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Quantitative analysis of the yield behavior of a ⟨1 1 1⟩/2 screw dislocation in α-iron

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ABSTRACT

In previous work, bond-order potentials (BOPs) have been used to establish a general yield criterion, different from the Schmid law, for the glide of ⟨1 1 1⟩/2 screw dislocations on {1 1 0} planes in body-centered cubic metals, while their applications are restricted to the 2D simulations at 0 K because of their low computational efficiency. On the other hand, embedded-atom-method (EAM) potentials have been generally employed for long dislocation segments at finite temperatures, but there is no study to clarify whether or not they can reproduce the yield criteria revealed by the BOPs. In this work, systematic atomistic simulations with an EAM potential have been performed to calculate the behaviors of ⟨1 1 1⟩/2 screw dislocations in α-iron under different loading conditions. We find that at 0 K, the simulation results can be well explained by the general yield criterion when the glide is restricted to {1 1 0} planes. Under uniaxial loadings, the activated slip systems are consistent with the experimental observations. At finite temperatures, as a preliminary attempt, the influence of the non-glide stress on the slip planes is presented, which could not be rationalized by the yield criterion at 0 K because extra effect from temperatures has come into the picture.

1. Introduction

Many experimental and theoretical studies of body-centered-cubic (BCC) metals show that ⟨1 1 1⟩/2 screw dislocations dominate the plastic deformation at low temperatures [1–3], and their non-planar core structures may cause the applied-stress-state, strong strain-rate and temperature dependence of yield behaviors [4,5]. Nevertheless, it is still a challenge to trace the core structure experimentally at atomic scale, while molecular static (MS) and dynamic (MD) simulations have been proved to be powerful to reveal the variations of core structures, as well as slip planes and the critical yield stress under external conditions such as the stress states, strain rates and temperatures [4,6–9]. However, their applicability and accuracy depend strongly on the empirical potentials to describe the interactions between atoms.

In order to explain the breakdown of the Schmid law for the low-temperature deformation of BCC metals, Gröger et al. [4,10] performed a series of MS simulations of the motion of a single ⟨1 1 1⟩/2 screw dislocations in two BCC metals, molybdenum (Mo) and tungsten (W), under a combination of two shear stresses, one parallel to the Burgers vector and the other perpendicular to the Burgers vector, and then constructed a general form of the yield criterion on the basis of the previous works by Qin and Bassani [11,12]. Besides the twinning-anti-twinning slip asymmetry, this yield criterion captures successfully the effect of the non-Schmid shear stresses (except the shear stress parallel to the Burgers vector on the glide plane) on the critical yield stress, and predicts the different activated slip systems in tension and compression. Chen et al. [13] found that this form of the yield criterion can be applied to α-iron (Fe) with a single ⟨1 1 1⟩/2 screw dislocation at 0 K. The interactions between atoms in these simulations are described with the bond-order potentials (BOPs) [14–16]. It is generally believed that the BOPs are more accurate than the embedded-atom-method (EAM) potentials since they contain the angular character of bonds in refractory BCC metals. However, because of the limited computational efficiency when using the BOPs, it is difficult to simulate dislocation dynamics at finite temperatures because long dislocation segments are required to capture kink-pair nucleation events. As a result, the effect of the non-glide stresses on the motion of ⟨1 1 1⟩/2 screw dislocations cannot be directly confirmed at finite temperatures by the BOPs. In contrast, the EAM potentials have been generally used to

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account for the dynamics of ⟨1 1 1⟩/2 screw dislocations with a length of several ten nanometers in BCC metals [8,9,17,18]. However, their accuracy at 0 K has not been testified integrally yet. Therefore, systematic simulations are needed with the EAM potentials at 0 K to calculate the yield behaviors of ⟨1 1 1⟩/2 screw dislocations in BCC metals, and to verify the yield criterion proposed by Gröger et al. [4,10].

