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# The elastic interaction between an edge dislocation and a loop in BCC systems

Taira Okita *, Naoto Sekimura

*Department of Quantum Engineering and Systems Science, University of Tokyo, Tokyo, Japan*

**Abstract**

We have evaluated the interaction between an edge dislocation and a loop in BCC metals. In this calculation, we used the linear elastic theory to estimate their long range interaction, and we incorporated the change in the normal vector of the loop in the stress field originating from the edge dislocation. The rotation of the loop significantly modifies the interaction and strongly affects the microstructural evolution and the irradiation hardening.


## 1. Introduction

The 14 MeV neutrons generated by DT fusion reactions produce high-energy collision cascades. Recent molecular dynamic (MD) simulations show that self-interstitial atoms produced in these cascades directly agglomerate into small dislocation loops [1,2], and many of them are glissile in nature [3,4]. Since the activation energies for migration of these small loops are much lower than that of the mono-interstitials, they will subsequently diffuse and interact with stress fields inside the material that arise from network dislocations or other loops. As a result, the evolution of the dislocation depends not only on the capture of individual self-interstitials but also on the capture rate of these small loops. The strain field of these mobile loops gives rise to a strong interaction with other dislocations that will impact the bias for void swelling. Ghoniem et al. demonstrated both the force and torque exerted on the loops by the strain field of a nearby dislocation [5]. In their study, the loops were assumed to be rigid and circular in shape even when the torque and force from the dislocation was relatively large. Wolfer et al. derived an equation for the change in normal vector in order to minimize the sum of the self-energy and interaction energy of the loop [6]. Okita et al. later applied their equations to various combinations of the Burgers vector for both types of the dislocations in FCC systems, and demonstrated that the rotation of the loop can significantly change the interaction, a conclusion which would not have been obtained without incorporating the rotation [7].

In this paper, we employ the derivation by Wolfer et al. [6] and apply it to the BCC system, where we evaluate the interaction between an edge dislocation and a glissile loop.

* Corresponding author. Tel.: +81 3 58416987; fax: +81 3 38183455.
*E-mail address:* okita@q.t.u-tokyo.ac.jp (T. Okita).

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## 2. Theoretical consideration of the loop rotation

Since the detailed derivations have been published elsewhere [6,7], we will only briefly summarize them in this paper.

It is possible to define the energy of a prismatic interstitial loop as

$$E = W - bA(\hat{n}) \cdot \left(\vec{t}(\vec{r}) \cdot \hat{n}\right), \tag{2-1}$$

where $W$ is the self-energy for the loop and $A$ is the area of the loop. The quantities $\vec{b}, \vec{t}$ and $\vec{n}$ are the Burgers vector of the loop, traction vector of the dislocation, and the normal vector of the loop, respectively. The loop normal vector $\vec{n}$ is in principle independent of $\vec{r}$, but it is correlated by virtue of its dependence on the stress field $\vec{t}(\vec{r})$. A derivation of this relation is required to evaluate the interaction. To minimize the total energy in terms of $\vec{n}$, the balance of the force and the balance of the torque exerted on the loop were calculated, and the final equation can be written as

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

where $\gamma$ is the angle between the traction vector $\vec{t}$, and the Burgers vector $\vec{b}$, and

$$\sqrt{k} = \sin\alpha, \tag{2-3}$$

$\alpha$ is the angle between the Burgers vector and the normal vector of the loop, defining the rotational angle.

$$\Lambda(k) = \frac{W_0}{A_0} \cdot \frac{2}{\pi k\sqrt{1-k}} \{(1 - 3k\eta + 2k^2\eta)E(k) - (1-k)(1-k\eta)K(k)\}, \tag{2-4}$$

$W_0$ and $A_0$ are the self-energy and the area of the circular loop, respectively, and $\eta$ is an empirical factor. We assume that the loop is circular in the absence of the stress field other than the loop itself, and $\eta$ is chosen to be 1/4. This assumption will not affect the calculation results, however. $K(k)$ and $E(k)$ are the complete elliptic integral of the first kind and second kind, respectively [8]. At a given position along the glide cylinder, the angle $\gamma$ between the traction vector and the Burgers vector is known, while $\alpha$ needs to be determined. Therefore, the Eq. (2-2) must be solved numerically for $k$, and hence for the angle $\alpha$.

We will now consider the interaction between a glissle loop and an edge dislocation in BCC systems, the Burgers vectors of which is $a_0/2\langle 1\,1\,1\rangle$.

