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Annihilation of Interstitial Atoms to Dislocations in Neutron-irradiated Cu and Ni at High Temperature

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Abstract

When Cu and Ni were irradiated at 300oC by neutrons in a reactor, interstitial clusters decorate dislocations at a low fluence such as 5 x 1017n/cm2. Computer simulation suggests that this is due to the accumulation of interstitial atoms in the dislocation strain field and also the difficulty of absorption of interstitials to extended dislocation which existed prior to irradiation. Interstitial clusters accumulated along dislocations coagulated to form dislocation loops in Cu and dipole loops which were along <112> direction with a <110> Burgers vector in Ni. These newly grown loops and dipoles can absorb interstitial clusters due to the unextended nature of these dislocations, and cause disappearance of decoration of interstitial clusters. Dislocations grew to a bow-out shape and was pinned at voids.

1. Introduction

Dislocations play an important role on the development of damage structure in Cu and Ni which are neutron-irradiated in a reactor at high temperature such as 300oC to 400oC [1]. By a collision between a metal atom and a neutron a displacement damage cascade forms. Interstitial atoms that are either a single interstitial and interstitial cluster are thought to move to dislocations and annihilate. Vacancies left in the crystal aggregates to form clusters such as stacking fault tetrahedra and voids [2]. It was observed by transmission electron microscopy (TEM) that interstitial clusters decorate dislocation lines [3, 1]. In 1997 Trinkaus et al. published a paper [4] in which a fundamental process of decoration of interstitial loops along dislocation was studied based on a model that interstitial clusters are not absorbed on dislocation lines and stay near dislocations. These interstitial clusters could modify the long range dislocation strain field and weaken further collections of point defects to dislocations. This occurs at low fluence range of neutron irradiations below 1018 n/cm2, whose range is important for the nucleation of voids at high temperature [5]. In the present work, we examined the development of dislocation structure in Cu and Ni with the neutron-fluence.

2. Experimental Procedures

A foil of Cu and Ni whose thickness was 50 microns was irradiated at KUR (Kyoto University Reactor) and JMTR (Japanese Materials Testing Reactor) of JAERI (Japan atomic energy research institute). Foils were irradiated in temperature-controlled capsules which were developed in both facilities [6,7,8]. Specimen temperature was controlled within 5 degrees during a whole range of irradiation [8]. The neutron fluence was between 7 x 1017 n/cm2 and 5 x 1018 n/cm2 in KUR irradiation and between 5 x 1018 n/cm2 and 1 x 1020 n/cm2 in JMTR irradiation. Specimens were thinned by electro-polishing and observed by transmission electron microscopy at 200 kV accelerating voltage.

3. Computer Simulations

To study the atomistic mechanism of annihilation of interstitial atoms at dislocations, computer simulation was carried out with an isotropic potential and using the embedded atom method (EAM) that was developed by Daw and Baskes [9, 10]. Dislocations in a form of dipole (two parallel extended dislocations with opposite Burgers vector) were introduced in a model crystal that was composed by 26598 atoms. An extended edge dislocation was at first introduced on a (111) plane with wider extended width and relaxed to the equilibrium structure by running a short period of molecular dynamics (MD) at 500 K. The periodic boundary condition was applied to all three surfaces. The

present EAM potential of Cu gives a stacking fault energy of 39 erg/cm2 which causes an extended width 13b of an edge dislocation, where b is the nearest neighbor distance of 2.56 A in copper. After the thermal equilibrium of the crystal was reached, 5 to 68 interstitial atoms were introduced at random positions in the crystal. A crystal was run by MD simulation for several hundreds of pico-seconds at 500 K. After this MD run, a crystal was energy-minimized by the conjugate gradient method. Partial dislocations were searched by observing the atom arrangement that was viewed from a <111> direction which is normal to the plane of extended dislocation and also from a <110> direction which is parallel to the extra half plane. If a single interstitial is absorbed on an extended dislocation and nucleates one step of extended jog, the latter should be detected as a displaced line of atoms in the <110> projection. Interstitial atoms were searched by counting a number of atoms which are included in the Wigner-Seitz cell [11]. The computer simulation of the present work was carried out only for Cu. The EAM potential of Ni of Daw & Baskes format give a relatively low stacking fault energy 30 erg/cm2 comparing to the experimental value 100 erg/cm2. The value of stacking fault energy is very important on the determination of width of extended dislocation and may also be important on the absorption of point defects to dislocation.

