First-principles Calculation for the Effect of Hydrogen Atoms on the Mobility of a Screw Dislocation in BCC Iron

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Effect of hydrogen atoms on the mobility of a screw dislocation in BCC iron has been evaluated using the first-principles calculation. The stable position of a hydrogen atom is found to be near the screw dislocation core and inside the core respectively when the dislocation is at the easy-core or hard-core configuration in BCC iron. The intrinsically unstable hard-core configuration of the screw dislocation is stabilized when a hydrogen atom is trapped inside the core. On the basis of this first-principles result, an elastic string model of a dislocation is developed to predict the kink motion in the presence of a hydrogen atom. It is found that a double-kink formation is facilitated when a hydrogen atom is located near a dislocation line, however, a kink motion is retarded when a hydrogen atom is behind the kink.

Keywords: first-principles calculation, screw dislocation, BCC iron, hydrogen atom

1. INTRODUCTION

Hydrogen in metals and alloys is known to have a significant effect on the fracture properties. In particular, the presence of hydrogen in steel can lead to embrittlement typically in two forms, intergranular and/or intragranular cracking, depending on the condition [1]. In some cases, hydrogen-induced decohesion, corresponding to intergranular cracking, can occur in the low stress region. This phenomenon is caused by the segregation of impurities and solutes to grain boundaries leading to the reduction of cohesive strength, in which there is experimental and numerical evidence to support this [2][3][4]. In all these fracture experiments of steel, plasticity is interwoven in various stages of the entire fracture process and is known to be enhanced and/or retarded due to the presence of hydrogen, in particular, in iron. Therefore, the interaction of a dislocation with hydrogen atoms in iron is especially needed for a complete understanding of hydrogen embrittlement in steels. A fundamental question is whether the presence of hydrogen in the core of a screw dislocation, which mainly controls plasticity in iron, can increase or decrease the mobility of screw dislocations. Firstly, a core structure and mobility of a screw dislocation in iron must be clarified by the first-principles method since atomistic calculations with empirical potential sometimes lead to erroneous core structures. A large-scale periodic quadrupolar array of dislocation cores in a parallelpiped cell is employed in the DFT (density functional theory) calculation to clarify the core structure and Peierls barrier map[5][6]. On the basis of these results, the interaction of a hydrogen atom with a screw dislocation core is evaluated using the first-principles method.

2. COMPUTATIONAL METHOD

Two screw dislocations with opposite helicity are placed in the cell to form a periodic quadrupolar array. Because of symmetric redundancy, the quadrupolar cell can be reduced to an equivalent dipolar cell (Fig. 1). The Cartesian coordinates X, Y, and Z are taken in the direction of $[11\bar{2}]$, $[1\bar{1}0]$, and [111].

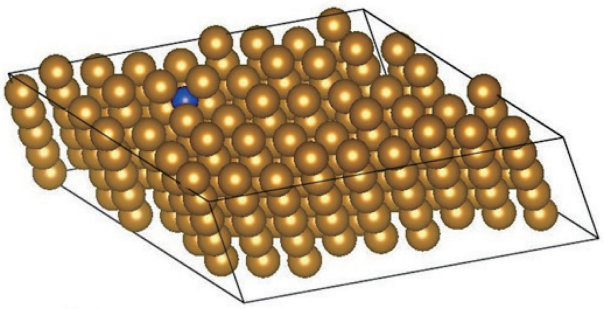

Fig. 1 Periodic quadrupolar array of screw dislocation cores in a parallelpiped cell of iron used in the DFT calculations.

The total number of atoms is 225 consisting of 45(=9×5) in the XY plane and 5 in the Z direction. The electronic structure calculations and the structure relaxations by force minimizations in DFT steps are performed using Vienna Ab initio Simulation Package (VASP) with Projector Augmented Wave (PAW) method and ultrasoft pseudopotentials. The exchange correlation energy is calculated by generalized gradient approximation (GGA). In all cases, spin-polarized calculations are employed. The Monkhorst Pack k-point of 1×1×5 mesh and the Methfessel-Paxton smearing method with 0.1-eV width are used. The cutoff energy for the plane wave basis set is 280 eV. Structural relaxation is terminated when maximum force acting on movable degree of freedom becomes less than 0.01 eV/Angstrom.

3. RESULTS AND DISCUSSION

Figure 2 (a) and (b) show the atom configurations in the core of a BCC iron screw dislocation. In the stable easy-core configuration (Fig. 2(a)), atoms are located spirally along the Burgers vector direction of <111> in accordance with the BCC structure, while a large space is created in the unstable hard-core configuration. The easy and hard-core configurations are alternately located in the {111} plane (Fig. 2(c)), the motion of a screw dislocation in BCC iron is inhibited by the large barrier of 40 meV/layer due to the presence of the hard-core configuration.

