§23. Dislocation Bias Effect in BCC Metals by Means of MD Simulation

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According to the model on the mechanism of dislocation bias reduction based on the interaction of dumbbell self-interstitial atoms(SIAs) with a dislocation[1,2], the bias is significantly affected by the configuration of an SIA in the dislocation strain field. A large scale molecular dynamics(MD) simulation is performed here to reveal the stability and the mechanism of diffusion of SIAs near edge dislocation core in BCC iron.

The interaction between the Fe atoms in the crystal is derived from long-range many-body Finnis-Sinclair type potential[3]. This potential represents the current state of the art for the description of the cohesive energies of Fe, Nb, Ta, Cr, Mo, and W. In each simulation, a large BCC crystal containing more than 30,000 Fe atoms is located in the three dimensional simulation box with size 79.5, 64.9, 70.3Å, respectively(Fig. 1). Initial atomic positions are determined by elastic calculation and equilibrated under constant pressure. All MD calculations are carried out under the constant temperature after the equilibration. To maintain the temperature of the system at a constant preset value during the simulation, the velocities of individual atoms were rescaled at every time step.

Most SIAs among six < 011 > dumbbell SIA take crowdion configuration parallel to the Burgers vector in the expansion side of the dislocation. Such crowdions are stable in the temperature range of this simulation, i.e. between 373K and 473K, making one-dimensional random to-and-fro motion parallel to the dislocation Burgers vector staying at several atomic layers "below" the dislocation core. They are known to be stable during the long simulation period reaching 56ps. This means that the SIA does not approach the dislocation core. While several SIAs diffuse toward upwards direction and absorbed by the dislocation during the equilibration stage.

Although it is known that the stable SIA in the dislocation-free BCC crystal is < 011 > dumbbell type, the results of the present simulation suggest that the stable configuration of SIAs is seriously affected by the dislocation resulting in the < 111 > crowdion type. Furthermore, diffusion of SIAs are suppressed by the dislocation strain field in a small region below the dislocation, resulting in a reduction of absorption efficiency of SIAs by dislocation. On the other hand, the absorption efficiency of vacancies are not seriously affected by the dislocation strain field compared to SIAs. This means that the dislocation bias factor is not so large as believed so far.

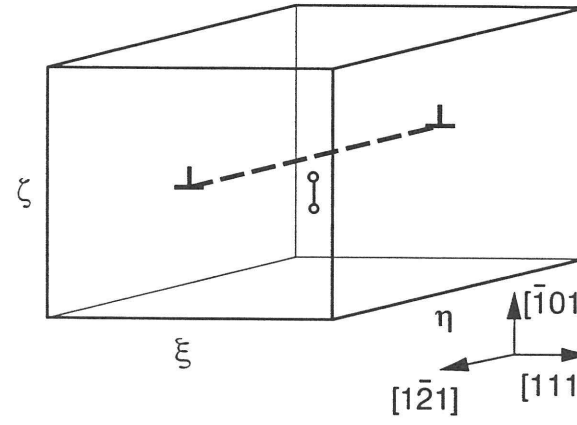

Fig. 1: Geometry of the crystal assumed in the present simulation. Each edge is denoted by ξ, η, ζ, and is parallel to [111], [$\bar{1}$01], [1$\bar{2}$1], respectively. Inside the crystal, straight edge dislocation is inserted parallel to [1$\bar{2}$1] direction. Dumbbell mark denotes the initial position of SIA.

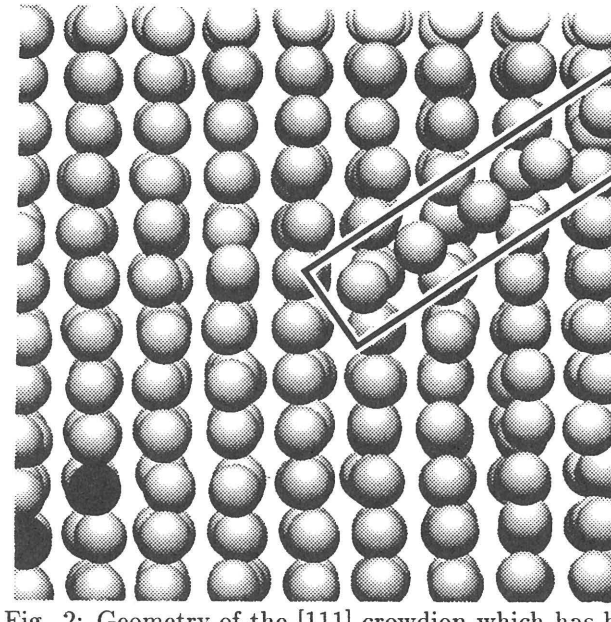

Fig. 2: Geometry of the [111] crowdion which has been transformed from [$\bar{1}$01] dumbbell(surrounded by solid rectangle). The position of initially introduced [$\bar{1}$01] dumbbell is denoted by two solid circles in the lower left corner.

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