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Line tension and configuration of a dislocation on the basal, prismatic, and pyramidal planes in zinc oxide

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The line tension and equilibrium configuration of a planer-dislocation shear loop on the basal, prismatic, and pyramidal planes in zinc oxide under an external stress are calculated. An extended version of the formulation of deWit and Koehler applicable to piezoelectric crystals is used, and the piezoelectric effects on the line tension and configuration are estimated. The results for zinc oxide are compared with those for zinc, and the characteristic features of zinc oxide are discussed.

I. INTRODUCTION

Dislocations in crystals under an external stress tend to be curved in order to be in equilibrium with the stress. The analysis of the equilibrium shapes of dislocations goes back to that of de Wit and Koehler.[1] In their formulation, the dislocation self-energy was approximated by the line integral of the energy per unit length of a straight dislocation, and their variational calculus results in the local equilibrium between the line tension and the Peach and Koehler force. The author[2] has recently given the extended version of the de Wit and Koehler formulation to piezoelectric crystals, in which the energy arising from the piezoelectricity has been incorporated into the dislocation self-energy. He has applied this method for dislocations in trigonal piezoelectric crystals, and visualized the piezoelectric effect on the line tensions and equilibrium shapes of dislocations.

On the other hand, dislocations in II-VI compounds have attracted much attention in the past two or three decades because of the photoplastic effect which was found in cadmium sulfide by Osip'yan and Savchenko.[3] In this phenomenon, the charges carried by dislocations play an important role, and the static fields produced by them inhibit further motion of other dislocations.[4] Another important characteristic of these crystals is piezoelectricity, and it brings about electric fields around dislocations. It is possible that these electric fields may affect the movements of other charged dislocations.

In this paper, we will investigate the line tension and equilibrium configuration of a planer-dislocation shear loop in zinc oxide. This crystal is a II-VI compound of wurtzite structure, and considered to be one of the most promising materials for bulk-wave supersonic transducers and surface-acoustic-wave devices. In addition, the piezoelectric effect in this crystal is expected to appear clearly because of its large piezoelectric coefficients. The orientation dependences of the prelogarithmic energy factors and prelogarithmic line tension factors will be shown, and the differences between their behavior and those for zinc, which has hexagonal crystal structure and no piezoelectricity, will be discussed. Because the detailed description of the formulation and the method of calculation has been given in Ref. 2, it is abbreviated for brevity in this paper.

II. SLIP SYSTEMS OF ZINC OXIDE

Slip systems of zinc oxide were investigated by several authors in the past. Osip'yan and Smirnova[5] gave a detailed analysis of hypothetically possible types of perfect dislocations in crystals of wurtzite structure. They studied the atomic crystal structure of the wurtzite lattice and presented 13 types of possible slip systems. However, all of these systems were not identified experimentally. Osip'yan, Petrenko, Zaretskii, and Whitworth[4] reviewed the structures and properties of moving dislocations in II-VI semiconductors, and they pointed out that the operative Burgers vectors are $[2\bar{1}\,\bar{1}0]$ and $[11\bar{2}0]$ for the (0001) slip, and that the $\{01\bar{1}0\}\langle\bar{2}110\rangle$ system is also possible in the wurtzite structure.

Hirth and Lothe[6] presented a table of a variety of slip systems observed in hcp metals by using electron-transmission microscopy or other experimental techniques. According to their discussion, an ideal ratio of c/a, where a and c are the lattice constants in hcp crystals, is 1.633 of the close packing of spheres, and the favored slip systems are different between the crystal groups of the larger and smaller c/a values than the ideal. For zinc oxide, c/a is 1.602,[7] and this is slightly smaller than the ideal. Their table shows that for the crystals of the slightly smaller c/a values than the ideal, the basal slip system $\langle 11\bar{2}0\rangle\{0001\}$ and the prismatic slip system $\langle 11\bar{2}0\rangle\{1\bar{1}00\}$ are predominant at room temperature, and the slip system $\langle 11\bar{2}0\rangle\{1\bar{1}01\}$ in the pyramidal plane is possible at high temperatures.

