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A study of the interaction between irradiation induced-defect and a line dislocation in bcc-iron

Satoshi Fujita [a,*], Taira Okita [b], Eiichi Kuramoto [b], Naoto Sekimura [b]

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

A B S T R A C T

We evaluate the interaction between a line edge dislocation and a self-interstitial atom cluster in α-iron by the molecular dynamics (MD) calculation. When the distance between the slip plane of the dislocation and the cluster centroid is more than twice as large as the cluster radius and the distance between the slip plane and the nearest part of the cluster is more than 1 nm, the results obtained by MD simulation agree well with that by the dislocation theory. The calculation temperature does not affect the stable position of the cluster near the dislocation. We discuss the difference in MD and the dislocation theory and the limitation of the infinitesimal small cluster approximation.

1. Introduction

The recent molecular dynamics (MD) simulations found that the high-energy particles injected into metals directly generate self-interstitial atom (SIA) clusters as well as mono-vacancies and interstitials [1,2]. In the fusion environments, most of the interstitials generated by 14 MeV neutrons are supposed to directly agglomerate into clusters. The MD simulations also clarified that these clusters are highly mobile along certain directions by the glide motion, specifically ⟨1 1 1⟩ direction in body-centered-cubic (BCC) metals and ⟨1 1 0⟩ direction in face-centered-cubic (FCC) metals [3,4]. After losing the ballistic energies from collision cascades, they will interact with strain fields inside of the metal, and glide to the stable positions according to the gradient in the interaction energy [5]. A line dislocation, the strain field of which is proportional to $1/r$ (r is the distance from the dislocation), tends to attract some of these clusters from quite far away. Therefore, the interaction between a line dislocation and a cluster is one of the key factors to determine the microstructural evolution under the fusion irradiation condition [6,7], especially in the initial stage of irradiation.

The length scale of their interaction which we should incorporate ranges from the atomistic scale up to some hundred nanometers, because of the long-range strain field of a line dislocation. When clusters are physically intersected with a line dislocation or their distance is as short as atomistic level, we will have to employ the MD simulations. On the other hand, they also interact by virtue of the strain field without touching each other. In most cases, we will have to treat the long-range interaction, as long as the interaction energy is equivalent with the thermal energy [6]. Thus, both the MD simulation and the simulation based on the dislocation theory (hereinafter, we call it dislocation model) have been used to evaluate the interaction. Recently, Okita et al. built up the modified dislocation model, detail of which was comprehensively described in [5], and verified the results obtained by the model agree well with that by MD simulation for the stable positions of the clusters [8], as shown in Fig. 1. Their study described that it is possible to integrate the results of MD with those of the dislocation model, and to build up the model from the atomistic scale to meso-scale with the physical consistency.

Based on these previous studies, we use the MD simulation to evaluate the short range interaction and temperature effects, both of which cannot be evaluated by the dislocation model. We calculate the stable position of a cluster around the edge dislocation, and verify the validity of the modified dislocation model at shorter distances.

2. MD simulation method

In this study, we use the α-iron single crystal and include a line edge dislocation and a circular-shaped SIA cluster into the crystal. The semiempirical many-body potential by Finnis and Sinclair [9] is used. The initial positions of the atoms are optimized by the steepest descent method so that total potential is approximately minimum. Schematic illustration of a simulated crystal is shown in Fig. 2. The free boundary condition is selected for the y direction and the periodic for the x and z. The temperatures are set just by the initial velocity of atoms with the Maxwell–Boltzmann distribution and not actively controlled during the simulations.

Firstly, the initial distances between the slip plane and the centroid of the SIA cluster, noted as h in Fig. 2, are set at several values

* Corresponding author.
E-mail address: fujita@n.t.u-tokyo.ac.jp (S. Fujita).

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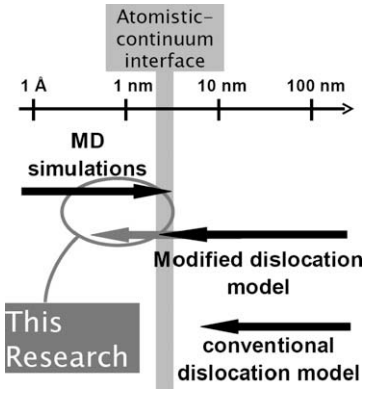

Fig. 1. Simulation methods to evaluate the interaction between a line dislocation and a cluster, and its applicable length scale.

