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DISLOCATION DYNAMICS SIMULATION OF DISLOCATION-VOID INTERACTION

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ABSTRACT

Structural materials in nuclear power plants, such as reactor pressure vessel (RPV) steels, are used under high-energy particle irradiation conditions, which cause a significant degeneration of material strength commonly known as neutron irradiation embrittlement. The main mechanism of the neutron irradiation embrittlement is known to be an extensive formation of point defects, such as vacancies and self-interstitial atoms (SIA), and the diffusion of the point defects as well as a subsequent formation of point defect clusters. The cluster works as an impediment to the motion of dislocations, which significantly affects and degenerates the material strength. Therefore, in order to clarify the detailed mechanism of the neutron irradiation embrittelement, the interaction between dislocations and point defect clusters must be accurately understood.

To deal with the interaction between dislocations and point defect clusters, there are several types of computational approaches. The most representative approach is the molecular dynamics (MD) simulation. The simulation can provide the information on the interaction from the atomistic viewpoint. However, the simulation has a huge limitation to large length-scale simulations, because a huge number of atoms must be used. Therefore, the method can only be applied to the simulation of the interaction between a single dislocation and a single point defect cluster, and cannot be used for studies on the interaction of dislocations with multiple point defect clusters. The other type of computational approach is based on the continuum mechanics. Takahashi and Ghoniem proposed a computational method for dislocation-preceipitate interactions, which is a combination of parametric dislocation dynamics (PDD) and boundary element method (BEM) based on the superposition principle[1]. The method has a potential to deal with the interaction of dislocations with a lot of precipitates.

In this work, as a first step for the investigation of the material strength degeneration due to the interaction between dislocations and point defect clusters, we focus on the interaction between an edge dislocation and a void, which is a cluster of vacancies, and study the critical resolved shear stress (CRSS) in the interaction. To study it, we first extend the PDD+BEM method to the dislocation-void interaction problem. Importantly, a local rule for the dislocation behavior along the void surface is introduced into the computational method to deal with the disappearance of a part of dislocation line and

the motion of dislocation ends along with the surface of void. To examine the accuracy and reliability of the PDD+BEM simulation of dislocation-void interactions, a dislocation-void interaction in iron is simulated by the PDD+BEM. In the simulation, CRSS for the dislocation to break away from the void is calculated, and is compared to MD simulation results given by Osetsky *et al.*[2] (Fig.1). The results of the PDD+BEM and MD are in excellent agreement, meaning that the method can be reliably used for studies on the dislocation-void interaction. The method is then applied to the investigation of the dislocation-void interaction problems. In the classical dislocation theory, pinning strength of tiny obstacle is dealt with using a very simple equation, which takes into account only the line tension effect[3]. However, the elastic interaction between dislocation arms originating from the void interface must play an important role in determining the pinning strength. In order to study the effect, we perform PDD+BEM simulation of the interaction with and without the elastic interaction between dislocation arms. The result without the elastic interaction is independent of the void diameter, and is much larger than that with the elastic interaction (Fig.2). Therefore, it could be revealed that the dependence of the CRSS on the void diameter is provided by the elastic interaction between the dislocation arms, and the elastic interaction pushes the dislocation to break away from the void. Finally, we perform the PDD+BEM simulation of the dislocation-void interaction in copper, and discuss the effect of the extended dislocation core on the CRSS

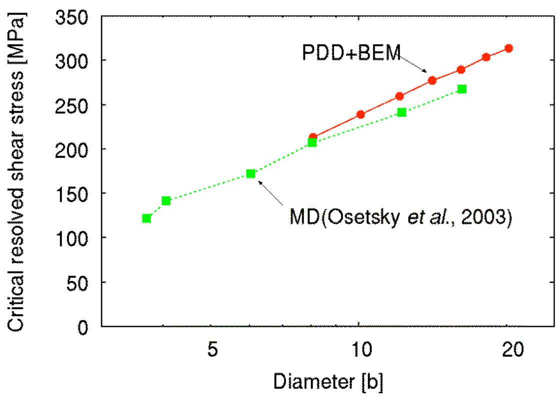

Fig.1 Critical resolved shear stress calculated By PDD+BEM and MD [2].

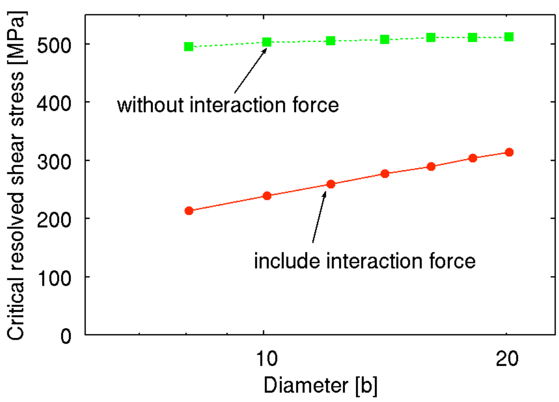

Fig.2 Critical resolved shear stress with and without elastic interaction.

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