In this work, the EAM potential developed by Ackland et al. [19] for Fe is chosen because it has been extensively utilized to simulate ⟨1 1 1⟩/2 screw dislocations in a large range of temperatures [8,9,18]. It can also reproduce the no-degenerate core structure of ⟨1 1 1⟩/2 screw dislocations as revealed by the first principle method [20,21]. Our first objective is to calculate the influence of non-glide stresses on the yield behaviors of a single ⟨1 1 1⟩/2 screw dislocation by applying different stress tensor at 0 K. Then, the yield criterion is established according to the proposal of Gröger et al. [10]. Finally, the new yield criterion is used to predict the activated slip systems under tension and compression and we draw a comparison between the predicted results and those from experiments. In addition, a series of MD simulations are performed and the influence of the non-glide stress perpendicular to the Burger vector on the slip planes is presented at finite temperatures.

2. Methodology

The simulation box we used is schematically presented in Fig. 1. The axis ***x*** is parallel to [1 1 1] direction, i.e., parallel to the Burgers vector and the dislocation line. The axes ***y*** and ***z*** are initially aligned along $[\bar{1}\,2\,\bar{1}]$ and $[\bar{1}\,0\,1]$, respectively. The box can be rotated around ***x*** by an angle χ, which can be generated by

$$\chi = \arctan\left(-\frac{\sqrt{2}n}{\sqrt{6}m}\right), \tag{1}$$

where m and n are integers ($m > 0$). It is sufficient to consider the range $-30° < \chi < 30°$ due to the crystal symmetry around the dislocation line [4]. When the maximum resolved shear stress plane (MRSSP) is located in the region bounded by $(\bar{2}\,1\,1)$ and $(\bar{1}\,0\,1)$ planes, $\chi > 0°$, while bordered by $(\bar{1}\,\bar{1}\,2)$ and $(\bar{1}\,0\,1)$ planes, $\chi < 0°$. As a result, ***y*** and ***z*** with χ are:

$$y//[-m-n\ 2m\ -m+n], \tag{2}$$

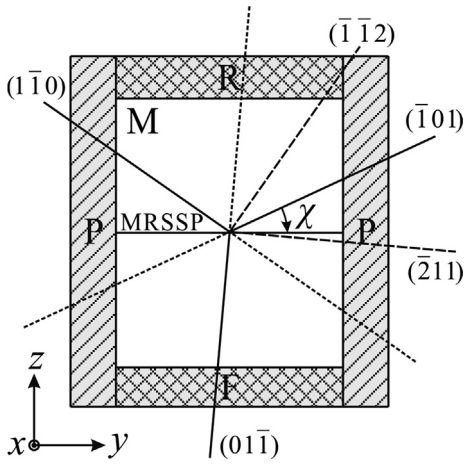

Fig. 1. Schematic picture of the simulation box. The ***x***-axis is always parallel to [1 1 1] direction. χ is the angle between the MRSSP and the $(\bar{1}\,0\,1)$ plane. Owing to the crystallographic symmetry, two {1 1 2} planes, $(\bar{1}\,\bar{1}\,2)$ and $(\bar{2}\,1\,1)$ planes, represent the boundaries of the angular region for all the orientations of the MRSSPs that are not related by symmetry.

$$z//[-3m+n\ -2n\ 3m+n]. \tag{3}$$

All the orientations in this work have been listed in Table 1. The box dimensions are $L_x = 3.46a$, $L_y = 80$–$90a$ and $L_z = 90$–$150a$ (the lattice parameter of Fe $a = 2.8553$ Å at 0 K) along ***x***, ***y*** and ***z***, respectively.

A screw dislocation is created by applying to all the atoms the isotropic elastic solution of the displacement field of [1 1 1]/2 screw dislocation [22] at the center of the box. Periodic boundary conditions (as indicated by '**P**' in Fig. 1) are applied along ***x*** and ***y***, while several atom layers normal to ***z*** are fixed near the top and bottom surfaces referred to as the rigid region '**R**' and the fixed region '**F**', respectively. The rigid region '**R**' can be moved as a whole along ***x*** and ***y*** freely to generate the stresses we need.

