The Role of Point Defect Clusters in Microstructure Formation in Fe-Cu Alloys

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1. Introduction

Neutron irradiation to reactor pressure vessel steels (RPV) leads to changes in the mechanical properties due to the formation of microstructures. In particular, the Cu precipitates are considered to be a major factor to induce the mechanical property changes. Many efforts have been made to understand the underlying mechanism of Cu precipitation in Fe-Cu binary alloys and RPV steels. We have performed Monte Carlo simulations in Fe-Cu binary alloys to investigate the microstructural features of Cu-containing clusters and to complement the experimental findings. Emphasis is placed on identifying the spatial distribution of and configuration of the Cu-containing microstructure under irradiation.

2. Methods

In this section we describe briefly the simulation techniques used, which include the molecular dynamics and Metropolis Monte Carlo method.

2.1 Molecular Dynamics Simulation

The molecular dynamics (MD) is useful for defining the state of the primary damage in a quantitative way. WE can obtain atomic-scale information and physical insight into the mechanisms of irradiation-induced displacements. The MOLDY code was used to quantify the primary damage parameters, including the number of point defects after the collisional phase and their locations [1]. The cascade simulation is initiated by giving one of the lattice atoms, which corresponds to the primary knock-on atom, a pre-defined amount of kinetic energy in a specified direction. The MD simulation continues until the phase of the recombination of the interstitials and vacancies is finished. The atomic block, however, does not return to the complete thermal equilibrium state because of the high temperature. Hence, the MD simulation is terminated when small changes occur to the number of the point defects.

2.2 Metropolis Monte Carlo Method

The Metropolis Monte Carlo (MMC) algorithm is an importance random sampling method for obtaining the thermodynamic equilibrium states of a system. In this work this method is applied to the canonical (NVT) ensemble where the number of particles (N), the system volume (V) and temperature (T) are conserved. In this ensemble, the initial number of each element – Fe, Cu, and vacancy is maintained constant throughout the simulation. The MMC simulation proceeds by randomly choosing a new trial state, based on the diffusion mechanisms. Atoms can exchange their position with neighboring vacant lattice sites or two different atoms, Fe and Cu, may rotate together. The atomic movement leads to the energy difference between the new and the previous state. For two ensemble states of $\square_{old}$ and $\square_{new}$, we can calculate the energy of the system before and after transition, denoted by $E(\square_{old})$ and $E(\square_{new})$ respectively. The new state $\square_{new}$ is accepted when $\square E$ ($= E(\square_{new})-E(\square_{old})$) is less than or equal to zero. If $\square E$ has a positive value, the new state is accepted according to the following rule. After generating a random number $\square$ between 0 and 1, we compare $\square$ with the term $\square$.

$$\xi = \exp(-\delta E / k_B T) \qquad (1)$$

where k_B is the Boltzmann constant and T is the temperature. If $\square > \square$, then we accept the new state $_{new}$.

The MMC can simulate a thermodynamics ensemble at the equilibrium state. Therefore, the basic assumption in this study is that the system will evolve towards the equilibrium state as the step number increases. After the specified number of Monte Carlo steps, the minimum-energy configuration of the atomic distribution is obtained. The energy difference $\square E$ depends on the interaction model for the Fe-Cu binary alloy. The Fe-Cu potential, derived by Ackland et al., was used as an interatomic potential in this study [2]. This potential is based on the framework of the Finnis-Sinclair formalism [3].

3. Results

3.1 Residual Damage

We performed displacement cascade simulations by using the MOLDY code. Prior to starting the cascade simulation, a block of 16000 iron atoms is equilibrated at 300°C for about 10 ps to obtain a phonon equilibrium mode. Then, the cascade simulation is initiated by giving a kinetic energy to an atom in a particular direction. In this simulation, the initial energy of PKA was set to be 3 keV and its direction was [135]. This cascade simulation has been performed at 300°C up to 8 ps. From the MD simulation results, the region around the damaged zone is selected for the subsequent MMC simulation. The residual defects are composed of the

interstitial- and vacancy-type point defects. Some are scattered as single point defects, and others exist in the form of clusters. The result of primary interest is the distribution of the point defects that survive from the displacement cascade. Fig. 1 shows the distribution of the vacancy-type point defects in the 20x20x20 block. Debris is left in the form of isolated defects or defect clusters. The role of these residual defects in forming the extended microstructure is the focal point in this study.

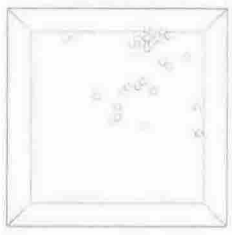

Figure 1. Vacancy-type defect configuration from a 3 keV cascade simulation in iron at 300°C.

3.2 Microstructural Evolution

The focal point in the MMC simulation is the role of the vacancies generated by the displacement cascades in the formation of the Cu-containing clusters. We investigate the atomic configuration of the system through the MMC simulation by changing two parameters, which are the initial Cu contents and the presence of residual defects. Generally, the formation of Cu clusters does not prevail in an alloy with low Cu contents (0.1 w/o) regardless of the inclusion of residual defects. Only a small size of Cu clusters, composed of a few Cu atoms, could be found from the simulation. For the alloys containing higher Cu contents (1.0 w/o), the tendency to form Cu clusters is apparent as can be seen in Figs. 2. Cu atoms have higher probabilities of encountering vacancies or other Cu atoms in the matrix during migration. When the residual vacancies are included, Cu atoms bind eagerly to the vacancies, which is shown in Fig. 2 (b). Although the shape of the Cu clusters is not a complete precipitate, these clusters take a transitional form which lie between the molecules and the bulk matter. The tendency to form small Cu-vacancy complexes is a very important to the radiation damage process. The vacancy clusters created by the displacement cascades can provide the nucleation sites for full-fledged Cu-rich precipitates.

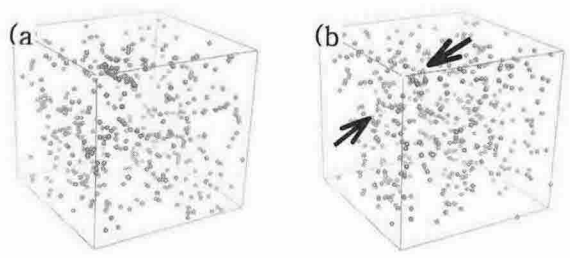

Figure 2. Atomic arrangement of the vacancies (*empty spheres on the RHS*) and copper atoms (*filled spheres*) at the end of the MMC simulations (a) no residual defects; (b) residual defects included. Note that the Cu-vacancy complexes in (b) are marked with arrows.

4. Conclusions

This paper has attempted to model the microstructural evolution in the Fe-Cu system under irradiation. Starting from the MD simulations of the displacement cascades, the MMC methods are applied to find the atomic configuration of the Cu clusters with the minimum system energy. The results show that the Cu clustering does not prevail for the Fe-Cu alloys of a lower Cu content (0.1 w/o) even when the residual defects are included. The vacancy clusters remained as they were at the end of the simulations. In the case of a higher Cu content (1.0 w/o), the formation of the Cu clusters is apparent regardless of the presence of the residual defects. In particular, the vacancy clusters in the Fe-Cu system are associated with the surrounding Cu atoms to form complexes. These calculation results are important for understanding the fundamental vacancy-solute interaction. Also, the computational approach in this study has shown that a combination of MD simulations and the Monte Carlo method can be used to predict the microstructural behavior under irradiation.

REFERENCES

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