The stable position of a hydrogen atom is searched near the screw dislocation core using the first-principles calculation, and it is found that the most stable place of a hydrogen atom is near the core for the easy-core configuration (Fig. 3(a)) and inside the core for the hard-core configuration (Fig. 3(b)). The total energy of the system for the easy-core configuration is lowered to -200 meV and for the hard-core configuration to -400 meV with respect to the reference state when the hydrogen atom is in the bulk state. This indicates that the intrinsically unstable hard-core configuration is stabilized with the absorption of a hydrogen atom in the large-spaced core.

On the basis of the first-principles results on the interaction of a hydrogen atom and the screw dislocation core, an elastic string model of dislocation is constructed to predict the nucleation of a double kink and its kink motion with and without the presence of a hydrogen atom. Due to the high Peierls barrier, the motion of an entire screw dislocation line in BCC iron is prohibited. The motion of a screw dislocation is facilitated by forming a double kink, and the movement to the next easy-core configuration is accomplished by the motion of these kinks. The barrier for the double-kink nucleation is estimated to be 600 meV (Fig. 4(a)). However, when a hydrogen atom is located just near a dislocation line, it reduces the barrier by 200 meV, thus the presence of a hydrogen atom promotes a double-kink formation (Fig. 4(b)). On the other hand, the motion of a kink

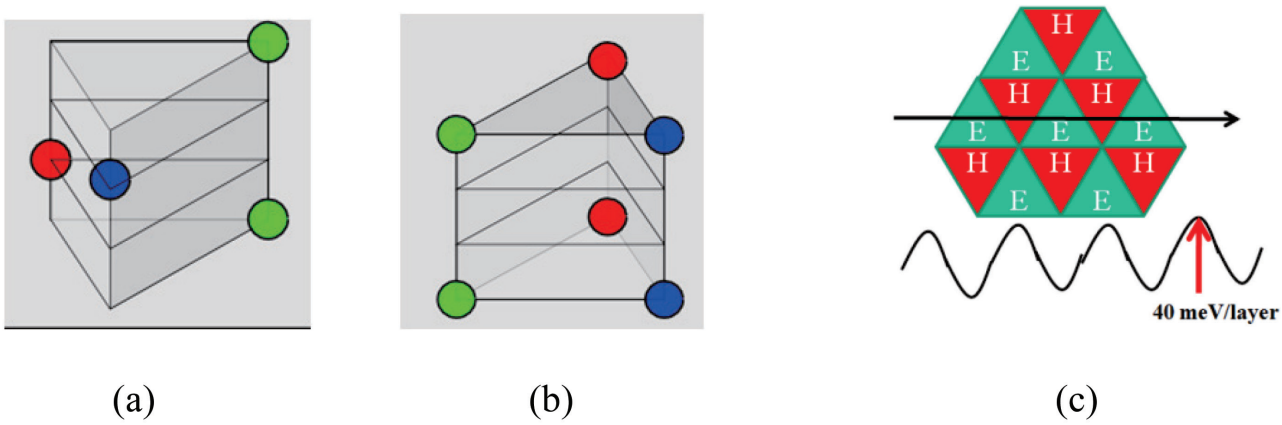

Fig. 2 Atomic positions in the core of a screw dislocation for the easy-core (a) and hard-core (b) configurations. (c) A plan view of {111} plane in BCC iron. Easy-core and hard-core configurations are alternately located.

