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# Size-dependent interaction of an edge dislocation with an elliptical nano-inhomogeneity incorporating interface effects

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ABSTRACT

The elastic behavior of an edge dislocation, which is positioned outside of a nanoscale elliptical inhomogeneity, is studied within the interface elasticity approach incorporating the elastic moduli and surface tension of the interface. The complex potential function method is used. The dislocation stress field and the image force acting on the dislocation are found and analyzed in detail. The difference between the solutions obtained within the classical-elasticity and interface-elasticity approaches is discussed. It is shown that for the stress field, this difference can be significant in those points of the inhomogeneity-matrix interface, where the radius of curvature is smaller and which are closer to the dislocation. For the image force, this difference can be considerable or dispensable in dependence on the dislocation position, its Burgers vector orientation, and relations between the elastic moduli of the matrix, inhomogeneity and their interface. Under some special conditions, the dislocation can occupy a stable equilibrium position in atomically close vicinity of the interface. The size effect is demonstrated that the normalized image force strongly depends on the inhomogeneity size when it is in the range of several tens of nanometers, in contrast with the classical solution where this force is always constant. The general issue is that the interface elasticity effects become more evident when the characteristic sizes of the problem (inhomogeneity size, interface curvature radius and dislocation-interface spacing) reduce to the nanoscale.



## 1. Introduction

Many advanced structural materials and solid device systems have inhomogeneous nanoscale structure which can be described in terms of matrix and nanoinhomogeneities (nanoscale inclusions with elastic constants different from those of the matrix). Addition of nanoinhomogeneities can greatly enhance some mechanical, electric, thermal, tribologic and other functional properties of the matrix that is for example the case with ceramic nanocomposites (Niihara, 1991; Bhaduri and Bhaduri, 1998; Zhan and Mukherjee, 2005; Moya et al., 2007; Mukhopadhyay and Basu, 2007, 2011; Cho et al., 2009). On the other hand, this can cause the appearance of new electronic and optical properties as is the case with quantum dots and quantum wires in semiconductor epitaxial layers (Ledentsov et al., 1998; Teichert, 2002; Bandyopadhyay and Nalwa, 2003). During fabrication, testing and use of these inhomogeneous solids, other crystalline defects, especially dislocations, are generated and elastically interact with the inhomogeneities, thus giving rise to the hardening, strengthening and toughening effects in ceramic nanocomposites (Niihara, 1991; Choi and Awaji, 2005) and misfit stress accommodation coupled with degradation of electronic and optical properties in semiconductor devices (Gutkin et al., 2003; Ovid'ko and Sheinerman, 2006). The study of dislocation-inhomogeneity interaction is thus a traditional topic in micromechanics and physics of plasticity of various composite materials and structures.

Theoretical description of the elastic interaction of dislocations with inhomogeneities is mainly based on solutions of appropriate boundary-value problems in the classical theory of elasticity (see, for example, Dundurs and Mura, 1964; Dundurs, 1967; Stagni and Lizzio, 1983; Warren, 1983; Gong and Meguid, 1994). The main result is quite predictable: in most of the cases, dislocations are attracted to (repelled off) the boundaries of elastically softer (harder) inhomogeneities. However, there exist some exclusions of this rule. For special set of material properties, edge dislocations

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with suitable Burgers vector orientations can occupy stable equilibrium positions near the interface of a circular (Dundurs and Mura, 1964) or elliptical (Stagni and Lizzio, 1983) inhomogeneity. It was also shown that this interaction is dependent on the Burger vector orientation and Poisson ratios of matrix and inhomogeneities. In most of the cases, the image forces drastically change due to slight changes in the inhomogeneity shape.

Such classical description of the dislocation-inhomogeneity interaction is sufficient when the characteristic sizes of the inhomogeneity are larger than some nanometers and/or the dislocation spacing from the interface is larger than the dislocation core radius. Otherwise, the approach of classical linear elasticity becomes incorrect, and one has to go out from its framework.

Two principal non-classical approaches have been applied in recent years to cope with these difficulties within the continuum description. The first one is the so-called strain-gradient elasticity approach (Gutkin et al., 2000a,b; Mikaelyan et al., 2000; Lazar, 2007; Davoudi et al., 2009, 2010; Song et al., 2009). This approach leads to elimination of all classical singularities from the dislocation elastic fields and image forces, to smoothing of jump discontinuities of the dislocation stresses at the matrix/inhomogeneity interfaces, to appearance of non-classical size effects and to some new features of image forces in close vicinity of the interface. However, the boundary conditions used in this approach are not still perfectly proved.

The second approach is the so-called surface/interface stress elasticity which considers the surfaces/interfaces as atomically thin layers of special phase with its own material properties and stressed state caused by peculiarities in the surface/interface atomic structures. This approach seems to be especially useful when one deals with nanoscopic solids or inhomogeneities. Indeed, when the sizes of such objects tend to a nanometer, the number of atoms in the surface/interface becomes comparable with the number of atoms in the bulk. Since the surface/interface atoms have different bonding situation than the bulk atoms, the effect of the surface/interface phase has to be taken into consideration.

