Proceedings of the 5th International Symposium on Steel Science (ISSS 2017)
Nov. 13-16, 2017, Kyoto, Japan: The Iron and Steel Institute of Japan

Interaction between a C/N atom and an edge dislocation in bcc iron analyzed by molecular dynamics simulation

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Abstract: Molecular dynamics (MD) simulations using Finnis-Sinclair potential were performed to analyze the interaction between a C/N atom and an edge dislocation in bcc iron. Three types of MD cells containing an edge dislocation were prepared for the analyses; (1) pure iron cell without any interstitial elements, (2) iron cell where a C atom was put on (110) slip plane, and (3) another iron cell where a N atom was put on the slip plane. Various magnitudes of shear stresses were applied to the three cells at a temperature of 300 K for monitoring the movement of the edge dislocation near the inserted interstitial solute atom. The critical shear stress that the dislocation could pass through the pinning (pinning force) was compared among these models. As a result, the pinning force by C atom was 1.5 times larger than that by N atom.

1. INTRODUCTION

C and N are interstitial atoms which increase the strength of steels by solid-solution strengthening. In most of previous studies, C and N have been believed to have similar effects on the strength of ferritic steels [1][2]. On the other hand, there are a few reports that demonstrated different strengthening abilities of them. For example, Fujii et al. showed that yield stress and work hardening rate of 60 ppm C steel are higher than those of 60 ppm N steel [3]. And besides, Ngo et al. clarified that Vickers hardness of 12%Cr martensite steel containing C was higher than that containing the same amount of N [4]. However, these reports are experimental facts which are difficult to explain theoretically. In this study, we evaluated the interaction between an edge dislocation moving in iron crystal and a C/N atom in the slip plane by means of molecular dynamics (MD) simulations and compared the pinning force of C and N atoms quantitatively. Moreover, the change in the interaction with increasing the distance from the slip plane was discussed on the basis of the calculation results.

2. CALCULATION PROCEDURE

The molecular dynamics (MD) is one of the simulation methods to treat the motion equations of a great number of atoms in crystals. In this study, Finnis-Sinclair potential was adopted as atomic interactions in the calculation of MD [5]. Total energy is:

$$U_{tot} = U_N + U_P. \tag{1}$$

U_N is the N-body term and U_P is a conventional central pair-potential summation. The equation for obtaining U_N is as follows:

$$U_N = -A\sum_i f(\rho_i), \tag{2}$$

$$\rho_i = \sum_j \phi(r), \tag{3}$$

$$\phi(r)=\begin{cases}(r-d)^2+\beta(r-d)^3/d, & r \le d \\ 0, & r > d\end{cases}. \tag{4}$$

And that for Up is as follows:

$$U_P = \frac{1}{2}\sum_{i\neq 0} V(r), \tag{5}$$

$$V(r)=\begin{cases}(r-c)^2\left(c_0+c_1r+c_2r^2\right), & r\le c\\ 0, & r>c\end{cases}. \quad (6)$$

where A, d, β, c, c_0, c_1 and c_2 are potential parameters. Table 1 shows the parameters of Fe-Fe, Fe-C, C-C, Fe-N and N-N. The potential parameters for Fe-C, C-C, Fe-N and N-N were calculated by Monte Carlo fitting method. First, target curves that show the cohesive energy depending on volume of various crystals consisting of Fe-C and Fe-N, such as Fe3C, Fe4N etc., were prepared. These curves were obtained by First-principles calculations by authors and other researchers [6][7]. The parameters for FS potentials were then obtained so that the curves calculated by MD using that FS potential could fit to the target curves. In the Monte Carlo fitting, the first parameters for them were set to Fe-Fe parameters, and then, the parameter values were slightly changed to find optimum values.

Table 1. Summary of potential parameters used for MD simulations

Parameter	Fe-Fe [5]	Fe-C	C-C	Fe-N	N-N
A	1.828905	1.802034	1.948782	1.945282	1.814085
d	3.569745	2.773918	3.610582	3.701081	3.528108
β	1.8	2.047524	1.705044	2.075628	1.793642
c	3.4	2.929438	3.362683	3.110501	3.437601
c_0	1.2371147	1.872488	0.8332333	1.3893607	1.248024
c_1	-0.3592185	0.2571113	-1.095113	-0.3669454	-0.3767342
c_2	-0.0385607	-0.7478457	-0.3379719	-0.5710205	-0.0556475

Langevin equation was used as the temperature control method. We made three models: First one is a bcc crystal with a size of $10.1\times10.5\times5.68$ nm^3 consisting of 51,030 iron atoms. An edge dislocation was introduced in the center of system. Fig. 1 shows the first model. the x, y and z axises correspond to $[1\bar{1}1]$, $[\bar{1}12]$ and $[110]$ directions. The x and y directions are set in the periodic boundary conditions. The dislocation exists on the (110) plane and the slip direction is set in $[1\bar{1}1]$ direction. In the second model, a carbon atom is inserted in an octahedral site (O site) just on the (110) slip plane of the first model. In the third model, a nitrogen atom is inserted similarly to the second model. To these model crystals, various magnitudes of shear stresses were applied at 300 K by giving forces of right and left directions to the Fe atoms consisting of the top two planes and bottom two planes, respectively. The movement of the edge dislocation was observed under various shear stresses, and average velocity was estimated from some snapshots for each stress. When the dislocation was pinned by the C/N atom and did not move for more than 1 ns, the shear stress was judged to be less than critical shear stress.