## 3. Results

### 3.1. Parallel Burgers vector, $\vec{B} = \frac{a_0}{2}[1\,1\,1]$, $\vec{b} = \frac{a_0}{2}[1\,1\,1]$

In this case, the loop moves along the glide cylinder. Alternatively, one may consider the center of the loop to be stationary while the edge dislocation moves on its glide plane. Within the stress field of the edge dislocation, the loop rotates. The rotational angle is plotted in Fig. 1 as a function of the distance ratio, $x/h$. In this calculation, $h$ is chosen to be 1.5 nm, and the loop radius is set to be 0.5 nm. It is notable that the loop remains rotated away from $\alpha = 0$ even at far distances, and that the loop suddenly flips and changes the orientation of the normal vector when it moves from the attractive area into

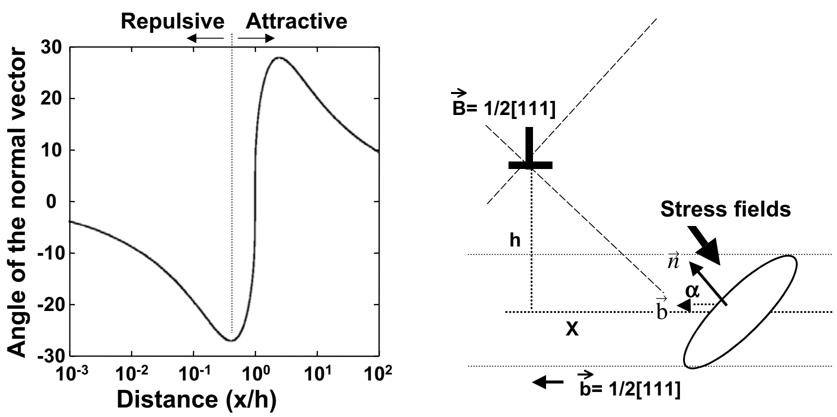


Fig. 1. The rotational angle of the loop as a function of $x/h$, where $h$ is chosen to be 1.5 nm, and the spatial relationship between the line dislocation and the glissile loop, the Burgers vectors of which are parallel. Note that the horizontal scale is logarithmic. In this calculation, the loop radius is chosen to be 0.5 nm.

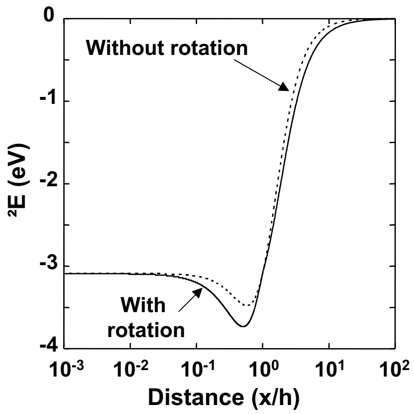


Fig. 2. The change in the energy as a function of $x/h$, where $h$ is chosen to be 1.5 nm. Note that the horizontal scale is logarithmic. The spatial relationship between a line dislocation and a loop is shown in Fig. 1. The Burgers vectors are parallel. In this calculation, the loop radius is chosen to be 0.5 nm.

the repulsive one. Fig. 2 shows the change in the interaction energy as a function of the distance, $x/h$. The change in the energy consists of two parts, namely the change in the self-energy of the loop as it rotates in the stress field, and the interaction energy. Although, the change in the energy is not so large in absolute term at far distances, it is sufficient to impose a drift on the otherwise random motion of a loop, leading to its eventual capture in the vicinity of the dislocation. The capture volume becomes measurably larger when the loop rotation is included.

### 3.2. Non-parallel Burgers vector, $\vec{B} = \frac{a_0}{2}[1\,1\,1]$, $\vec{b} = \frac{a_0}{2}[1\,1\,\bar{1}]$

There are several slip planes in BCC systems, and we choose the $(1\,0\,\bar{1})$ in this paper. Correspondingly, the line vector of the dislocation is $[1\,\bar{2}\,1]$. Fig. 3 shows the spatial relationship between an edge dislocation and a loop. The intersection between the glide cylinder and the extrapolation of the inserted half plane is chosen to be the origin, with the signs of the direction defined as shown in Fig. 3. Fig. 4 shows the rotational angle as a function of $x/h$. Even at far distances, the loop rotates, and the angle increases as it approaches the dislocation. It rotates most at the closest approach. Fig. 5 shows the change in the energy as a function of the distance ratio, $x/h$. There are two stable points along the glide cylinder. Since the absolute value of the interaction energy is much larger than the thermal energy even at far distances, glissile loops generated directly by collision cascades at far distances will eventually be captured by the dislocation and move to the stable point along the glide cylinder. When we include the rotation, the

