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One dimensional motion of interstitial clusters in Ni–Au alloy

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Abstract

The activation energy for one dimensional motion of the interstitial clusters was calculated in Ni–Au alloy by a static method. An EMT potential was used, which was tuned to fit the experimental volume size factor and heat of solution. The number of interstitials contained within the clusters was 1, 7 and 19. In pure Ni, the activation energies of clusters were less than 0.1 eV, and they increased with the size of the interstitial clusters. After the addition of the oversized solute atoms the activation energies increased from 0.49 eV to 0.97 eV. In neutron irradiated Ni with oversized solute atoms, the defect structures near grain boundaries, and the accumulation and absorption of interstitial clusters along the dislocations can be explained by the interactions between interstitial clusters and the oversized atoms.

1. Introduction

One dimensional (1D) motion of interstitial clusters is important for the microstructural evolution in metals [1–6]. 1D motion of interstitial clusters was first observed during the electron irradiation with high voltage electron microscopy [2,7]. Movement of interstitial clusters was also often observed in neutron irradiated metals by transmission electron microscopy (TEM) [8]. The movement of interstitial clusters produced by cascade damage was shown by molecular dynamics [9]. The activation energy required for overcoming the Peierls barrier for the motion of dislocation loops in Fe and Ni calculated by computer simulation was less than 0.2 eV, with the smaller interstitial clusters having the lower activation energies [4,10].

Alloying elements are expected to affect the motion of interstitial clusters. Yoshiie et al. have studied the effect of alloying elements in Ni [11–15]. For example, in neutron irradiated pure Ni, well-developed dislocation networks and voids were observed at 573 K at a dose of 0.026 dpa by TEM. The existence of microvoids was detected by positron annihilation lifetime measurements even at a low dose level of 0.001 dpa. After the addition of 2 at.% Si (−5.81% volume size factor to Ni [16]) and Sn (74.08% volume size factor), no voids were detected by TEM observation and positron annihilation lifetime measurement. Alloying elements of Si and Sn were expected to prevent the 1D motion of the interstitial clusters.

In this paper, the effect of extremely oversized alloying elements on the motion of interstitial clusters was investigated by computer simulation using

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a Ni–Au (63.60% volume size factor [16]) alloy. The effective medium theory (EMT) potential was fitted for Ni–Au alloy [17], and the migration energy of the interstitial clusters was calculated by a static method [4,10].

2. Method of calculation

For the computer simulations, we employed the EMT potential for Ni and Au, which is one of *N*-body potentials like EAM type potential. The potential is based on the idea that the binding energies of the atoms are determined by the embedding energies of the atoms in the electron jellium. The parameters were fitted by Jacobsen et al. to the cohesive energy, the equilibrium Wigner–Seitz radius, the bulk modulus, the shear modulus, and so on [17]. The formation energies of a vacancy, a dumb-bell and a crowdion are shown in Table 1. Fig. 1 shows the size and orientation of the model lattice we used. Interstitial clusters were introduced into the central region of the model lattice, which were made by bundling the ⟨1 1 0⟩ crowdions on {1 1 0} atomic planes. The interstitial clusters were fully relaxed under the fixed boundary conditions (five atomic layers) by the static method. The method did not take temperature effects into account.

The activation energy for a motion of the interstitial clusters was calculated by the same way as Refs.

Table 1
The formation energies of a vacancy and an interstitial obtained by the EMT potential

	Formation energy (eV)
Vacancy	1.90
⟨1 0 0⟩ dumb-bell	5.05
⟨1 1 0⟩ corwdion	5.44

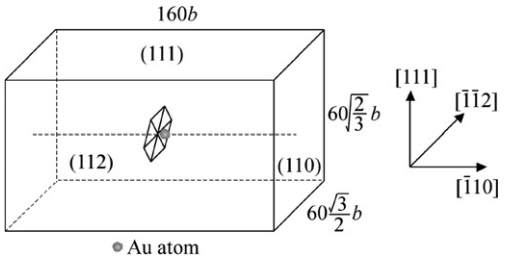

Fig. 1. The size and orientation of the model lattice ('*b*' denotes atomic distance). Interstitial clusters were introduced into the central region of the model lattice, which were made by bundling the ⟨1 1 0⟩ crowdions on {1 1 0} atomic planes. Alloying element Au was placed to prevent the motion of the interstitial clusters.

