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Simulation of the effect of volume size factor of solute atoms and their clusters on one dimensional motion of interstitial clusters in Ni binary alloys

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ABSTRACT

The effect of the volume size factor of solute atoms and their clusters on the one-dimensional motion of interstitial clusters was studied by computer simulations. Solute atoms were placed on the migration path of the interstitial clusters, and the change in the migration energy of the interstitial clusters was obtained by the static method. The volume size factor of Au atoms in a Ni-Au binary alloy was systematically changed from −30% to +100%. When the volume size factor of the solute atoms was larger or smaller than Ni atoms, the migration energy of the interstitial clusters increased. The average migration energy required for the interstitial clusters to pass through one, two, three, and four solute atoms (volume size factor: +63.7%) was 0.57, 1.28, 2.09, and 2.47 eV, respectively. If the solute atom clusters grow and their density is sufficiently high, the jump frequency of the interstitial clusters is so low that the interstitial clusters cannot move through the solute atom clusters under an irradiation temperature of 573 K.

1. Introduction

One-dimensional (1-D) motion of interstitial clusters (interstitial-type dislocation loops) was first observed during electron irradiation with high voltage electron microscopy [1,2]. Arakawa et al. reported that nanometer-sized dislocation loops with the Burgers vector of 1/2 ⟨1 1 1⟩ moved back-and-forth in α-Fe [3,4]. They suggested that the small 1/2 ⟨1 1 1⟩ dislocation loops have a structure consisting of a bundle of crowdions. Satoh et al. reported that the 1-D motion of interstitial clusters is influenced by the purities of α-Fe specimens [5,6]. The effect of solute atoms on the 1-D motion of interstitial clusters is important in bcc metals. Satoh et al. also reported 1-D motion of interstitial clusters in austenitic stainless steel SUS316L and its model alloys [7,8]. The difference in the frequency and distance of the 1-D motions was not observed under 1250 keV electron irradiation at room temperature [7]. The authors suggested that the 1-D motion of interstitial clusters was induced by interatomic mixing and suppressed by solute segregation under electron irradiation at 673 K [8]. The effect of solute atoms on the 1-D motion of interstitial clusters is also important in fcc metals.

The movement of interstitial clusters produced by cascade damage has also been shown by molecular dynamics [9–16], which was reported earlier than the experimental reports of Arakawa et al. mentioned above [3,4]. The activation energy for 1-D motion of interstitial clusters was less than 0.1 eV in α-Fe, and was almost constant or slightly decreased with increasing cluster size (1–20 interstitials) [10,13–15]. Kuramoto et al. calculated the activation energy of dislocation loops (7–219 interstitials) in α-Fe and Ni by a static method. The energy was less than 0.2 eV, with the smaller interstitial clusters having lower activation energies [17–19]. We have previously proven the comparability between molecular dynamics and the static method in the case of vacancy migration [20]. In fact, the difference between molecular dynamics and the static method was small when the size of the interstitial clusters was small. The large dislocation loops show dislocation-like motion and the small ones show point-defect-like migration [19].

1-D motion of interstitial clusters has a significant effect on the microstructural evolution in metals [2,21–24]. 1-D motion of interstitial clusters has also been often observed in neutron-irradiated metals by transmission electron microscopy (TEM) [25]. Alloying elements also affect the motion of interstitial clusters. Yoshiie et al. investigated the effect of alloying elements in Ni [26–30]. In neutron-irradiated pure Ni, Ni-2 at.%Cu (+7.18% volume size factor to Ni [31]), and Ni-2 at.%Ge (+14.76% volume size factor [26]),

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well-developed dislocation networks and voids were observed at 573 K at a dose of 0.026 dpa by TEM. Microvoids were detected by positron annihilation spectroscopy (PAS) even at a low dose level of 0.001 dpa. In Ni-2 at.%Si (−5.81% volume size factor [31]) and Ni-2 at.%Sn (+74.08% volume size factor [31]), no voids were detected by TEM and PAS. These results suggest that Si and Sn alloying elements prevent 1-D motion of interstitial clusters.

Marian et al. and Terentyev et al. reported interactions between interstitial clusters and solute atoms in Fe-Cu alloys and Fe-Cr alloys [14,32]. The solute atoms act as obstacles for the motion of interstitial clusters. Substitutional He atoms also slow the motion of interstitial clusters [33]. Sato et al. also reported that the oversized solute atoms led to an increase in the activation energy in the Ni-Au alloy system (+63.60% volume size factor [31]) [34]. However, one Au atom was not sufficient to prevent the motion of interstitial clusters. In this study, the following two effects were examined by computer simulation. The first was the size effect of solute atoms, and the other was the effect of oversized solute clusters. Solute atoms with a simulated volume size factor of −30% to +100% and solute atom clusters with an experimental volume size factor of +63.60% were introduced into the model lattice by modifying the effective medium theory (EMT) potential for the Ni-Au alloy [34,35]. The migration energy of the interstitial clusters was calculated using a static method [17,18].