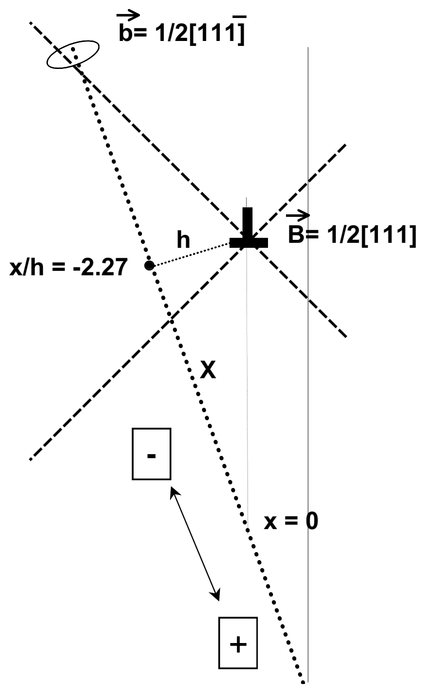


Fig. 3. The spatial relationship between the line dislocation and the loop, and the definition of the origin and sign for the results in Figs. 4 and 5. The Burgers vector of the line dislocation, the glide plane and the line vector are $\vec{B} = \frac{a_0}{2}[1\,1\,1]$, $(1\,0\,\bar{1})$ and $[1\,\bar{2}\,1]$, respectively. The Burgers vector of the loop is $\vec{b} = \frac{a_0}{2}[1\,1\,\bar{1}]$.

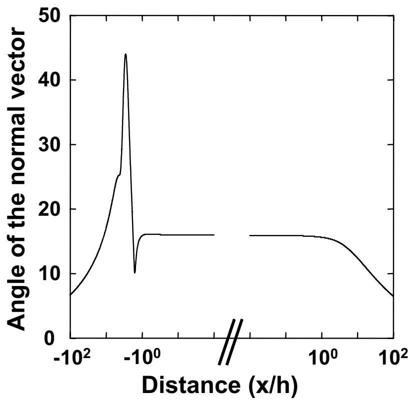


Fig. 4. The rotational angle as a function of $x/h$. The spatial distribution of the line dislocation and the loop is shown in Fig. 3. The Burgers vectors of the dislocation and the loops are $\vec{B} = \frac{a_0}{2}[1\,1\,1]$ and $\vec{b} = \frac{a_0}{2}[1\,1\,\bar{1}]$, respectively. Note that the horizontal scale is logarithmic. $h$ and the loop radius are chosen to be 1.5 nm and 0.5 nm, respectively.

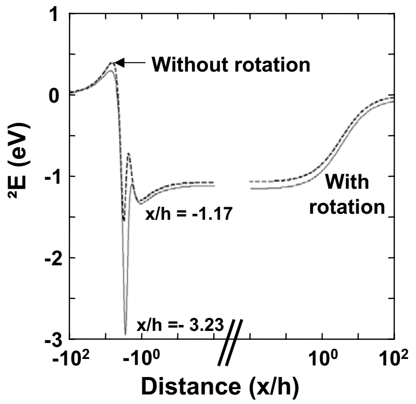


Fig. 5. The change in the energy as a function of $x/h$. The spatial distribution of the line dislocation and the loop is shown in Fig. 3. The Burgers vectors of the dislocation and the loops are $\vec{B} = \frac{a_0}{2}[1\,1\,1]$ and $\vec{b} = \frac{a_0}{2}[1\,1\,\bar{1}]$, respectively. Note that the horizontal scale is logarithmic. $h$ and the loop radius are chosen to be 1.5 nm and 0.5 nm, respectively.

activation barrier to come into the most stable point ($x/h = -3.23$) decreases, and some of the loops will move into the most stable point. The absolute value of the interaction energy is much stronger when we include the loop rotation. The loop cannot easily escape from the most stable position, because the activation barrier is much larger.

## 4. Discussions and conclusions

In this paper, we used the elastic theory and evaluated the interaction between a loop and a line dislocation. One of the major points of this study is that we include the change in the normal vector of the loop in order to make contact with atomistic simulations [9]. We demonstrated that the rotation of the loop can strongly change the interaction.

Recent MD simulations showed that loops or clusters can be obstacles to dislocation motion without physically touching the dislocations [10], and can thereby induce irradiation hardening. The absolute value of the interaction energy becomes larger by including the loop rotation; hence the stress required for the line dislocation to move against the interaction becomes larger.

In this calculation, we do not consider the core energy of the loop, which is a function of the rotational angle of the loop. Further studies are necessary using by MD simulations to evaluate the effect of the rotation on the core energy of a loop, although the core energy may not change significantly by the rotation.

We showed that the loop can come to the close vicinity of the dislocation with the one-dimensional glide motion along the glide cylinder. However, with only glide motion, the loop will most likely not be absorbed by the dislocation. There would be no bias unless the loop moves perpendicular to its Burgers vector direction and be absorbed by the dislocation. Further studies are required to clarify this mechanism.

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