Available online at www.sciencedirect.com
SCIENCE DIRECT®
Journal of Nuclear Materials 329–333 (2004) 929–932
journal of nuclear materials
www.elsevier.com/locate/jnucmat

Anisotropic motion of point defects near edge dislocations

K. Sato [a,*], T. Yoshiie [a], T. Ishizaki [b], Q. Xu [a]

[a] Research Reactor Institute, Kyoto University, Noda, Kumatori-cho, Sennan-gun, Osaka 590-0494, Japan
[b] Toyota Central R&D Labs., Inc., 41-1, Aza Yokomichi, Oaza Nagakute, Nagakute-cho, Aichi-gun, Aichi-ken 480-1192, Japan

Abstract

We calculated the formation energy and the migration energy of vacancies near perfect edge dislocations in Cu. Effective vacancy volume in the most compressive site (the dislocation core) was 94.3% of that in the perfect lattice. The vacancy formation energy only in the most compressive site was conspicuously low (0.74 eV), and the energy in other sites was almost equal to that in the perfect lattice. As the vacancy got close to the dislocation core from the compression side, the vacancy migration energy in the direction of the Burgers vector and also on the extra half plane decreased. Calculated migration energies suggest the trapping of vacancies on the compression side of the edge dislocation and the de-trapping at high temperatures.
© 2004 Published by Elsevier B.V.

1. Introduction

Interaction between point defects and dislocations is important for the understanding of void growth because it brings about the bias effect. Usually we assume that point defects near edge dislocations are absorbed easily and annihilated. Recently we have obtained interesting results which suggest the formation of vacancies during annealing of Fe and Ni deformed with high-speed (strain rate: 4.3×10^5/sec) at room temperature using positron annihilation spectroscopy [1]. If specimens contain vacancy clusters a lot, the long lifetime of positron annihilation is detected. By annealing, the lifetime increases and the intensity which indicates the density of clusters decreases with a coalescence of clusters. In our experiment, however, the constant intensity of 35% was observed as well as the increase of lifetime from 150 to 250 psec in Fe at the temperature range of 473 and 573 K. The temperature range is too low to form vacancies by thermal emission. The same result was also obtained in Ni. One of possible explanations is the de-trapping of vacancies near edge dislocations. Near dislocations, a high strain state is achieved and vacancies are deformed. The positron annihilation lifetime at deformed vacancies is lower than that in perfect lattice [2–4] and it is not easy to separate the lifetime component from the dislocation component.

In order to check the validity of our assumption, the volume, the formation energy and the migration energy of vacancies near perfect edge dislocations in Cu were calculated by computer simulation employing the Finnis–Sinclare potential and the energy calculation of model lattice by the static method [5–9].

2. Method of calculation

The Finnis–Sinclare potential for Cu, which was fitted by Ackland et al. [10], was used for computer simulation. Fig. 1 shows the size and orientation of the model lattice we employed. We defined the [$\bar{1}$ 1 0], [1 1 $\bar{2}$] and [1 1 1] direction as x-, y- and z-axis, respectively. The edge dislocation line parallel to the y-axis was introduced at the center of the model lattice by displacing the atoms according to the elasticity theory. The Burgers vector was $a/2[\bar{1}\,1\,0]$, where a is the lattice constant. The periodic boundary condition for the y-axis direction and the fixed boundary conditions at surfaces perpendicular to x-axis and z-axis were employed [2–4]. The lattice was relaxed by the static method, which did not take into account temperature effects [5,6].

* Corresponding author. Tel.: +81-724 51 2404; fax: +81-724 51 2620.
E-mail address: ksato@rri.kyoto-u.ac.jp (K. Sato).

0022-3115/$ - see front matter © 2004 Published by Elsevier B.V.
doi:10.1016/j.jnucmat.2004.04.062

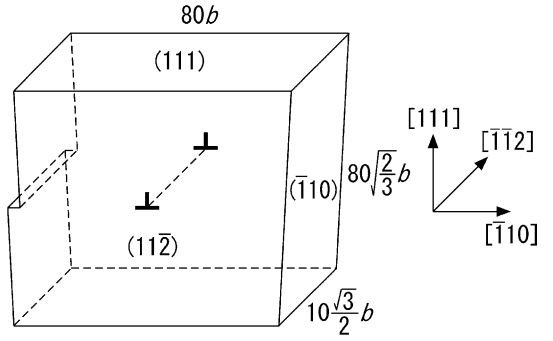

Fig. 1. The size and orientation of the model lattice ('b' denotes atomic distance).