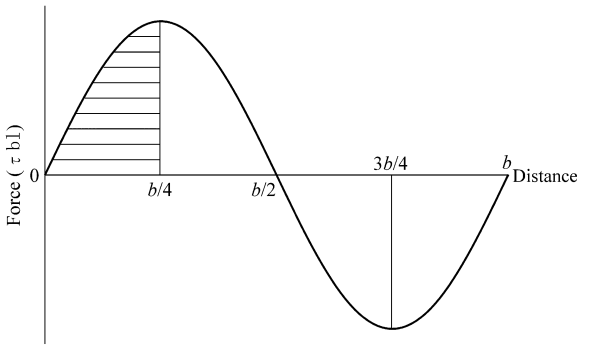

Fig. 2. The ideal force–distance curve. '*b*' denotes atomic distance. In this study, the activation energy for a motion of the interstitial clusters was obtained as twice of the shadowed area.

[4,10]. We consider that the cluster which has a higher thermal energy than the Peierls barrier can move. The results that the migration energy obtained by molecular dynamics simulation [18,19] and this static method [4,10] is almost the same in Fe support our method. The interstitial clusters were identified as perfect dislocation loops. The above relaxation process was repeated at stepwise increases in the applied shear stress, which results in the movement of loops. The activation energy required for the motion of the dislocation loops was calculated by integrating the force–distance curve $\sum_i \tau_i b l \Delta d_i$, where τ_i is the shear stress applied on the dislocation loop at point i, b is the magnitude of Burgers vector, τb is the force acting on the unit length of a loop, l is a total length of circumference of a loop and Δd_i is a short distance between two adjacent points. Fig. 2 shows the ideal force–distance curve. The activation energy was obtained as twice the value of the shadowed area. The number of interstitials contained within the clusters was 1, 7 and 19. In this study, the migration of an interstitial was regarded as the ⟨1 1 0⟩ crowdion. Because the migration mechanism of the crowdion is almost similar to that of the interstitial clusters, and that of the ⟨1 0 0⟩ dumb-bell is not similar. A single atom of the alloying element Au was placed to prevent the motion of interstitial clusters. Detailed positions are shown in Fig. 3.

3. EMT potential for Ni–Au alloy

Jacobsen et al. reported how to fit the parameters of the EMT potential for the two-component metal systems [17]. They fitted two parameters to the

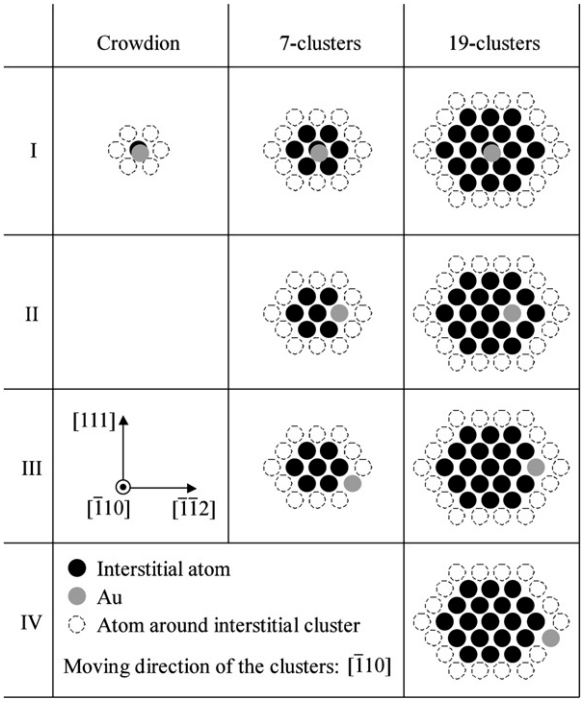

Fig. 3. Position of alloying element Au to prevent the motion of the interstitial clusters. Black circle is the interstitial atom, gray circle is Au atom and dotted circle is atom around interstitial clusters. Moving direction of interstitial clusters is [$\bar{1}$10] direction.

experimental heats of solution for the A–B alloy and the B–A alloy. But, in this method, the calculated volume size factor of Au to Ni was different from the experimental one. Because the effect of volume size factor is very important in this study, two parameters were fitted to the experimental volume size factor of Au to Ni [16] and to heat of solution for the Ni–Au alloy [20]. Fig. 4 shows the change

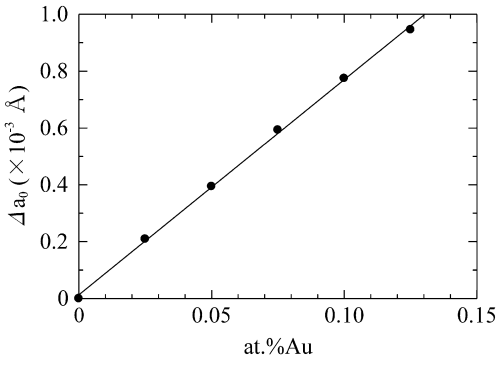

Fig. 4. The change in lattice parameter of Ni with concentration of Au in solution obtained with the new potential developed here.