The basic concept of surface/interface stress in solids was first proposed by Gibbs (1906). Later, Gurtin and Murdoch (1975, 1978) and Gurtin et al. (1998) elaborated a framework for solving elastic problems within this model. This approach is based on the quantity called "surface free energy", which is defined as the reversible work per unit area to create a new surface. This quantity leads to a tensor of elastic stresses acting on the surface/interface as follows:

$$\sigma_{\alpha\beta} = E\delta_{\alpha\beta} + \frac{\partial E}{\partial \varepsilon_{\alpha\beta}}. \tag{1}$$

Here $E$ is the surface free energy, $\delta_{\alpha\beta}$ is the Kronecker delta, and $\sigma_{\alpha\beta}$ and $\varepsilon_{\alpha\beta}$ are the stress and strain tensors, respectively, in which the components normal to the surface/interface are excluded.

In the framework of the surface/interface elasticity approach, a number of classical thin film, inclusion and inhomogeneity problems have been resolved in nanoscale and some size effects have been found for relevant nanoscale materials (Cammarata, 1994; Sharma et al., 2003; Sharma and Ganti, 2004; Duan et al., 2005; Sharma and Wheeler, 2007; Tian and Rajapakse, 2007; Goldstein et al., 2010).

Recently, the same approach has been used in revisiting the problems of the dislocation-inhomogeneity interaction. Fang and Liu (2006a,b) have recalculated the image forces acting upon screw and edge dislocations near circular inhomogeneities and shown that (i) the contribution of the interface stress becomes significant when the inhomogeneity radius is reduced to nanoscale (smaller than about of 50 nm), (ii) the interface stress can add repelling or attracting extra forces to the classical image forces on dislocations, and (iii) it can cause an extra equilibrium position for a dislocation in very close vicinity of the interface (spaced by about of 0.3 nm from it). Similar results have been obtained later by Luo and Xiao (2009) for the case of a screw dislocation interacting with an elliptical nanoinhomogeneity. Fang et al. (2009) and Ou and Pang (2011) have studied the image forces on screw dislocations near core-shell nanowires of circular cross-sections embedded to infinite matrix. Chen et al. (2011) have described in detail the features of the image force acting on an edge dislocation near a coated elliptic inhomogeneity in a matrix within the classical theory of elasticity. These solutions (Fang et al., 2009; Luo and Xiao, 2009; Chen et al., 2011; Ou and Pang, 2011) have given the results rather similar to the aforementioned data (i)–(iii), however with some specific features caused by the elliptic shape of the inhomogeneity (Luo and Xiao, 2009; Chen et al., 2011) and the influence of coating layers (Fang et al., 2009; Ou and Pang, 2011). The authors of all these works have been concentrated on the image force and have not studied the dislocation stress fields.

Shodja et al. (2011) and Moeini-Ardakani et al. (2011) have recently applied the surface elasticity approach to the problems of screw and edge dislocations in the wall of a nanotube and investigated the elastic stresses and the image forces in detail. In particular, it has been demonstrated that in tiny nanotubes with wall thickness in the order of a few nanometers, the surface stresses noticeably affect the bulk stress fields over the nanotube cross section, while in coarser nanotubes, the surface stress effect is negligibly small. Moreover, an edge dislocation produces the stress fields which oscillate in subsurface layers of the nanotube (Moeini-Ardakani et al., 2011). This result is in contrast with the classical solution for shear and normal stress components which vanishes on both the free surfaces. In the bulk of the nanotube wall, the classical and surface-stress solutions coincide well. Moeini-Ardakani et al. (2011) have treated the stress oscillations as if caused by surface rippling due to the presence of edge dislocations. Further, unlike the case of classical elasticity, the dislocation can be repelled from the free surfaces and occupy stable equilibrium positions in atomically thin subsurface layers.

Although the aforementioned works have revealed many features in elastic interaction of dislocations with curved interfaces and free surfaces, they are still some questions to answer. In the case of elliptic nanoinhomogeneity, for example, this is the interface stress effect on the elastic stress distribution when an edge dislocation has the Burgers vector of arbitrary orientation and is located out of the principal axes of the inhomogeneity. It is also very desired to find out under which circumstances this effect should either be taken into account or not.

In using the surface/interface elasticity approach, the material constants of surfaces and interfaces are of primary importance. Miller and Shenoy (2000), Shenoy (2005) proposed a detailed formulation for determining the free surface properties of aluminum and some other materials [Ag, Au, Cu, Ni…] by means of the embedded atom method. Later, Mi et al. (2008) computed the interface properties of some non-coherent metallic interfaces like Ag–Ni, Au–Ni, and Ag–Cu. Recently, Pahlevani and Shodja (2011) used the same formulation as Mi et al. (2008), but with the other interatomic potential suggested earlier by Rafii-Tabar and Sutton (1991), and composed detailed tables for surface energies, surface stresses and elastic moduli of FCC metal surfaces and interfaces.

In the present work, we apply the interface elasticity approach to the case of an edge dislocation located outside of an elliptical nanoinhomogeneity. The governing equations of the interface elasticity are solved by means of complex potential functions expanded in Laurent series. To numerically calculate the stress fields and image forces, we have taken the material characteristics of InAs (nanoinhomogeneity) and GaAs (matrix) which are commonly used in quantum dot fabrication.