It is worth mentioning that in virtually all MS calculations on BCC crystals [4,6,8,13,23], the non-Schmid behaviors were investigated by means of researching the effect of the orientation of the MRSSP and the shear stress perpendicular to the Burger vector which is in fact a combination of two normal stresses of opposite sign. Once glide occurs on {1 1 0} planes such as $(\bar{1}\,0\,1)$ plane, the stress tensor applied can be converted to the orientation of $\chi = 0°$. Then we can observe the effect of non-glide stresses mutually independent on the Schmid stress in the stress tensor transformed. Gröger et al. [24,25] have studied the effect in detail apart from σ_{23} for which they only indirectly provided the proof that its presence promotes the composite slip of the dislocation on two {1 1 0} planes. However, to be exact, σ_{23} is the stress perpendicular to the Burger vector on slip plane. Therefore, the loading method for which σ_{23} is the predominant non-glide stress has been selected in our study, then we can accomplish our objectives in the previous section as well as getting an overall comprehension of the effect of the non-glide stresses. The strain tensor applied in this study has the form

$$\mathrm{E} = \begin{bmatrix} 0 & 0 & \frac{1}{2}\gamma_{31} \\ 0 & 0 & \frac{1}{2}\gamma_{23} \\ \frac{1}{2}\gamma_{31} & \frac{1}{2}\gamma_{23} & 0 \end{bmatrix} \tag{4}$$

In all cases, the MRSSP is always parallel to the x-y plane. It is not difficult to obtain that when $\chi > 0°$ ($\chi < 0°$) the positive loading (γ_{31}) will produce shearing in anti-twinning (twinning) sense for the nearest {1 1 2} plane. The applied strain increases incrementally and after any strain increment a full relaxation has been carried out in the '**M**' region. The relaxation is thought to be completed when the force on each atom falls below 10^{-5} eV·Å^{-1}. While loading, γ_{23} will be firstly applied to a predetermined value γ^f_{23} and then γ_{31} is applied until the dislocation starts to move. At this moment, the strain state is recorded as (γ^f_{23}, γ^c_{31}), which is regarded as the critical condition necessary for the dislocation motion. When the applied strain is given in Eq. (4), the corresponding stress tensor can be given as:

Table 1
The simulation boxes with different orientations generated by the integers m and n, see the text.

Number	m	n	χ (°)	y	z
1	7	6	−26.3295	$[\bar{1}\,\bar{3}\,14\,\bar{1}]$	$[\bar{5}\,4\,9]$
2	3	2	−21.0517	$[\bar{5}\,6\,\bar{1}]$	$[\bar{7}\,4\,11]$
3	2	1	−16.1021	$[\bar{3}\,4\,\bar{1}]$	$[\bar{5}\,2\,7]$
4	7	2	−9.3670	$[\bar{9}\,14\,\bar{5}]$	$[\bar{1}\,\bar{9}\,\bar{4}\,23]$
5	6	1	−5.4964	$[\bar{7}\,12\,\bar{5}]$	$[\bar{1}\,\bar{7}\,\bar{2}\,19]$
6	1	0	0	$[\bar{1}\,2\,\bar{1}]$	$[\bar{1}\,0\,1]$
7	6	−1	5.4964	$[\bar{5}\,12\,\bar{7}]$	$[\bar{1}\,\bar{9}\,2\,17]$
8	7	−2	9.3670	$[\bar{5}\,14\,\bar{9}]$	$[\bar{2}\,\bar{3}\,4\,19]$
9	2	−1	16.1021	$[\bar{1}\,4\,\bar{3}]$	$[\bar{7}\,2\,5]$
10	3	−2	21.0517	$[\bar{1}\,6\,\bar{5}]$	$[\bar{1}\,\bar{1}\,4\,7]$
11	7	−6	26.3295	$[\bar{1}\,14\,\bar{1}\,\bar{3}]$	$[\bar{9}\,4\,5]$