Suzuki, Ichihara, Takeuchi, Nakagawa, Maeda, and Iwanaga[8] have observed *in situ* the dislocation motion in the II-VI compounds CdS, CdSe, and ZnO by transmission electron microscopy at room temperature. In their experiment, the nonscrew and screw dislocations were observed in $\{1\bar{1}00\}$ ZnO crystals. Recently, Czernuszka and Pratt[9] have used the cathodoluminescence mode in the scanning electron microscope to image bands of dislocations in zinc oxide. They have concluded that dislocations beneath indentations on $\{0001\}$ surfaces lie on

second-order pyramidal planes $\{1\bar{1}02\}$, and indentations on $\{1\bar{1}00\}$ surfaces cause slips on basal and prismatic planes. In the work of Peng and Czernuszka,[10] reflection electron microscopy has been used, and individual dislocations on $(1\bar{1}00)$, $(11\bar{2}0)$, and (0001) surfaces of a single crystal of zinc oxide have been observed, and as for the dislocations on $(1\bar{1}00)$, the Burgers vectors of the type $\frac{1}{3}\langle 11\bar{2}0\rangle$ have been identified. Reflecting on all of these studies cited above, we adopt the basal slip system $\langle 11\bar{2}0\rangle\{0001\}$, the prismatic slip system $\langle 11\bar{2}0\rangle\{1\bar{1}00\}$,

