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Analysis of displacement and strain fields of a screw dislocation in a nanowire using gradient elasticity theory

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Displacement and strain fields of a screw dislocation in a nanowire are considered within the theory of gradient elasticity. The gradient solution of the corresponding boundary value problem is derived and discussed in detail. It is shown that the dislocation fields do not contain classical jumps and singularities at the dislocation line. The maximum values of the dislocation displacement and elastic strain strongly depend on both the dislocation position and nanowire radius, thus demonstrating a nonclassical size effect.

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Deformation phenomena and behavior of defects in quasi-one-dimensional nanostructures (nanowires, nanotubes, nanorods, etc.) have attracted much attention in recent years. In particular, much effort has been spent studying the basic mechanisms of plastic deformation in single- and polycrystalline nanowires and nanorods [1–4], and stress relaxation in bicrystalline [5], core-shell [6–14] and axially [15] heterogeneous nanowires, as well as in pentagonal nanorods [16–21]. The theoretical description of defects (dislocations and disclinations) in such nanostructures is normally based on appropriate solutions of boundary-value problems within the framework of classical elasticity. This approach gives reliable results unless one considers the defect core region or the defect behavior near free surfaces and interphase boundaries. It is well known that in the latter situations, the classical theory of elasticity gives unphysical singularities in the defect elastic fields or in the image forces acting on the defects, respectively. The use of strain-gradient elasticity theory is a simple way to dispense with these problems.

Strain-gradient elasticity is one of theories of the so-called generalized elastic continuum with weak nonlocality (see Refs. [22–25] for reviews and details). The simplest version of this theory is governed by the constitutive law [26]:

$$\boldsymbol{\sigma} = (1 - \ell^2\nabla^2)[\lambda(\mathrm{tr}\boldsymbol{\varepsilon})\boldsymbol{I} + 2\mu\boldsymbol{\varepsilon}], \tag{1}$$

where $(\boldsymbol{\sigma}, \boldsymbol{\varepsilon})$ denote the stress and elastic strain, (λ, μ) are the Lamé constants, $\boldsymbol{I}$ the unit tensor, ∇^2 the Laplacian, and $\ell \geqslant 0$ is the gradient coefficient, a new extra material constant. For an atomic lattice, an estimate of $\ell \approx 0.25h$ can be used, where h is the lattice constant [26]. Recently, ℓ has been determined from atomic simulation [27] and experimental observations [28] of dislocation cores in GaN. The constitutive law (1) has already been applied to the problems of cracks [26,29] (see also Refs. [22,23] for more references), screw [30] and edge [31] dislocations, and wedge and twist disclinations [32] in an infinite solid. Substitution of Eq. (1) into the equilibrium equation, $\nabla \cdot \boldsymbol{\sigma} = 0$, leads to a forth-order partial differential equation for the displacement

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vector $\boldsymbol{u}$. It is readily shown that $\boldsymbol{u}$ is the solution of the inhomogeneous Helmholtz equation [29]:

$$(1-\ell^2\nabla^2)\boldsymbol{u}=\boldsymbol{u}^0, \tag{2}$$

where $\boldsymbol{u}^0$ denotes the displacement field calculated in the theory of classical elasticity. Recently Eq. (2) has also been derived from a variation principle [24]. Based on the earlier work of Mindlin [33], the following extra boundary condition was introduced [26,29] to apply Eq. (2) to a traction boundary value problem in the gradient elasticity described by Eq. (1):

$$\frac{\partial^2\boldsymbol{u}}{\partial n^2}=0, \tag{3}$$

where the vector $\boldsymbol{n}$ is a unit outward normal to the boundary. With Eq. (3) and $\ell^2>0$, the uniqueness of the solution would be guaranteed [34]. The governing differential Eq. (2) and the extra boundary condition (3) have been applied to some problems of fracture mechanics [26,29,35,36], composite materials [37], line forces and the Flamant problem [38]. The aim of the present work is to consider the elastic properties of a screw dislocation in a nanowire in terms of the strain gradient elasticity described by Eqs. (1)–(3).

Let a screw dislocation lie at the point $(c,0)$ in an infinite elastically isotropic cylinder of the radius a which is considered as the continuum model of a very long nanowire with fixed ends (Fig. 1). In classical elasticity, this problem was first considered by Eshelby [39], who introduced an image screw dislocation at the inverse point $(a^2/c,0)$ to satisfy the classical traction boundary condition on the free surface. Recently, the approach of image dislocations has been extended to the cases of screw dislocations in the walls of hollow centric [40,41] and eccentric [42] cylinders.

