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Screw dislocations in piezoelectric nanowires

Xu Wang[a], Ernie Pan[a,b,*]

[a] School of Mechanical Engineering, Zhengzhou University, Zhengzhou, Henan 450001, PR China
[b] Department of Civil Engineering, University of Akron, OH 44325, USA

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ABSTRACT

In this article, we extend Eshelby's classic work (Eshelby, 1953) on screw dislocation in an elastic rod to the corresponding piezoelectric case. In our study the screw dislocation suffers a displacement jump and an electric potential jump across the slip plane, and the surface of the piezoelectric cylinder is traction-free and charge-free. Our results demonstrate that this extension is not trivial because under some conditions the screw dislocation cannot be ejected from the piezoelectric cylinder by applying an external torque to the cylinder and the stress–strain curve in torsion possesses a nonlinear region due to the movement of the screw dislocation. These observations are quite different than those predicted by Eshelby (1953) for the elastic rod case, and should be particularly interesting to piezoelectric nanowire structures involving Eshelby twist.

1. Introduction

Eshelby (1953) demonstrated that when all boundary conditions were taken into consideration, the image force acting on the screw dislocation would keep the dislocation along the axis of the cylinder (i.e., the center of the cylinder is a stable equilibrium position for the dislocation). He observed that only when the screw dislocation was displaced more than 0.54 of the rod radius from the axis did the image force tend to pull it out of the rod. He also predicted that the screw dislocation would cause a twist of the cylinder (the so-called "Eshelby twist") and that the dislocation could be ejected from the rod by twisting or bending it suitably. Interestingly the "Eshelby twist" was only experimentally verified in nanowires very recently (Bierman et al., 2008; Zhu et al., 2008; Deppert and Wallenberg, 2008). It is added that the "Eshelby twist" was also observed by Mann (1949). Thus, the objective of this work is to extend Eshelby's classical work to piezoelectric cylinders. In our study the screw dislocation suffers a displacement jump and an electric potential jump across the slip plane, and the surface of the piezoelectric cylinder is traction-free and charge-free. Physically the jump in the electric potential (or the so-called "electric-potential-dislocation") corresponds to the electric dipole layer along the slip plane (Lee et al., 2000). Our results show that some new phenomena emerge if the dislocation possesses an electric potential jump.

2. Screw dislocations in piezoelectric rods

Now we consider a homogeneous piezoelectric rod containing a screw dislocation (Fig. 1). The rod has 6 mm point group symmetry about the rod axis (i.e., the z-axis is along the $c[0\,0\,0\,1]$ direction of the crystalline) before the introduction of dislocations. This symmetric material corresponds to the hexagonal crystal system (2 dielectric constants, 3 piezoelectric constants, 5 elastic constants). The screw dislocation is assumed to be straight and infinitely long in the z-axis, suffering a displacement jump $b = b_z$ and an electric potential jump $\Delta\phi$ across the slip plane. The jump in the electric potential corresponds to the electric dipole layer along the slip plane (i.e., Soh et al., 2005). We first discuss the problem within the framework of antiplane shear deformation. When the surface of the infinite cylinder $x^2 + y^2 = R^2$ is traction-free and charge-free, the displacement $w = u_z$ and electric potential ϕ due to the piezoelectric screw dislocation $(b, \Delta\phi)$ at the point $x = \xi$ and $y = 0$ can be easily obtained by using the method of images such that

$$w = \frac{b}{2\pi}\tan^{-1}\frac{y}{x-\xi} - \frac{b}{2\pi}\tan^{-1}\frac{y}{x-R^2/\xi},$$
$$\phi = \frac{\Delta\phi}{2\pi}\tan^{-1}\frac{y}{x-\xi} - \frac{\Delta\phi}{2\pi}\tan^{-1}\frac{y}{x-R^2/\xi}. \quad (1)$$

The non-convex electric enthalpy per unit length of the cylinder can be calculated (Suo et al., 1992)

* Corresponding author at: Department of Civil Engineering, University of Akron, Akron, OH 44325, USA. Tel.: +1 330 972 6739; fax: +1 330 972 6020.
E-mail address: pan2@uakron.edu (E. Pan).

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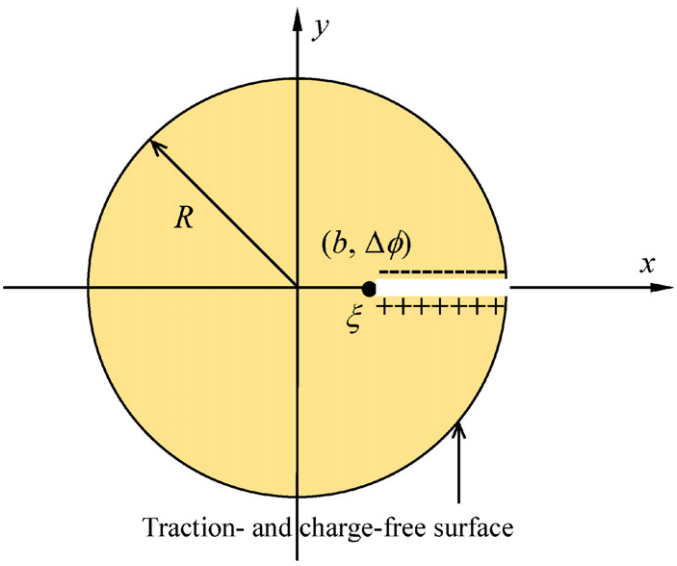

Fig. 1. A piezoelectric screw dislocation $(b, \Delta\phi)$ within a piezoelectric rod of radius R. The slip plane is along the x–z plane and it passes through the source point ξ. The electric potential jump $\Delta\phi$ across the slip plane physically corresponds to an electric dipole layer.

$$W = \frac{1}{2}\int\left[c_{44}\left(\frac{\partial w}{\partial x}\right)^2 + 2e_{15}\left(\frac{\partial w}{\partial x}\right)\left(\frac{\partial \phi}{\partial x}\right) - \epsilon_{11}\left(\frac{\partial \phi}{\partial x}\right)^2 + c_{44}\left(\frac{\partial w}{\partial y}\right)^2 + 2e_{15}\left(\frac{\partial w}{\partial y}\right)\left(\frac{\partial \phi}{\partial y}\right) - \epsilon_{11}\left(\frac{\partial \phi}{\partial y}\right)^2\right]\mathrm{d}x\,\mathrm{d}y = \frac{c_{44}b^2 + 2e_{15}b\Delta\phi - \epsilon_{11}\Delta\phi^2}{4\pi}\ln(R^2-\xi^2), \tag{2}$$

where c_{44}, e_{15} and ϵ_{11} are, respectively, the elastic modulus measured in a constant electric field, the piezoelectric constant, and the dielectric permittivity measured at a constant strain. With regard to Eq. (2), we remark that: (i) it contains the dielectric medium as a special case ($e_{15} = 0$) and (ii) the energy corresponding to the dislocation core has been neglected in writing the electric enthalpy.

As a result the image force on the piezoelectric screw dislocation is

$$F = -\frac{\mathrm{d}W}{\mathrm{d}\xi} = \frac{c_{44}b^2 + 2e_{15}b\Delta\phi - \epsilon_{11}\Delta\phi^2}{2\pi}\frac{\xi}{R^2-\xi^2}, \tag{3}$$

which indicates that $\xi = 0$ is an equilibrium position. However this equilibrium position is not necessarily unstable as in the purely elastic case (Eshelby, 1953) in view of the fact that the sign of the term $(c_{44}b^2 + 2e_{15}b\Delta\phi - \epsilon_{11}\Delta\phi^2)$ can be positive as well as negative. It is observed that the image force derived in this section is by means of the energy method, which is different than the direct one (Wang et al., 2010).

On any cross-section of the cylinder there is a torque M

$$M = c_{44}\int\left(x\frac{\partial w}{\partial y} - y\frac{\partial w}{\partial x}\right)\mathrm{d}x\,\mathrm{d}y + e_{15}\int\left(x\frac{\partial \phi}{\partial y} - y\frac{\partial \phi}{\partial x}\right)\mathrm{d}x\,\mathrm{d}y = \frac{c_{44}b + e_{15}\Delta\phi}{2}(R^2-\xi^2). \tag{4}$$

If we drop the anti-plane deformation requirement, we can apply a torque $-M$ to cancel out M. As a result, the twist of the rod per unit length can be calculated as

$$\alpha(\xi) = -\frac{2M}{c_{44}\pi R^4} = -\frac{c_{44}b + e_{15}\Delta\phi}{c_{44}\pi R^4}(R^2-\xi^2). \tag{5}$$

Table 1
The minimum and maximum of the image force and their corresponding locations.