4. Results

(a) TEM observations

Figures 1(a) to (d) show a dislocation structure in Cu which were irradiated at 300oC to the fluence of (a) 7 x 1017 n/cm2, (b) 3 x 1018 n/cm2, and (c) 1 x 1020 n/cm2 at 400oC. It can be seen in Fig. 1(a) that interstitial clusters accumulated in the form of a decoration along straight dislocations at the low fluence. During further irradiation these interstitial clusters coagulated along dislocations to form interstitial loops of irregular shapes as seen in Fig. 1(b). Dislocations resulting from this coalescence can not be extended significantly. During further irradiation, these loops grew to bowed shape by absorbing interstitial atoms [5]. Voids grew to a large size at the stage of 1019 n/cm2 irradiation. Dislocations were pinned at voids as seen in Fig. 1(c). At a heavy neutron-irradiation, dislocation density increased in regions connecting nearby voids as seen in Fig. 1(d).

Figures 2(a) to (c) show the development of a dislocation structure which was observed in neutron-irradiated Ni. Interstitial clusters are accumulated along dislocations at a low fluence as seen in Fig. 2(a). Interstitial clusters grew close to a straight dipole dislocation which aligns along <112> directions with a Burgers vector which is parallel to <110> directions. This means that the Burgers vector of these dipoles is not parallel to the dipole. These dipoles did not change their shape during TEM observation. These dipoles were thought to be formed by agglomeration of interstitial clusters. On further irradiation, dipoles developed to a bundle of parallel dipoles as seen in Fig. 2(b). After further increase of the neutron fluence dislocations grew to well isolated lines as seen in Fig. 2(c). Significant characteristics of dislocation structure in neutron-irradiated Ni was a low density of dislocations at high fluence. Many large voids were observed while the number of dislocations was very low.

(b) Computer Simulation

In a model crystal of 26598 Cu atoms, we introduced a dislocation and 10 interstitial atoms. Figures 3(a) and (b) show the final configuration of interstitial atoms which arrived near the dislocation. As is shown in Fig. 3, interstitial atoms were found on a (111) plane, which is parallel to the plane on which the dislocation line is extended. Interstitial atoms near partial dislocation has a <110> crowdion structure as shown by a bar in Fig. 3. Interstitial atoms locate on the expansion side of the dislocation. An interstitial atom is trapped to a dislocation line as extra-atoms which locate immediately outside of stacking fault. By close examination of the structure, it was found that a trapped interstitial atom does not relax to an extended jog between two partial dislocations. This tendency of accumulation of interstitial on a (111) plane near dislocation was observed for the number of introduced interstitials which is between 5 and 20. With increasing the number of introduced interstitial atoms, they grew to a small platelet which locates immediately outside and along <110> partial dislocation lines as shown in Figs. 4(a) and (b). With further increase of interstitial atoms, they form interstitial clusters along a dislocation which is similar to the decoration of interstitial clusters as observed experimentally.

5. Discussions

The present experimental results show that a straight dislocation which existed in crystal prior to a neutron-irradiation does not grow to an irregularly curved shape by absorbing interstitial atoms. Interstitial atoms are accumulated near dislocations because of their elastic interaction with a dislocation and as a consequence, they cluster along dislocations. This is due to the difficulty of absorbing interstitial atoms through the nucleation of extended jog on the dislocation. Interstitial atoms are trapped as small interstitial platelets on a plane which is parallel and

outside the extended straight dislocations in Cu. These small interstitial clusters grew to larger interstitial clusters by coalescence [5]. In Cu these interstitial clusters grow to complicated shape of dislocation loops. These dislocations have a high sink efficiency on the absorption of point defects for both of interstitial atoms and vacancies. In Ni, interstitial clusters did not form a complicated structure of dislocation loops along pre-existed dislocations. They grew to dislocation dipole of interstitial clusters whose direction is <112> and a <110> Burgers vector. These dipoles grew to a form of bundle and finally developed to dislocation structure as observed in Fig. 3(b).

