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Screw dislocation in a Bi-medium within strain gradient elasticity revisited

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Abstract: In this paper, we consider a straight screw dislocation near a flat interface between two elastic media in the framework of strain gradient elasticity (as studied by Gutkin et. al. [1]) by now taking care of some incomplete calculations). Closed form solutions for stress components and the Peach-Koehler force on the dislocation have been derived. It is shown that the singularities of the stress components at the dislocation line are eliminated and both components are continuous and smooth across the interface. The effect of the distance of the dislocation position from the interface on the maximum value of stress is investigated. Unlike in the case of classical solution, the image force remains finite when the dislocation approaches the interface. It is shown that the dislocation is attracted by the medium with smaller shear modulus or smaller gradient coefficient.

Keywords: Strain gradient elasticity; Screw dislocation; Bi-medium; Image force

1 Introduction

The study of the elastic interaction of dislocations and inclusions is of considerable importance for understanding the strengthening and hardening mechanism of crystalline materials, especially composite materials [2, 3]. Several investigations have been conducted to assess dislocation-inclusion interaction of a straight dislocation with a semi-infinite interface between two dissimilar media [1, 4–7]; interactions of edge and screw dislocations

with a circular inclusion [8–11]; and the interaction of dislocations with coated fibers [12–16]. Most of these attempts have been made in the context of conventional or classical elasticity. However, classical elasticity solutions are characterized by singularities in the components of the stress and strain fields. In addition, the force acting on the dislocation due to the existing interface becomes infinite as the dislocation approaches the interface, and some components of the stress field experience abrupt jumps at the interface. Gutkin et. al. [1, 7] indicated that these jumps can be justified only from a macroscopic point of view, and these solutions are inadmissible from a nanoscopic point of view. Thus, classical elasticity breaks down at the dislocation core and at the interface.

Additionally, it has been experimentally and computationally shown that elastic (see, e.g., [17–21]) and plastic (see, e.g., [21–30]) responses of materials at small length scales can be size dependent. Classical continuum theories are, however, scale-free and, hence, they cannot predict the behavior of materials at very small scales. In order to remedy this critical shortcoming, one or more material length scales are incorporated into the continuum constitutive equations. One of these fortified continuum theories is strain gradient elasticity where strain energy density or Hooke's law contains gradients of elastic strain and/or stress fields.

The constitutive equation of a simple theory of strain gradient elasticity proposed by the second author and coworkers (for a recent review see [31] and refs quoted therein) reads

$$(1 - l^2 \nabla^2) \sigma = (1 - c^2 \nabla^2) [\lambda (tr \epsilon) 1 + 2\mu \epsilon], \quad (1)$$

where ϵ and σ denote the elastic stress and strain tensors, λ and μ are the usual Lamé constants, 1 the unit tensor, ∇^2 the Laplacian, and l and c are two different gradient coefficients with the dimension of length. The stress and strain gradients are added to dispense the singularity of the stress and strain at the dislocation core and the crack tips. In analogy with what is now commonly known as the Ru-Aifantis theorem [31], a simple approach to solve boundary-value problems (BVPs) associated with Eq. (1) is to use existing solutions of classical elasticity for the same (traction) BVP. In fact, providing that appropriate care is

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taken for extra boundary conditions (on account of the higher order terms) or conditions at infinity, u and σ can be found through the inhomogenous Helmholtz equations

$$\begin{aligned} (1 - c^2 \nabla^2) u &= u^0, \\ (1 - l^2 \nabla^2) \sigma &= \sigma^0, \end{aligned} \quad (2)$$

where u^0 and σ^0 are the solutions of the same BVP in classical elasticity. Eqs. (2) have been successfully applied to study the interaction between a dislocation and an interface [1, 7, 11, 32–34].

In this paper, we use the theory of strain gradient elasticity described by Eq. (1) to study the interaction between a straight screw dislocation and a flat interface. The same problem was studied by Gutkin et. al. [1] with some deficiencies. For example, the stress components were not smooth or continuous despite the additional boundary conditions they imposed. In addition, it was not explained why the behavior of screw and edge dislocations near the interface of two materials with different gradient coefficients are different. These motivated us to reconsider this problem and calculate the stresses and the image force acting on the dislocation.

2 Classical solution

Consider two elastic isotropic, perfectly bonded semi-infinite bodies denoted by region 1 ($x \geq 0$) and region 2 ($x \leq 0$) with different Lamé coefficients and gradient constants. Such a solid is called a bi-medium. Super- and subscripts 1 and 2 are exclusively used for reference to these two regions and the omission of super- or sub-script indicates that the relationship is true for both regions. Suppose a straight screw dislocation with the Burgers vector $b = (0, 0, b)$ is situated in region 1 on the x -axis at $x = x_0$, and the dislocation line is parallel to the interface of the media (Fig. 1).