λ	1	1.5	2	3	4	10
ξ/R	±0.3226	±0.3926	±0.4299	±0.4705	±0.4929	±0.5391
$\tilde{F}$	∓0.2180	∓0.5321	∓0.8744	∓1.5938	∓2.3341	∓6.8885

Note: $\tilde{F} = \frac{2\pi RF}{c_{44}b^2 + 2e_{15}b\Delta\phi - \epsilon_{11}\Delta\phi^2}$.

Remark. When a piezoelectric circular cylinder is under torsion, we have $E_\theta = 0$ (i.e., the circumferential component of the electric field is zero) (Tarn, 2002). Thus the classical formula for torsion can still be adopted by just replacing the shear modulus μ by the elastic modulus c_{44}.

It is observed from the above expression that $\alpha = 0$ if the condition $c_{44}b + e_{15}\Delta\phi = 0$ is satisfied. When taking into consideration the twist of the cylinder, the electric enthalpy W per unit length of the cylinder can now be modified as

$$W = \frac{c_{44}b^2 + 2e_{15}b\Delta\phi - \epsilon_{11}\Delta\phi^2}{4\pi}\ln(R^2-\xi^2) - \frac{(c_{44}b + e_{15}\Delta\phi)^2}{4\pi c_{44}}\frac{(R^2-\xi^2)^2}{R^4}. \tag{6}$$

Due to the fact that at $\xi = 0$, we have

$$\frac{\mathrm{d}W}{\mathrm{d}\xi} = 0, \qquad \frac{\mathrm{d}^2W}{\mathrm{d}\xi^2} = \frac{(c_{44}b + e_{15}\Delta\phi)^2 + \tilde{c}_{44}\epsilon_{11}\Delta\phi^2}{2\pi R^2 c_{44}} > 0, \tag{7}$$

with $\tilde{c}_{44} = c_{44} + e_{15}^2/\epsilon_{11} \geq c_{44}$ being the piezoelectrically stiffened elastic constant, then $\xi = 0$ is always a *stable* equilibrium position for the piezoelectric screw dislocation when taking into consideration the twist of the cylinder. In this case, the image force on the screw dislocation is

$$F = -\frac{\mathrm{d}W}{\mathrm{d}\xi} = \frac{(c_{44}b^2 + 2e_{15}b\Delta\phi - \epsilon_{11}\Delta\phi^2)\xi}{2\pi R^2}\left[\frac{R^2}{R^2-\xi^2} - 2\lambda\frac{R^2-\xi^2}{R^2}\right], \tag{8}$$

where

$$\lambda = \frac{(c_{44}b + e_{15}\Delta\phi)^2}{c_{44}(c_{44}b^2 + 2e_{15}b\Delta\phi - \epsilon_{11}\Delta\phi^2)}, \quad (\lambda \leq 0 \ \text{ or } \ \lambda \geq 1). \tag{9}$$

Remark. There is a typo in Eq. (4) in Eshelby (1953). The factor 4π in the denominator should read 2π.

It can be easily observed from Eq. (8) that:

(i) When $c_{44}b^2 + 2e_{15}b\Delta\phi - \epsilon_{11}\Delta\phi^2 \leq 0$ (in this case $\lambda \leq 0$), a dislocation at any position of the cylinder will always be *attracted* to the center;

(ii) On the other hand when $c_{44}b^2 + 2e_{15}b\Delta\phi - \epsilon_{11}\Delta\phi^2 > 0$ (in this case $\lambda \geq 1$), if the screw dislocation is displaced further than

$$\xi_{\max} = \left[1 - (2\lambda)^{-(1/2)}\right]^{1/2}R \tag{10}$$

from the center the screw dislocation will be pulled out of the cylinder by the image force. The existence of the component $\Delta\phi$ in the screw dislocation and/or the piezoelectric effect will make $\xi_{\max} > 0.54R$, the value obtained by Eshelby (1953) for an elastic screw dislocation with $\Delta\phi = 0$. In addition the minimum and maximum of the image force take place at the point determined by the following algebraic equation

$$6\lambda\left(\frac{\xi}{R}\right)^6 - 14\lambda\left(\frac{\xi}{R}\right)^4 + (10\lambda+1)\left(\frac{\xi}{R}\right)^2 + 1 - 2\lambda = 0. \tag{11}$$

Table 1 lists the calculated results for six different values of λ. It is observed from Table 1 that an increment in λ will cause the location to move toward the surface of the cylinder, accompanying with an increase in the magnitude of the maximum and minimum image force.

In the following we discuss the possibility of ejecting the dislocation by applying an external torque M' to the cylinder. According to Eshelby (1953), the external energy per unit length due to the external torque is $V = -\alpha(\xi)M' = -(c_{44}b + e_{15}\Delta\phi)M'\xi^2/c_{44}\pi R^4$ (here we have omitted the trivial constant). Thus the total energy Π, which is the sum of the electric enthalpy W and the external energy V, can be expressed as

$$\Pi = \frac{c_{44}b^2 + 2e_{15}b\Delta\phi - \epsilon_{11}\Delta\phi^2}{4\pi}\ln(R^2 - \xi^2) - \frac{(c_{44}b + e_{15}\Delta\phi)^2}{4\pi c_{44}}\frac{(R^2-\xi^2)^2}{R^4} - \frac{c_{44}b + e_{15}\Delta\phi}{c_{44}\pi R^4}M'\xi^2. \quad (12)$$

In order to obtain the critical value of M' at which the screw dislocation at the center of the cylinder can be possibly ejected, we must have $d^2\Pi/d\xi^2 = 0$ at $\xi = 0$. This is a necessary but not sufficient condition. We finally arrive at the critical value as follows

$$M'_c = \frac{R^2}{4}\left[c_{44}b + e_{15}\Delta\phi + \frac{\tilde{c}_{44}\epsilon_{11}\Delta\phi^2}{c_{44}b + e_{15}\Delta\phi}\right] = \frac{R^2}{2}(c_{44}b + e_{15}\Delta\phi)[1 - (2\lambda)^{-1}]. \quad (13)$$

When there is no piezoelectric effect, the above reduces to

$$M'_c = \frac{c_{44}b^2 + \epsilon_{11}\Delta\phi^2}{4b}R^2, \quad (14)$$

which can further reduce to the result of Eshelby (1953) if $\Delta\phi = 0$.

In the presence of the critical value of M' given by Eq. (13), the image force on the screw dislocation is

$$F = -\frac{d\Pi}{d\xi} = \frac{(c_{44}b^2 + 2e_{15}b\Delta\phi - \epsilon_{11}\Delta\phi^2)\xi^3}{2\pi R^2}\left(\frac{1}{R^2-\xi^2} + \frac{2\lambda}{R^2}\right) \quad (15)$$

It follows from Eq. (15) that:

(i) When $c_{44}b^2 + 2e_{15}b\Delta\phi - \epsilon_{11}\Delta\phi^2 < 0$ and $-1/2 \le \lambda \le 0$, there is no way to eject the screw dislocation at the center of the cylinder due to the fact that $\xi F < 0$ for $\xi \neq 0$.
(ii) When $c_{44}b^2 + 2e_{15}b\Delta\phi - \epsilon_{11}\Delta\phi^2 < 0$ and $\lambda < -1/2$, the screw dislocation may find two new non-central stable equilibrium positions at $\xi = \pm R\sqrt{1 + (2\lambda)^{-1}}$.
(iii) When $c_{44}b^2 + 2e_{15}b\Delta\phi - \epsilon_{11}\Delta\phi^2 \ge 0$, the screw dislocation will be ejected from the cylinder due to the fact that $\xi F > 0$ for $\xi \neq 0$.

Observations (i) and (ii) are quite different than that by Eshelby (1953). In fact when $c_{44}b^2 + 2e_{15}b\Delta\phi - \epsilon_{11}\Delta\phi^2 < 0$, we have $\xi F < 0$ as $\xi \to \pm R$ (in this case the traction-free and charge-free surface always repels the dislocation; Lee et al., 2000; Pak, 1990). Thus no matter what value of the external torque M' is applied, there are only two possibilities if $c_{44}b^2 + 2e_{15}b\Delta\phi - \epsilon_{11}\Delta\phi^2 < 0$: (i) there is always no way to eject the screw dislocation at the center of the cylinder if $\lambda = 0$ (i.e., $c_{44}b + e_{15}\Delta\phi = 0$); (ii) the screw dislocation may find two new non-central stable equilibrium positions in the presence of M' if $\lambda < 0$ ($c_{44}b + e_{15}\Delta\phi \neq 0$). Moreover the two new stable equilibrium positions can be explicitly given by

$$\xi = \pm R\left[1 + \frac{(2\lambda)^{-1}}{\tilde{M} + [\tilde{M}^2 + (2\lambda)^{-1}]^{1/2}}\right]^{1/2}, \quad (\lambda < 0) \quad (16)$$

where $\tilde{M} = M'/(R^2(c_{44}b + e_{15}\Delta\phi)) \ge (1 - (2\lambda)^{-1})/2$ (the equality establishes when $M' = M'_c$). It is clearly observed from Eq. (16) that when the dimensionless torque $\tilde{M}$ increases starting from its critical value of $(1 - (2\lambda)^{-1})/2$, (i) the two new stable equilibrium positions move outward from the origin $\xi = 0$ toward the surface $\xi = \pm R$ if $-1/2 \le \lambda < 0$; (ii) the two new stable equilibrium positions move outward from $\xi = \pm R\sqrt{1 + (2\lambda)^{-1}}$ toward the surface $\xi = \pm R$ if $\lambda < -1/2$. Two typical cases of $\lambda = -1/4 > -1/2$ and $\lambda = -1 < -1/2$ are illustrated, respectively, in Figs. 2 and 3 to verify the above analysis.

In short we observe that when $c_{44}b^2 + 2e_{15}b\Delta\phi - \epsilon_{11}\Delta\phi^2 < 0$, the screw dislocation cannot be ejected from the cylinder by apply-

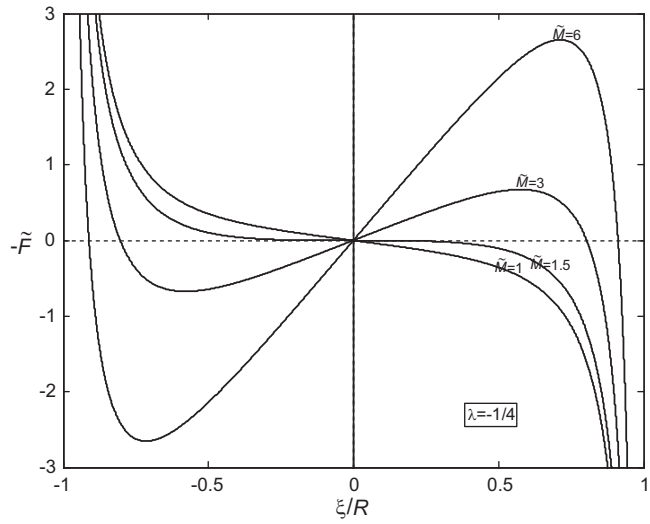

Fig. 2. The image force $\tilde{F} = 2\pi RF/(c_{44}b^2 + 2e_{15}b\Delta\phi - \epsilon_{11}\Delta\phi^2)$ on the screw dislocation with $\lambda = -1/4$ under different values of external torque $\tilde{M}$. The two new stable equilibrium positions move outward from the origin $\xi = 0$ to the surface $\xi = \pm R$ as $\tilde{M}$ increases from its critical value of $\tilde{M} = 1.5$.

