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Atomic simulation for influence of helium atom on movement of edge dislocation in nickel

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Abstract: The molecular dynamics (MD) simulation and the modified analytical embedded-atom method (MAEAM) were used to study the influence of a He atom on the movement of the $(a/2)\langle 110\rangle\{1\,\bar{1}\,1\}$ edge dislocation in Ni. First, the calculated Burgers vector distribution shows that the equilibrium dissociation distance (D_{ed}) and the stacking fault energy (E_{sf}) between two partial edge dislocations are about 25.95 Å and 108 mJ/m^2, respectively. Then, the obtained formation energies (E_f) of a He atom at some different sites demonstrate that the He atom is attracted and repelled in the tension and compression regions, respectively. And the He−dislocation interaction reveals that an interstitial He atom plays a more significant role in the dislocation movement than a substitutional He atom. Finally, it is found that the movement of an interstitial He atom is apparent as the first partial dislocation bypasses and the edge dislocation offers fast-diffusion path for the migration of a He atom.

Key words: movement; edge dislocation; He; atomic simulation; Ni

1 Introduction

It is known that the crystalline material generally contains abundant dislocations, which are dramatically responsible for the variation in the mechanical properties [1,2]. In particular, the movement of the dislocation and its interaction with other defects are important to understand the irradiation damage and mechanical properties. The degradation in the mechanical strength with a long-term exposure to irradiation has been enslaved to produce abundant defects, which could form some effective blocking barriers to hinder the dislocation movement under the external stress [3−5]. And the plastic deformation of materials results mainly from the movement of the dislocation in the crystal [6]. Hence, it is interesting to study the movement of the dislocation and its interaction with other defects [7−11].

With the development of the computational technique, molecular dynamics (MD) simulation has been proved to be a useful tool to study the impeditive influence of defect obstacles on the movement of the dislocation [12,13]. MORISHITA et al [14,15] used MD to study the migration energy and the binding energy of a He atom and its interaction with other defects in α-Fe, which demonstrated that the He atom was strongly trapped in a single vacancy. HEINISCH et al [16] studied the formation energy and the binding energy of the interstitial He atom in or near a dislocation core. The obtained results indicated that the interstitial He atom had a negative binging energy in the compression region and a strongly positive binding energy in the tension region. NEDELCU et al [17] found that a H atom in the Fe matrix could block the dislocation movement, and the stress exerted on the dislocation could reach 15.5 MPa. The interstitial H atom strongly impeded the movement of the dislocation and gave a maximal value of stress (~38.2 MPa) before the dislocation passing by. OSETSKY et al [18−20] constructed an atomic-level model to interpret the dislocation movement and the inherent mechanisms of the dislocation−obstacle interaction.

In fact, at low temperatures, He atoms also induced the irradiation hardening phenomenon [21] and the degradation of material lifetime [22], which could be deduced from the reaction between He and dislocation. He atom assembled to form a cluster and impeded the dislocation movement [23]. Moreover, the irradiation hardening phenomenon of structural materials in the nuclear reaction was primarily affected by the

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interactions between dislocation and other obstacles [24,25]. The effect of the He atom on the decrease of fracture toughness of the reduced-activation steels was so crucial that the He atom further resulted in a significant change in the mechanical properties of nuclear materials. In addition, since its solubility in metallic material was extremely low, He tended to precipitate into clusters or bubbles and produced void swelling and surface roughing. Ni, as a corrosion-resistant material with very good formability, was usually used to improve the mechanical properties of Fe material [26,27].

2 Methodology

A simulation system, where about 20000 Ni atoms are assigned in a simulation box, is first constructed. The sizes of the simulation box are about $21a\times17a\times17a$ in the x, y and z directions, respectively. The alphabet a=0.3156 nm represents the lattice parameter of the crystalline Ni. The coordinate axes x, y and z of the simulation box are oriented in [110], $[1\bar{1}1]$ and $[\bar{1}12]$ directions, respectively. The real length of the box is about 7.5, 6 and 6 nm, respectively. The method of obtaining the edge dislocation was described in detail in Ref. [28]. The stable configuration with two straight edge partial dislocations along the $\langle\bar{1}12\rangle$ direction is shown in Fig. 1. Periodic boundary conditions are applied in the x-axis and z-axis directions, whereas fixed boundary condition is employed in the y-axis direction. The atoms in the region of upper and lower three $(1\bar{1}1)$ crystalline planes are rigidly fixed, whereas other atoms can move freely. The glide force acting on the dislocation is generated by the relative displacement of the rigid blocks in the x direction.