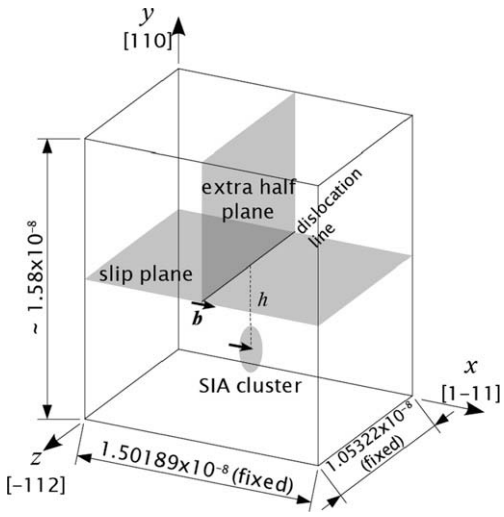

Fig. 2. Simulated crystal in the MD calculation. Note that the Burgers vectors are set to be parallel, $\boldsymbol{b} = (a_0/2)\,[1\,1\,1]$. '*r*', and '*h*' denote the cluster radius and the distance between the slip plane and a cluster, respectively. $r = 5.0 \times 10^{-10}$ or 1.0×10^{-9}. The length is shown in meters.

from 3.0×10^{-9} m down to 8.0×10^{-10} m, while the temperature is set to 100 K.

Then, we choose several temperatures up to 600 K while the initial distance '*h*' is fixed to be 3.0×10^{-9} m in order to investigate the temperature dependence.

3. Results and discussion

The positions of the cluster are shown by x/h, where x is the position of the cluster along its glide cylinder. When the centroid of the SIA cluster is just beneath the position of the extra half plane, we set $x = 0$.

3.1. The initial distance 'h' dependence of the position of the cluster

Fig. 3(a) and (b) show the position of the cluster, x/h. In that set of calculations, the distance '*h*' ranges from 8.0×10^{-10} to 3.0×10^{-9} m, and we choose two different cluster radii, $r = 5.0 \times 10^{-10}$ m and $r = 1.0 \times 10^{-9}$ m. There are approximately 17 atoms in the $r = 5.0 \times 10^{-10}$ m cluster and approximately 66 atoms in the $r = 1.0 \times 10^{-9}$ m cluster. The difference of the sign in x/h arises from the first direction of the thermal fluctuation at

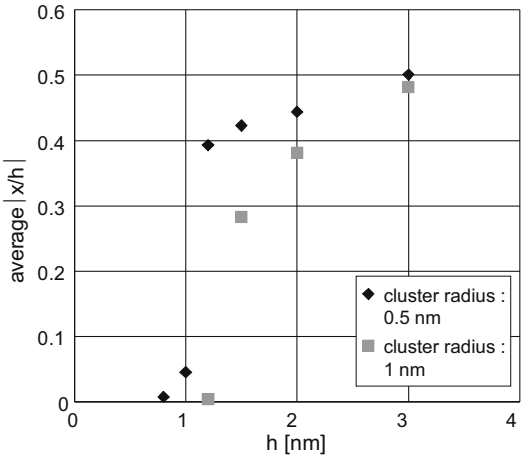

Fig. 4. *h* dependence of average $|x/h|$. Temperature is 100 K. Stable x/h is almost 0.5 in the modified dislocation model.