Trinkaus et al. [4] modeled that the decoration of interstitial loops around dislocations is due to the difficulty of absorption of interstitial loops. We observed the similar decoration of interstitial clusters in electron-irradiated gold [12]. A foil of gold of 50îm

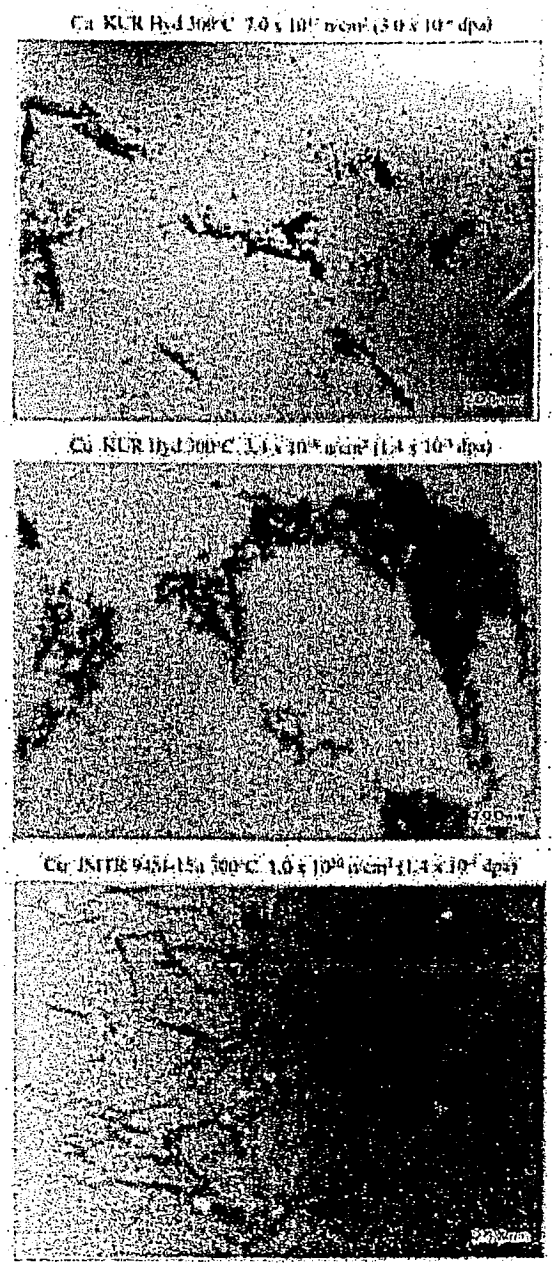

Fig. 1 Dislocation structure observed in neutron-irradiated Cu at various stages of neutron irradiation. (a) Decorated dislocation by interstitial clusters. 7 x 1018 n/cm2. (b) 3.4 x 1018 n/cm2. (c) 1 x 1020 n/cm2 at 300oC.