The formation energy of vacancies was determined according to the following processes. First, we relaxed the model lattice with the dislocation, and calculated the total energy of it (E_1). Next, we introduced a vacancy into the relaxed model lattice by removing one atom, and calculated the total energy after relaxation (E_2). The vacancy formation energy was obtained as the difference between E_1 and the sum of E_2 and the cohesive energy E_c because one atom was removed by the introduction of the vacancy. The vacancy was introduced into ten positions, at which numbers 1–10 are written as shown in Fig. 2.

We considered vacancy migration as the movement of a neighboring atom nearest to the vacancy into the vacancy site. A point where the total energy of the model lattice was at its maximum for the particular migration route was defined as saddle point. The atom was fixed at the saddle point and the other atoms were relaxed. The migration energy was determined as the difference between the total energy of the model lattice before the migration of the atom and that at the saddle point.

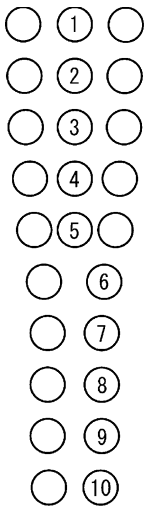

Fig. 2. A view showing a frame format of the dislocation. The vacancy was introduced into ten positions, at which numbers 1–10 are written.

The dislocation and the vacancy were relaxed only near the atomic site determined by the elasticity theory. Because the perfect edge dislocation extends into two partial dislocations by the relaxation with large atomic displacement. The obtained formation energy and migration energy of vacancies far from the dislocation core were 1.22 and 1.44 eV, respectively. While relaxed ones with large atomic displacement were 1.20 and 0.98 eV, respectively. Although the values of migration energies were different, they show the same trends of change near the dislocation core.

3. Results and discussion

Fig. 3(a) shows the structure of the slip plane of a perfect edge dislocation. A view showing a frame format of the dislocation and the calculated elastic strain are shown in Fig. 3(b). The elastic strain was obtained by $(d-d_0)/d_0$ (d: atomic distance near the dislocation obtained in this calculation, d_0: atomic distance in the perfect lattice). The elastic strain of the dislocation core was about ±10%. We defined effective vacancy volume as the third power of the average distance from vacancy site to first nearest-neighbor atoms. The effective vacancy volume in the most compressive site decreased to 94.3% of that in the perfect lattice. In Fe, the vacancy volume in this site was smaller than that in Cu [2].

Fig. 4 shows the vacancy formation energy obtained near the edge dislocation. Horizontal axis denotes the position of the vacancy as shown in Fig. 2. The vacancy formation energy only in the most compressive site, position 5 in Fig. 2, was 0.74 eV. The formation energy of vacancy in other sites was almost equal to that in the perfect lattice. The formation energy of vacancy in the most expanded site, position 6 in Fig. 2, was not high. This result is explained as follows. Though the vacancy volume was expanded in the Burgers vector direction, the atom in one upper layer of the slip plane was very close to the vacancy site.

We named directions of vacancy migration as (i), (ii) and (iii) in Fig. 5. The directions(i), (ii) and (iii) are the $[\bar{1}\,1\,0]$ direction, the $[1\,1\,0]$ direction and the $[\bar{1}\,\bar{1}\,0]$ direction, respectively. Fig. 6 shows the vacancy migration energy near the edge dislocation. As the vacancy gets closer to the dislocation core, the vacancy migration energy towards direction (i) on the compression side decreases. The other noticeable point is that the energy required for vacancies to migrate up and down on the slip plane was also lower than other migration energies. There is a strong possibility that the vacancy exists at position 5, because the formation energy at position 5 is

