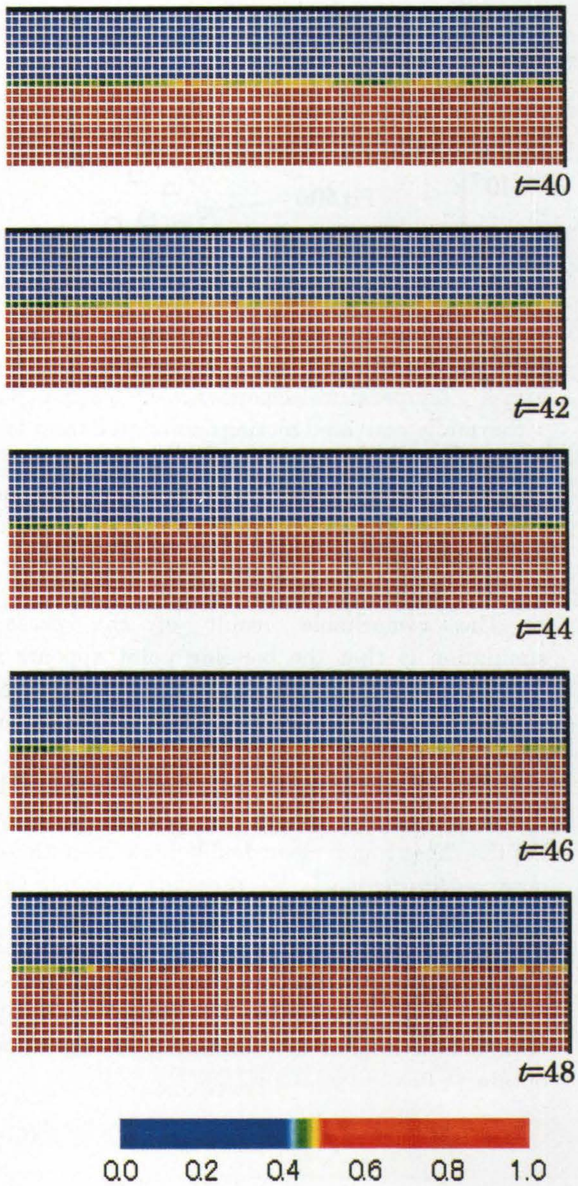

Fig. 5 (a) Transitions of strain field on the slip plane at $1/T$=20000 in high temperature side.

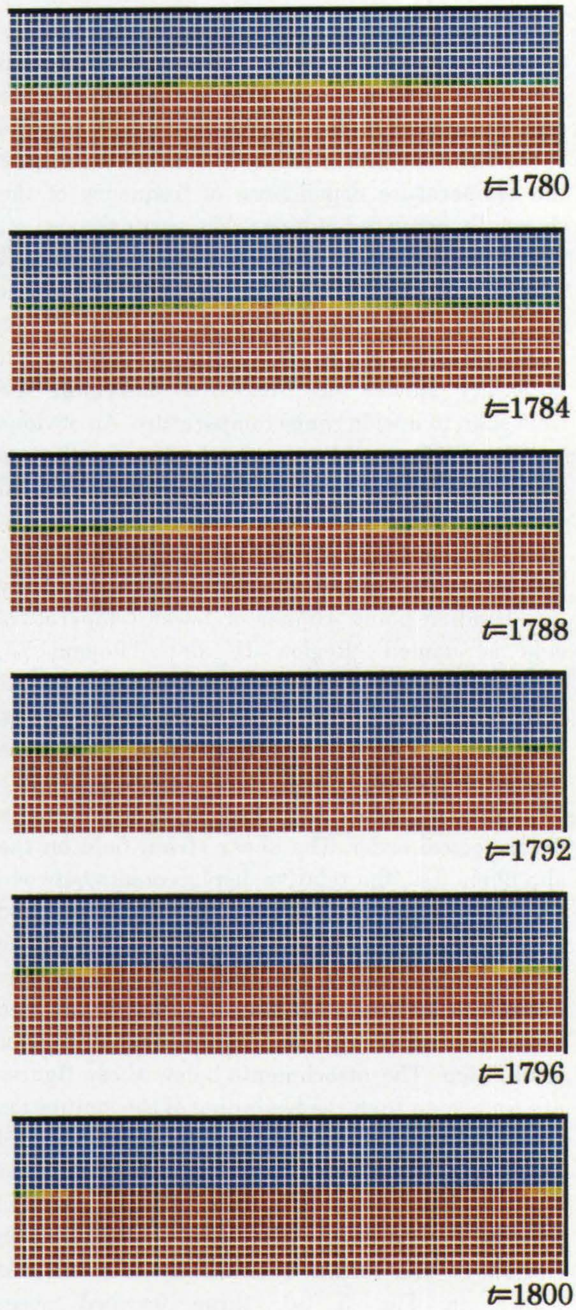

Fig. 5 (b) Transition of strain field on the slip plane at $1/T$=46000 in low temperature side.

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