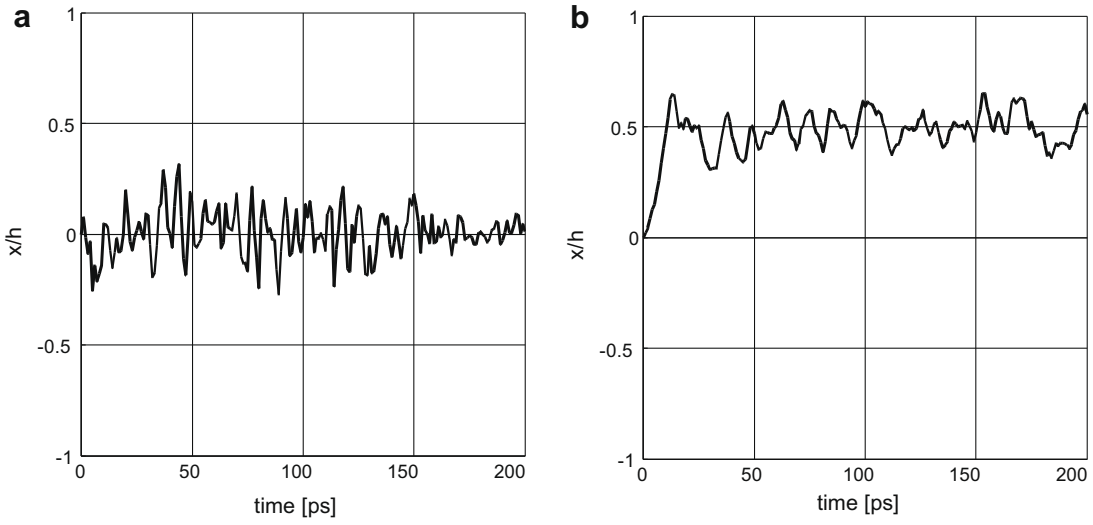

Fig. 3. x/h dependence of the MD calculation time. Temperature is 100 K. (a) $r = 5.0 \times 10^{-10}$ m, $h = 8.0 \times 10^{-10}$ m, (b) $r = 5.0 \times 10^{-10}$ m, $h = 3.0 \times 10^{-9}$ m.

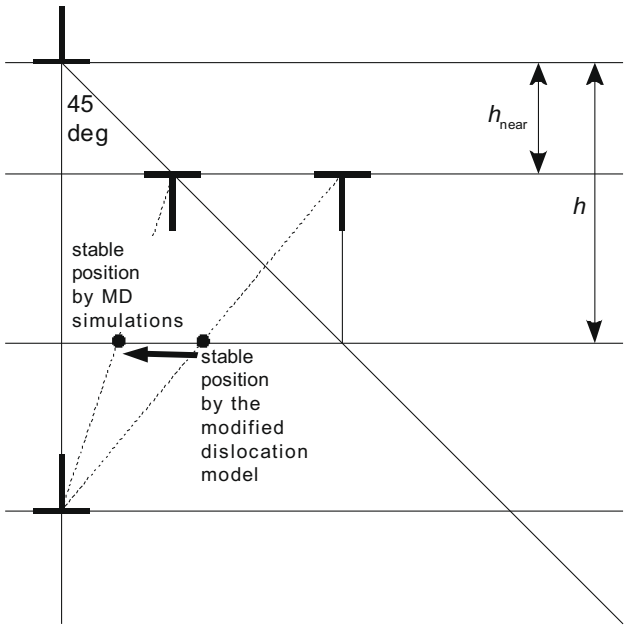

Fig. 5. An illustration of the stable position of a cluster beneath a line dislocation.

the initial step of the simulation. It is clear, however, by the geometrical symmetry that there are two stable positions of the cluster; one in $x > 0$, and the other in $x < 0$.

Fig. 4 shows $\langle|x/h|\rangle$, which denotes the average $|x/h|$ between $t = 5.0 \times 10^{-11}$ s and $t = 2.0 \times 10^{-10}$ s, as functions of h. When h is more than twice the cluster radius and h is longer than r at more than 1 nm, $\langle|x/h|\rangle$ is approximately 0.5, and it agreed well with the modified dislocation model [6]. $\langle|x/h|\rangle$, however, becomes smaller than 0.5 when the distance h is shorter. This confirms the limitation of the infinitesimal small cluster approximation or the linear elasticity itself, where the modified dislocation model based on these approximations is quantitatively invalid. When $h = 8.0 \times 10^{-10}$ m, the stable $|x/h|$ is very small and the two stable positions are not distinctive. In the infinitesimal small cluster approximation, we represent the strain by the centroid, and the strain exerted on the cluster is determined by the distance h. According to the dislocation theory, the nearest portion of the cluster tends to move toward $|x| = h$, while the farther portion of the cluster toward $x = 0$. By the modified dislocation model, the stable position of the cluster is determined by the balance of the nearest portion toward $|x| = h$ and the farther portion toward $x = 0$, while the distance h is described by the centroid. When the distance h is extremely short, h_{near}, the distance between the slip plane and the nearest portion of the cluster, is remarkably smaller than h.