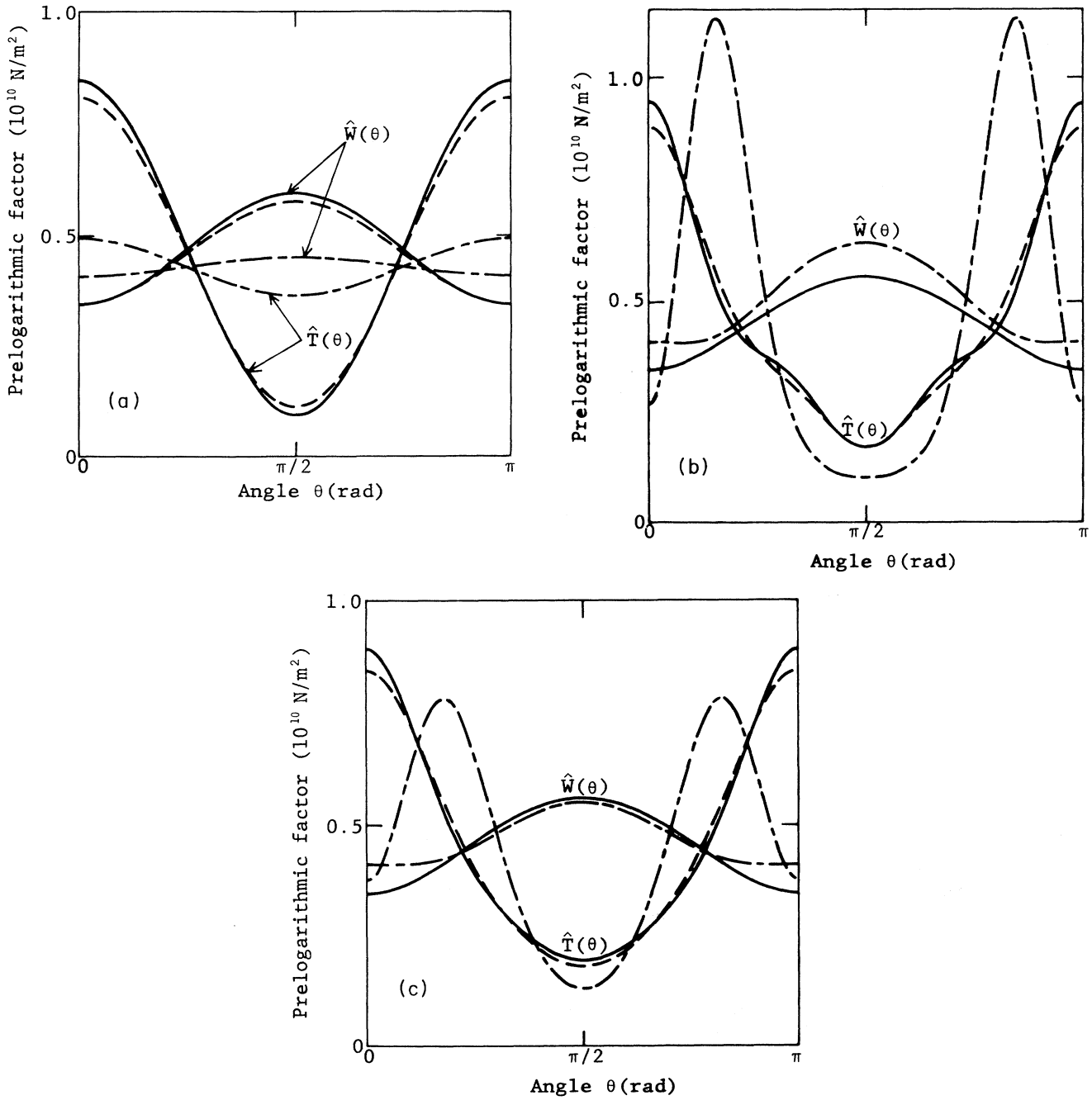

FIG. 1. The orientation dependences of the prelogarithmic energy factor $\hat{W}(\theta)$ defined by Eq. (1) and the prelogarithmic line tension factor $\hat{T}(\theta)$ defined by an equation analogous to Eq. (1). The solid lines represent the factors for zinc oxide, the dashed lines for zinc oxide, its piezoelectricity being neglected, and the dotted-dashed lines for zinc. $\theta=0$ and π correspond to the points of pure screw character on the loops and $\theta=\frac{1}{2}\pi$ to the point of pure edge character. (a) is for the basal slip system $\langle 11\bar{2}0\rangle\{0001\}$, (b) is for the prismatic slip system $\langle 11\bar{2}0\rangle\{1\bar{1}00\}$, and (c) is for the pyramidal slip system $\langle 11\bar{2}0\rangle\{1\bar{1}02\}$.

and the two pyramidal slip systems $\langle 11\bar{2}0\rangle\{1\bar{1}01\}$ and $\langle 11\bar{2}0\rangle\{1\bar{1}02\}$ as the slip systems for the numerical calculations.

III. RESULTS AND DISCUSSION

Based on the de Wit and Koehler formulation, Bacon and Scattergood[11] calculated the line tensions and loop configurations of dislocations in nonpiezoelectric crystals of cubic and hexagonal structures; they obtained the results for the prismatic slip system $\langle 11\bar{2}0\rangle\{1\bar{1}00\}$ and the pyramidal slip system $\langle 11\bar{2}0\rangle\{1\bar{1}01\}$ in zinc as an example of hexagonal crystals. The ratio of its lattice constants c/a is 1.86,[12] and its favorable slip systems are the basal $\langle 11\bar{2}0\rangle\{0001\}$ and the prismatic $\langle 11\bar{2}0\rangle\{1\bar{1}00\}$ slip systems according to Hirth and Lothe. For the sake of comparison, we have recalculated the line tension and energy factors of zinc in the same slip systems as adopted for zinc oxide. The numerical data of the lattice, elastic, piezoelectric stress, and dielectric constants for zinc oxide are taken from Refs. 7, 13, and 14, and those of the lattice and elastic constants for zinc from Refs. 12 and 15.

