First-principles Calculation on Peierls Stress of a Screw Dislocation in BCC Molybdenum

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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 molybdenum have been studied over the years using the first-principles and empirical methods, however, their conclusions vary due to the inefficiency of the methods. We have executed the first-principles calculation based on the density functional method, employing the most accurate 1 × 1 × 20 **k**-point samplings, to determine Peierls stress of the $a_0/2$[111] screw dislocation of molybdenum. We have determined the value of 1.8GPa for the simple shear stress along (–110)<111>.

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

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 associated with 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 BCC metals, in particular, the dislocation core structure and Peierls stress. Numerous first-principles and empirical atomistic simulation studies have been carried out 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]; the 3-fold structure (Fig. 1(a)) is obtained using the Finnis-Sinclair potential and the modified generalized pseudopotential theory (MGPT) potential, while the 6-fold 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 sizes of its supercells are severely limited. Since a screw dislocation has a long-range strain field around the core, 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 DFT calculations using the supercell of this size and concluded that the core of the $a_0/2$[111] screw dislocation in BCC molybdenum has a 6-fold structure [4]. In this calculation, we confirmed the convergence on the number of **k**-point samplings, using the 1 × 1 × 20, 2 × 2 × 40, and 3 × 3 × 60 **k**-points. In this paper, we report the result of the most accurate determination of Peierls stress for the screw dislocation in BCC molybdenum.

2. COMPUTATIONAL METHOD

We have employed the VASP (Vienna *ab-initio* simulation package) code [5], which implements the density functional theory with the ultrasoft pseudopotential and the generalized gradient approximation (GGA) for the exchange correlation

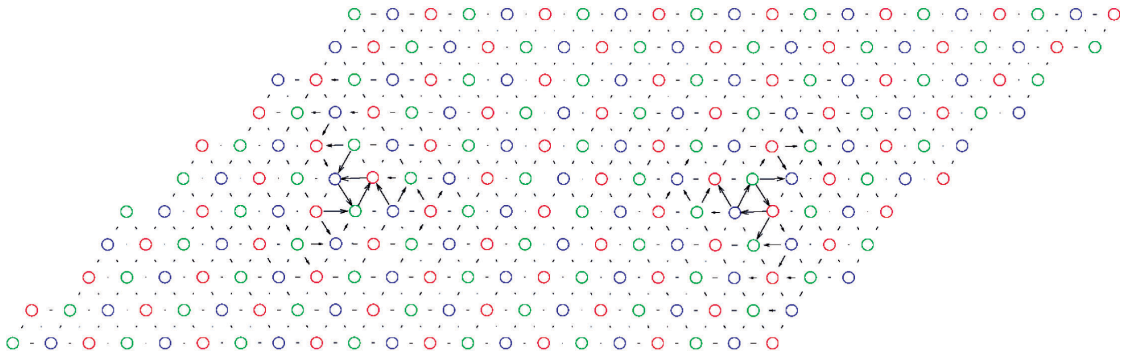

Fig. 1(a)Differential displacement map of 3-fold structure.

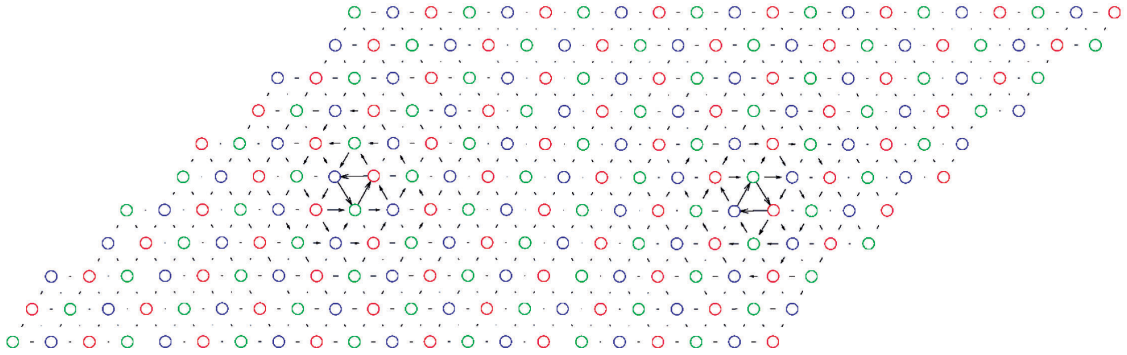

Fig. 1(b)Differential displacement map of 6-fold structure.

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

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 6-fold 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 1 × 1 × 20 **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. Figure 3 shows that new 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 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.

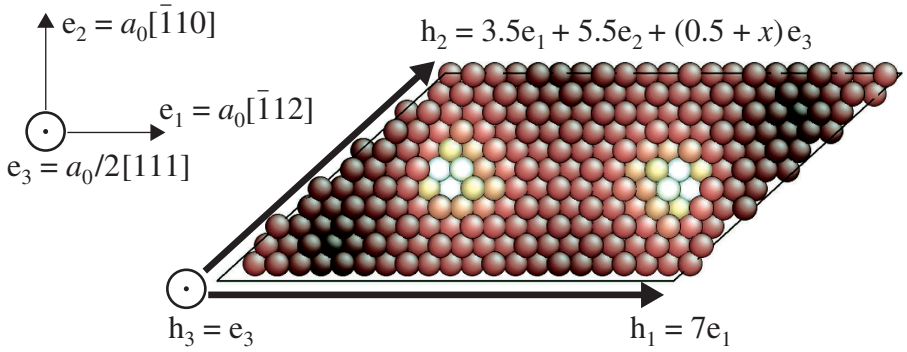

Fig. 2 The BCC Mo supercell consisting of 231 atoms.

