First-principles Calculation on Peierls Potential of an Isolated Screw Dislocation in BCC Iron

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Peierls potential of an isolated screw dislocation in BCC iron is calculated using first-principles method. We have found that the Peierls barrier is 0.04 eV per Burger's vector, and that the two dimensional Peierls potential around a hard-core position is nearly flat. These results significantly differ from currently available molecular dynamics potentials, and indicate that improved molecular dynamics potential is necessary for the simulations of plastic deformation.

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

1. Introduction

Plasticity in BCC metals is mainly mediated by thermal activation of kink-pair nucleation in screw dislocation lines which are required to overcome strong lattice friction, and shows strong dependence on the direction of the applied stress and temperature [1]. Therefore it is crucial to estimate the lattice friction of a dislocation from atomistic calculations to model plasticity in BCC metals. The Peierls potential which causes lattice friction in BCC iron has been calculated using the density functional theory (DFT) with localized basis [2] [3]. In the present work we employ more accurate plane-wave basis DFT to calculate Peierls potential of an isolated screw dislocation core to obtain more reliable estimate.

2. Computational method

The effect of long-range strain field generated by a dislocation is incorporated into calculation using the so-called flexible boundary condition [4]. The system is divided into three concentric hexagonal regions 1, 2, and 3 as shown in Fig. 1. First, region 1 and 2 are used in DFT calculations and atoms in region 1 are relaxed to account for non-linear forces around a core, while atoms in region 2 are fixed. After the DFT relaxation, region 1, 2, and 3 are used in the second step where atoms in region 2 and 3 are relaxed according to linear elastic forces. These steps are repeated alternately until convergence. The number of atoms in region 1 and 2 is 48 and 99, respectively.

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. Monkhorst Pack k-point of 1x1x24 mesh is used, and convergence of Peierls barrier energy with respect to the increasing mesh number at 1x1x24 is confirmed. The Methfessel-Paxton smearing method with 0.1-eV width is used. The cutoff energy for the plane wave basis set is 400 eV. Structural relaxation is terminated when maximum force acting on movable degree of freedom becomes less than 0.01eV/Angstrom.

In the present work we investigate two-dimensional energy landscape of Peierls potential which determines the mobility and migration path of a screw dislocation. To investigate two-dimensional energy landscape, we use the drag method in which displacements of three atoms around the screw dislocation core are fixed in the Burger's vector direction to control the dislocation position. All other atoms in region 1 are relaxed in the DFT calculations, and the energy of a relaxed configuration gives Peierls potential at the dislocation position.

Note that the same boundary condition must be used for each dislocation position to calculate an energy difference between them. Since the flexible boundary condition is optimized for the easy-core position, other dislocation configurations have excess energy which comes from incompatibility between the core region and the boundary region. This excess energy mostly consists of linear elastic energy which can be easily calculated without DFT calculations. This elastic excess energy

is subtracted from the obtained energy difference between a reference state and the target dislocation position to eliminate the effect of boundary condition.

3. Results and discussion

Peierls energy at several dislocation points shown in Fig. 2 (a) are calculated, and the results are summarized in Fig. 2 (b). Approximate energy contour lines are also shown. The main findings from the result are as follows:

(1) The barrier height is 0.04 eV, which is consistent with the previous DFT calculations.

(2) The energy landscape along the migration path is single-humped, which is also consistent with the previous calculations.

(3) The energy difference between a hard-core position and the midpoint of two easy-core position is extremely subtle.

