First-principles Calculation on Core Structures and Peierls Stress of a Screw Dislocation in BCC Iron

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Predicting atomistic properties of a dislocation is a first step toward an understanding of plastic behavior of materials, in particular BCC metals. The core structure and Peierls stress of a screw dislocation in BCC iron have been determined using the first-principles calculations based on the density functional theory with the large-scale supercell containing 231 atoms. For the $a_0/2$[111] screw dislocation of BCC iron, the core structure was found, using 1 × 1 × 4 k-point samplings, to be a symmetric displacement field with no broken symmetry, and the Peierls stress was determined to be 1.1GPa for the simple shear stress along (–110)<111>.

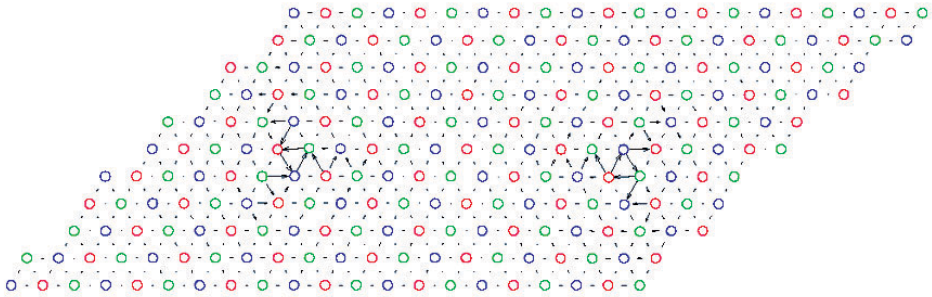
Keywords: first-principles calculation, screw dislocation, Peierls stress, BCC, iron

1. INTRODUCTION

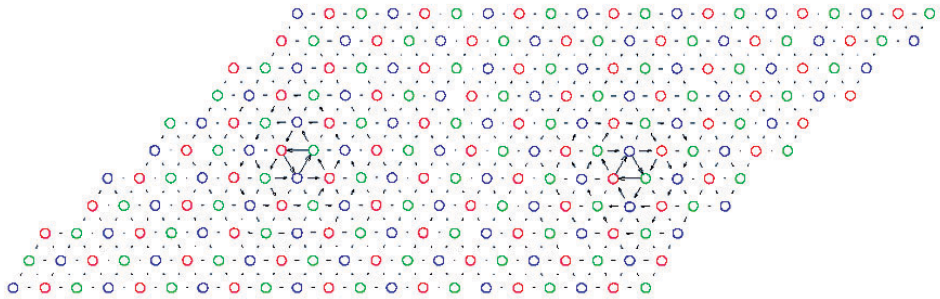
Electronic and atomistic bonding states of materials are required to understand fundamental mechanical properties of nuclear materials, in particular, embrittlement and fracture due to irradiation. Hydrogen embrittlement in BCC metals is one of the important fundamental phenomena for understanding the cause of the stress corrosion cracking observed in light-water nuclear reactors. Before studying the interaction of a hydrogen atom and a dislocation, it is first necessary to understand a behavior of a screw dislocation, in particular, the dislocation core structure and Peierls stress, which is considered to control the low temperature deformation of BCC metals.

Atomistic simulations using the empirical interatomic potentials have been performed to determine the accurate core properties of a screw dislocation in BCC metals, and it was commonly understood that it has a degenerate core structure with a broken symmetry about the <-110> axis. A core displacement field, extended along the (-1-12) directions, has a threefold symmetry, and this property is considered to explain the anisotropy of the plasticity in BCC metals. With the progress of computational power around and after the year of 2000, the results of the first principles calculations based on the density functional theory (DFT) appear and predict a different non-degenerate core structure with no preferential extension of the displacement field along the (-1-12) directions[1][2][3]. Although the method of the first principle calculations is the most accurate in evaluating the total energy of the system, it has limitations. Since the total number of atoms used in this method is limited to approximately 100 and the strain field of a screw dislocation has a long-range character, a configuration of one or more screw dislocations in the computational region and a boundary condition must be devised to predict an accurate core structure [4]. Moreover, the effect of k-point samplings along the direction of the Burgers vector on the convergence of this method, must be confirmed, in particular for the case of iron, by taking into consideration of the effect of spin polarization.

