Peierls stress of a screw dislocation in a piezoelectric medium

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In this letter, the Peierls-Nabarro (PN) model is extended to describe dislocation mobility in piezoelectric materials. The Peierls stress of a screw dislocation in a piezoelectric material is calculated based on the generalized PN model and linear piezoelectricity theory. © *2004 American Institute of Physics*. [DOI: 10.1063/1.1790030]

Piezoelectric materials have been extensively used to manufacture thin films and other components in sensors, transducers, integrated circuits, and various other electric devices. There has been a keen interest to study the dislocation mobility in piezoelectric materials.

Nevertheless, only a few analytical studies regarding dislocation mechanics of piezoelectric materials have been reported in the literature.[1–5] Moreover, it seems to us that the issues regarding the mobility of dislocations in such materials have not been resolved. In this letter, an analytical expression for the Peierls stress in a piezoelectric crystal is obtained.

Consider a piezoelectric screw dislocation in a hexagonal crystal ($6mm$). Assume that the x-y plane is the isotropic basal plane and the z axis is the out-plane axis. Consider an infinitely long screw dislocation with Burgers vector b_m lying along the z axis.

The dislocation mechanics in piezoelectric materials is more complicated than the dislocation mechanics in purely elastic media. In a piezoelectric medium, dislocations often coexist with discontinuous charge distributions. Similar to the dislocation representing displacement discontinuity, the electrical potential discontinuity is represented by the electric dipole. In this analysis, it is assumed that there is an electric dipole vector b_e along the z axis.

For simplicity, we consider the following coupled antiplane strain and in-plane electric potential problem:

$$u_x = u_y = 0,\ u_z = u_z(x,y), \tag{1}$$

$$E_x = -\phi_{,x}(x,y),\ E_y = -\phi_{,y}(x,y),\ E_z = 0, \tag{2}$$

where $\phi = \phi(x,y)$ is the electrical potential, E_i $(i = x,y,z)$ are the electric-field components, and u_i $(i = x,y,z)$ are the displacement components.

A set of nontrivial constitutive equations can be obtained for the present purpose.[4] For a hexagonal crystal of $6mm$ class, they are given as

$$\sigma_{xz} = c_{44}\gamma_{xz} - e_{15}E_x, \tag{3}$$

$$\sigma_{yz} = c_{44}\gamma_{yz} - e_{15}E_y, \tag{4}$$

$$D_x = e_{15}\gamma_{xz} + \epsilon_{11}E_x, \tag{5}$$

$$D_y = e_{15}\gamma_{yz} + \epsilon_{11}E_y, \tag{6}$$

where σ_{xz}, σ_{yz} are the two out-plane shear stresses, γ_{xz}, γ_{yz} are the related shear strains, D_x, D_y are in-plane electrical displacements, and c_{44}, e_{15}, ϵ_{11} are shear elastic modulus, piezoelectric coefficient, and dielectric constant, respectively.

Because the electrostatic charge equation is decoupled with the stress equilibrium equation, the screw dislocation solution has the same form as the classical Burgers' solution,[4]

$$u_z = \frac{b_m}{2\pi} \arctan \frac{y}{x}, \tag{7}$$

$$\phi = \frac{b_e}{2\pi} \arctan \frac{y}{x}, \tag{8}$$

$$\sigma_{xz} = -\frac{(c_{44}b_m + e_{15}b_e)y}{2\pi(x^2 + y^2)}, \tag{9}$$

$$\sigma_{yz} = \frac{(c_{44}b_m + e_{15}b_e)x}{2\pi(x^2 + y^2)}, \tag{10}$$

$$D_x = \frac{(-e_{15}b_m + \epsilon_{11}b_e)y}{2\pi(x^2 + y^2)}, \tag{11}$$

$$D_y = \frac{(e_{15}b_m - \epsilon_{11}b_e)x}{2\pi(x^2 + y^2)}. \tag{12}$$

To extend the original Peierls-Nabarro (PN) model[6,7] to piezoelectric materials, we distribute a single mechanical dislocation and a single electrical dipole along the glide plane, such that the nonlocal dislocation system has an equivalent displacement jump w and an equivalent electric potential jump φ along the upper half of the crystal ($y > 0$) with respect to the lower half ($y < 0$). These jumps are assumed to result from the distribution of an infinitesimal dislocation, b'_m, and an infinitesimal jump in electric potential, b'_e, respectively. Such infinitesimal quantities are determined by the following equivalency conditions:

$$b'_m = \left(\frac{\partial w}{\partial x}\right)\bigg|_{x=x'},\quad b'_e = \left(\frac{\partial \varphi}{\partial x}\right)\bigg|_{x=x'}, \tag{13}$$

and

$$b_m = \int_{-\infty}^{\infty} b'_m(x)dx,\quad b_e = \int_{-\infty}^{\infty} b'_e(x)dx. \tag{14}$$

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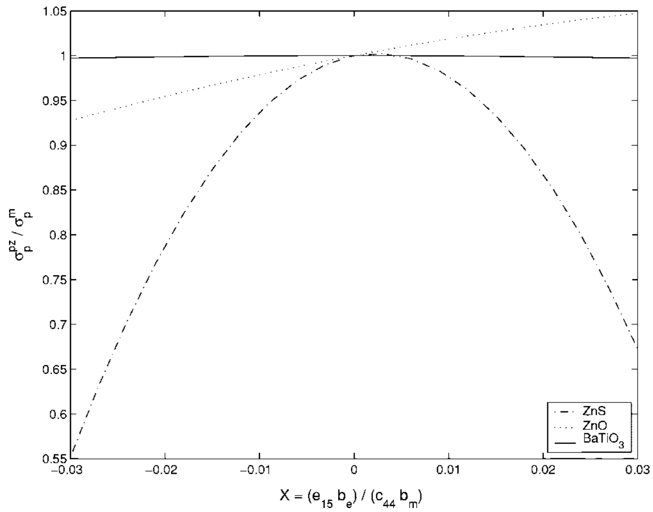

FIG. 1. The Peierls stress in piezoelectric materials.

By doing so, we create a cohesive strip that connects two perfect crystal half spaces. Comparing with the two perfect crystal half spaces, the cohesive strip may be viewed as a phase of a *lower order symmetry*, because of the presence of the topological defect and the biased charge distribution. As an analog to Landau's potential,[8] it is then plausible to speculate that the excess free energy inside the cohesive strip could be expressed by an even-order polynomial expansion of some *order parameters*.[9] In an equilibrium state, these order parameters may be proportional to nondimensional misfit variables, w/b_m and φ/b_e. The stress and the electric displacement field, caused by the misfit and derived from the above-mentioned free energy will be an odd function of the order parameters. In the spirit of original PN model, we assume these fields by the following expressions:

$$\sigma_{yz}(x,0) = \frac{c_{44}b_m}{2\pi d}\sin\left(\frac{2\pi w}{b_m}\right) + \frac{e_{15}b_e}{2\pi d}\sin\left(\frac{2\pi\varphi}{b_e}\right), \tag{15}$$

$$D_y(x,0) = \frac{e_{15}b_m}{2\pi d}\sin\left(\frac{2\pi w}{b_m}\right) - \frac{\epsilon_{11}b_e}{2\pi d}\sin\left(\frac{2\pi\varphi}{b_e}\right), \tag{16}$$

where d is the width of dislocation. It should be noted that the validness of the above assumption hinges on the fact that the Taylor expansion of a sinusoidal function is a series of odd order polynomials.

Using Eqs. (14) and (16) and considering the fact that the smeared dislocation and the electrical dipole are along $y=0$, we may obtain the stress field σ_{yz} and the electric displacement field D_y,

$$\sigma_{yz}(x,0) = \frac{c_{44}}{2\pi}\int_{-\infty}^{\infty}\frac{b'_m}{x-x'}dx' + \frac{e_{15}}{2\pi}\int_{-\infty}^{\infty}\frac{b'_e}{x-x'}dx', \tag{17}$$

$$D_y(x,0) = \frac{e_{15}}{2\pi}\int_{-\infty}^{\infty}\frac{b'_m}{x-x'}dx' - \frac{\epsilon_{11}}{2\pi}\int_{-\infty}^{\infty}\frac{b'_e}{x-x'}dx'. \tag{18}$$

Comparing Eq. (19) with Eq. (21) and Eq. (20) with Eq. (22), we obtain two nonlinear integral equations,

$$\int_{-\infty}^{\infty}\frac{(\partial w/\partial x)_{x=x'}}{x-x'}dx' = \frac{b_m}{d}\sin\left(\frac{2\pi w}{b_m}\right), \tag{19}$$

$$\int_{-\infty}^{\infty}\frac{(\partial\varphi/\partial x)_{x=x'}}{x-x'}dx' = \frac{b_e}{d}\sin\left(\frac{2\pi\varphi}{b_e}\right). \tag{20}$$

The solutions of these nonlinear integral equations are,

$$w(x) = \frac{b_m}{\pi}\arctan\frac{2x}{d} + \frac{b_m}{2}, \tag{21}$$

$$\varphi(x) = \frac{b_e}{\pi}\arctan\frac{2x}{d} + \frac{b_e}{2}. \tag{22}$$

A standard procedure is now followed to calculate the total misfit enthalpy generated by the dislocation-dipole system and to obtain an analytical expression for the Peierls stress.[10]

Let a be the spacing of atomic planes in x direction (in the absence of a dislocation). If the dislocation is translated by u, then the planes at a position na (where n is an integer) in the upper half of the crystal will be displaced with respect to lower half by $w(na-u)$. Also the planes at na in the upper half of crystal will then experience a potential shift $\varphi(na-u)$, with respect to the lower half. The misfit enthalpy between a pair of atomic planes can be written as

$$\begin{aligned}\delta H &= ad\int(\sigma_{yz}d\gamma_{yz} - D_y dE_y)\\ &= a\int(\sigma_{yz}dw + D_y d\varphi)\\ &= \frac{c_{44}b_m a}{2\pi d}\int\sin\left(\frac{2\pi w}{b_m}\right)dw + \frac{e_{15}b_e a}{2\pi d}\int\sin\left(\frac{2\pi\varphi}{b_e}\right)dw\\ &\quad + \frac{e_{15}b_m a}{2\pi d}\int\sin\left(\frac{2\pi w}{b_m}\right)d\varphi - \frac{\epsilon_{11}b_e a}{2\pi d}\int\sin\left(\frac{2\pi\varphi}{b_e}\right)d\varphi\\ &= \delta H_1 + \delta H_2 + \delta H_3 + \delta H_4.\end{aligned} \tag{23}$$

Summing δH_1 from $n=-\infty$ to $+\infty$, one has

$$\begin{aligned}H_1(u) &= \frac{c_{44}b_m^2 a}{4\pi^2 d}\sum_{n=-\infty}^{\infty}\left\{1+\cos 2\left[\arctan\frac{2(na-u)}{d}\right]\right\}\\ &= \frac{c_{44}b_m^2}{4\pi} + \frac{c_{44}b_m^2}{2\pi}\exp(-\pi d/a)\cos\left(\frac{2\pi u}{a}\right).\end{aligned} \tag{24}$$

The limit for wide dislocations ($d/a \gg 1$) has been used in the above calculation.[10] Similarly, it may be found that

$$H_4(u) = -\frac{\epsilon_{11}b_e^2}{4\pi} - \frac{\epsilon_{11}b_e^2}{2\pi}\exp(-\pi d/a)\cos\left(\frac{2\pi u}{a}\right), \tag{25}$$

which is the contribution due to the electric dipole distribution.

Considering the relation,

$$\tan\frac{\pi\varphi}{b_e} = \tan\frac{\pi w}{b_m}, \tag{26}$$

one may find that

$$H_2(u) = \frac{e_{15}b_m b_e}{4\pi} + \frac{e_{15}b_m b_e}{2\pi}\exp(-\pi d/a)\cos\left(\frac{2\pi u}{a}\right),$$

$$H_3(u) = \frac{e_{15}b_m b_e}{4\pi} + \frac{e_{15}b_m b_e}{2\pi}\exp(-\pi d/a)\cos\left(\frac{2\pi u}{a}\right).$$

The Peierls potential in the cohesive strip (or the total misfit enthalpy) is

$$H(u) = \sum_{i=1}^{4} H_1(u) = \frac{1}{4\pi}\{c_{44}b_m^2 + 2e_{15}b_m b_e - \epsilon_{11}b_e^2\} \cdot \left[1 + 2\exp(-\pi d/a)\cos\left(\frac{2\pi u}{a}\right)\right]. \quad (27)$$

The Peierls stress for a screw dislocation in a piezoelectric crystal class is then obtained by finding the maximum stress,

$$\sigma_P^{pz} = \max\left[\frac{1}{b_m}\frac{\partial H(u)}{\partial u}\right]. \quad (28)$$

We therefore obtain

$$\sigma_P^{pz} = \left(\frac{c_{44}b_m}{a} + \frac{2e_{15}b_e}{a} - \frac{\epsilon_{11}b_e^2}{ab_m}\right)\exp\left(-\frac{\pi d}{a}\right), \quad (29)$$

where the superscript *pz* denotes the Peierls stress for piezoelectric materials. When $b_e=0$, we recover the classical Peierls stress for a purely elastic crystal,[10]

$$\sigma_P^m = \frac{c_{44}b_m}{a}\exp\left(-\frac{\pi d}{a}\right), \quad (30)$$

where superscript *m* denotes the Peierls stress for a purely mechanical system (i.e., for which $b_e=0$).

Let

$$X := \frac{e_{15}b_e}{c_{44}b_m}, \quad k := \frac{c_{44}\epsilon_{11}}{e_{15}^2}. \quad (31)$$

Then,

$$\frac{\sigma_P^{pz}}{\sigma_P^m} = 1 + 2X - kX^2. \quad (32)$$

We plot the ratio, σ_P^{pz}/σ_P^m, against the nondimensional variable X for some typical semiconductor piezoelectric materials. The results are displayed in Fig. 1.

We notice from the figure that the ratio σ_P^{pz}/σ_P^m depends on the ratio b_e/b_m for a particular semiconductor (see Table I for material properties of some semiconductors). This implies that depending on the magnitude of mechanical dislocation and electrical dipole vector, the Peierls stress for the considered piezoelectric material may increase or decrease (with respect to mechanical Peierls stress), and therefore result in a decrease or increase of dislocation mobility. These curves vary with material properties and will be different for different piezoelectric materials.

TABLE I. Material properties of some semiconductors (Ref. 11).

Compound	ρ (density) (10^3 kg/m^3)	ϵ_{11} (10^{-9} F/m)	c_{44} (10^{10} N/m^2)	e_{15} (C/m^2)
ZnS	3.98	0.0770[b]	2.28	−0.0638
ZnO	5.68	0.0757[a]	4.247	−0.48
$BaTiO_3$	5.7	9.8722[a]	4.4	11.4

[a]Constant strain.
[b]Constant stress.

As a second example we investigate the mobility of a dislocation in a 180° domain-wall structure of a ferroelectric material by using the modified Peierls-Nabarro developed in this paper. We consider only those ferroelectric materials that possess the symmetry of transversely isotropy, and thus we can describe the above-mentioned structure by the same set of field equations developed above. A slight modification is required in calculating the total misfit enthalpy. Since the piezoelectric coefficient e_{15} changes sign across the 180° domain wall, the interaction terms δH_2 and δH_3 will vanish after being added along the two atomic planes. The other two terms in the expression for total enthalpy remain unchanged (they are independent of the piezoelectric coefficient). Following the usual algebra we can then obtain the expression for the Peierls stress for the considered case as

$$\frac{\sigma_P^{pz}}{\sigma_P^m} = 1 - kX^2. \quad (33)$$

From Eq. (33), we conclude that unlike piezoelectric materials, the presence of an electric dipole in a 180° domain-wall structure of a ferroelectric material will always result in a decrease of the Peierls stress and thus result an increase in dislocation mobility. This is illustrated by plotting the Peierls stress of $BaTiO_3$ versus nondimensional electric dipole density, X, in Fig. 1.

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