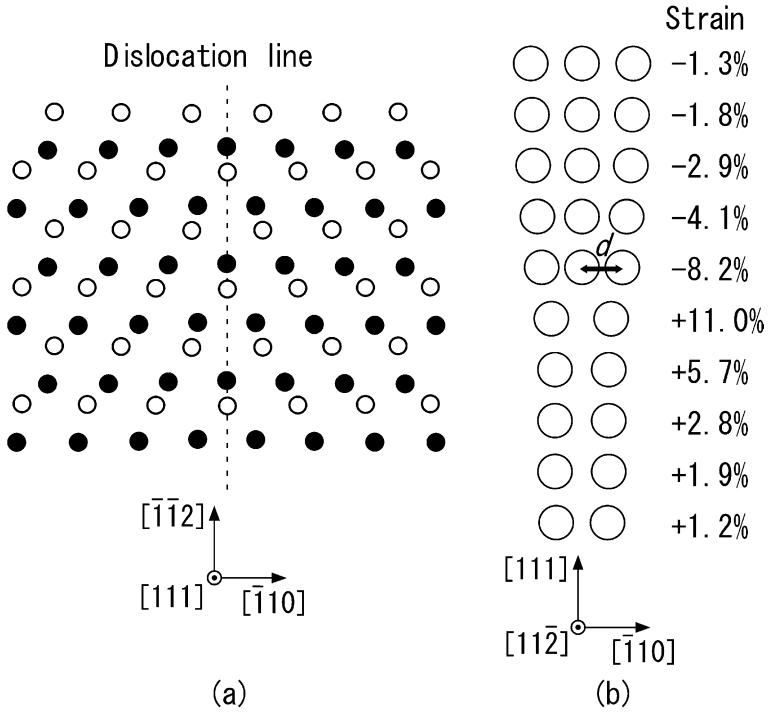

Fig. 3. (a) The structure of the slip plane of a perfect edge dislocation. Dotted line denotes dislocation line. Black and white circles are atoms of upper and lower layer of the slip plane, respectively. (b) A view showing a frame format of the dislocation and the elastic strain nearby. '*d*' denotes the atomic distance of core atoms of the dislocation. The plus and minus signs indicate tensile and compressive strain, respectively.

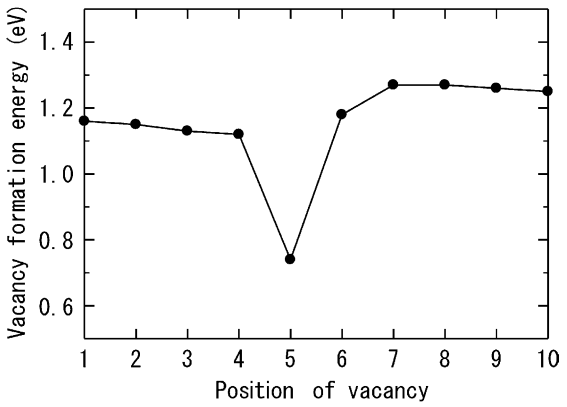

Fig. 4. The vacancy formation energy near the perfect edge dislocation in Cu. The horizontal axis denotes vacancy sites as shown in Fig. 2.

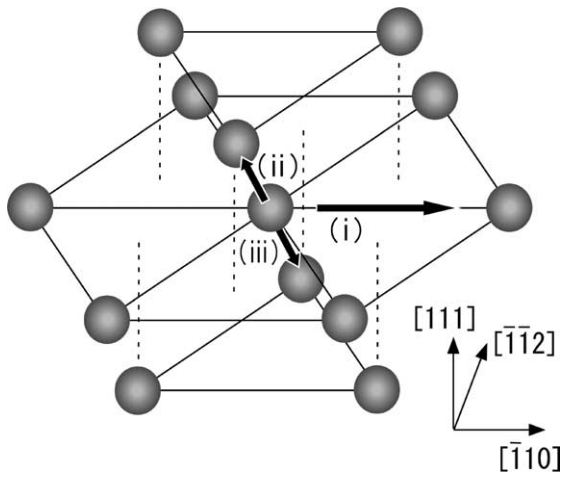

Fig. 5. The direction of vacancy migration. The directions (i), (ii) and (iii) are the [$\bar{1}$ 1 0] direction, the [1 1 0] direction and the [$\bar{1}$ $\bar{1}$ 0] direction, respectively.

lower than that at position 6 and the migration energy from position 6 to 5 is lower than that from position 5 to 6. Another possible migration direction is parallel to the dislocation line (so called pipe diffusion). The migration energy of vacancy at position 5 in this direction is, however, 1.46 eV, and is almost the same as the vacancy migration energy in the perfect lattice.

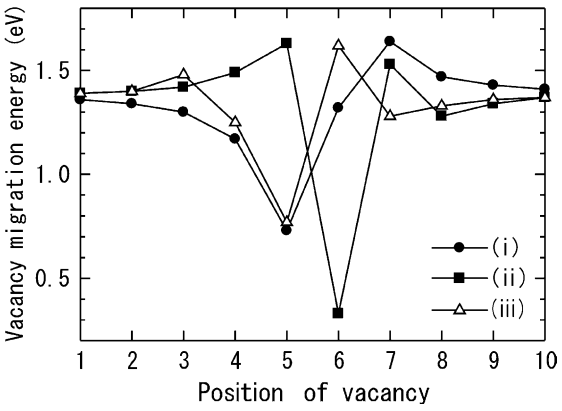

Fig. 6. The vacancy migration energy near the perfect edge dislocation in Cu. The horizontal axis denotes vacancy sites as shown in Fig. 2. (i), (ii) and (iii) in the figure correspond to the directions (i), (ii) and (iii) shown in Fig. 5, respectively.