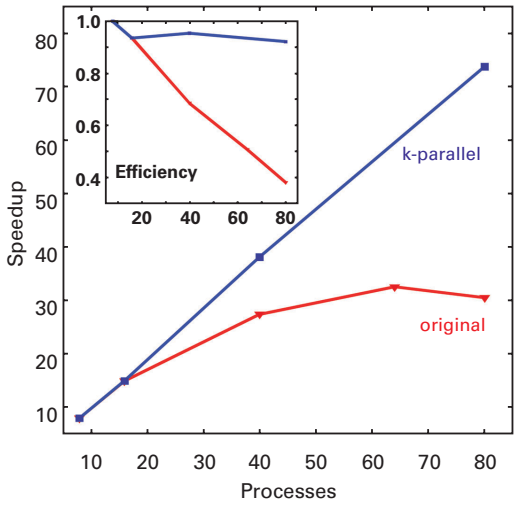

Fig. 3 Performance of **k**-point-parallelized VASP code.

3. RESULTS AND DISCUSSION

Figure 4 shows the result of calculation for stress-driven instability of the dislocation core in the (–110)<111> slip system of BCC molybdenum. At a critical value of $x_c \approx 0.146$, which corresponds to the shear strain of $\gamma_c \approx 1.6\%$, it is found that the core structures can no longer be stabilized and the Peierls stress is estimated to be $\tau_p \approx 1.8$GPa. At the value of $x = 0.16$, 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. 4. (c)). Under the same supercell setup, Li *et al.* [3] gave the Peierls stress of $\tau_p \approx$ 2.4GPa and ≈ 3.8GPa using the Finis-Sinclair potential and the tight-binding model, respectively. Using the different boundary condition where the supercell contains one dislocation, Xu and Moriarty [1] used the MGPT and obtained the value of $\tau_p \approx 3.4$GPa, while Woodward and Rao [2] derived $\tau_p \approx 2.1$GPa by the DFT calculation with four special **k**-points. In comparison with these previous results, no correlation between core structures and Peierls stresses predicted by various methods could be found, that is, higher and lower τ_p values are estimated with the core structure of both the 3-fold and 6-fold. In this work, we have performed the most accurate DFT calculations with twenty **k**-points using the periodic boundary condition where the supercell contains two screw dislocations, and obtained the 6-fold core structure and the lowest τ_p value of 1.8GPa in BCC molybdenum. Although we use the different boundary condition and **k**-points sampling, our result generally comes close to the DFT result of Woodward and Rao.

4. SUMMARY

We have implemented the VASP (Vienna ab-initio simulation package) code on the Earth Simulator by parallelization in terms of **k**-point samplings and achieved a good parallel performance. Using this code and the largest 1 × 1 × 20 **k**-point samplings, we have performed DFT calculations and obtained Peierls stress of 1.8GPa for the $a_0/2$[111] screw dislocation in BCC molybdenum under the simple shear stress condition in the (–110)<111> slip system.

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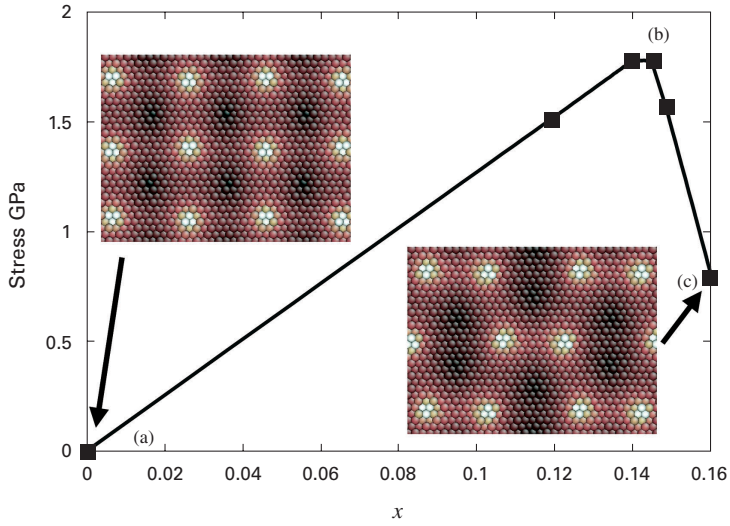

Fig. 4 Stress-driven instability of dislocation cores: (a) an initial position, (b) a critical position, and (c) a moved position of the cores. The parameter x corresponds to the shear strain γ_{23}. Positions of dislocation cores are seen as highlighted atoms in the inset images.

第一原理計算によるBCCモリブデン中らせん転位のパイエルス応力の決定

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転位の原子レベルの性質を予測することは、物質の塑性変形挙動の機構を理解するために重要である。特に、BCC金属においてはらせん転位のパイエルス応力が大きいこともあり、原子レベルからのその挙動の理解が求められている。BCC結晶構造をもつモリブデン金属においては、第一原理計算及び経験的手法を用いてらせん転位の芯の構造を決定する計算が数年来行われてきたが、計算手法が十分でないこともあり、手法により異なる結果が得られていた。我々はこの問題に決着をつけるべく、密度汎関数法に基づく第一原理計算を実施した。計算は**k**点サンプリング及び波動関数の平面波展開におけるエネルギーカットオフ値に特に注意を払って行ない、BCCモリブデン中のらせん転位芯は6回軸構造を持っていることを確認した後、転位の移動に必要なパイエルス応力τ_p = 1.8GPaの値を得ることに成功した。これらの結果を得るには膨大な計算量が必要であったため、計算に先立ってコードの並列化および地球シミュレータ向けのチューニングを実施し、高いベクトル化率と並列化効率の両立を実現している。

キーワード：第一原理計算, らせん転位, パイエルス応力, 体芯立方格子(BCC), モリブデン