Numerous first-principles and empirical atomistic simulation studies have been carried out so far to determine the accurate core properties, however, the results of the core structure and Peierls stress differ depending on the simulation methods. Essentially, two core structures have been proposed for a screw dislocation in BCC molybdenum by various computational approaches [1][2][3][4][5]; the threefold structure (Fig. 1(a)) is obtained using the Finnis-Sinclair potential and the modified generalized pseudopotential theory (MGPT) potential, while the symmetric structure (Fig. 1(b)) is obtained by the tight-binding and the density functional theory (DFT) methods. Although the DFT method gives the most accurate energy among these methods, the



(a) Differential displacement map of threefold degenerate core structure



(b) Differential displacement map of symmetric non-degenerate core structure

Fig. 1 Two proposed core structures of a screw dislocation in BCC metals.

sizes of its supercells are severely limited, and the effects of core overlapping and image stress can be significant. Woodward and Rao [2] proposed a boundary condition for the supercell containing one screw dislocation, in which atomic displacements due to a screw dislocation in the cell are allotted by the Green function method. Li *et al.* [3] introduced a pair of screw dislocations in the supercell and proposed a shape of the supercell in such a way as to cancel the strains among supercells. They evaluated the accuracy of the core energy by changing the size of the supercell, and concluded that the supercell containing 231 atoms is good enough. We performed the most accurate DFT calculations using the supercell of this size by confirming the convergence on the number of k-point samplings, and concluded that the core of the $a_0/2[111]$ screw dislocation in BCC molybdenum has a symmetric non-degenerate structure [6]. The results of the core structure and Peierls stress of a screw dislocation in BCC iron are meager [3]. The recent calculations using the DFT method and the empirical EAM potential [7] suggest a symmetric non-degenerate core [8], respectively, similar to the result by Frederiksen and Jacobsen [3]. However, the accuracy of the DFT method is not fully confirmed due to the limitation of the number of atoms and k-point samplings.

In this paper, we report results of the accurate determination of a core structure and Peierls stress for a screw dislocation in BCC iron using the supercell containing 231 atoms with $1 \times 1 \times 4$ k-sampling points, as a first trial simulation.

2. COMPUTATIONAL METHOD

We have employed the VASP (Vienna *ab-initio* simulation package) code [9], which implements the density functional theory with the ultrasoft pseudopotential and the generalized gradient approximation (GGA) for the exchange correlation energy, for calculating accurately the total energy of the system. In order to exploit the vector processors on the ES system, we have tuned the code by using the one-dimensional FFT routine in the numerical library ASL/ES. For the problem with the supercell containing 231 atoms, the VASP code achieved 66.4% of the peak performance on the ES.

Using the configuration of the symmetric non-degenerate core structure obtained by the previous work as an initial condition, we applied the additional shear strain along the e_3 direction in Fig. 2 to study the stress-driven instability of the dislocation core. The parameter x in Fig. 2 corresponds to the shear strain γ_{23}. With each value of x being increased, atoms are relaxed to a minimum energy state by the conjugate gradient or the quasi Newton algorithm. Using the supercell consisting of 231 atoms with various k-point samplings, this procedure requires considerable amounts of calculation time, which invalidates the original implementation of parallel coding on the VASP code. To overcome this situation, we have re-parallelized the code in terms of k-point samplings. The result shows that the parallel code achieves almost linear speedup. Analyzing the detailed profile data of the code, we found that the k-point parallelization has almost no influence on the average vector length. We have obtained the average

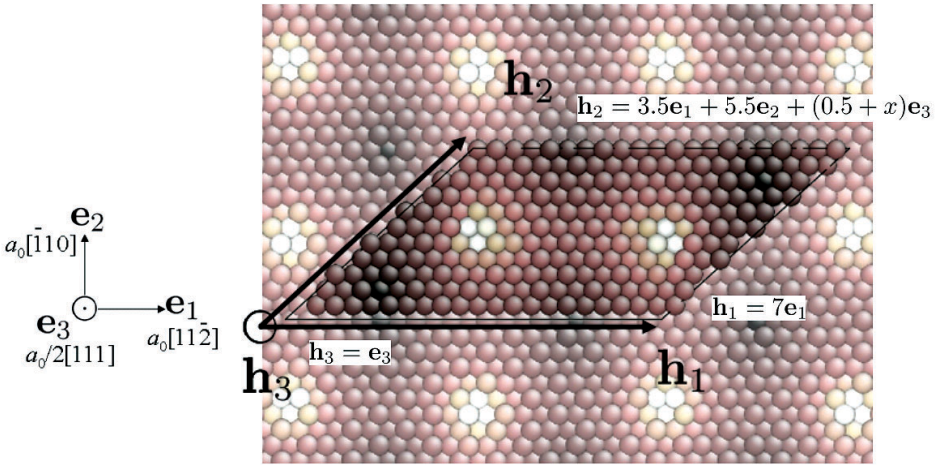


Fig. 2 The BCC iron supercell consisting of 231 atoms. The parameter x corresponds to the shear strain γ_{23}.