The classical nonvanishing displacement component is $u_z^0=(b/2\pi)w^0$, where b is the Burgers vector magnitude and

$$w^0=\theta_1-\theta_2=\theta(x_1,y)-\theta(x_2,y). \tag{4}$$

Here $x_1=x-c$, $x_2=x-a^2/c$ and the angle θ is a single-valued function associated with the material point (x,y), which is given by [43]:

$$\theta=\theta(x,y)=\tan^{-1}\left(\frac{y}{x}\right)+\frac{\pi}{2}\mathrm{sgn}(y)[1-\mathrm{sgn}(x)]. \tag{5}$$

The total strain $\boldsymbol{\varepsilon}^{\mathrm{T}}$ is the symmetric part of the displacement gradient $(\nabla\boldsymbol{u})$ and may be represented by the sum of the elastic $(\boldsymbol{\varepsilon})$ and plastic $(\boldsymbol{\varepsilon}^*)$ strains [43]. Their classical components (in units of $b/4\pi$) are:

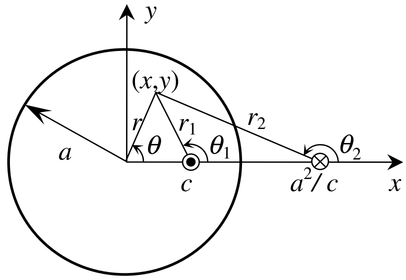

Figure 1. A screw dislocation parallel to the nanowire axis.

$$\begin{aligned}&\varepsilon_{zx}^0=-\frac{y}{r_1^2}+\frac{y}{r_2^2},\quad \varepsilon_{zy}^0=\frac{x_1}{r_1^2}-\frac{x_2}{r_2^2},\\&\varepsilon_{zx}^*=0,\quad \varepsilon_{zy}^*=-2\pi\delta(y)H(x_1),\end{aligned} \tag{6}$$

where $H(x_1)$ is the Heaviside step function and $\delta(y)$ is Dirac's delta function. The classical stress is $\boldsymbol{\sigma}^0=2\mu\,\boldsymbol{\varepsilon}^0$. It is an interesting feature of the gradient theory given by Eqs. (1)–(3) that the gradient solution for the stress field, in contrast to the displacement and strain fields, coincides with the classical solution [26,29–32]. Therefore, we do not consider the stress field here. We also omit the cumbersome calculation procedure and report the final results only.

Within the gradient theory, it is convenient to decompose the gradient solution for the displacement field $w=[2\pi/b]u_z$ into a particular solution, w_{p}, and the complementary solution, w_{c}, i.e. $w=w_{\mathrm{p}}+w_{\mathrm{c}}$. The first term results in:

$$w_{\mathrm{p}}=w^0-\ell^2\int_0^\infty s\sin sy[\Psi(s,x_1)-\Psi(s,x_2)]\mathrm{d}s \tag{7}$$

with $\Psi(s,x_i)=\left[\mathrm{sgn}(x_i)\exp\left(-|x_i|\sqrt{\frac{1}{\ell^2}+s^2}\right)+2H(-x_i)\right]\Big/(1+s^2\ell^2)$, $i=1,2$. The second term reads:

$$w_{\mathrm{c}}=\sum_{n=1}^{\infty}p_nI_n(r/\ell)\sin n\theta, \tag{8}$$

where $I_n(r/\ell)$ is the modified Bessel function of the first kind of the order n. The unknown coefficients p_n, $n=1,2,\ldots$ are obtained by imposing the extra boundary condition $(\partial^2 w/\partial r^2)|_{r=a}=0$:

$$p_n=\frac{-1}{\pi I_{n,rr}(a/\ell)}\int_{-\pi}^{\pi}\left[\frac{\partial^2 w_{\mathrm{p}}}{\partial r^2}\right]_{r=a}\sin n\theta\,\mathrm{d}\theta \tag{9}$$

where $I_{n,rr}(a/\ell)\equiv\left[\partial_{rr}^2 I_n(r/\ell)\right]_{r=a}$.

