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DISLOCATION DYNAMICS MODELING OF INTERACTION BETWEEN SUPER DISLOCATION AND γ-PRECIPITATES IN NICLE-BASED SUPERALLOYS

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ABSTRACT

Nickel-based superalloy is a technologically important class of commercial engineering alloy, and is used as a material of gas turbine blade in nuclear power plants. The most notable property of the superalloys is to provide a better mechanical strength at an elevated temperature, which is commonly known as the inverse temperature dependence. The major mechanism of the inverse temperature dependence is well explained by a characteristic behaviour of super dislocations in γ' phases. Recently three-dimensional atom probe observations have provided information on the existence of spherical γ-precipitates at a central region of γ' phases [1]. The γ-precipitates are believed to be an obstacle to the super dislocation motion and a factor to change the mechanical property of the material. Pretorius *et al*. studied the relationship between the critical resolved shear stress (CRSS) and the diameter of γ-precipitates, and found that the increase of the CRSS is proportional to the diameter of γ-precipitates [2]. The relationship must result from the interaction between the γ-precipitates and the super dislocation in γ' phases. Therefore, it is very important to figure out the physical picture of the interaction between the super dislocations and the γ-precipitates.

In this study, at first, the core structure of super dislocations in γ' phases are modelled using the Parametric Dislocation Dynamics (PDD) with the Peierls-Nabarro (PN) model[3]. The PN model can describe the dislocation core structure based on the continuum elasticity theory, and uses the elastic interaction between displacements in the dislocation core and the lattice restoring stress. The lattice restoring stress can be calculated by taking a spatial derivative of generalized stacking fault (GSF) energy. In this work, the GSF energy of the γ' phase is calculated using an interatomic potential for nickel-aluminum binary system developed by Mishin[4]. Also, the other type of dislocation models, such as super partial dislocation model and partial dislocation model, are used to compare with the PDD+PN model. In the models, constant energies of complex stacking fault and anti-phase boundary are used to express the total energy of the super dislocation, and are used as a lattice restoring stress force. To examine the

accuracy of the models, the atomistic core structure of the super dislocation is simulated using the Molecular Dynamics (MD) method, and is compared to the other dislocation models. As the result, the PDD+PN model gives us the best approximation of the atomistic core structure of the super dislocation in the models (Fig.1).

The shape of the super dislocation interacting with a γ-precipitate in a γ' phase is then simulated using the PDD+PN model. An infinitely straight edge super dislocation is placed at the middle of the γ-precipitate, and then, the super dislocation is relaxed to find the energetically stable shape. In the stable shape, the leading dislocation of the super dislocation lies along with the interface between the γ-precipitate and the γ' phase. The trailing dislocation is likely to be away from the leading dislocation, and lies along with the interface at the opposite side of the leading dislocation. Also, we performed a MD simulation of the interaction between a super dislocation and a γ-precipitate, to compare with the PDD+PN result, and found that the two results are in good agreement. Then, the CRSS in the interaction is calculated using the PDD+PN model. In the simulation, the diameter of the γ-precipitate and the position of the interaction are changed. The effect of the parameters on the CRSS is finally discussed.

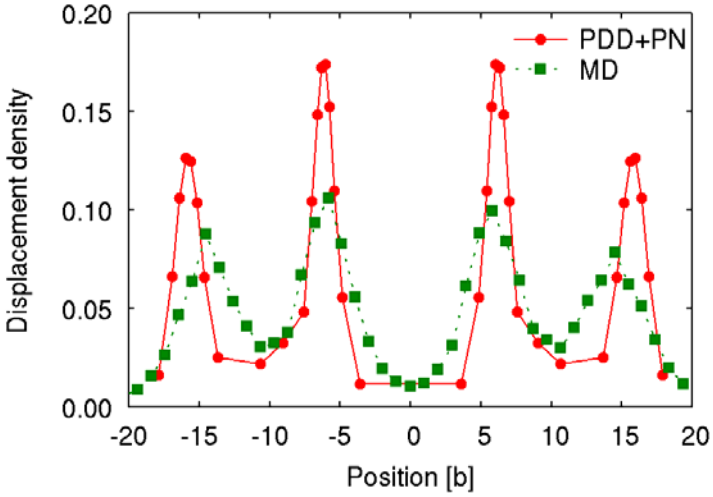

Fig.1 Displacement density distributions in a super dislocation in a γ' phase calculated by MD and PDD+PN model.

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