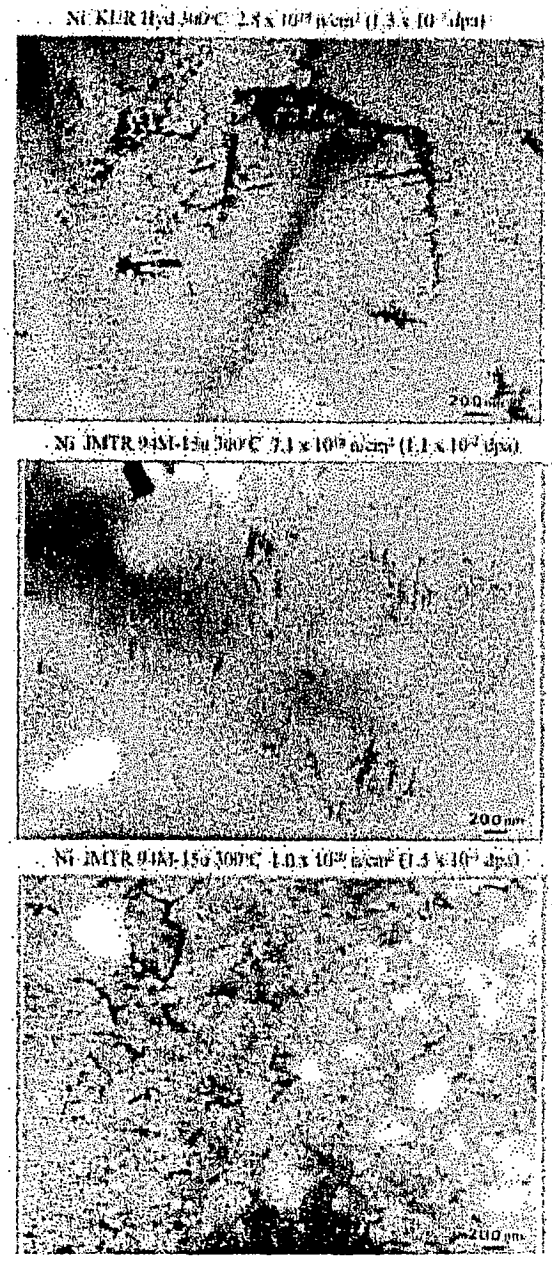

Fig. 2 Dislocation structure observed in neutron-irradiated Ni at various stage of neutron irradiation. (a) Formation of dipoles observed along dislocation. 2.8 x 1018 n/cm2. (b) 7.1 x 1018 n/cm2. (c) 1 x 1020 n/cm2 at 300oC.

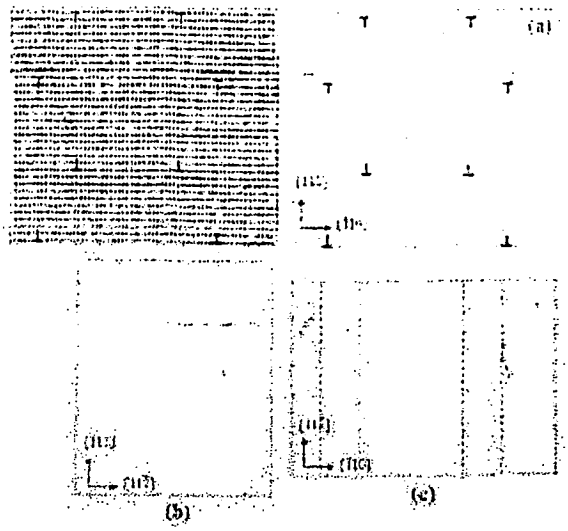

Fig. 3 Ten interstitial atoms introduced in dislocated copper of 26598 atoms. The configuration of interstitial atoms vas obtained after prolonged MD run. (a) Atom arrangement viewed from <112> direction. (b) and (c) show an interstitial atom with a structure of <110> crowdion on a (111) plane near a partial dislocation.

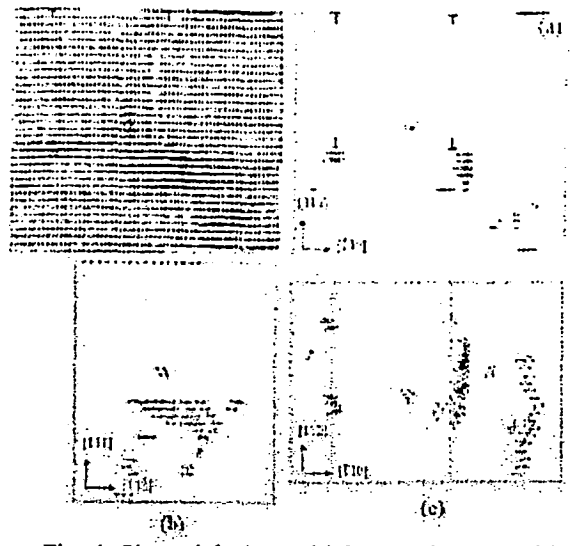

Fig. 4 Sixty eight interstitial atoms introduced in dislocated copper of 26598 atoms. The configuration of interstitial atoms vas obtained after prolonged MD run. (a Atom arrangement viewed along <112> direction. (b) and (c) show a projected view of interstitials near dislocation lines.

thickness were irradiated at 78 K to the fluence of 1 x 1018 e/cm2 of 30 MeV electrons with Linac acceralator and polished at –20oC and observed at 100 K. Also the decoration of interstitial clusters along a dislocation was observed in gold of 50lm thickness which was irradiated at 78 K with 3MeV electrons to 3 x 1018 e/cm2 [13]. Specimen was thinned at –20oC and observed at 100 K.

6. Summary

The development of dislocation structure in irradiated Cu and Ni was studied by TEM observation and by a computer simulation. The decoration of interstitial clusters along dislocations is found at low fluence of irradiation. The decoration is due to the difficulty of absorption of interstitial atoms by dislocations. It was shown that the sink efficiency of dislocations on the point defects absorption varies with the neutron fluence. This is due to the trapping of interstitial atoms at extended dislocation at low fluence, while absorption of point defects on climbed dislocation is operative at high fluence. The difference of the dislocation sinks strength on point defect absorption affects the development of damage structure.

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