In comparing the classical (w^0) and gradient (w) solutions for the displacement field, some important differences can be found. First, when $x\to c>0$, the classical displacement given by Eqs. (4) and (5) has an abrupt jump at the dislocation line $y=0$, while the gradient solution, Eqs. (7)–(9), is smooth there (Fig. 2). The classical and gradient solutions practically coincide far from the dislocation line, when $|y|>5\ell$. Similar results have been obtained in the case of an infinite medium [22,30,44]. Second, the maximum magnitude of $w^0(c,y)$ is always $\pi/2$ regardless of the dislocation position

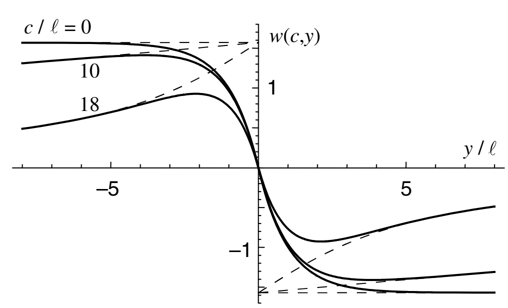

Figure 2. The normalized displacement $w(c,y)$ near the screw dislocation placed in different positions $c/\ell=0$, 10 and 18 in an infinite cylinder of radius $a/\ell=20$. Solid and dashed lines correspond to the gradient and classical solutions, respectively.

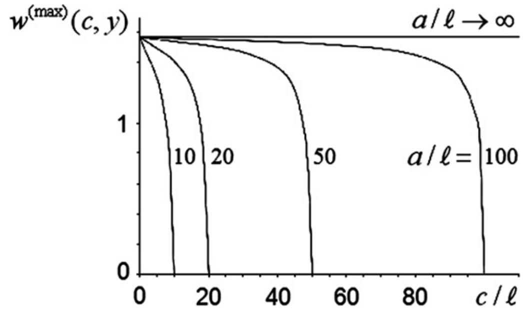

Figure 3. Dependence of the maximum magnitude $w^{\max}(c, y)$ of the normalized displacement near the screw dislocation on its position c/ℓ for different values of the cylinder radius $a/\ell = 10$, 20, 50, 100 and ∞.

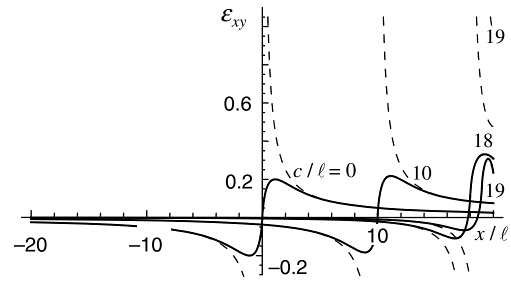

Figure 4. The elastic strain $\varepsilon_{zy}(x, y = 0)$ distribution in an infinite cylinder of radius $a/\ell = 20$ due to a screw dislocation placed at different positions $c/\ell = 0$, 10, 18 and 19. Solid and dashed lines correspond to the gradient and classical solutions, respectively. The strain values are given in units of $b/(2\pi\ell)$.

(Fig. 2). In contrast, the maximum magnitude of $w(c, y)$ is approximately $\pi/2$ only when the dislocation lies in the cylinder center, but attains a smaller value as the dislocation is placed closer to the cylinder free surface (Figs. 2 and 3). For a fixed dislocation position c/ℓ, the bigger radius a of the cylinder produces the bigger value of $w^{(\max)}(c, y)$ (Fig. 3). These observations may be treated as a specific size effect appearing within the gradient elasticity.

With Eqs. (7)–(9), it follows from $\varepsilon^{\mathrm{T}}_{zk} = (1/2)\partial_k u_z$ $(k = x, y)$ that the elastic strains (in units of $b/4\pi$) are

$$\varepsilon_{zx} = \varepsilon^0_{zx} + \frac{y}{\ell r_1} K_1\left(\frac{r_1}{\ell}\right) - \frac{y}{\ell r_2} K_1\left(\frac{r_2}{\ell}\right) + \frac{1}{2r}\sum_{n=1}^{\infty}\left\{p_n r I_{n,r}\left(\frac{r}{\ell}\right)\cos\theta\sin n\theta - n p_n I_n\left(\frac{r}{\ell}\right)\sin\theta\cos n\theta\right\}, \quad (10)$$

$$\varepsilon_{zy} = \varepsilon^0_{zy} - \frac{x_1}{\ell r_1} K_1\left(\frac{r_1}{\ell}\right) + \frac{x_2}{\ell r_2} K_1\left(\frac{r_2}{\ell}\right) + \frac{1}{2r}\sum_{n=1}^{\infty}\left\{p_n r I_{n,r}\left(\frac{r}{\ell}\right)\sin\theta\sin n\theta + n p_n I_n\left(\frac{r}{\ell}\right)\cos\theta\cos n\theta\right\}, \quad (11)$$

where ε^0_{zk} is given by Eq. (6) and K_n denotes the modified Bessel function of the second kind of the order n. The plastic strains are

$$\varepsilon^*_{zx} = 0, \quad \varepsilon^*_{zy} = \int_0^{\infty} \cos sy[\Psi(s, x_1) - \Psi(s, x_2)]\mathrm{d}s \quad (12)$$

in the same units.

