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Analytical formulations of image forces on dislocations with surface stress in nanowires and nanorods

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ABSTRACT

The interaction between dislocations and surfaces is usually characterized by image forces. Most analytical solutions to image forces could be found in literatures for two-dimensional (2D) solids with or without the consideration of surface stress. This work provides alternative analytical formulations of image forces for nanowires which are in more flexible forms compared with the infinite power series solutions from complex variable method. Moreover, this work proposes analytical formulations of image forces for nanorods (3D) by approximating the 3D shape effect as a height-dependent shape function, which is obtained through curve fitting of the finite element results of image forces without surface stress. The results of nanowires are demonstrated to be acceptable compared with the classical solution and complex variable method. More importantly, the analytical formulation of nanorods has not been found in other literatures so far. This work could contribute to nanostructure design and provide guidance for the fabrication of high quality nanostructures.

1. Introduction

Dislocations in solids play an important role in determining the mechanical and electronic properties of materials (Du and Srolovitz, 2004; Liu et al., 2004; Luryi and Suhir, 1986; People and Bean, 1985; Schwarz, 1999; Srinivasan et al., 2003; Zhong and Zhu, 2008), due to the fact that the atoms of the dislocations have different bonding and environment from the other atoms buried in the bulk. More importantly, when the dislocation is embedded in nanostructures with dimensions on the order of tens of nanometers, the behavior of the dislocation becomes highly sensitive to the surrounding environment because the atoms near the dislocation will interact more actively in such extremely small domain. Generally, external loads, grain boundaries, inclusions and surfaces/interfaces, etc. will affect the behavior of the dislocation. This influence might be crucial in determining the way that the dislocation behaves in nanostructures, thus it should be taken into consideration in comprehensive studies.

Classical studies (Hirth and Lothe, 1982; Hull and Bacon, 2011) showed that a fictitious image dislocation needs to be imposed to enforce the stress-free surface boundary condition when a dislocation is embedded in a semi-infinite solid. The image dislocation has the same magnitude but opposite direction of the Burgers vector of the original dislocation. Based on the concept of the image dislocation, Dundurs and coworkers (Dundurs and Mura, 1964; Dundurs and Sendeckyj, 1965) studied the elastic fields and image forces with the consideration of the interaction between an edge dislocation and a circular inclusion. Lubarda (2011) obtained the stress fields for screw and edge dislocations emitted from a cylindrical void and provided analytical formulations for image forces on dislocations. A different scheme to analyze the displacement and strain fields of a screw dislocation in a nanowire is by using gradient elasticity theory (Aifantis, 2003, 2009, 2011; Davoudi et al., 2009, 2010; Shodja et al., 2008). They provide more complete solutions for non-singular stresses and strains in dislocations compared with the classical nonlocal approach (Eringen, 1977, 1984, 2001). It was employed to derive the solution to the image force in an integral form on a screw dislocation near a flat interface (Gutkin et al., 2000). The study of dislocations in gradient elasticity theory was revisited and extended by Lazar and coworkers (Lazar and Maugin, 2006; Lazar et al., 2006) to the second gradient elasticity theory to analyze the stress and strain field of the edge or screw dislocation. Another distinct approach to investigate image forces acted on dislocations is through the complex variable method or complex potential method (Muskhelishvili, 1977). This approach is based on the analogy (Smith, 1968) between the anti-plane strain deformation and the 2D perfect fluid motion, so it is mainly used in 2D situations. Smith (1968) pioneered to study the interaction between screw dislocations and circular cylindrical inhomogeneities. By using conformal transformation techniques, elliptical inclusions were considered by Stagni and Lizzio (1983)

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for the dislocation in the matrix and Warren (1983) for the dislocation in the inclusion. Moreover, anisotropy was also taken into consideration through Stroh's formalism (Stroh, 1958) and image forces on dislocations in anisotropic elastic half-spaces with a fixed boundary was obtained by Ting and Barnett (1993). However, in these mentioned formulations and many more, there is no intrinsic length scale associated in these constitutive relationships. Therefore, these results should be considered only in macroscopic cases.

In the past few decades, nanotechnology has been developed rapidly and it discloses that the behaviors of nano-materials differ from the conventional materials dramatically. Nanostructures have at least one of its dimensions below tens of nanometers. Due to the large surface to volume ratio, the surface stress begins to play an important role in changing the constitutive laws seen in the classical elastic theory. In this case, nanostructures usually demonstrate some size-dependent properties that could not be seen in conventional materials. This significant difference could be critical in fabrications and designs, so great efforts have been devoted to investigating the effect of surface stress. Relationship of the deformation-dependent surface energy with the surface stress was first described by the Shuttleworth's equation (Shuttleworth, 1950). Gurtin and coworkers (Gurtin and Ian Murdoch, 1975; Gurtin et al., 1998) linked the surface stress to the bulk stress at the vicinity of the surface by regarding the surface as a negligibly thin object adhering to the underlying material without slipping. Aifantis et al. (2007) adopted the strain gradient approach for nucleation of misfit dislocations and plastic deformations in core/shell nanowires. They also considered the interface contribution to the gradient dependent potential energy of polycrystals in terms of interfacial strain (Aifantis and Askes, 2007). Fang and Liu (2006a,b) combined the surface stress model with complex variable method to solve the image force for a screw or edge dislocation located in materials of a circular nanowire embedded in an infinite matrix. Luo and Xiao (2009) extended this analysis to the case of an elliptical nanowire embedded in an infinite matrix with conformal mappings. Recently, Ahmadzadeh-Bakhshayesh et al. (2012) adopted the same method to analyze the surface/interface effect on the image force of a screw dislocation in an eccentric core–shell nanowire. However, these results based on the complex variable method provide the results of image forces as infinite power series, which are difficult to manipulate in further situations. The influences of the size parameter and surface elasticity are also hard to interpret clearly. Beside this limitation, their solutions by using the complex variable method are limited to 2D elastic plane stress or strain problems and mainly used for isotropic materials.