Table 2
The volume size factor and heat of solution of Au to Ni obtained by the experiments [16,18] and this study

	Volume size factor (%)	Heat of solution (eV)
Experiments	63.60	0.34
This study	63.74	0.34

in lattice parameter of Ni with the concentration of Au in solution. Table 2 shows the volume size factor and heat of solution obtained by the experiments and this study.

4. Results and discussion

Table 3 shows the activation energy for the motion of the interstitial clusters. The activation energy increased with the size of the interstitial clusters in pure Ni. The activation energy also increased due to the presence of the oversized solute atoms. For the cases examined, the maximum value of the activation energy was 0.97 eV at the center of the 7-loop. There are several works which calculated the migration energy for an interstitial cluster in Fe by molecular dynamics [18,19,21,22]. The activation energy for 1D motion of interstitial clusters was approximately 0.06 eV, and was almost constant or slightly decreased with increase in the size of the clusters. But, in these calculations, the migration energies were obtained in interstitial clusters of non-hexagonal shape, and it is doubtful that the clusters act like dislocation loops. It is impossible therefore to directly compare the above molecular dynamics calculations with our calculations.

Yoshiie et al. reported that no voids were detected by both TEM observation and positron lifetime measurement in Ni–Sn alloy under fission neutron irradiation [14]. The interstitial type dislocation loops were observed preferentially near grain

Table 3
The activation energy for one dimensional motion of the interstitial clusters

	The activation energy for motion of interstitial clusters (eV)		
	Crowdion	7-Clusters	19-Clusters
Without Au	0.02	0.05	0.08
I	0.67	0.97	0.65
II		0.49	0.85
III		0.06	0.52
IV			0.18

Roman numerals correspond to the ones in Fig. 3.

boundaries [15]. They claimed these loops to be evidence of no 1D motion of interstitial clusters. The result of the present calculation shows that the mobility of interstitial clusters decreased by the oversized solute atoms. However, the highest migration energy of interstitial clusters with a solute atom, 0.97 eV, was too low to explain no-migration of the solute-trapped defects at the 573 K neutron irradiation experiments. Stronger trapping sites for the interstitial clusters are required to stop the motion. One of possible explanations is that the larger volume size factor of Sn, 74.08%, may have a significant effect. The other is the existence of solute rich areas or solute clusters. Especially, the effect of the latter is expected at 2 at.% concentration of Sn. The larger the loops are, the higher the probability of interacting with multiple solute atoms. We will report the effect of the solute clusters on the 1D motion of the interstitial clusters in next paper.

Trinkaus et al. reported that the dislocation decoration was due to the strain field of the dislocation itself and the trapped dislocation loops [5]. Impurities are also considered to contribute to the decoration. Mukouda et al. reported that dislocations in Cu and Ni were decorated with a large number of interstitial clusters under neutron irradiation at 573 K at a dose of about 0.001 dpa. When the irradiation dose was increased to 0.1 dpa, no decorated interstitial clusters around dislocations were observed [23]. The size of the decorated dislocation loops grows with increase of the neutron dose, and our calculation indicates the tendency that the activation energy for migration of clusters to overcome the oversized solute atom decreased with increasing cluster size. Therefore, if cluster migration is prevented by impurities, with increasing the cluster size by irradiation, the activation energy to overcome the impurities decreases, and finally at higher doses clusters can move and be absorbed by dislocations as reported by Mukouda et al.

5. Conclusion

The activation energy for the motion of the interstitial clusters was calculated in Ni–Au alloy using the EMT potential, which was tuned to fit the experimental volume size factor and heat of solution. The existence of oversized solute atoms leads to an increase of the activation energy. But, one solute atom is not enough to prevent the motion of the interstitial clusters. Solute clusters may play an important role for the trapping of clusters. The interaction between the interstitial clusters and solute atoms including the clusters is considered to be one of mechanisms for the damage structure near grain boundaries in Ni containing oversized elements like Sn and the decoration of dislocations by interstitial clusters in Cu and Ni.

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