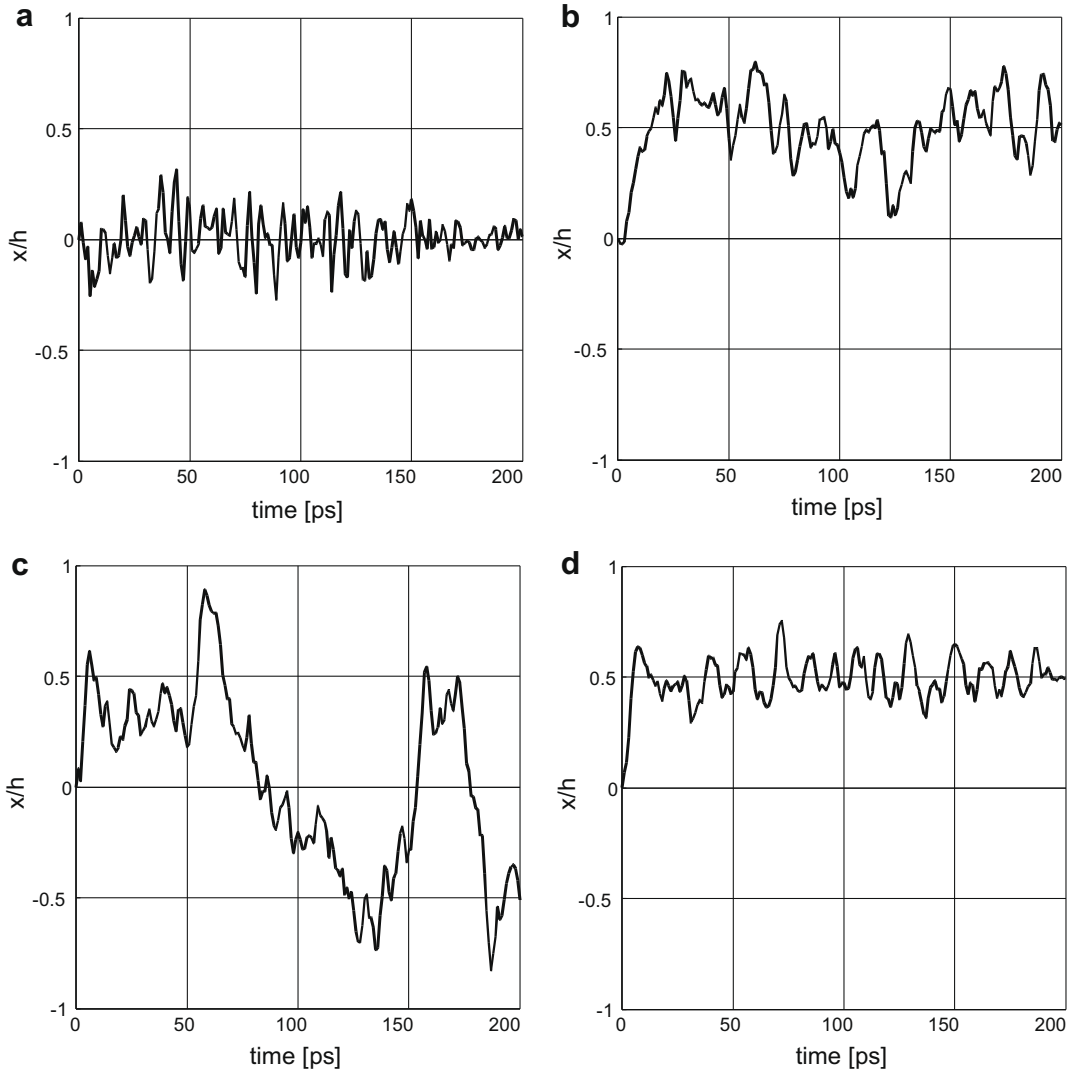

Fig. 6. x/h as functions of time. In all calculations, h is set to be 3.0×10^{-9} m. (a) $r = 5.0 \times 10^{-10}$ m, $T = 100$ K, (b) $r = 5.0 \times 10^{-10}$ m, $T = 400$ K, (c) $r = 5.0 \times 10^{-10}$ m, $T = 600$ K, (d) $r = 1.0 \times 10^{-9}$ m, $T = 400$ K.

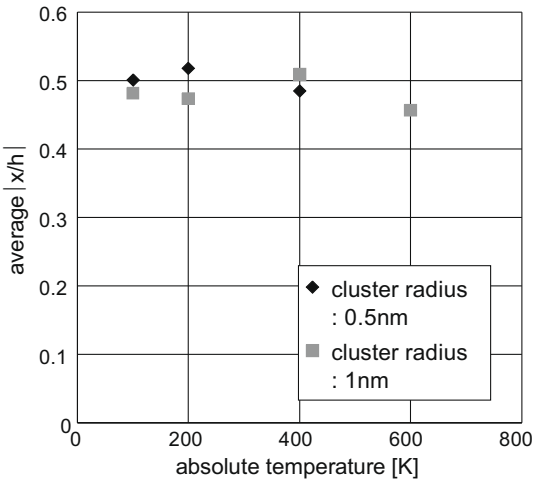

Fig. 7. Temperature dependency of $\langle|x/h|\rangle$. $h = 3.0 \times 10^{-9}$ m.

