Monte-Carlo Simulation of Defect Behavior in Cascade Damage

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Monte-Carlo simulations of point-defect behavior in Fe during the annealing stage of cascades are performed at 290°C. The fractions of freely migrating defects, recombined defects and clustered defects are estimated for various initial defect distributions. Most of interstitials escape from the cascade region, and vacancies tend to form clusters in the cascade region. The difference in behaviors between interstitials and vacancies may play a significant role on microstructural evolution.

1. Introduction

Changes in mechanical properties of the materials exposed by energetic particles are strongly related with irradiation-induced microstructural changes, such as formation of point-defects, defect clusters and microstructural and microchemical evolution from cascade damage. Both the macrosopic and microscopic changes under irradiation are usually complicated and non-linear functions of irradiation parameters, such as energy, mass, flux, fluence of incident particles and irradiation temperature. In this study, a Monte-Carlo simulation study is performed to investigate how the cascade defect distribution in a localized and segregated fashion evolved in BCC Fe by diffusion processes of point-defects which occur within greater spatial and time scales than Molecular Dynamics simulations.

2. Monte-Carlo Method

A conventional 'Metropolis method' is applied to describe the kinetics of defect migration, where one of the defects in computational volume is randomly chosen and moved at the nearest neighbor position. Many-body interatomic potential by Finnis and Sinclair is used for a BCC Fe crystal.

3. The effect of vacancy density on defect clustering and migration

Interactions and diffusion of point-defects in a cascade damage region are simulatied at 290°C to investigate the dependence of defect behavior on initial vacancy densities within a constant cascade size. The simulations are continued up to about 10^{-4} sec, when all mobile defect clusters, i.e., single and di-defect clusters, disappear from the cubic simulation volume. During the annealing simulation, a mobile defect cluster that jumped outside this volume is assumed to escape the cascade to be a freely migrating defects (FMD). The number of the FMDs and recombined defects in the volume are estimated as a function of initial number of Frenkel pairs and initial vacancy

density. Figs. 1 and 2 show the calculated results for the cascade-type and random-type intitial distributions, respectively.

The annealing behavior of point-defects from the cascade-type distribution is strongly dependent on an initial vacancy density in the cascade region. It is indicated that vacancies are likely to form clusters inside the cascade volume, resulting in the reduction of escaping vacancies. However, with increasing the initial vacancy density, the fraction of escaping interstitials decreases very slightly.

In the case of random initial distribution of point-defects, on the other hand, the fraction of escaping vacancies is similar to that of escaping interstitials. The densities of both types of defects for the random-type distribution were so small, compared with the case for the cascade resulting in smaller recombination and greater escaping efficiencies. The difference in these defect behaviors between the two initial distributions is mainly due to the clustering of vacancies in the cascade volume.

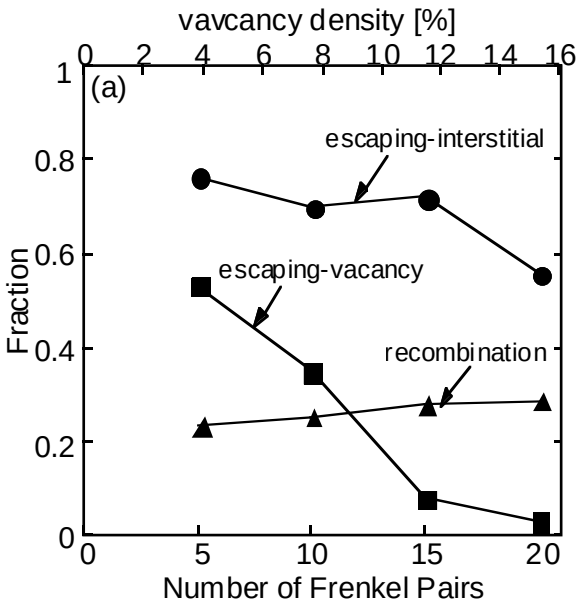

Fig. 1 The fraction of escaping interstitials, escaping vacancies and recombination under cascade damage.

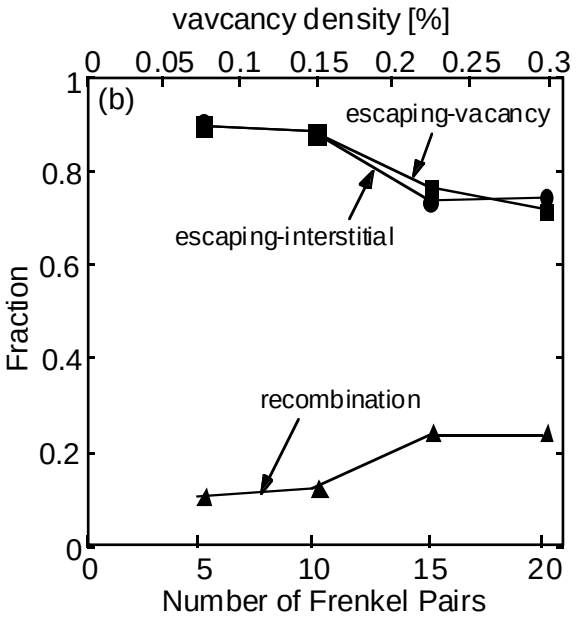

Fig. 2 The fraction of escaping interstitials, escaping vacancies and recombination under randam production of point-defects.