2. General formulation of image force

The calculation of the image force mainly falls into two categories: the nonlocal approach and the energy approach. The "nonlocal" concept was introduced by Kröner (1967) and followed by Eringen (1977, 1984, 2001) to tackle the mathematical singularity due to the discrete field of dislocations. In the nonlocal approach, one can calculate the image force along the dislocation line using the Peach–Koehler equation (Hirth and Lothe, 1982):

$$\vec{f} = (\sigma^{NL} \bullet \vec{b}) \times \vec{\xi}, \tag{1}$$

where $\vec{f}$ is the image force density vector along the dislocation line, σ^{NL} is the nonlocal stress exerted on the dislocation, and $\vec{\xi}$ is the unit vector along the direction of the dislocation line.

The nonlocal stress requires a volumetric integration of the stress tensor over the whole crystal space (Kröner, 1967):

$$\sigma^{NL}(\vec{x}) = \int_V \kappa(\vec{x} - \vec{x}')\sigma(\vec{x}')dV', \tag{2}$$

where $\kappa(\vec{x} - \vec{x}')$ is a correlation kernel that links the local point ($\vec{x}$) on the dislocation line to the nonlocal point ($\vec{x}'$) in the rest crystal space.

The nonlocal stress σ^{NL} should be the sum of the contribution from all other portions of the crystal to the dislocation, which accounts for the long range effects from the free surfaces. Usually a volumetric integration over the whole crystal space should be calculated for σ^{NL}.

Recently, Colby et al. (2010) investigated the dislocation filtering behavior in GaN nanodots by selective area growth through a nanoporous template. This dislocation dissipation mechanism has been studied numerically through finite element method based on the nonlocal approach (Liang et al., 2010; Ye et al., 2012), in which the surrounding surfaces are considered only as free surfaces and the evaluation the nonlocal stress in Eq. (2) only considers the largest contribution from the linear integral of the stress part in the plane perpendicular to the dislocation.

The energy approach is based on the virtual work principle. In mechanics, a general force is defined as the change of the total energy relative to a general configuration coordinate change:

$$f = -\frac{\partial W}{\partial a}, \tag{3}$$

where ∂a can be seen as the change of the dislocation position in this case, and W is the total energy stored in the solid.

Similar to the nonlocal approach, the calculation of the total energy usually requires a volumetric integration of the energy density over the whole crystal space. This is quite cumbersome in most cases and it is often approximated as the same energy to introduce the dislocation into the crystal (Ahmadzadeh-Bakhshayesh et al., 2012; Dundurs and Mura, 1964; Dundurs and Sendeckyj, 1965; Fang and Liu, 2006a, b; Luo and Xiao, 2009). The approximation is carried out by evaluating the work done by stresses on the cut surface of the dislocation to move the slip plane. It could avoid the energy integration directly but somehow neglect the stress contributions from other part of the material.

This work adopts the energy approach to formulate analytically image forces on dislocations with surface stress in nanowires and nanorods. First, the analytical stress and strain fields are derived in case of isotropic circular nanowires. The results are fed into the energy approach to obtain the analytical formulation of image forces of nanowires. Second, this work proposes to study image forces of nanorods by approximating the 3D shape effect as a height-dependent shape function, which could be obtained through curve fitting of the finite element data without surface stress. This work provides explicitly analytical formulations of image forces on dislocations in nanowires and nanorods with surface stress. The results of nanowires are demonstrated to be acceptable compared with the classical solution and complex variable method. More importantly, the analytical formulation of nanorods has not been found in other literatures so far. This work could contribute to nanostructure design and provide guidance for the fabrication of high quality nanostructures.

3. Stress field

In Fig. 1, consider an elastic solid of domain (V) with an inclusion (Ω) prescribed with an eigenstrain ε^*. The surface of the solid is denoted by (S).

The constitutive relationship of the stress and the strain is:

$$\sigma_{ij} = L_{ijkl}(\varepsilon_{kl} - \varepsilon^*_{kl}), \tag{4}$$

where L_{ijkl} is the stiffness tensor of the material.

The strain is related to the displacement through compatibility condition: