Journal of Nuclear Materials 386–388 (2009) 188–190

Contents lists available at ScienceDirect

Journal of Nuclear Materials

journal homepage: www.elsevier.com/locate/jnucmat

Interaction mechanisms of glissile loops in FCC systems by the elastic theory

T. Okita [a,*], S. Fujita [b], Y. Yang [a], N. Sekimura [a]

[a] Department of Nuclear Engineering and Management, Graduate School of Engineering, The University of Tokyo, Tokyo, Japan
[b] Department of Quantum Engineering and Systems Science, Graduate School of Engineering, The University of Tokyo, Tokyo, Japan

ABSTRACT

The elastic theory calculations are conducted to clarify the interaction between a large dislocation loop and a small glissile loop in face-centered-cubic systems. In the parallel Burgers vector case, the interaction force changes from repulsive to attractive when the small loop moves along its glide cylinder. In the perpendicular Burgers vector cases, the interaction strongly depends on the spatial position of the glide cylinder of the small loop from the center of the large loop. There are attractive regions in any combinations of the Burgers vectors and spatial positions calculated in this study, which may induce the loop decoration.

1. Introduction

The production and formation of irradiation-induced defects under high energetic particle injections are quite different from that under the electron and light ion irradiation [1], as recent MD simulations demonstrate that high damage energy irradiation directly produces defect clusters as well as Frenkel pairs [2,3]. These clusters, when no longer subject to the rapid Brownian motion, are synonymous with dislocation loops [4]. They are still highly mobile because of their low activation energies, or low Peierls potentials [5,6], and interact with other loops or line dislocations [7–10]. As a result, the growth of larger loops as well as the evolution of network dislocations depends also on the capture rate of these small glissile loops rather than of individual self-interstitials only. Since the mobile directions of the small loops are constraint to specific directions, the growth kinetics of the larger loops under collision cascades are strongly different from that by three-dimensional defect migrations. Therefore, the loop–loop interaction is a mechanism which we should clarify in order to build up models for the microstructural evolution, and resultant macroscopic changes such as void swelling or irradiation hardening, especially under 14 MeV fusion neutrons [3].

In this study, the elastic theory is used to elucidate the loop behavior under the stress field of other loops in face-centered-cubic (FCC) systems. We incorporate the glide motion and rotation of the loop into the model.

2. Calculation methods

We use the equation derived by Wolfer et al. [4], which describes the interaction of a loop with any kinds of stress field. In their study, they remove the constraint of a fixed orientation of the loop, and allow the loop to rotate in order to minimize the energy under the stress field by assuming elastically isotropic solid, the detail of which is written in [4]. The equations used in this study are written as follow:

$$\mathrm{sgn}(\gamma)\sqrt{k(1-k)}\Lambda(k) = |\vec{t}| \cdot sin\gamma \tag{2-1}$$

where γ is the angle between the traction vector $\vec{t}$, and the Burgers vector of the loop $\vec{b}$, the mobile and rotational loop, which we call 'loop A', and

$$\sqrt{k} = sin\alpha \tag{2-2}$$

α is the angle between the Burgers vector and the normal vector of the loop A, defining the rotational angle.

$$\Lambda(k) = \frac{W_0}{A_{a0}} \cdot \frac{2}{\pi k\sqrt{1-k}}\{(1-3k\eta+2k^2\eta)E(k) - (1-k)(1-k\eta)K(k)\} \tag{2-3}$$

W_0 and A_{a0} are the self-energy and the area of the circular loop A, respectively, and η is an empirical factor, chosen to be 1/4. $K(k)$ and $E(k)$ are the complete elliptic integral of the first kind and second kind, respectively. At a given position along the glide cylinder, the angle γ between the traction vector and the Burgers vector is known, while α needs to be determined. Therefore, Eq. (2-1) must be solved numerically for k, and hence for the angle α.

The traction vector exerted on the loop originating from the other loop (hereinafter, we call this loop 'loop B') can be written with the infinitesimal dislocation loop approximation [11],

* Corresponding author.
E-mail address: okita@q.t.u-tokyo.ac.jp (T. Okita).

0022-3115/$ - see front matter © 2009 Elsevier B.V. All rights reserved.
doi:10.1016/j.jnucmat.2008.12.310

$$\vec{t} = \sum_{j=1}^{3} \tilde{\sigma}_{ij} n_j = \frac{\mu A_b}{4\pi(1-\nu)} \cdot \frac{1}{|\vec{r}|^3} \left[\begin{array}{l} \left\{ \frac{3(1-\nu)(\vec{B}\cdot\vec{r})(\vec{N}\cdot\vec{r})}{|\vec{r}|^2} - (1-4\nu)(\vec{B}\cdot\vec{N}) \right\} \vec{b} + (1-2\nu)\{(\vec{N}\cdot\vec{b})\vec{B} + (\vec{B}\cdot\vec{b})\vec{N}\} \\ + \frac{3\nu}{|\vec{r}|^2} [(\vec{B}\cdot\vec{r})\{(\vec{r}\cdot\vec{b})\vec{N} + (\vec{N}\cdot\vec{b})\vec{r}\} + (\vec{N}\cdot\vec{r})\{(\vec{r}\cdot\vec{b})\vec{B} + (\vec{B}\cdot\vec{b})\vec{r}\}] \\ + \frac{3(1-2\nu)}{|\vec{r}|} (\vec{B}\cdot\vec{N})(\vec{b}\cdot\vec{r})\vec{r} - \frac{15}{|\vec{r}|^4} (\vec{B}\cdot\vec{r})(\vec{N}\cdot\vec{r})(\vec{b}\cdot\vec{r})\vec{r} \end{array} \right] \tag{2-4}$$

μ, A_b and ν denote the shear modulus, the area of the loop B, and the poisson's ratio, respectively. $\vec{b}$, $\vec{B}$, $\vec{N}$ and $\vec{r}$ describe the Burgers vector of the loop A, the Burgers vector of the loop B, the normal vector of the loop B and the distance vector between the loop A and loop B, respectively. The infinitesimal small loop approximation will be quantitatively valid when the distance is more than twice as large as the loop radii [10].

In this study, we assume that the loop B, which is a larger loop, does not glide nor does change the normal vector by the stress originating from the loop A, and $\vec{B} = a_0/2[1\ 1\ 0]$, $\vec{N} = \sqrt{2}/2[1\ 1\ 0]$.The shear modulus and the poisson's ratio are set to be 6.50×10^{10} Pa and 0.30, respectively.

3. Results and discussion

In this study, we choose the radius of the loop A (r_a) and loop B (r_b) to be 5.0×10^{-10} m and 2.0×10^{-9} m, respectively, while the closest distance between the centroids of the loops is set to be 3.0×10^{-9} m, which is shown as h in Fig. 1. The preliminary calculations confirm that the change in the energy is proportional to h^{-3}, r_a^2 and r_b^2, which is exactly agreed with the conventional dislocation theory [12]. Even when we include the loop rotation, although the stable position of the loop A is changed by its rotation, the change in the energy at the stable position reveals mostly the same dependencies. This indicates that the calculations conducted in this study by using the specific values of h, r_a, and r_b can be extended to any sizes of loops and any distances.

In both cases shown in the followings, when the Burgers vector of one loop is reversed, only the sign of the interaction energy changes without loop rotation. On the other hand, when we include the loop rotation, the absolute value also changes and the interaction energy becomes smaller.

3.1. Parallel Burgers vectors case, $\vec{B} = a_0/2\ [1\ 1\ 0]$, $\vec{b} = a_0/2\ [1\ 1\ 0]$

Fig. 2 describes the change in the energy as a function of $|x|/h$, which is defined in Fig. 1(a). The interaction can be almost negligible when $|x|/h > 10$, which demonstrates the short-range interaction of the loops. When $|x|/h > 2.0$, the compressive stress of the loop B repels the loop A, and there is an activation barrier at $|x|/h \sim 2.0$, where the stress field of the loop B changes from the compressive to tensile. The loop A comes to the stable position of $|x|/h \sim 0.5$. In this case, the loops never coalesce only by the glide motion. Therefore, when a collision cascade occurs inside of the tensile field of the loop B and directly generates a loop, it will tend to be attracted and come to be aligned near the loop B [13], unless the Burgers vector is changed or climb motions occur.

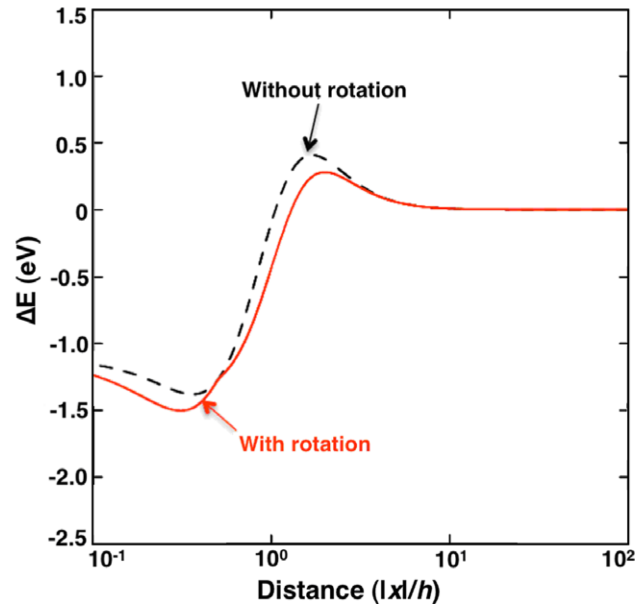

Fig. 2. The change in the energy as a function of $|x|/h$, when $\vec{B} = a_0/2\ [1\ 1\ 0]$, and $\vec{b} = a_0/2\ [1\ 1\ 0]$. x and h are defined in Fig. 1(a).

The activation barrier at $|x|/h \sim 2.0$ becomes smaller when we include the rotation of the loop A, hence some of the loops can overcome the barrier and come into the stable position at higher probability. This indicates that the rotation of the loop enhances loop alignments.

3.2. Perpendicular Burgers vector case, $\vec{B} = a_0/2\ [1\ 1\ 0]$, $\vec{b} = a_0/2\ [1\ 1\ 0]$

In this case, the spatial position for the glide cylinder of the loop A is determined by the angle θ as well as the distance h, as shown in Fig. 1(b). In this study, we choose the specific angles, namely $\theta = 90°$ and $\theta = 0°$. Fig. 3(a) shows the change in the energy at $\theta = 90°$as a function of $|x|/h$. In this case, the potential shows the

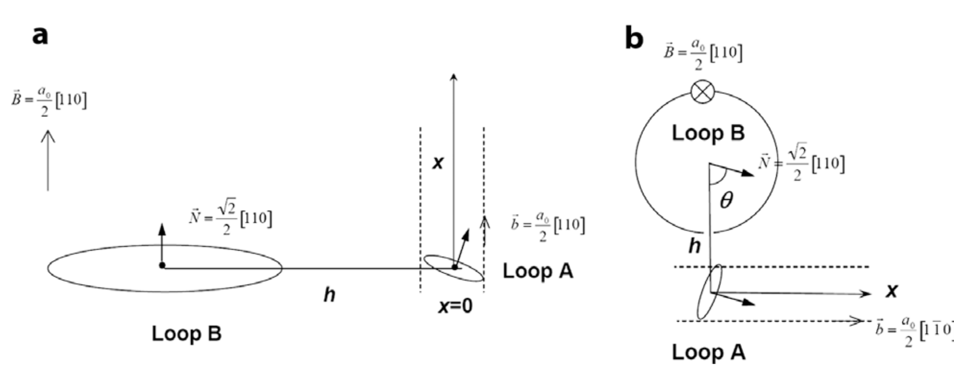

Fig. 1. The spatial relationships between the small mobile loop (loop A) and large loop (loop B). x denotes the glide direction of the loop A, and h the closest distance between the centroids of the loops. (a) the parallel Burgers vectors, and (b) the perpendicular Burgers vectors.