To reveal the effect of distance between the interstitial site and slip plane on the C/N-dislocation interaction, the position of N atom in the third model was changed: Since O sites exist in the $[110]$ plane as well as between two adjacent $[110]$ planes, the positions of N atoms were described with the layer number as

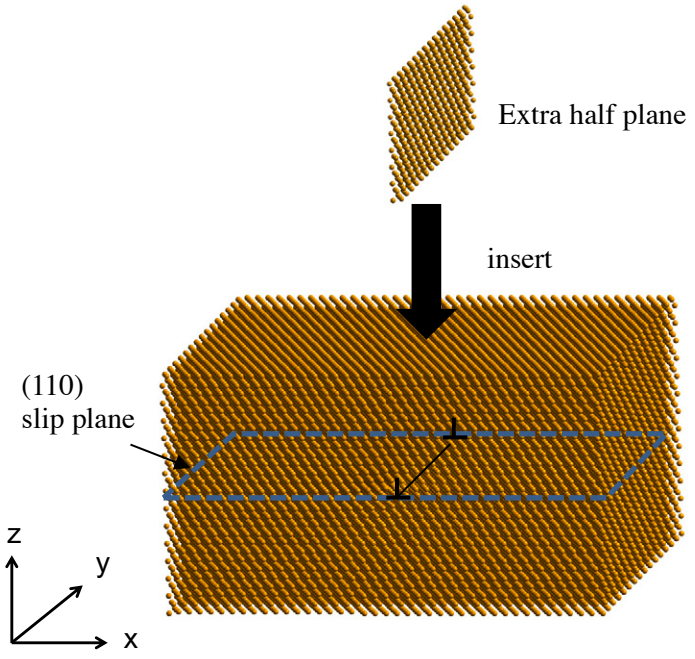

Fig. 1. System of the first model.

shown in Fig. 3. It should be noted here that there are three types of N position for the 0 layer, namely, upper, middle and lower.

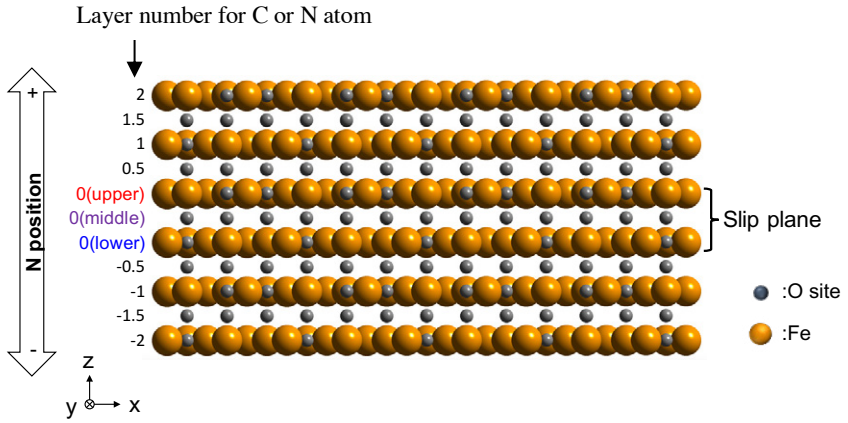

Fig. 2 Magnified iron crystal of Fig. 1 showing positions of Fe atoms and O sites. C or N atom is located at an O site in each layer.

3. RESULT AND DISCUSSION

3.1. Comparison between experimental and calculation results on edge dislocation velocity in pure iron

Fig. 3 shows the relation between applied shear stress and velocity of edge dislocation on (110) plane. The black points are experimental data obtained by Urabe et al. [8], while the red points are the calculation results obtained by MD calculation in this study. The calculation data are agreed well with the experimental data, meaning that FS potential used for the MD calculation in this study is reliable for predicting dislocation movement in ferritic steel.