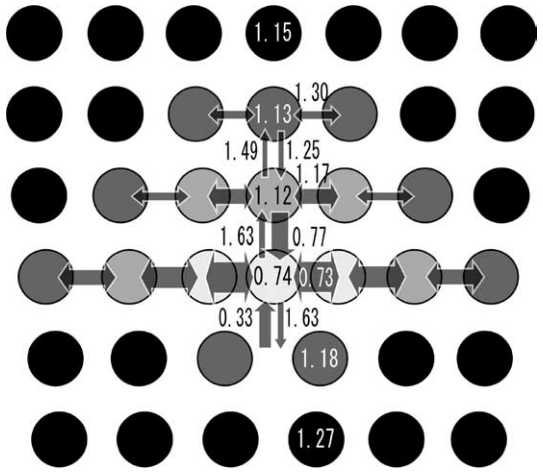

Fig. 7. The trapping model of vacancies in the perfect edge dislocation. Arrow width denotes the easiness of the vacancy migration. The pale circles denote the position at which the vacancy is trapped. The values in circles denote vacancy formation energies, and other values denote vacancy migration energies.

From these results, we devise the trapping model of vacancies in the edge dislocation as shown in Fig. 7. Arrow width denotes the easiness of the vacancy migration determined by the calculated formation energy and migration energy of vacancies. Vacancies are mainly trapped on the compression side of dislocations at low temperature. The vacancy can migrate a few atomic distances on the extra half plane and on the slip plane. The probability of vacancy existence is highest in the most compressive site (position 5 in Fig. 2), because the migration energy to the dislocation core is low. The vacancy volume decreased in the trapped site. So, the positron annihilation lifetime is shorter than that in the perfect lattice. When the specimen is annealed, vacancies are de-trapped and contribute to the growth of the vacancy clusters.

4. Conclusion

The formation energy and the migration energy of vacancies near the perfect edge dislocation core were calculated in Cu. Strong anisotropic motion of vacancies was obtained near the dislocation. On the compression side near the core, the migration energy in the Burgers vector direction is lower than that in the perfect lattice, but that in the direction perpendicular to the close-packed layer is higher. The vacancies are trapped on the compression side of the edge dislocation with vibration of the Burgers vector direction. As the vacancy volume decreases, the positron annihilation lifetime of vacancies at the trapped position is low. If vacancies are de-trapped from the dislocation, an increase of positron annihilation lifetime is expected.

In fcc metals, the vacancy trapping in the extended edge dislocation is also important because of the easy extension of edge dislocations. We will report about it in the future.

References

[1] K. Sato, T. Ishizaki Q. Xu, T. Yoshiie, submitted for publication.
[2] Y. Kamimura, T. Tsutsumi, E. Kuramoto, Phys. Rev. B 52 (1995) 879.
[3] Y. Kamimura, T. Tsutsumi, E. Kuramoto, J. Phys. Soc. Jpn. 66 (1997) 3090.
[4] E. Kuramoto, H. Abe, M. Takenaka, F. Hori, Y. Kamimura, M. Kimura, K. Ueno, J. Nucl. Mater. 239 (1996) 54.
[5] E. Kuramoto, K. Ohsawa, T. Tsutsumi, M. Koyanagi, J. Nucl. Mater. 271&272 (1999) 26.
[6] E. Kuramoto, J. Nucl. Mater. 276 (2000) 143.
[7] K. Sato, T. Yoshiie, Y. Satoh, Q. Xu, E. Kuramoto, M. Kiritani, Radiat. Eff. Def. Sol. 157 (2002) 171.
[8] K. Sato, T. Yoshiie, Y. Satoh, Q. Xu, M. Kiritani, Mater. Sci. Eng. A 350 (2003) 220.
[9] K. Sato, T. Yoshiie, Y. Satoh, Q. Xu, Mater. Trans. 45 (2004) 833.
[10] G.J. Ackland, G. Tichy, V. Vitek, M.W. Finnis, Philos. Mag. A 56 (1987) 735.