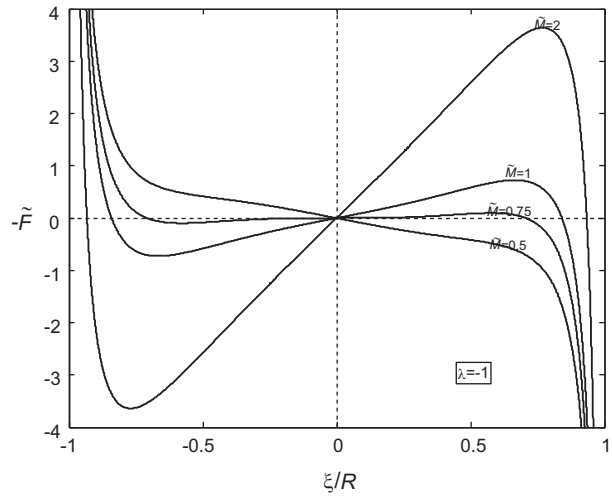

Fig. 3. The image force $\tilde{F} = 2\pi RF/(c_{44}b^2 + 2e_{15}b\Delta\phi - \epsilon_{11}\Delta\phi^2)$ on the screw dislocation with $\lambda = -1$ under different values of external torque $\tilde{M}$. The two new stable equilibrium positions move outward from $\xi = \pm 0.707R$ toward the surface $\xi = \pm R$ as $\tilde{M}$ increases from its critical value of $\tilde{M} = 0.75$.

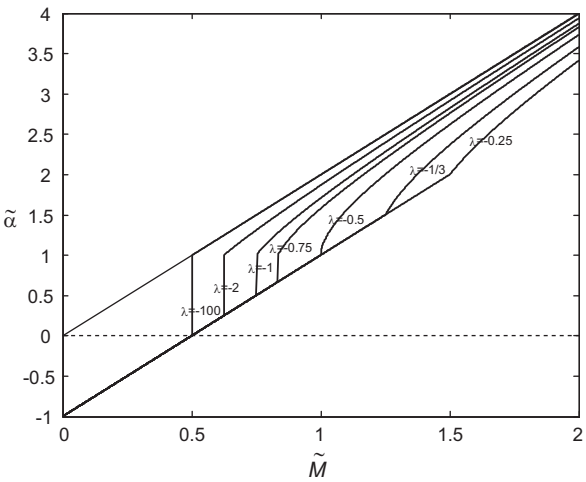

Fig. 4. The torsional stress–strain curve of a piezoelectric cylinder containing a screw dislocation for different values of $\lambda < 0$.

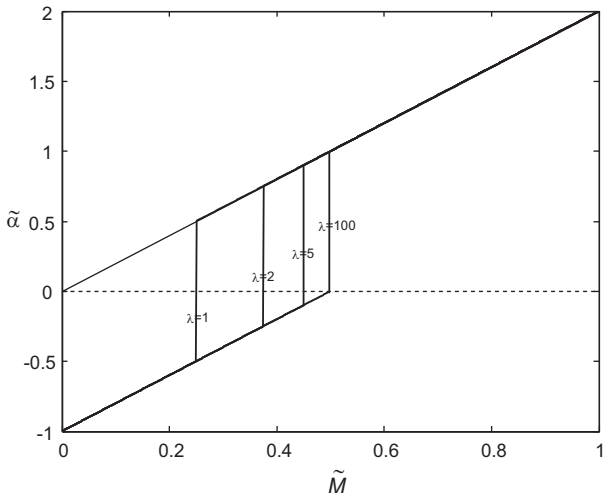

Fig. 5. The torsional stress–strain curve of a piezoelectric cylinder containing a screw dislocation for different values of $\lambda \geq 1$.

ing any external torque and it can at most be moved to some new equilibrium positions within the cylinder.

Next we discuss the induced twist α under the external torque M':

(i) When $c_{44}b + e_{15}\Delta\phi = 0$ ($\lambda = 0$), the screw dislocation will always be lodged at the center of the cylinder under any external torque M'. Thus the twist can be simply determined as

$$\alpha = \frac{2M'}{c_{44}\pi R^4}, \tag{17}$$

which indicates that the induced twist is proportional to the external torque.