2. Calculation method

We employed the EMT potential for Ni and Au, which is one of *N*-body potentials [35]. The parameters were fitted by Jacobsen et al. to the cohesive energy, the equilibrium Wigner-Seitz radius, the bulk modulus, the shear modulus, etc. [35]. The size and orientation of the model lattice are shown in Fig. 1. The model lattice was composed of 576,000 ($160 \times 60 \times 60$) atoms. Interstitial clusters were introduced into the center of the model lattice, which were made by bundling the ⟨1 1 0⟩ crowdions on the {1 1 0} atomic planes. The interstitial clusters were fully relaxed under the fixed boundary conditions (five atomic layers) by the static method, which did not take the effects of temperature into account.

The activation energy for a motion of the interstitial clusters was calculated by the same static method as that presented in Refs. [17,18,34]. The migration energies obtained by molecular dynamics simulation [10,13–15] and this static method [17–19] were almost the same for α-Fe, which supports the validity of our method. The aforementioned relaxation process was repeated with stepwise increments in the force applied to the interstitial clusters, which results in their movement. The migration energy of the interstitial clusters was obtained by integrating the force–distance curve $\sum_i f_i \Delta d_i$, where f_i is the force applied to the interstitial clusters at point i, and Δd_i is the shortest distance between two adjacent points. Fig. 2 shows the ideal force–distance curve. The migration energy was obtained as shown by the shaded area. The number of interstitials contained within the clusters was 1, 7, and 19. In this study, the migration of an interstitial was seen as

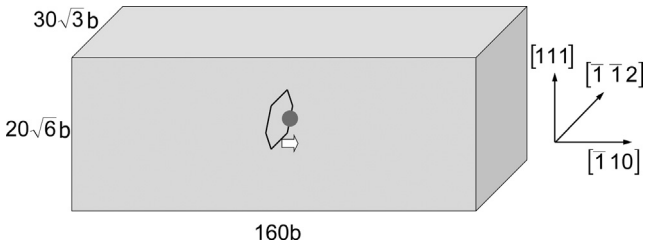

Fig. 1. The size and orientation of the model lattice, where 'b' denotes the atomic distance.

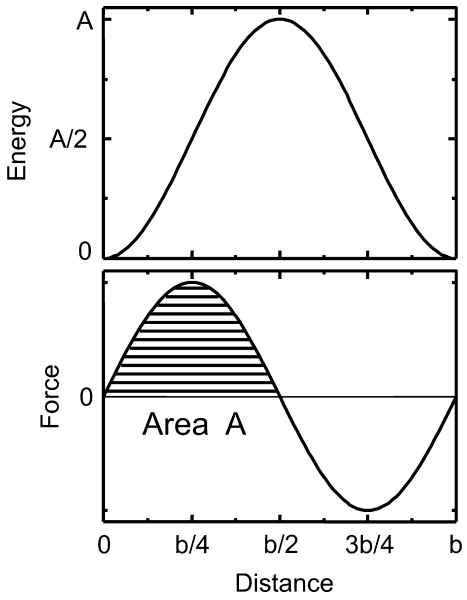

Fig. 2. The ideal force–distance curve in the migration of the interstitial clusters, where 'b' denotes the atomic distance. The migration energy was obtained, as shown by the shaded area.

the ⟨1 1 0⟩ crowdion. This is because the migration mechanism of the crowdion is similar to that of the interstitial clusters. The migration energy of the crowdion, 7 clusters, and 19 clusters obtained by the method described above was 0.02, 0.05, and 0.08 eV, respectively [34].

To obtain the effective medium theory potential for a Ni–Au alloy system, the parameters were adjusted to realize the volume size factor and heat of the solution. In Ref. [34], the parameters were tuned to an experimental volume size factor of +63.60% [31] and a heat of solution of 0.34 eV [36]. The atomic volumes of solution A (Ω_A) change linearly with the atomic concentration of the solute B at low concentration. The effective atomic volume of the solute B (Ω_B^*) is obtained by a linear extrapolation of the volume plot of one hundred percent solute. The volume size factor is given as $(\Omega_B^* - \Omega_A)/\Omega_A \times 100$ (%). For estimation of the effect of the solute clusters, the same parameters were used. To evaluate the effect of the volume size factor of the solute atoms, the parameters were adjusted to five volume size factors of −30%, 0%, +30%, +63.60%, +100% and a heat of solution of 0.34 eV. Table 1 shows the real volume size factors after the tuning.

3. Results and discussion

3.1. The effect of volume size factors

Fig. 3 shows the migration energy of the crowdion, 7 clusters, and 19 clusters to overcome the energy barrier of one solute atom with different volume size factors. Regardless of the size of the interstitial clusters and the location of the solute atom, the migration energy of the interstitial clusters increased with the absolute value of the volume size factor. The migration energy of the interstitial clusters exceeded 1 eV for the +100% volume size factor. It is expected that the strain field formed by the oversized solute atoms suppresses the 1-D motion of the interstitial clusters.

It is interesting to note that the solute of the volume size factor −30% has higher migration energy than that of the +30% solute. In previous experiments [26–30], Ni-2 at.%Si (−5.81%) prevented void formation at doses of 0.2 dpa, although Ni-2 at.%Ge (+14.76%) did not prevent void formation. The results indicated a strong suppres-