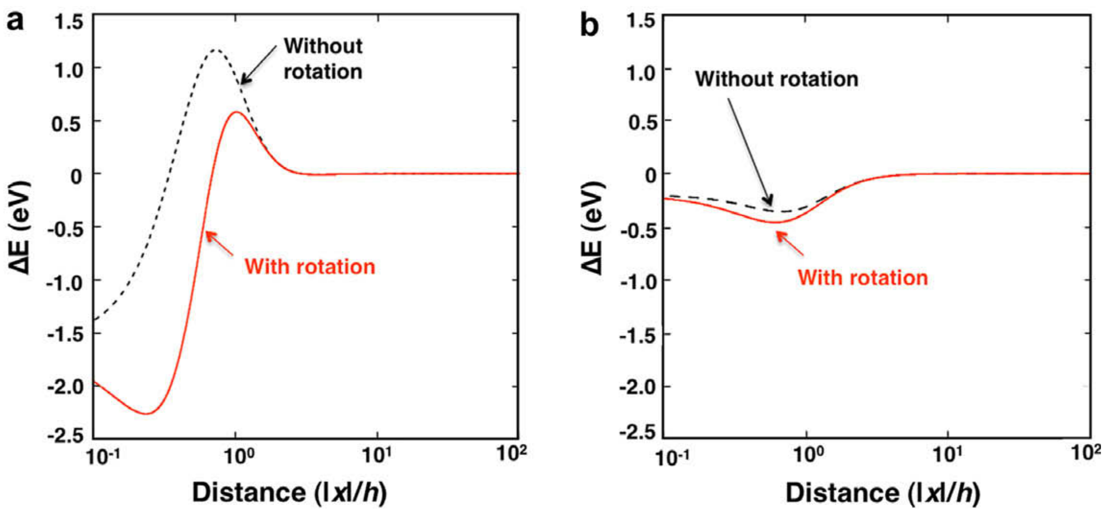

Fig. 3. The changes in the energy as a function of $|x|/h$, when $\vec{B} = a_0/2$ [1 1 0], and $\vec{b} = a_0/2$ [1 $\bar{1}$ 0]. x, h and θ are defined in Fig. 1(b). (a) $\theta = 90°$ and (b) $\theta = 0°$.

qualitatively similar dependence as the parallel Burgers vectors case, shown in Fig. 2. The interaction changes from the repulsive to the attractive when $|x|/h \sim 1.0$. When we include the rotation of the loop A, there is a stable position at $|x|/h \sim 0.2$, which could not be observed without rotation. We have obtained the similar results by molecular dynamics simulations [14]. Fig. 3(b) shows the change in the energy at $\theta = 0°$, when the glide cylinder of the loop A passes just above the inserted plane of the loop B. There is an attractive interaction, although the absolute value of the energy is very small and the interaction is short-range. In this case, the glide motion of the loop B may possibly be the major interaction and the loops may coalesce each other, which is not included in this model. We also clarified that when θ ranges between 0° and 90°, the changes in the energy vary between these two extreme cases.

4. Conclusions

We have evaluated the change in the energy by the glide motion of a loop exerted by the stress field originating from another loop, and incorporate the rotation of the loop under the stress field in FCC systems. When the Burgers vectors are parallel, the loop formed in the tensile region is attracted by the other loop, and they will be aligned nearby. When the Burgers vectors are perpendicular, the interaction depends on the angle between the position vector of the glide cylinder and the normal vector of the other loop. In any cases, however, there exist attractive regions, which moves loops to be aligned and the loops may coalesce each other. In this calculation, we do not include the loops split into two partials and the energy contributions of the core tractions [15], which are remained for further studies.

Acknowledgements

The authors gratefully appreciate Dr. W.G. Wolfer in Lawrence Livermore National Laboratory and Prof. E. Kuramoto for their fruitful discussions and advices.

References

[1] B.N. Singh, J. Nucl. Mater. 258–263 (1998) 18.
[2] R.S. Averback, T. Diaz de la Rubia, in: H. Ehrenreich, F. Spaepen (Eds.), Solid State Physics, vol. 51, Academic Press, 1998, p. 281.
[3] A.J.E. Foreman, W.J. Phythian, C.A. English, Philo. Mag. A 66 (1992) 671.
[4] W.G. Wolfer, T. Okita, D.M. Barnett, Phys. Rev. Lett. 92 (8) (2004) 085507.
[5] R.E. Stoller, G.R. Odette, B.D. Wirth, J. Nucl. Mater. 251 (1997) 49.
[6] Y.N. Osetsky, D.J. Bacon, A. Serra, B.N. Singh, S.I. Goulubov, J. Nucl. Mater. 276 (2000) 65.
[7] N.M. Ghoniem, B.N. Singh, L.Z. Sun, T. Diaz de la Rubia, J. Nucl. Mater. 276 (2000) 166.
[8] T. Okita, S. Fujita, E. Kuramoto, N. Sekimura, Philo. Mag., submitted for publication.
[9] T. Okita, N. Sekimura, J. Nucl. Mater. 367–370 (2007) 368.
[10] S. Fujita, T. Okita, E. Kuramoto, N. Sekimura, these proceedings.
[11] F. Kroupa, in: B. Gruber (Ed.), Theory of Crystal Defects, Proceedings, Academic Press, New York, 1966, p. 275.
[12] D. Hull, D.J. Bacon, Introduction to Dislocation, third Ed., Pergamon, Oxford, 1984. chapt.5.
[13] B.N. Singh, A.J.E. Foreman, H. Trinkaus, J. Nucl. Mater. 249 (1997) 103.
[14] S. Fujita, unpublished data.
[15] R. Bullough, A.J.E. Foreman, Philo. Mag. 22 (1970) 31.