(ii) When $c_{44}b^2 + 2e_{15}b\Delta\phi - \epsilon_{11}\Delta\phi^2 < 0$ and $c_{44}b + e_{15}\Delta\phi \neq 0$ ($\lambda < 0$), the screw dislocation may find new equilibrium positions under external torque M'. Thus the twist can be determined as

$$\tilde{\alpha} = \begin{cases} 2\tilde{M} - 1, & \text{if } \tilde{M} < \dfrac{1-(2\lambda)^{-1}}{2} \\ \tilde{M} + [\tilde{M}^2 + (2\lambda)^{-1}]^{1/2}, & \text{if } \tilde{M} \geq \dfrac{1-(2\lambda)^{-1}}{2} \end{cases} \tag{18}$$

where $\tilde{\alpha} = c_{44}\pi R^2\alpha/(c_{44}b + e_{15}\Delta\phi)$.

Eq. (18) demonstrates that when $\tilde{M} \geq (1-(2\lambda)^{-1})/2$, a nonlinear function exists between the twist and the external torque. Furthermore when $M' = M'_c$, $\tilde{\alpha}$ undergoes a jump from $-(2\lambda)^{-1}$ to 1 if $\lambda < -1/2$; whereas $\tilde{\alpha}$ is still *continuous* at $M' = M'_c$ if $-1/2 \leq \lambda < 0$. We illustrate in Fig. 4 the stress–strain curve in torsion for different values of $\lambda < 0$. In this figure the straight dashed line $\tilde{\alpha} = 2\tilde{M}$ is the asymptotic line as $\tilde{M} \to \infty$. It is clearly observed from Fig. 4 that the stress–strain curve is continuous when $-1/2 \leq \lambda < 0$; whereas it undergoes a jump when $\lambda < -1/2$.

(iii) When $c_{44}b^2 + 2e_{15}b\Delta\phi - \epsilon_{11}\Delta\phi^2 \geq 0$ ($\lambda \geq 1$), the screw dislocation will be ejected from the cylinder once $M' = M'_c$. Thus the induced twist can be determined as

$$\tilde{\alpha} = \begin{cases} 2\tilde{M} - 1, & \text{if } \tilde{M} < \dfrac{1-(2\lambda)^{-1}}{2} \\ 2\tilde{M}, & \text{if } \tilde{M} \geq \dfrac{1-(2\lambda)^{-1}}{2} \end{cases} \tag{19}$$

The above expression corresponds to Fig. 3 in Eshelby (1953). Furthermore when $M' = M'_c$, $\tilde{\alpha}$ undergoes a jump from $-(2\lambda)^{-1}$ to $1-(2\lambda)^{-1}$ due to the ejection of the screw dislocation. The stress–strain relation satisfying Eq. (19) can be more clearly observed in Fig. 5 for different values of $\lambda \geq 1$, where the curve for fixed λ is similar to Fig. 3 in Eshelby (1953). However, Eshelby's curve passed the origin, which we believe is a minor error in Fig. 3 (Eshelby, 1953).

3. Conclusions

We addressed a screw dislocation in a homogeneous piezoelectric cylinder. Our results demonstrated that: (i) when all the boundary conditions are taken into consideration, the center of the piezoelectric cylinder is a stable equilibrium position; (ii) when $c_{44}b^2 + 2e_{15}b\Delta\phi - \epsilon_{11}\Delta\phi^2 \geq 0$, the screw dislocation will be ejected from the cylinder by applying a critical value of the torque given by Eq. (13); (iii) when $c_{44}b + e_{15}\Delta\phi = 0$, there is no way to eject the screw dislocation at the center of the cylinder by applying any value of torque to the cylinder; (iv) when $c_{44}b^2 + 2e_{15}b\Delta\phi - \epsilon_{11}\Delta\phi^2 < 0$ and $c_{44}b + e_{15}\Delta\phi \neq 0$, the screw dislocation may find two new non-central stable equilibrium positions [given by Eq. (16)] by applying a certain value of torque to the cylinder; (v) the stress–strain curve of a piezoelectric rod in torsion [see Eqs. (17)–(19)] will no longer simply be Fig. 3 in Eshelby (1953), and when $c_{44}b^2 + 2e_{15}b\Delta\phi - \epsilon_{11}\Delta\phi^2 < 0$ and $c_{44}b + e_{15}\Delta\phi \neq 0$, a nonlinear region in the curve exists due to the lodged screw dislocation [see Eq. (18)]. It is believed that our striking theoretical predictions will be useful to piezoelectric nanowire growth where the interesting Eshelby twist exists.

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