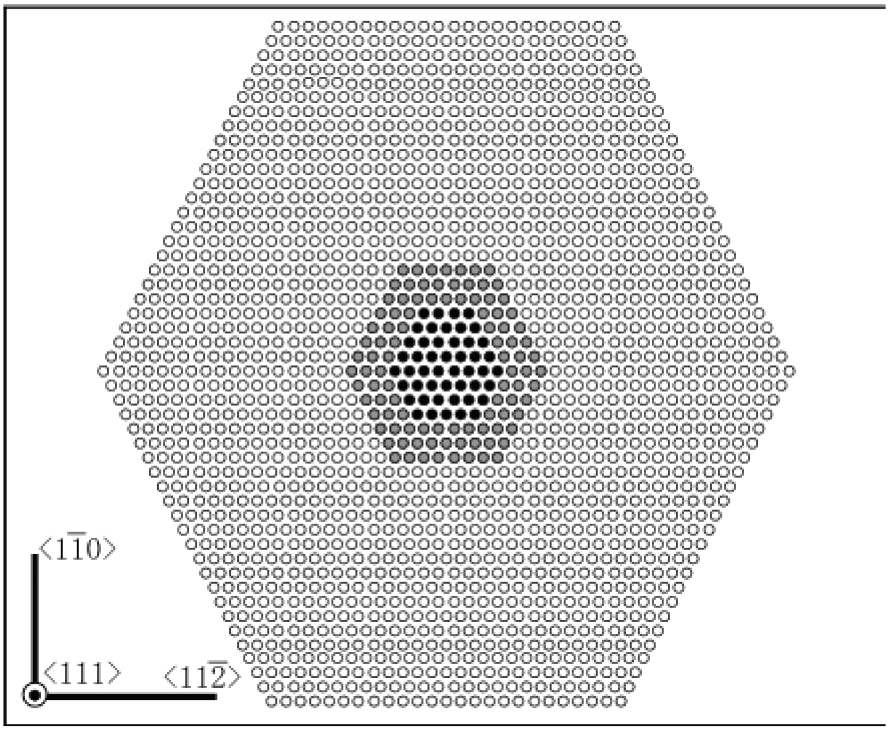

Fig. 1 Atom configuration used in the present study. Black, gray, and white disks denote atoms in region 1, 2, and 3, respectively. Region 1 and 2 are used in DFT calculations and only atoms in region 1 are relaxed. In the linear relaxation step, region 3 is added and atoms in region 2 and 3 are relaxed using linear elastic forces. See the main text for details.

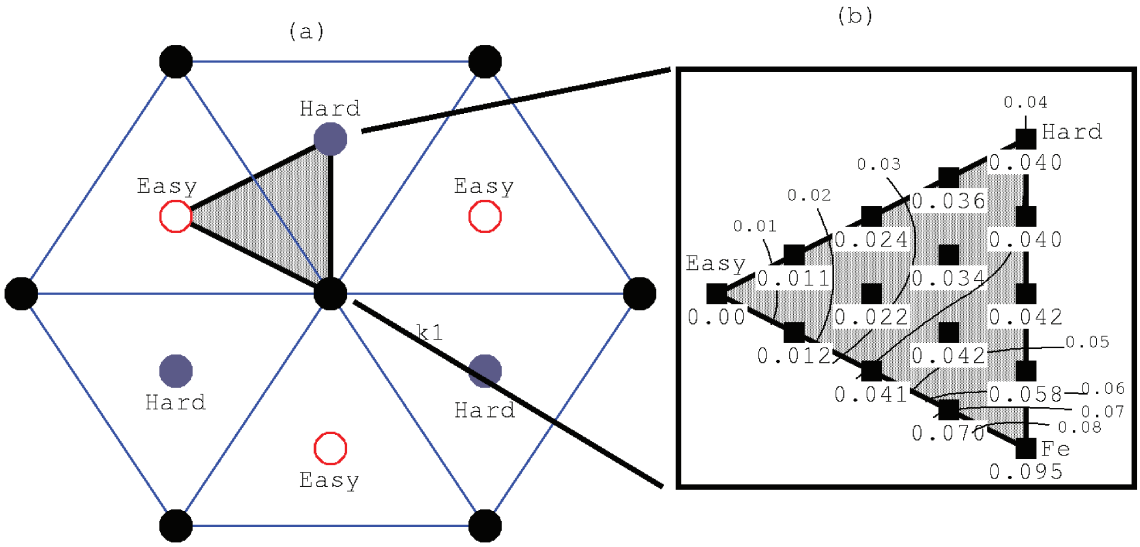

Fig. 2 (a) Iron atoms and dislocation positions seen from the <111> direction. Iron atoms, easy-core positions, and hard-core positions are shown by black, white, and gray disks, respectively. Peierls potential energy at each position shown in (b) is calculated, and relative energy with respect to the easy-core position (in eV per Burger's vector) is shown in the figure. Approximate energy contour lines are also shown.

(4) Iron atom position is highly unstable, in contrast to molecular dynamics result based on EAM potentials.

The subtle energy change along the line between a hard-core position and an iron atom position indicates that migration path can fluctuate widely even at very low temperature. In actual situations, a screw dislocation migrates by thermally forming a kink-pair so that one must calculate a kink formation energy to estimate dislocation velocity. The estimate of a kink formation energy by the DFT calculation is unfeasible in the present computing environment, since it requires thousands of atoms. Therefore, we are now developing a multiscale model of kink pair formation and dislocation migration based on the present work. Our present results indicate that currently available EAM potentials [5] are not suitable for molecular dynamics simulations which include plastic deformation, since their Peierls potential shape is qualitatively incorrect. Improvements of EAM potentials based on the DFT calculations of Peierls potential are highly expected.

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第一原理計算による BCC 鉄中らせん転位のパイエルスポテンシャルの計算

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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パイエルスポテンシャルを計算した。パイエルス障壁は転位のバガースベクトルの長さあたり 0.04eV であった。また、ハードコアの転位位置の周囲では二次元パイエルスポテンシャルがほぼ平坦になることが分かった。これらの結果は現在使われている分子動力学ポテンシャルの性質とは顕著に異なり、塑性変形を含む分子動力学計算のためには改良されたポテンシャルが必要であることが分かった。

キーワード: 第一原理計算, らせん転位, BCC 鉄, パイエルスポテンシャル