Displacement fields around 1/2[111] screw dislocations in bcc metals and their defocus convergent-beam electron diffraction patterns

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Abstract

Displacement fields have been calculated around 1/2[111] screw dislocations with various types of core structures in bcc metals. Three types of cores are studied: two types of polarized cores with large and small extensions of the displacement fields and an isotropic core. The difference in the displacement along the [111] direction \( \Delta u_z \) from that for the elastic solution has been evaluated for each type of dislocation. In the outside of the core region, the \( \Delta u_z \) values are close to zero along the six \(< 110 >\) directions and the regions with \( \Delta u_z > 0 \) and \( \Delta u_z < 0 \) are alternately arranged, lying between those directions. Appreciable difference in \( \Delta u_z \) has been detected between the polarized cores and the isotropic core up to large distance from the core region. The defocus convergent-beam electron diffraction patterns have been calculated for the dislocations with the incident beam parallel to the dislocation line. Winding and spiral features have been shown in the higher-order Laue zone (HOLZ) lines for the dislocated structures, which have been confirmed by a preliminary experiment. In addition, small shifts of the HOLZ lines have been shown by the calculation between the polarized cores and the isotropic one.

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1. Introduction

Since about 1970, the core structure of a 1/2[111] screw dislocation in bcc metals and its behavior under stress have been extensively investigated by computer simulation, as reviewed by Vitek [1] and by Duesbery [2]. Most of the simulations have shown that the stable core structure is of polarized type (Fig. 1(a) and (b)), characterized by an extended displacement field spreading along the three \(< 112 >\) directions. Therefore, for many years, it has been widely believed that such a polarized core structure is the origin of the plastic anisotropy and the immobility of the screw dislocation in bcc metals.

On the contrary, Takeuchi and his co-workers [3–5] showed that an isotropic core (Fig. 2(c)), which is accompanied by a displacement field nearly identical with that of the solution of the elastic theory, can also be a stable structure. Here, they adopted a model in which the atomic rows parallel to the dislocation line interact with each other and can relax only along the row direction. Subsequently, the isotropic core was also found to be stable in some full 3D relaxation models [2,6] using non-central potentials derived by Finnis and Sinclair [7]. In addition, very recently, Ismail-Beigi and Arias [8] attempted for the first time ab initio density-functional calculations for the screw dislocation cores in Mo and Ta and showed that the stable core is of the isotropic type. Subsequent ab initio studies also showed the stable isotropic core in Mo and Ta [9] and in Fe and Mo [10].

The convergent-beam electron diffraction (CBED) technique is useful for investigating strain induced by defects in material because it is very sensitive to local lattice distortion. Rackham and Steeds [11] showed that the higher-order Laue zone (HOLZ) lines in the CBED pattern split when the electron beam probe illuminates a dislocation line. Later, Carpenter and Spence [12] studied in detail the splitting of the HOLZ line caused by the displacement field around a dislocation and shown that the splitting is useful for determining the Burgers vector of the dislocation. However, because the displacement field of a dislocation varies from place to place, features in a CBED pattern changes sensitively to the exact position of the beam probe which is generally difficult to experimentally determine.
This fact makes a simple and accurate interpretation of the pattern difficult. This drawback can be overcome by the use of defocus CBED or large-angle CBED method (the Tanaka method)\[13–15\], in which the beam is focused at a point apart from the sample (Fig. 2). By this method, not only it becomes easy to locate the exact position of the beam probe on the sample, but also real and reciprocal space information are brought together, which makes the defocus CBED method much more informative than the usual CBED method.

The purpose of the present paper is to investigate in detail the displacement fields around 1/2[111] screw dislocation with various types of core structures shown by computer simulation and to examine the possibility for experimentally determining the core structure of the dislocation in real material by the defocus CBED method. Most of the CBED and defocus CBED studies of dislocations have been done so far in the geometry where the electron beam crosses the dislocation line. However, for the present purpose, parallel incidence of the beam to the dislocation line is expected to be more suitable because in such a geometry the interpretation of the pattern should be rather straightforward. In the present study, we have simulated the HOLZ lines bent by the displacement fields around the dislocation in defocus CBED patterns.