In classical elasticity, the zx -component of the stress field and the z -component of the displacement field due to the interaction of the screw dislocation and the interface should be continuous across the interface ($x = 0$). Imposing these boundary conditions, the classical stresses (in the units of $\mu_1 b / 2\pi$) are given by Head [4] as

$$\begin{aligned} \sigma_{zx}^{0(1)} &= -\frac{y}{r_1^2} + \gamma \frac{y}{r_2^2}, & \sigma_{zx}^{0(2)} &= -(1 + \gamma) \frac{y}{r_1^2}, \\ \sigma_{zy}^{0(1)} &= \frac{x - x_0}{r_1^2} + \gamma \frac{x + x_0}{r_2^2}, & \sigma_{zy}^{0(2)} &= (1 + \gamma) \frac{x - x_0}{r_1^2}, \end{aligned} \quad (3)$$

Figure 1: A screw dislocation near a bi-medium interface

where $r_1 = \sqrt{(x - x_0)^2 + y^2}$, $r_2 = \sqrt{(x + x_0)^2 + y^2}$ as depicted in Fig. 1 and γ is defined by

$$\gamma = \frac{\mu_2 - \mu_1}{\mu_2 + \mu_1}. \quad (4)$$

As indicated earlier, the zx -component of the classical stress field should be continuous on $x = 0$, while the component σ_{zy} has an abrupt jump across the interface:

$$\sigma_{zy}^{0(1)}(x = 0, y) - \sigma_{zy}^{0(2)}(x = 0, y) = 2\gamma \frac{x_0}{x_0^2 + y^2}. \quad (5)$$

It is worthwhile to note that this jump goes to infinity when the dislocation nears the interface. Since the zy -component of the stress field does not contribute to the traction vector, this jump is justified in classical elasticity. Gutkin et al. [1, 7] indicate that this jump is unphysical and the nature of it is quite unclear in nanoscopic point of view: In fact, the jump in zy -component is a consequence of the approximation of classical continuum models, which may become insufficient for describing nanoscale phenomena [1, 7]. It may, thus, be desirable for the interface stress jump to be eliminated from the solution of this problem within any generalized theory of elasticity aiming to consider nanoscale phenomena.

3 Gradient solution

Let us consider the same problem within the theory of strain gradient elasticity. Equations (2) must be solved for both regions 1 and 2. Also as mentioned in section 2, due to the presence of higher gradient terms, prescription of extra boundary conditions is required.

To find the zx -component of the stress field, it is convenient to decompose it into a particular part, $\sigma_{zx}^{p(j)}$ ($j = 1, 2$) and the homogeneous part, $\sigma_{zx}^{h(j)}$. It can easily be shown that

$$\begin{aligned}\sigma_{zx}^{p(1)} &= \sigma_{zx}^{0(1)} + \frac{y}{l_1 r_1} K_1 \left(\frac{r_1}{l_1} \right), \\ \sigma_{zx}^{p(2)} &= \sigma_{zx}^{0(2)},\end{aligned}\quad (6)$$

where $\sigma_{zx}^{0(1)}$ and $\sigma_{zx}^{0(2)}$ are the classical solutions given by Eq. (3). Using the Fourier transform with respect to y

$$\begin{aligned}\hat{\sigma}_{zx}^{h(j)}(x, s) &= F \left\{ \sigma_{zx}^{h(j)}(x, y); y \rightarrow s \right\} \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \sigma_{zx}^{h(j)}(x, y) e^{-isy} dy,\end{aligned}\quad (7)$$

the corresponding equation of the homogeneous part is reduced to the following ordinary differential equation

$$\left(1 - l^2 s^2 - l^2 \frac{d^2}{dx^2} \right) \hat{\sigma}_{zx}^{h(j)} = 0. \quad (8)$$

Considering the fact that the stress components approach zero as x approaches ∞ or $-\infty$, and using the inverse of Fourier transform, the homogenous solutions read as follows

$$\begin{aligned}\sigma_{zx}^{h(1)} &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(s) e^{-x\sqrt{s^2 + \frac{1}{l_1^2}}} e^{isy} ds, \\ \sigma_{zx}^{h(2)} &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} a(s) e^{x\sqrt{s^2 + \frac{1}{l_2^2}}} e^{isy} ds,\end{aligned}\quad (9)$$

where $A(s)$ and $a(s)$ are to be determined by the boundary conditions proposed and used by Gutkin et al. [7]:

$$\begin{aligned}\sigma_{zx}^{(1)}(x=0, y) &= \sigma_{zx}^{(2)}(x=0, y), \\ \frac{\partial \sigma_{zx}^{(1)}}{\partial x}(x=0, y) &= \frac{\partial \sigma_{zx}^{(2)}}{\partial x}(x=0, y).\end{aligned}\quad (10)$$

