§8. Development of Simulation Models for Irradiation Performance of Fusion Materials

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(i) Introduction

The development of fusion materials must be performed without any experimental evidence derived from truly prototypic neutron flux-spectra, because, at the present time, there exists no fusion reactors or test reactors operating at fusion relevant flux-spectra. Therefore, it is very important to develop the multi-scale models for material behavior under 14 MeV neutron irradiation, and to make predictions of irradiation performance of fusion materials.

Toward these objectives and challenges, we have three approaches in this project; (1) Simulations for fundamental processes of defect production and agglomeration under irradiation, (2) Simulations and comparisons of material behavior under irradiation between pure materials and their alloys, and (3) Simulations for plastic deformation of irradiated materials.

(ii) The outline in this fiscal year

In this fiscal year, we had mainly three accomplishments, corresponding to the approaches shown in the previous section.

(1) We have evaluated the factors which control the one-dimensional motion of interstitial clusters directly generated by collision cascade.

(2) We have improved the methods to simulate the effects of transmutant helium and/or other impurities on defect agglomeration and cluster formation. We have also made a more quantitative evaluation for the circumstances of fusion reactor.

(3) We have evaluated the current issues to improve the dislocation dynamics simulations for material deformations, and to clarify the roles for defect clusters in the initial stage of the plastic deformation.

Among these three, we will mainly discuss the defect behavior under the plastic deformation, because we consider that it is one of the most difficult problems to complete the multi-scale modeling.

(iii) The accomplishments

In the previous enormous studies for plastic deformations by dislocation dynamics, the behaviors of the stacking-fault tetrahedral (SFT) had not been well clarified, and they had been treated the similar way just as other defects or impurities comprised in the matrix. This used to be the local rule of SFT for the dislocation dynamics, and this too much simplified model had been input into the simulations and the effects of SFT on plastic deformation had been evaluated.

However, since the SFT is one of the major defects observed in the irradiated materials for fcc metals, especially for materials with low stacking-fault energy such as Cu, it is essential to fully and precisely evaluate the mechanisms of interaction between SFT and line dislocations by MD simulations, and compare the results with the linear elastic theory.

We have used the Mishin potential, the advantage of which is that it can reproduce the phase stability for both FCC and HCP, and that it is suitable for the deformation simulations. SFT can be obstacles for dislocation motion, because there are interactions between line dislocations and stair-rod dislocations in the SFT. Figure 1 shows one snapshot describing the interaction between the line dislocation and SFT. The strength as the obstacles for the dislocation motion appears to strongly depend on the cross section between SFT and the line dislocation, because the cross section determines the length of the stair-rod dislocation physically intersecting the line dislocation, and the bowing angles of the line dislocations.

Therefore, the cross section is an essentially good indicator to describe the strength of the obstacles for dislocation motion. And, the angle between the SFT and the glide plane appears to also affect the interaction and to be an important parameter.

In the previous local rule for the dislocation dynamics, only the size of the clusters and the bowing angles of the line dislocations were taken as the local rules. We have improved and modified them with the physical base model and developed the new local rule by incorporating the cross section and the angle between SFT and the glide plane.

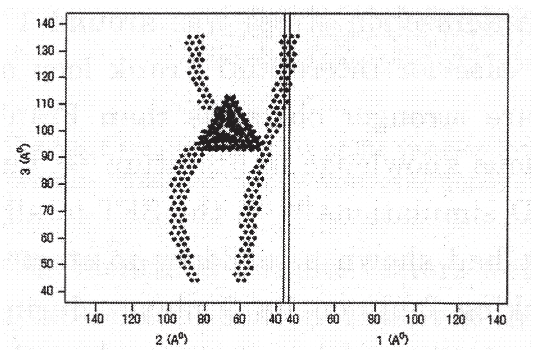

Figure 1. Interaction between line dislocation and an overlapping 28-vacancies SFT. The inserted edge dislocation was $a_0/2[101]$, but it dissociated into two partial dislocations.