2. Computational procedures

The size of the model bcc lattice prepared was about 65b × 65b in a (111) plane, where \( b \) denotes the length of the Burgers vector \( \mathbf{b} = 1/2[111] \). First, a screw dislocation was introduced at the center by giving atomic displacements according to the solution of the elastic theory. Then, the structure was relaxed by use of empirical potentials. Here, periodic boundary condition with the period of \( b \) was applied to the [111] direction, i.e. the dislocation line direction, and the atoms whose distance from the dislocation line exceeds 30\( b \) were fixed to the elastic solution during relaxation. The interatomic potentials used were the Vitek’s \( J_3 \) potential for Fe [16] (potential A), the Finnis–Sinclair’s potential [7] for Mo (potential B) and Ta (potential C) to obtain different types of core structures. After the relaxation, all the three structures were rescaled to \( b = 0.273 \) nm that corresponds to \( b \) for Mo. For the resultant structures, the displacement fields were calculated.

The distribution of HOLZ lines was calculated in the defocus CBED bright-field (BF) disc. In Fig. 2, the geometry in the defocus CBED is illustrated schematically. Here, the dislocation is located at the center of the illuminated circular area with the radius of \( r_0 \). The incident beam is exactly parallel to [111] at the center and it deviates from [111] linearly as the distance from the center increases, the deviation reaching the maximum semi-angle of \( \alpha \) at the boundary of the illuminated area. HOLZ lines were calculated in a kinematical approximation and in a local column approximation. In the latter approximation, we assumed that whether a given position on the BF disc is on a HOLZ line or not is determined only by the strain at the corresponding position on the sample and the corresponding incident beam direction. In the calculation, only the first-order Laue zone (FOLZ) lines were taken into account.
3. Results and discussion

The core structures obtained are shown as (111) projections using differential displacement (DD) maps [16] in Fig. 1(a)–(c). Here, the arrow centered between any two atoms indicate the relative [111] displacement and the arrow lengths are scaled such that a displacement of b/3 produces a vector connecting nearest-neighbor atoms in this projection. The core structures obtained by the potential A and by the potential B are of the polarized type, characterized by extending displacement field along the three <112> directions. We notice that the degree of the extension of the displacement field is much larger in the former than that in the latter. On the other hand, the structure obtained by the potential C is almost identical with that before relaxation, i.e. the elastic solution. This type of core is called the isotropic core. We hereafter abbreviate the dislocations obtained by the potentials A, B and C as the type A, B and C dislocations, respectively.

In Fig. 3, the displacement field around each dislocation is shown as a contour plot in a large area surrounding the dislocation. Here, the difference in the displacement along the [111] direction, $\Delta u_{\text{z}}(x,y) = u_\text{z}(x,y) - u_\text{z}^0(x,y)$, is depicted, where $u_\text{z}(x,y)$ denotes the displacement in each structure and $u_\text{z}^0(x,y)$ the displacement in the elastic solution, i.e. $u_\text{z}^0(x,y) = \frac{b}{2\pi} \tan^{-1}(\frac{y}{x})$. The areas with $|\Delta u_\text{z}| > 0.01b$ extend up to about 6.3b and 3.2b from the center for the type A and B dislocations, respectively, whereas there is no area with $|\Delta u_\text{z}| > 0.01b$ for the type C dislocation. In the outside of the core region, $\Delta u_\text{z}$ values are close to zero along [110], [011], [101], [011] and [101] directions in all the structures and the regions with $\Delta u_\text{z} > 0$ and $\Delta u_\text{z} < 0$ are alternately arranged, lying between those directions. Although appreciable difference in $\Delta u_\text{z}$ can be detected between the polarized dislocations and the isotropic one up to large distance from the core region and that the difference in $\Delta u_\text{z}$ between the two polarized dislocations is relatively small in the outside of the core region. For example, the areas with $|\Delta u_\text{z}| > 0.004b$ extend up to about 11.7b, 9.1b and 3.8b from the center, and the areas with $|\Delta u_\text{z}| > 0.002b$ extend up to about 16.4b, 14.3b and 7.6b for the type A–C dislocations, respectively.