vector length of 229.3 with 8 processors (1 node) and 229.1 with 80 processors (10 nodes), and the vectorization ratio of 99.3% and 99.1%, respectively. In the case of iron, spin polarization must be taken into consideration, and the convergence of the iterative electronic structure calculation is found to be degraded compared to the molybdenum case. The number of iterations for the iron case requires approximately five times more than that for the molybdenum case. Therefore, the numerical condition for the supercell containing 231 iron atoms with the 1 × 1 × 4 k-point samplings is adopted as a first trial numerical simulation.

3. RESULTS AND DISCUSSION

The core structure of a screw dislocation for BCC iron is predicted by starting with the threefold degenerate structure and relaxing the structure. The result is found to be a symmetric non-degenerate structure with no preferential spreading along the (-1-12) directions, as shown in Fig. 1(b), which is in agreement with the results of the previous calculations using equal to or less than 100 atoms [3][8]. It is probable that a symmetric non-degenerate core structure is obtained for a screw dislocation in BCC iron using the first principles calculations, however, the convergence of the k-point samplings must be critically checked for a final determination.

Figure 3 shows the result of calculation for stress-driven instability of the dislocation core in the (-110)<111> slip system of the previous result for BCC molybdenum [6] and the present result for BCC iron. The shear modulus derived from the inclination of the stress versus strain curve mostly agrees with the existing data. At a critical value of around $x_c \approx 0.15$, which corresponds to the shear strain γ_c of around 1.6%, it is found that the core structures can no longer be stabilized and the Peierls stress for BCC iron is estimated to be $\tau_p \approx 1.1$GPa. Above the critical value of x_c, the two cores move toward each other by $a_0/3$[-112], and the shear stress as well as the energy of the system decreases significantly

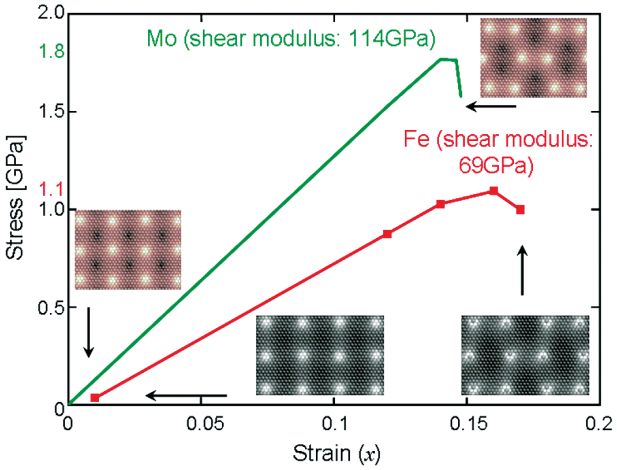


Fig. 3 Stress-driven instability of dislocation cores for BCC Mo and Fe: The shear modulus is derived from the inclination of the stress versus strain curve, and Peierls stress is determined from the maximum value of stress. The inset pictures show the positions of dislocation cores before and after the instability occurs.

(see the inset picture of Fig. 3). This result is the first direct determination of the Peierls stress of a screw dislocation in BCC iron. As in the case of the determination of the core structure, the convergence of the k-point sampling must be confirmed.

In this work, we have performed the large-scale DFT calculations using the periodic boundary condition where the supercell, consisting of 231 atoms, contains two screw dislocations with 1 × 1 × 4 k-points, and obtained the symmetric non-degenerate core structure and the Peierls stress τ_p value of 1.1GPa in BCC iron. A further study on the convergence of k-point samplings in the DFT calculation of a screw dislocation is necessary for a final determination of the core structure and Peierls stress.

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第一原理計算によるBCC鉄中らせん転位の機械的性質

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原子レベルから転位の構造を知ることは、特に体心立方格子(BCC)構造の金属の塑性を理解するために重要である。密度汎関数理論に基づく第一原理計算により231個の原子から構成される大規模なスーパーセルを用いて、BCC鉄のらせん転位の芯構造及びパイエルス応力を決定した。1 × 1 × 4のk-点サンプリングの計算では、BCC鉄のa_0/2[111]のらせん転位の芯構造は対称的な変位場を持っていることが分かった。また、単純な(–110)<111>方向のせん断に対して、パイエルス応力は1.1GPaであると決定した。

キーワード：第一原理計算, らせん転位, パイエルス応力, 体心立方格子, 鉄