§19. Dynamical Process of Damage Formation and Its Evolution in BCC Metals Irradiated by Fusion Neutron

Shimomura, Y., Sugio K. (Faculty of Engineering, Hiroshima University), Nishiguchi, R. (Hiroshima Jogakuin University)

Body centered cubic (bcc) metal such as Vanadium, Molybdenum and Tungsten is accumulating an attention as fusion reactor materials due to their high melting temperature and superior mechanical properties. In the present work we studied fundamental physical properties of a point defect and point defect clusters such as an interstitial atom and a vacancy by computer simulation

Computer simulations were carried out for point defects (interstitial atoms and vacancies) in V and Mo. Utilized potentials of V and Mo are an empirical isotropic potential of embedded atom method due to Johnson and Oh and an angular dependent potential of modified embedded atom method (MEAM) due to Baskes. The migration of single interstitial (1i) in V and Mo was determined by calculating the mean square deviation (msd) of atoms in crystal during molecular dynamics (MD) run. A model crystal consists of 2000 atoms which was subjected by the condition of periodic boundary and constant volume. A crystal was attained at first to a thermal equilibrium at high temperature by running a MD simulation under a periodic boundary condition of zero pressure. After thermal equilibrium was attained, a MD simulation was continued for much longer time under conditions of a constant energy and constant volume. During a time t_i of MD run an interstitial makes jumps and the mean square displacement of atoms $\bar{}(r_i - r_{i0})^{**}2$ was calculated, where r_i and r_{i0} are the position coordinates of the atom i at the time t_i and zero. With the value of msd obtained and the Einstein equation of diffusion coefficient, the pre-exponential coefficient and the activation energy of the migration of 1i was obtained [1]. The values obtained for a migration of single interstitial in V and Mo are as follows.

$D = 5.61 \times 10^{-4} \exp(-0.17\ eV/kT)\ (cm^2/sec)$ for V

$D = 7.37 \times 10^{-4} \exp(-0.38\ eV/kT)\ (cm^2/sec)$ for Mo

The value of activation energy of migration of 1i of V reasonable agrees with experimental data by Klabunde et at [2]. On the other hand, the value of Mo does not agree with the experimental value 0.083 eV by Shultz et al [3]. It was found that a remarkable difference of migration energy of single interstitial in V and Mo which were obtained in the preset work was due to the difference of core structure of an interstitial atom. The most stable structure of single interstitial atom is <110> dumbbell in both V and Mo. During their migration, interstitial relaxes to a configuration of <111> crowd-ion which is the saddle point configuration of energy during migration. In Mo, a <110> dumbbell makes a jump through a saddle point configuration of a <111> crowdion. That is, an interstitial makes a zig-zag movement. The row of atoms along a <111> crowdion is straight in Mo, while it collapse in the core of interstitial in V as shown in Fig. 1. Central two atoms of this relaxed sprit configuration align to several different directions which compose meta-stable configurations of single interstitial atom in V. By jumping between these meta-stable configuration, single interstitial atom in V makes successive jumps along a <111> direction and also rotate to different direction of either <110> or <111> directions with low activation energy as listed in Table I. The same type of simulation is carrying out with MEAM to study the anisotropic bond nature of bcc metals.

Reference

[1] K. Sugio, Y. Shimomura and H. Huang, Submitted to JIMS

[2] C. E. Klabunde, R. R. Coltman, Jr., and J. M. Williams,

[3] H. Schultz, "Point Defects and Defect Interaction in Metals" Kyoto Japan p. 183

Process	Activation energy
<110> → <553>	0.33 eV
<110> → <211>	0.25 eV
<110> → <511>	0.25 eV
<511> → <110>	0.22 eV
<511> → <211>	0.18 eV
<511> → <100>	0.15 eV
<211> → <553>	0.09 eV

Table I

The activation energy of various processes.

Fig. 1