The line tensions and loop shapes in nonpiezoelectric crystals cannot be obtained by making the piezoelectric stress and dielectric constants tend to zero in the energy expression for piezoelectric crystals because of the singularity of a matrix which appears in the calculation of the energy per unit length of a straight dislocation. The energy factors of no piezoelectricity can be calculated by using the formula of Eshelby, Read, and Shockley,[16] as was shown by Foreman.[17]

In Figs. 1 and 2, the solid lines are for zinc oxide, the dashed lines are for zinc oxide, its piezoelectricity being neglected, and the dotted-dashed lines are for zinc. In Fig. 1, the orientation dependences of the prelogarithmic energy factor and the prelogarithmic line tension factor are shown: (a) is for the basal slip system $\langle 11\bar{2}0\rangle\{0001\}$, (b) is for the prismatic slip system $\langle 11\bar{2}0\rangle\{1\bar{1}00\}$, and (c) is for the pyramidal slip system $\langle 11\bar{2}0\rangle\{1\bar{1}02\}$. The prelogarithmic energy factor $\hat{W}(\theta)$ is defined by

$$W(\theta)=\hat{W}(\theta)b^2\ln\frac{R}{r_0}\ , \tag{1}$$

where $W(\theta)$ is the self-energy per unit length of a straight dislocation, θ is the angle between the dislocation line element and the Burgers vector, b is the magnitude of the Burgers vector, and r_0 and R are the inner and outer cutoff radii, respectively. The line tension can be expressed in terms of $W(\theta)$, and its prelogarithmic factor is defined by an equation analogous to Eq. (1). Because the prelogarithmic factors for the pyramidal slip system $\langle 11\bar{2}0\rangle\{1\bar{1}01\}$ behave in nearly the same manner as for the prismatic slip system $\langle 11\bar{2}0\rangle\{1\bar{1}00\}$, they have been omitted. The dashed lines representing the energy factors of no piezoelectricity in Figs. 1(b) and 1(c) are very close to the solid lines, and one cannot discriminate between them.

In Fig. 1(a), the functional forms of the factors are similar to those for isotropic materials because of the isotropic character of the basal plane; the energy factor of no piezoelectricity for the basal slip system is expressed in terms of the isotropic relation, as shown by Foreman. The piezoelectric effect on the line tension at $\theta=0$ (pure screw) is opposite to that at $\theta=\frac{1}{2}\pi$ (pure edge). According to the local force balance [Eq. (9) in Ref. 2], which is the essence of the line tension approximation theory, the radius of curvature of the dislocation line element is in proportion to the line tension for a given external stress. This means that the radius of curvature of the dislocation increases at $\theta=0$ and decreases at $\theta=\frac{1}{2}\pi$.

In Figs. 1(b) and 1(c), the outstanding difference between the prelogarithmic line tension factors of zinc oxide and those of zinc appears. As pointed out by Bacon and Scattergood, the line tension factor of zinc has a maximum between $\theta=0$ and $\frac{1}{2}\pi$ and the loop becomes flat there. It was shown by the author[2] that by the