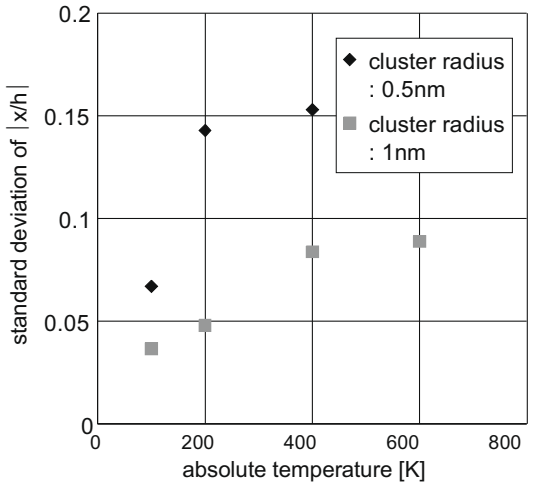

Fig. 8. Temperature dependency of $\sigma(|x/h|)$. $h = 3.0 \times 10^{-9}$ m.

Thus, the stable position of the nearest portion determined by the h_{near} is much closer to the $x = 0$, compared with that determined by the h. That is the reason for the difference for the stable position between MD and the modified dislocation model when h is very small. The above explanations are illustrated in Fig. 5. The interaction between core of the dislocation and the cluster is another possible reason to explain the difference between the MD and the modified dislocation model, which cannot be taken into account by the linear elasticity and may become significant when the distance between the dislocation and the nearest part of the cluster is smaller than a few nanometers.

3.2. Temperature dependence of the position of the cluster

Fig. 6(a)–(d) show the positions of the cluster, x/h. In that set of calculations, absolute temperature T is set up to 600 K, the initial distance h is fixed to 3.0×10^{-9} m, $r = 5.0 \times 10^{-10}$ m or 1.0×10^{-9} m. $\langle|x/h|\rangle$ and $\sigma(|x/h|)$ are shown in Figs. 7 and 8, respectively as functions of T, here $\sigma(|x/h|)$ is standard deviation of $|x/h|$ between $t = 5.0 \times 10^{-11}$ s and $t = 2.0 \times 10^{-10}$ s. These results demonstrate that the stable position of the cluster is almost independent of temperature, although thermal fluctuations become significant at higher temperature. The fluctuations of x/h are smaller for larger clusters, since fluctuations of average position of atoms in the clusters are proportional to $N^{-0.5}$ when N is the number of atoms in the clusters and each atom is assumed to vibrate independently. $\langle|x/h|\rangle$ are approximately 0.5 and well agree with the modified dislocation theory. In the case of $r = 5.0 \times 10^{-10}$ m, $T = 600$ K and $h = 3 \times 10^{-9}$ m, the fluctuation of the cluster position is so high that it jumps from one stable position to the other even in the time scale of MD calculations.

At the higher temperature when the vacancy migration becomes significant, the climb motion of the cluster and/or the dislocations would have been expected. However no climb motion is observed in the short time scale explored by the MD simulations.

4. Conclusions

(1) The stable position of the cluster evaluated by the modified dislocation model agrees well with that by MD simulation, when the distance between a slip plane of an edge dislocation and a cluster is more than twice as large as the cluster radius and the distance between the slip plane and the nearest portion of the cluster is more than 1 nm. The stable position of the cluster by MD simulation is closer to just beneath the line dislocation when the distance is smaller, however.
(2) In the MD simulation, the stable position of the cluster is not affected by the calculation temperature.

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References

[1] R.S. Averback, T. Diaz de la Rubia, in: H. Ehrenreich, F. Spaepen (Eds.), Solid State Physics, vol. 51, Academic Press, 1998, p. 281.
[2] A.J.E. Foreman, W.J. Phythian, C.A. English, Philos. Mag. A 66 (1992) 671.
[3] D.J. Bacon, F. Gao, Y.N. Osetsky, J. Nucl. Mater. 276 (2000) 1.
[4] Y.N. Osetsky, D.J. Bacon, A. Serra, B.N. Singh, S.I. Goulubov, J. Nucl. Mater. 276 (2000) 65.
[5] W.G. Wolfer, T. Okita, D.M. Barnett, Phys. Rev. Lett. 92 (8) (2004) 085507.
[6] T. Okita, N. Sekimura, J. Nucl. Mater. 367–370 (2007) 368.
[7] T. Okita, S. Fujita, E. Kuramoto, N. Sekimura, submitted for publication.
[8] T. Okita, S. Fujita, N. Sekimura, submitted for publication.
[9] M.W. Finnis, J.E. Sinclair, Philos. Mag. 50 (1) (1984) 45.