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MOLECULAR DYNAMICS SIMULATION FOR CLUSTERS OF COPPER ATOMS IN FE-CU ALLOY UNDER RADIATION

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ABSTRACT

The behavior of copper atoms for the micro-structural changes that occur in ferrite vessel steels containing trace copper under fast-neutron irradiation. A molecular dynamics simulation of displacement cascades in Fe-3atÿCu alloy has been carried out with various primary knocked on atom(PKA)energies and temperature. The results showed that if PKA energy (E) was less 20keV and/or temperature was below 1000K, no stable clusters of copper atoms was found, but when EP = 20keV, T = 1000K, clusters of copper atoms contain over seven Cu atoms were formed and stabilized after 5ps later, the process forming the clusters has been described and the mechanism forming the clusters has been discussed.

***Keywords*:** Fe-Cu alloy, neutron radiation, molecular dynamics, cascade simulations

1. INTRODUCTION

Various defects are created by displacement cascades during heavy-ion and fast neutron irradiation on structural components in nuclear reactors. The point defects created by cascades have effects on the microstructure changes, and eventually cause irradiation induced embrittlement, hardening and void swelling [1-5] which are connected with the safety and life-time of nuclear structural steels. Copper is well known to cause embrittlement in nuclear reactor pressure vessel steels by forming Cu-rich precipitates [6-7]. Thus, it is important to understand the processes and mechanisms by which Cu solute Cu atoms effect irradiation defect formation in Fe, and the Cu-point defect interactions that determine copper diffusion. Because of the difficulties in handling irradiated materials and in experimental examination of atomic scale structural changes, recent molecular dynamics (MD) have been widely used for investigation of irradiation effects in Fe-Cu alloy materials. For example, Becquart C. S. *et al.* have studied the role of Cu in Fe-0.2at.%Cu and Fe-2at.%Cu alloy with different primary knocked-on atom (PKA) energies [8]. Marian J. *et al.* have studied the Cu solute-atom diffusion in the Fe-0.9at.%Cu alloy[9]. Lee Byeong-Joo *et al.* used the modified embedded-atom method inter-atomic potential have investigated the primary irradiation defect formation in pure Fe and Fe-0.5at.%Cu alloy with PKA energy of 2keV at 573K[10]. Jang Je-Wook *et al.* have investigated the effects of alloying elements, Cu, Cr and C, on the number of residual point defects, their clustering tendency and constitution in pure Fe, Fe-0.5 at.%Cu, Fe-10 at.%Cr and Fe-0.1 at.%C alloy[11]. Even though these studies provide valuable information on the effect of Cu on the primary irradiation defect formation in Fe, they all not find Cu cluster, while it is important to Cu-rich precipitates [6-7]. Therefore, it is necessary to investigate the Fe-Cu alloy again and examine the effect of Cu on the irradiation defect formation from a mechanistic perspective.

2. SIMULATION METHOD

The inter-atomic potentials used in the present work are the many-body functions of Ackland *et al.* [12-13]. This potential describes all three possible atomic interactions, namely, Fe-Fe, Fe-Cu and Cu-Cu, of the metallic Fe-Cu

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binary alloy and was in fact developed to describe both the coherent metal stable bcc. phase of the early Cu precipitation stage (a0 = 2.961Å). Cutoff radii were set at the midpoint between second and third nearest-neighbor distance (1.20Å) for the Fe-Fe and Fe-Cu interactions, i.e. 3.4Å, and between the third and fourth coordination spheres for the Cu-Cu interactions (4.3Å). Adjustment to the universal screened Coulomb function of Biersack and Ziegler[14] for interaction within normal nearest-neighbor distance was also performed to permit investigating atomic collisions in radiation damage. A modified version of the XMD computer code is employed, and all simulations are carried out with periodic boundary conditions and constant volume. The number of atoms involved in each simulation is 250000 (50 × 50 × 50 unit cells). It is believed that the simulation box size effect is negligible as far as the box size is large enough not to allow the overlapping of cascade region due to the periodic boundary condition. Prior to a cascade, Fe atoms are randomly replaced by Cu atoms, forming substitutional Cu atoms in body-centered-cubic Fe. Cu concentration is 3 at.%. The concentration is a little bit higher compared to typical concentration of elements in nuclear structural steels, but it was chosen to see the alloying effect more clearly. All the displacement cascade was initiated by giving a kinetic energy to a selected Fe atom, for primary PKA energies ranging from 5keV and 20keV, the initial equilibration temperature ranging from 573K and 1000K. At the beginning of the simulation, the system of particles is let to equilibrate, for 5ps, at the chosen temperature, to be close to the vessel irradiation temperature.