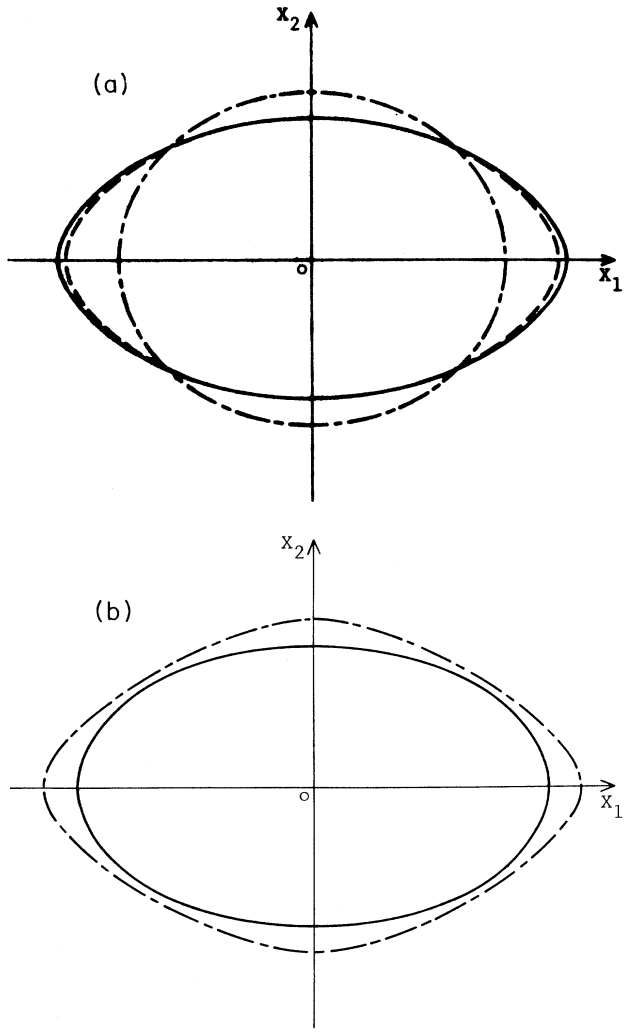

FIG. 2. The equilibrium shapes of dislocation shear loops. The solid lines represent the loop shape for zinc oxide, the dashed line for zinc oxide, its piezoelectricity being neglected, and the dotted-dashed lines for zinc. (a) is for the basal slip system $\langle 11\bar{2}0\rangle\{0001\}$, and (b) is for the prismatic slip system $\langle 11\bar{2}0\rangle\{1\bar{1}00\}$.

piezoelectric effect, the line tension factors of lithium niobate, which is of trigonal crystal structure, also have a local maximum and a local minimum between $\theta=0$ and $\frac{1}{2}\pi$ or the maximum points move from those obtained neglecting piezoelectricity. Although the slip systems adopted for lithium niobate are different from the present hexagonal case, no appearance of local maximum and minimum is peculiar to zinc oxide. In Fig. 1(b), it is seen that, instead of maxima, the inflection points appear at about $\theta=\frac{1}{4}\pi$ and $\frac{3}{4}\pi$ by the piezoelectric effect.

We show the equilibrium configurations of dislocations in Fig. 2: (a) is for the basal slip system and (b) is for the prismatic slip system. The configurations for the two pyramidal planes are very similar to that shown in Fig. 2(b). The coordinates are being normalized by $(b/\sigma_{31})\ln(R/r_0)$, where σ_{31} is the applied shear stress.

In Fig. 2(a), the loop shape on the basal slip plane in zinc, which Bacon and Scattergood did not obtain, is shown; its shape slightly deviates from a circle. The loop shape for zinc oxide is drastically different from that for zinc. The piezoelectric effect on the loop shape is noticeable at the pure edge parts, and makes the loop further distorted into the direction of the external shear stress σ_{31}. Brown, Spring, and Ipohoroski[18] computed the shapes of Frank loops on the basal plane in copper and nickel by the Wulff construction; the resulting loop shapes resemble hexagons, reflecting the hexagonal lattice structure. In contrast with their result, there appears to be no hexagonal structure in the configurations presently obtained, which is a consequence of the de Wit and Koehler formulation, viz., the line tension approximation.

In Fig. 2(b), the solid and dashed lines are so close to one another that the two lines cannot be distinguished. The loop shape for zinc has flat parts corresponding to the maxima of the line tension, and that for zinc oxide resembles an ellipse.

IV. CONCLUSIONS

The line tension and loop shape on the basal plane in zinc oxide are of isotropic character, and the loop shape is distorted into the direction of the external shear stress by the piezoelectric effect. The orientation dependences of the line tensions of the dislocations in the prismatic $\langle 11\bar{2}0\rangle\{1\bar{1}00\}$ and the pyramidal $\langle 11\bar{2}0\rangle\{1\bar{1}01\}$ slip systems resemble each other; they have no local maximum or local minimum which appears for zinc, and they have inflection points by the piezoelectric effect. The loop shapes for the prismatic slip system $\langle 11\bar{2}0\rangle\{1\bar{1}00\}$ and the two pyramidal $\langle 11\bar{2}0\rangle\{1\bar{1}01\}$ and $\langle 11\bar{2}0\rangle\{1\bar{1}02\}$ slip systems are the same and close to an ellipse.

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