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Analysis of stress field of a screw dislocation inside an embedded nanowire using strain gradient elasticity

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The stress field of a screw dislocation inside an embedded nanowire is considered within the theory of strain-gradient elasticity. It is shown that the stress singularity is removed and all stress components are continuous and smooth across the interface, in contrast with the results obtained within the classical theory of elasticity. The maximum magnitude of dislocation stress depends greatly on the dislocation position, the nanowire size, and the ratios of shear moduli and gradient coefficients of the matrix and nanowire materials.

Keywords: Strain gradient elasticity; Screw dislocation; Nanowire

Fabrication, characterization and application of embedded nanowires are among the hottest topics in materials science and applied physics. Nanowire-based structures and devices are developed for wide use in various fields of nanoscience (e.g. biology, electronics, medicine, optics, optoelectronics, photonics and sensors). It is well known that the structure and properties of embedded nanowires depend greatly on their environment. In particular, much attention has been paid to the elastic strains and stresses that arise in or near the embedded nanowires due to the presence of defects [1] and differences in the material properties of the nanowires and surrounding matrix [1,2]. The theoretical consideration of these questions is commonly based on the classical theory of elasticity; however, this cannot be applied to extremely (atomically) thin nanowires, interface areas and defect cores. There are two ways to overcome these limitations. The first is to discard the continuum description and use atomic simulations [3,4]. The second is to still exploit the continuum approach but within an extended theory of elasticity that could cope with classical difficulties (singularities, jump discontinuities, etc.). The theory of strain-gradient elasticity seems to be the most simple and effective extension of classical elasticity in this sense.

The governing equation of the simple isotropic theory of gradient elasticity proposed by Ru and Aifantis [5] reads

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

where $\boldsymbol{\sigma}$ and $\boldsymbol{\varepsilon}$ are the elastic stress and strain tensors, respectively, λ and μ are the Lamé constants, $\mathbf{I}$ is the unit tensor, ∇^2 is the Laplacian and $\ell, c \geqslant 0$ are two gradient coefficients (different in a general case) which represent intrinsic length scales within the gradient theory. It was strictly proved [5,6] that the solution of Eq. (1) boils down to the independent solution of the following inhomogeneous Helmholtz equations for the stress $\boldsymbol{\sigma}$ and displacement $\mathbf{u}$ fields:

$$(1-\ell^2\nabla^2)\boldsymbol{\sigma} = \boldsymbol{\sigma}^0 \quad (2)$$

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$$(1 - c^2\nabla^2)\mathbf{u} = \mathbf{u}^0 \tag{3}$$

where $\boldsymbol{\sigma}^0$ and $\mathbf{u}^0$ denote the corresponding fields calculated in the theory of classical elasticity. For a crystalline solid with the lattice parameter a, numerical estimates have been made for ℓ and c based on theoretical models [7–12] and experimental observations [13]. For example, Eringen [7,8] obtained Eq. (2) in his version of the theory of nonlocal elasticity and found that $\ell \approx 0.39a$. Altan and Aifantis [9] derived Eq. (3) and came up with $c \approx 0.25a$.

Eqs. (2) and/or (3) have been applied to the problems of dislocations [7,8,14–23], disclinations [20,24,25], cracks [5,6,9,26,27], composite materials [28], inclusions [29], line forces and the Flamant problem [30]. Some of these works were extensively reviewed in Refs. [31,32]. The main general result is the elimination of classical singularities from the solutions for elastic fields and energies. For dislocations placed near interphase boundaries, the image forces have also been regularized [17–19,23]. Moreover, it has been shown that in the problems for inclusions [29], dislocations inside free-surface nanowires [22] and outside embedded nanowires [23], the maximum values of elastic fields become size-dependent, in contrast with the corresponding classical solutions, which are size-independent. The aim of the present paper is to consider the elastic stress of a screw dislocation placed inside an embedded nanowire in the framework of the strain gradient elasticity described by Eqs. (1)–(3).

Let a screw dislocation lie at the point $(\xi, 0)$ inside an infinite cylinder (nanowire) Ω embedded in an infinite elastic medium (matrix) D (Fig. 1). In classical elasticity, this problem was solved in displacements by Dundurs [33]. The nonvanishing stress components yield (in units of $b/2\pi$) the following:

$$\sigma_{zx}^{0(D)} = -\mu_D(1+S)\frac{y}{r_1^2} + \mu_D S\frac{y}{r^2},$$

$$\sigma_{zy}^{0(D)} = \mu_D(1+S)\frac{x_1}{r_1^2} - \mu_D S\frac{x}{r^2},$$

$$\sigma_{zx}^{0(\Omega)} = -\mu_\Omega\frac{y}{r_1^2} + \mu_\Omega S\frac{y}{r_2^2}, \quad \sigma_{zy}^{0(\Omega)} = \mu_\Omega\frac{x_1}{r_1^2} - \mu_\Omega S\frac{x_2}{r_2^2}, \tag{4}$$