3.2. Effect of C and N atoms on critical shear stress for (110) slip

Fig. 4 shows the effect of C and N atoms on the velocity of edge dislocation obtained with the second and third models. The C and N atoms were put on the 0(lower) layer shown in Fig. 2 for this calculation. The broken line draws the relation between shear stress and dislocation velocity in pure iron shown in Fig. 3. In both C and N steels, the dislocation velocity exhibits almost same trend as that of pure iron in the shear stress range more than 200 MPa, suggesting that a single C and N atom gives little effect on the movement of edge dislocation when the applied shear stress is sufficiently larger than the critical shear stress. However, with decreasing shear stress less than 200 MPa, the dislocation velocity in C and N steels begins to deviate from that of pure iron due to pinning effect. Then it rapidly drops at around 100 MPa, resulting in zero velocity. The critical shear stresses of C and N steels, at which the dislocation velocity becomes zero, are 80 MPa and 120 MPa, respectively. Therefore, it is concluded that the pinning force by C atom is 1.5 times larger than that by N atom in the case of this slip model.

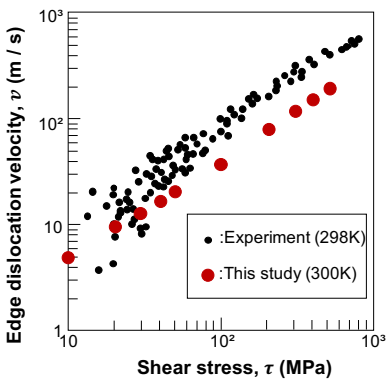

Fig. 3. Edge dislocation velocity in changing shear stress in iron.

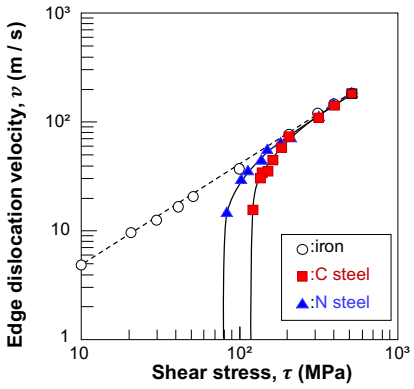

Fig. 4. Change in edge dislocation velocity as a function of shear stress in C or N steel.

3.3. Effective range of pinning force on a N atom

Fig. 5 shows the dependence of the position of interstitial O site on the critical shear stress (pinning force) in N steel calculated with the second model. The pinning force is the largest when the N atom is located just on the slip plane (0 layer), particularly when it is the upper site. However, the pinning force is markedly decreased with increasing the distance from the slip plane. When the N position becomes 2 layers away from the slip plane (0.4 nm), the pinning force due to a N atom almost disappears. This result suggests that solid-solution strengthening by an interstitial atom originates from the interaction between the solute atom and the edge dislocation core.

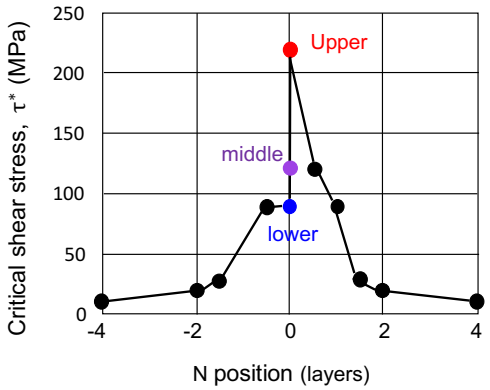

Fig. 5. Change in the effect of a N atom on the critical shear stress of ferritic steel as a function of the distance of N atom from (110) slip plane.

4. CONCLUSION

The velocity of an edge dislocation moving on (110) slip plane in iron crystal is validly simulated by MD calculation with the FS potential which is cited from [5]. Therefore, the results of MD simulation obtained in this study is suggested to be reliable.

The pinning force by a C atom against the moving edge dislocation is 1.5 times larger than that by a N atom. This difference is a possible explanation for different abilities of solid-solution strengthening by C and N.

The pinning force by a N atom almost disappears when the distance of N position becomes 0.4 nm away from the slip plane. This result indicates that solid-solution strengthening by the interstitial element originates from the interaction between the solute atom and the edge dislocation core rather than the wider stress field of edge dislocation.

Acknowledgements: This work was supported by JSPS KAKENHI Grant Number 15H05768.

REFERENCES

[1] A. Cracknell and N. J. Petch: Acta Metall., 3 (1955), 186-189.
[2] G. Lütjering and E. Hornbogen: Z. Metallk., 59 (1968), 29-46
[3] K. Fujii, D. Akama, N. Nakada, T. Tsuchiyama and S. Takaki: CAMP-ISIJ, 25 (2012), 281.
[4] Ngo Huynh Kinh Luan: Kyushu University, (2012), Doctoral thesis.
[5] M. W. Finnis and J. E. Sinclair: Phil. Mag. A, 50 (1984), 45-55.
[6] L. S. I. Liyanage, S. G. Kim, J. Houze, S. Kim, M. A. Tschopp, M. I. Baskes and M. F. Horstemeyer: Phys. Rev. B, 89 (2014), 094102.
[7] A. V. dos Santos and J. V. Santos: Materials Research, 16 (2013), 1260-1265
[8] N. Urabe and J. Weertman: Mater. Sci. Eng., 18 (1975), 41-49