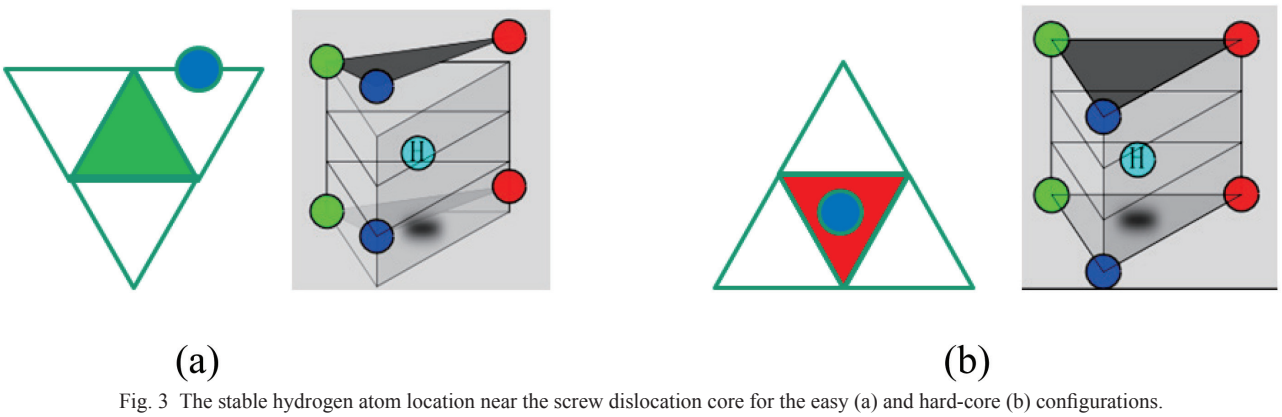

Fig. 3 The stable hydrogen atom location near the screw dislocation core for the easy (a) and hard-core (b) configurations.

is retarded when it passes near the hydrogen atom, as shown in Fig. 4(b), and the barrier for the kink to move is found to be 200 meV. And even when a kink escapes from this barrier, a hydrogen atom follows the kink to retard its motion because hydrogen atoms move easily in the bulk BCC iron. Thus, it is concluded from the above results that the motion of a screw dislocation in the environment of dispersed hydrogen atoms is difficult in BCC iron.

Lastly, it is emphasized that a transformation of a screw dislocation core occurs depending on the density of absorbed hydrogen atoms. It is found from the first-principles calculations that a hydrogen atom is trapped near the dislocation core when the screw dislocation is in the easy-core configuration. The energy reduction of one absorbed hydrogen atom in this case is 200 meV. On the other hand, in the case that a screw dislocation moves to the hard-core configuration and absorb hydrogen atoms, dislocation core energy increases by 40 meV per layer but the absorption energy increases to 400 meV. If we denote the number of absorbed hydrogen atoms per one atom layer by C, the total energy of the easy-core and hard-core configuration with absorbed hydrogen atoms is -200C meV and 40-400C meV, respectively. When C is greater than 0.2, the hard-core configuration becomes more stable and it is predicted that the core position changes from the easy-core to the hard-core, as shown in Fig. 5(a), (b).

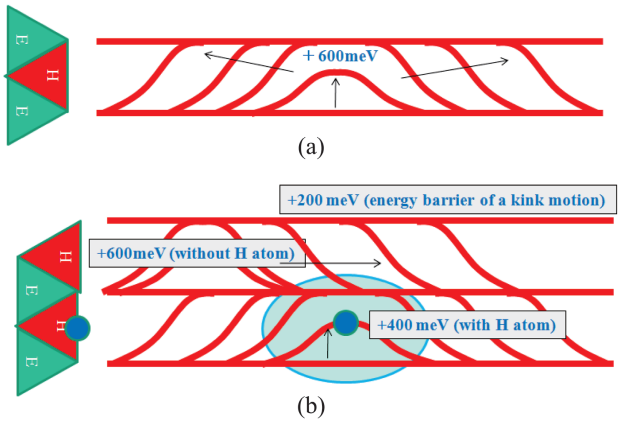

Fig. 4 (a) The process of a double-kink nucleation and its motion when a screw dislocation is in the easy-core configuration in BCC iron. (b) A double-kink nucleation and its subsequent motion when the hydrogen atom is located near a screw dislocation line.

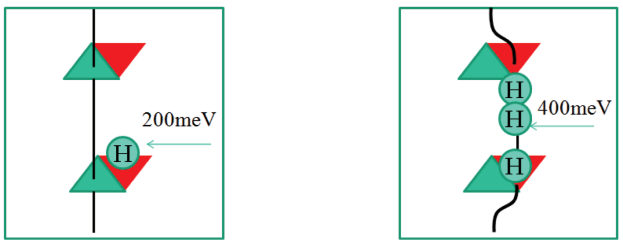

Fig. 5 Transformation of a core structure of a screw dislocation when the density of absorbed hydrogen atoms per atom layer is below (a) and above (b) 20% (C=0.2).

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第一原理計算による BCC 鉄中らせん転位の移動への水素の影響

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第一原理計算により BCC 鉄中の一本のらせん転位の移動度に与える水素原子の影響を調べた。BCC 鉄中の一本のらせん転位において、1 個の水素原子の安定位置は、転位が easy core の位置にいる場合は転位芯の外にあるが、不安定な hard core にいる場合は転位芯の中心の大きな空間にいる方が安定であることが分かった。この第一原計算に基づき、転位キンクの弾性ひもモデルを構築し、水素原子との相互作用を計算した。その結果、転位運動の前方に水素原子が存在する時はキンクの形成が助長されるが、水素原子が後方に存在する時はキンク運動を阻害することが分かった。

キーワード:第一原理計算, らせん転位, BCC鉄, 水素原子