Fig. 4(a)–(d) shows the defocus CBED patterns in the BF disc calculated for the perfect crystal without dislocation and the structures containing the type A–C dislocations, respectively. Here, the radius $r_0$ (Fig. 2) of the illuminated area on the sample is 5.0 nm, which is the same as those of the displayed area in Fig. 3, and the convergent angle $\alpha$ is $2 \times 10^{-3}$ rad. For the calculation, only the strain components $e_x$, $e_y$, $e_{xy}$ were taken into account because the other components were sufficiently small, compared with them. In the central region in the patterns (b)–(d), where no lines are drawn, no continuous HOLZ lines were obtained due to large spatial dependence of strain. Comparing the pattern in Fig. 4(a) with those in Fig. 4(b)–(d), we notice the following effects on the HOLZ lines by the displacement fields induced by the dislocations: (1) those HOLZ lines whose position for the perfect crystal (Fig. 4(a))
is relatively far from the dislocation center show a winding feature for the dislocated structures (Fig. 4(b)-(d)) and (2) those lines whose position in (a) pass the central area appear to go toward the center in a spiral fashion in (b)-(d). The HOLZ lines indicated by circles in Fig. 4(a) are classified into the former group while those indicated by triangles are into the latter group.

In Fig. 5, the rectangular region in Fig. 4(b) is magnified and shown together with the HOLZ-line pattern in the same region in Fig. 4(d). We find small shifts of the HOLZ lines between the two patterns. The region where appreciable difference is observed is located at about 2.0 nm from the center and we notice a considerable difference in the magnitude of the displacement field between the two structures in Fig. 3(a) and (c). In contrast, we could detect no noticeable difference between the patterns for the type A and B dislocations, i.e. the two polarized dislocations.

We calculated the defocus CBED patterns in the BF disc using different values of the accelerating voltage \( E \) with the range 97–105 kV, and the convergent angle \( \alpha \) with the range \( 10^{-3} - 10^{-2} \) rad. With changing \( E \), the defocus CBED pattern itself changed sensitively. However, we could always detect the winding and spiral features of the HOLZ lines for the dislocated structures and the small shifts of the HOLZ lines between the polarized and isotropic dislocations. On the other hand, with changing \( \alpha \), the density of the HOLZ lines changed. We found that for large \( \alpha \) the shifts of HOLZ lines between the polarized and isotropic dislocations become small: for the \( \alpha \) values larger than about 0.007 rad, no noticeable shifts were detected. The winding and spiral features of the HOLZ lines were always found, irrespective of the \( \alpha \) value.

We attempted a preliminary experiment for a deformed sample of Ta and succeeded in obtaining defocus CBED patterns from area containing a 1/2[111] screw dislocation. Here, we confirmed the winding and spiral features of the HOLZ lines in the vicinity of the dislocation position. However, the patterns obtained up to now appear to be unsuitable for analyzing the difference between the different types of dislocation cores for the following reasons: (1) the dislocation center and the beam center do not coincide exactly and (2) the HOLZ lines are not sharp enough to detect small positional shifts expected by the calculation. As for (1), careful adjustment of the beam and sample positions would be possible, referring to the fact that the exact coincidence of the beam and sample positions makes the pattern 3-fold symmetric. On the other hand, as for (2), we need to examine further the conditions under which the small shifts of the HOLZ lines between the different types of dislocations can be detected by more precise calculations taking into account the dynamical effects.

As described in the Section 1, the dispute on the core structure of the 1/2[111] screw dislocation in bcc metals is still far from settled in spite of many computational works done so far. We believe that experimental approach such as the defocus CBED discussed in the present paper is crucially important to give a final solution to this problem.

4. Conclusions

Displacement fields were calculated around 1/2[111] screw dislocations with various types of core structures in bcc metals. Three types of cores were studied: two types of polarized cores with large and small extensions of the displacement fields and an isotropic core. The difference in the displacement along the [111] direction \( \Delta u_1 \) from that for the elastic solution was evaluated for each type of dislocation. We found that in the outside of the core region the \( \Delta u_1 \) values are close to zero along the six \( < 110 > \) directions and the regions with \( \Delta u_1 > 0 \) and \( \Delta u_1 < 0 \) are alternately arranged, lying between those directions. Applicable difference in \( \Delta u_1 \) was detected between the polarized cores and the isotropic core up to large distance from the core region while the difference in \( \Delta u_1 \) between the two types of polarized cores was relatively small in the outside of the core region. The defocus CBED patterns in the BF disc were calculated for the dislocations with the incident beam parallel to the dislocation line. For the dislocated structures, the HOLZ lines showed winding or spiral feature, which was confirmed by our preliminary experiment. In addition, small shifts of the HOLZ lines were shown by the calculation between the polarized cores and the isotropic one. To detect such small shifts of the HOLZ lines experimentally, we need careful adjustment of the beam and sample positions and suppression of the broadening of the HOLZ lines due partly to dynamical effects.
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