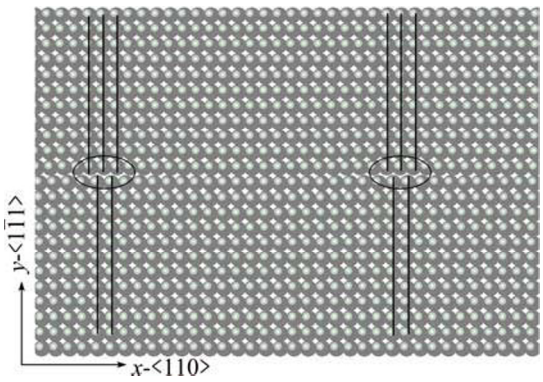

Fig. 1 Planar structure of $(a/2)\langle110\rangle\{1\bar{1}1\}$ edge dislocation perpendicular to $\langle\bar{1}12\rangle$ direction (Black lines denoted sites of partial dislocations)

Two potential functions are introduced to depict the atomic interactions. The modified analytical embedded-atom method (MAEAM) potential, which has been successfully used to study the physical properties of metallic materials [29,30], is adopted to describe the metallic atom interactions. And the interactions between He and Ni atoms are treated by the Morse potential [31]. These empirical potentials and the corresponding technical details were explicitly reported elsewhere [29].

3 Results and discussion

3.1 Distribution of burgers vector

After the simulation system is adequately relaxed at 0 K, the rearranged atoms in double $(1\bar{1}1)$ planes adjacent to the slip plane are plotted in Fig. 2, where two partial dislocations are clearly confirmed by the different stacking segments as surrounded by rectangles. Here, the position of each partial dislocation could be accurately identified by the distribution of the Burgers vector [32], which is defined as the disregistry of the misfit displacement between neighbor atoms in both adjacent $(1\bar{1}1)$ glide planes with respect to the x coordinate, as shown in Fig. 3. The maximal disregistry

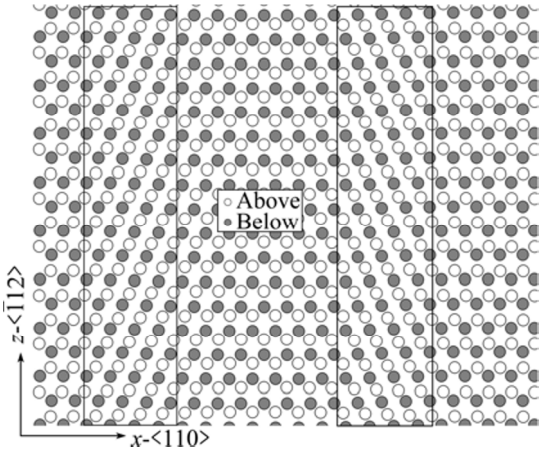

Fig. 2 Equilibrium crystalline sites of atoms in two adjacent $(1\bar{1}1)$ planes below (open circles) and above (solid circles) slip plane

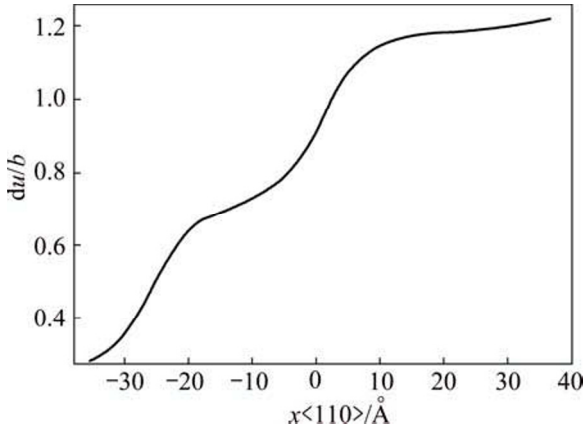

Fig. 3 Disregistry of differential displacement between atoms in two neighbor atomic planes adjacent to slip plane in $\langle110\rangle$ direction