3. RESULTS AND DISCUSSION

With the increase in the spacing *H* of the two plates, the liquid bridge may lose its stability and be split into two droplets, both of which have the shape of spherical cap, as shown in Fig. 3.

We performed MD simulations of displacement cascades at different temperature, with different PKA energy, while only at 1000K and PKA energy was 20keV, the stable cluster of Cu atoms containing seven Cu atoms was found. Fig. 1. Presents the process of Cu cluster evolution with a PKA energy of 20 keV at 1000K. The process associate with a displacement cascade, during 0ps~1ps the energy of PKA is distributed by multiple collisions among many atoms, with the result that Cu atoms leave their lattice sites and to region new lattice sites. Some Cu atoms regain new lattice sites, while others are unable to regain lattice sites form self-interstitial atoms (SIAs). As the results of redistributes of Cu atoms, the cluster form partially at 3 ps. With the cascade successive the cluster formed completely and stabilized. The same state can be seen at 6ps, 7ps, 8ps.

Table 1 show the previous and this work simulate condition and results of Fe-Cu alloy. The results show that if Cu concentration is below 3 at.%0PKA energy is less 20keV and/or temperature is below 1000K, no stable clusters of Cu atoms was found, but when Cu concentration is 3 at.%0EP=20keV and T=1000K, cluster of Cu atoms containing seven Cu atoms were formed. In other words only high Cu concentration0high PKA energy and high temperature can obtain Cu clusters.

The Cu cluster has been observed in this study. However, the role of displacement cascades on the Cu clusters formation has not been well understood. Some people think Cu atoms were transported by the numerous vacancies created by the cascades[15], while others people consider the interstitials atoms play a role in transporting Cu atoms either [16]. Because of the very strong binding energies between Cu atoms and vacancies, we believe that the occurrence of many vacancies created by cascades will affect the Cu atoms significantly. However, more work should be done to clarify this point. The further study of this point will be documented elsewhere. From the First-principles calculations we find the total energy of a vacancy in the middle of two Cu atoms is -5536.064eV. The total energy of two Cu atoms bonded is -5536.362eV. The difference of the two results is about 0.3eV. So the status of two Cu atoms bonded is more stable.

Table 1
Previous and this Work Simulate Condition and Results of Fe-Cu alloy

	Cu concentration	*PKA energy*	*Temperature*	*Cu cluster*
Becquart C.S.	0.2at.%, 02 at.%	5keV, 10keV, 20keV	600K	-
Lee Byeong-Joo	0.5 at.%	2keV	573K	-
Jang Je-wook	0.5 at.%	2keV	573K	-
This work	3 at.%	5keV	573K	-
This work	3 at.%	10keV	1000K	-
This work	3 at.%	20keV	1000K	7 Cu atomic