where b is the Burgers vector, μ_D and μ_Ω are the shear moduli of the matrix and the nanowire, respectively, $S = (\mu_\Omega - \mu_D)/(\mu_\Omega + \mu_D)$, $x_1 = x - \xi$, $x_2 = x - R^2/\xi$, R is the nanowire radius, $r^2 = x^2 + y^2$ and $r_{1,2}^2 = x_{1,2}^2 + y^2$. This solution clearly demonstrates limitations of the classical theory. First, near the dislocation line, when $r_1 \to 0$, the stress components $\sigma_{zx}^{0(\Omega)}$ and $\sigma_{zy}^{0(\Omega)}$ are singular. Secondly, the stress component $\sigma_{zr}^0 = \sigma_{zx}^0\cos\theta + \sigma_{zy}^0\sin\theta$ is continuous across the interface, $\sigma_{zr}^{0(D)}|_{r=R} = \sigma_{zr}^{0(\Omega)}|_{r=R} = -(\mu_D b/2\pi)(1+S)\ \ \xi\sin\theta/(R^2 - 2R\xi\cos\theta + \xi^2)$, and also becomes singular there when the dislocation reaches the interface ($\xi \to R,\ \theta = 0$). Thirdly, the stress component $\sigma_{z\theta}^0 = -\sigma_{zx}^0\sin\theta + \sigma_{zy}^0\cos\theta$ suffers an abrupt jump at the interface, $[\sigma_{z\theta}^0]_-^+ = \sigma_{z\theta}^{0(D)}|_{r=R} - \sigma_{z\theta}^{0(\Omega)}|_{r=R} = -(S/R)[\mu_D + \mu_\Omega(R^2 - \xi^2)/(R^2 - 2R\xi\cos\theta + \xi^2)]$, which depends on the dislocation position. When the dislocation approaches the interface ($\theta = 0, \xi \to R$), the stress jump, $[\sigma_{z\theta}^0]_-^+ \to -2\mu_\Omega S/(R - \xi)$, drastically increases and becomes singular. All these features make it impossible to use the classical solution (4) in the case of dislocations in atomically thin nanowires. As was discussed previously in detail [17,18], the stress jump at the interface, $[\sigma_{z\theta}^0]_-^+$, is justified in the classical theory of elasticity aimed at describing macroscopic elastic solids because it does not contribute to the traction vector that should be in balance at the interface. However, from the nanoscopic point of view, this assumption does not seem to be valid. Indeed, the stress jump is doubtful in view of the fact that atoms forming the interface interact with other atoms belonging to both the materials in contact. Hence, the assumption of a transitional region near the interface, where the interaction between atoms varies gradually from stronger in more rigid material to weaker in other materials, is unavoidable. It can be concluded from this assumption that the stress jump is only a consequence of the approximation of classical continuum models, which often become insufficient for describing nanoscale phenomena.

Let us consider the same problem within the gradient theory described by Eqs. (1)–(3). The full solution procedure and results for all elastic fields and image forces will be given elsewhere [34]. Here we concentrate on the main peculiarities of the gradient solution for stress field. Thus, the stress equation (2) must be solved for both regions D and Ω. Due to the existence of higher-order derivatives, some additional boundary conditions are needed. Following Refs. [17–19,23], we have used the following conditions of balance for stresses and stress gradients at the interface:

$$[\sigma_{zr}]_-^+ = 0, \quad [\sigma_{z\theta}]_-^+ = 0, \quad \left[\frac{\partial\sigma_{zr}}{\partial r}\right]_-^+ = 0, \quad \left[\frac{\partial\sigma_{z\theta}}{\partial r}\right]_-^+ = 0. \tag{5}$$

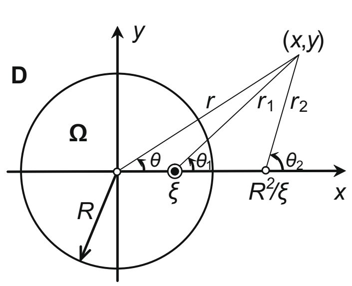

Figure 1. A screw dislocation inside an embedded nanowire.

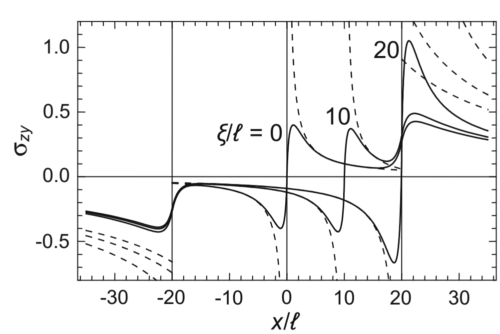

Figure 2. The stress component $\sigma_{zy}(x, 0)$ of a screw dislocation placed at the position $\xi/\ell_\Omega = 0$, 10, and 20 in the case of $R = 20\ell_\Omega$, $\mu_D/\mu_\Omega = 10$, and $\ell_\Omega = \ell_D$. Solid and dashed curves correspond to the gradient and classical solutions, respectively. The stress values are given in units of $\mu_\Omega b/(2\pi\ell_\Omega)$.