Let us briefly discuss the main features of the gradient solution for the strain field. First, in the limit $\ell \to 0$, it is transformed into the classical solution given by Eq. (6). Second, when $a \to \infty$, the gradient solution tends to that for a screw dislocation in an infinite isotropic solid [22,30,44]. Third, while the classical elastic strains possess unphysical singularities $\sim 1/r_1$ as $r_1 \to 0$, the appearance of the modified Bessel function in the gradient elastic strains eliminates these singularities, since $K_1(r_1/\ell) \sim \ell/r_1$ when $r_1 \to 0$. On the other hand, when $r \to 0$, $I_n(r/\ell) \sim (r/\ell)^n$ and this cancels out the singular term $1/r$ behind the summation sign in Eqs. (10) and (11). Thus, the gradient solution is not singular anywhere, as can also be seen from Figure 4. Far from the dislocation line, when $|x - c| > 5\ell$, the classical and gradient solutions practically coincide. All these results are similar to those obtained earlier for a screw dislocation in an infinite medium [22,30]. Fourth, the maximum value of the ε_{zy} component, $\varepsilon^{(\max)}_{zy}$, is $\approx 0.2b/(2\pi\ell) \approx 0.127$ (at $b \approx h \approx 4\ell$ [26]) when the dislocation is located at the cylinder center as is also the case for an infinite solid. However, $\varepsilon^{(\max)}_{zy}$ first increases when the dislocation is shifted to the free surface (Fig. 4). Closer than $\approx 1.5\ell$ to the free surface, $\varepsilon^{(\max)}_{zy}$ begins to decrease and reduces to zero when the dislocation reaches the surface (Fig. 5). Thus, within the gradient elasticity, one can estimate the maximum possible shear strain in an infinite nanowire due to the screw dislocation. For example, it follows from Figure 5 that in the nanowire of radius $a = 100\ell \approx 25h \approx$ 7–8 nm, the maximum strain reaches its peak at $c \approx a - 1.5\ell$, which is estimated as $\varepsilon^{(\max)}_{zy} \approx 0.35b/(2\pi\ell) \approx 0.222$. The peak value of $\varepsilon^{(\max)}_{zy}$ decreases with the nanowire radius a (see the dashed curve in Fig. 5), thus demonstrating one more nonclassical size effect, this time for the elastic strain. Obviously, this size effect becomes stronger with decreasing a and disappears when $a/\ell \to \infty$.

In summary, strain-gradient elasticity gives smooth and nonsingular solutions for the displacement and strain fields of a screw dislocation in a nanowire. Moreover, it allows us to observe a nonclassical size effect, namely the strong dependence of the maximum displacement and strain on both the dislocation position and

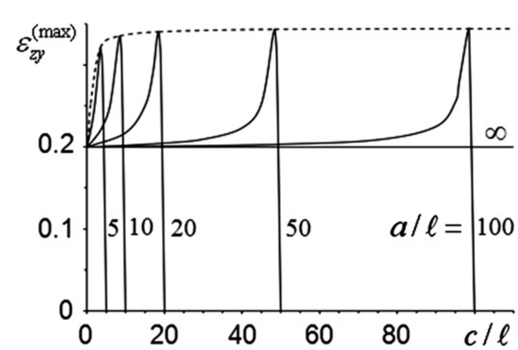

Figure 5. Dependence of the maximum elastic strain $\varepsilon^{(\max)}_{zy}$ on the dislocation position for different values of the cylinder radius $a/\ell = 5$, 10, 20, 50, 100 and ∞. The dashed curve shows the effect of the cylinder radius on the peak value of $\varepsilon^{(\max)}_{zy}$.

nanowire radius. In particular, it is shown that the maximum strain reaches its peak value when the dislocation is located near the free surface, and this peak value grows with the nanowire radius until the latter becomes rather big. The maximum possible elastic shear strain caused by a screw dislocation in a nanowire is in direct proportion with the ratio b/ℓ. For a perfect lattice dislocation ($b/\ell \approx 4$) in a nanowire with radius $a \approx 10$ nm, this maximum strain ranges from ≈12.7% (when the dislocation is in the center of the nanowire) to ≈22.2% (when it is near the free surface). Strictly speaking, these results are rather approximate since our elastically isotropic model is still a first step in describing dislocation fields in a real nanowire.

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