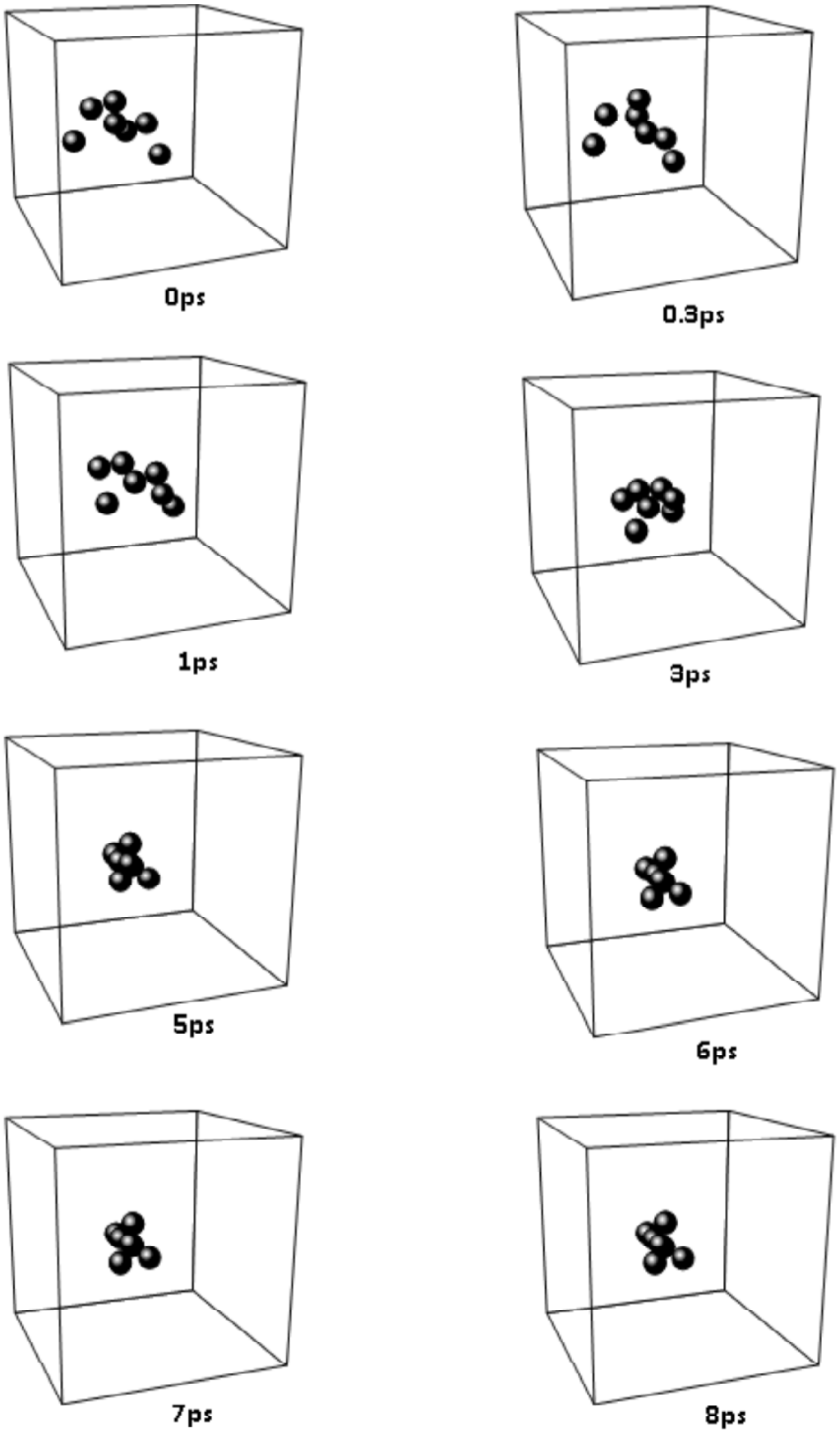

Figure 1: Process of Cu Cluster Evolution with a PKA Energy of 20 keV at 1000K

4. CONCLUSIONS

We performed MD simulations of displacement cascades in Fe-3 at.%Cu at different temperature, with different PKA energy. If PKA energy (EP) is less 20keV and/or temperature is below 1000K, no stable clusters of copper atoms was found, but when EP=20keV, T=1000K, clusters of copper atoms contain over seven Cu atoms were formed and stabilized after 5ps later. Because of the very strong binding energies between Cu atoms and vacancies, we believe that the occurrence of many vacancies created by cascades will play important role in transporting Cu atoms.

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