The above boundary conditions provide not only a continuous but also a smooth transition of the profile of σ_{zx} across the interface. If $\hat{\sigma}_{zx}^{(j)}(x, s) = F \left\{ \sigma_{zx}^{(j)}(x, y); y \rightarrow s \right\}$, the above boundary conditions will be equivalent to

$$\begin{aligned}\hat{\sigma}_{zx}^{(1)}(x=0, s) &= \hat{\sigma}_{zx}^{(2)}(x=0, s), \\ \frac{\partial \hat{\sigma}_{zx}^{(1)}}{\partial x}(x=0, s) &= \frac{\partial \hat{\sigma}_{zx}^{(2)}}{\partial x}(x=0, s).\end{aligned}\quad (11)$$

The Fourier transform of gradient solutions are

$$\begin{aligned}\hat{\sigma}_{zx}^{(1)} &= -i \sqrt{\frac{\pi}{2}} \operatorname{sgn}(s) \left(e^{-|s(x-x_0)|} - \gamma e^{-|s(x+x_0)|} \right) \\ &+ i \sqrt{\frac{\pi}{2}} \frac{s}{\lambda_1} e^{-|x-x_0|\lambda_1} + A(s) e^{-x\lambda_1},\end{aligned}\quad (12)$$

and

$$\hat{\sigma}_{zx}^{(2)} = -(1+\gamma) i \sqrt{\frac{\pi}{2}} \operatorname{sgn}(s) e^{-|s(x-x_0)|} + a(s) e^{x\lambda_2},$$

where $\lambda_j = \sqrt{s^2 + \frac{1}{l_j^2}}$. Substitution of $\hat{\sigma}_{zx}^{(1)}$ and $\hat{\sigma}_{zx}^{(2)}$ into Eqs. (11) gives us the unknown functions $A(s)$ and $a(s)$. After some simplifications, we obtain

$$\begin{aligned}\sigma_{zx}^{(1)} &= \sigma_{zx}^{0(1)} + \frac{y}{l_1 r_1} K_1 \left(\frac{r_1}{l_1} \right) \\ &+ \int_0^{\infty} \frac{\sin(sy)}{\lambda_1 + \lambda_2} e^{-x\lambda_1} \left[\frac{\lambda_1 - \lambda_2}{\lambda_1} s e^{-x_0\lambda_1} - 2\gamma \lambda_2 e^{-x_0 s} \right] ds, \\ \sigma_{zx}^{(2)} &= \sigma_{zx}^{0(2)} + 2 \int_0^{\infty} \frac{\sin(sy)}{\lambda_1 + \lambda_2} e^{x\lambda_2} \left[s e^{-x_0\lambda_1} + 2\gamma \lambda_1 e^{-x_0 s} \right] ds.\end{aligned}\quad (13)$$

Figure 2 compares the classical and gradient solutions of the zx -component of the stress field. Both $\sigma_{zx}^0(x, y = 2l_1)$ and $\sigma_{zx}(x, y = 2l_1)$ are continuous across the interface. Unlike $\sigma_{zx}^0(x, y = 2l_1)$, $\sigma_{zx}(x, y = 2l_1)$ is also smooth at the interface.

Figure 2: The profile of $\sigma_{zx}(x, y = 2)$ when $\mu_2/\mu_1 = 10$ and $l_2/l_1 = 2$ with the dislocation being placed at $x_0/l_1 = 5$. Solid and dashed curves correspond to the gradient and classical solutions, respectively. The stress values are given in units of $\mu_1 b / (2\pi l_1)$.

In the same manner, the gradient solution of the zy -component of the stress field can be obtained

$$\begin{aligned}\sigma_{zy}^{(1)} &= \sigma_{zy}^{0(1)} - \frac{x-x_0}{l_1 r_1} K_1 \left(\frac{r_1}{l_1} \right) + \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} D(s) e^{-x\lambda_1} e^{isy} ds, \\ \sigma_{zy}^{(2)} &= \sigma_{zy}^{0(2)} + \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d(s) e^{x\lambda_2} e^{isy} ds.\end{aligned}\quad (14)$$

The unknown functions, $D(s)$ and $d(s)$, can be given by imposing the following boundary conditions

$$\begin{aligned}\sigma_{zy}^{(1)}(x=0, y) &= \sigma_{zy}^{(2)}(x=0, y), \\ \frac{\partial \sigma_{zy}^{(1)}}{\partial x}(x=0, y) &= \frac{\partial \sigma_{zy}^{(2)}}{\partial x}(x=0, y),\end{aligned}\quad (15)$$

or in terms of their Fourier transforms

$$\begin{aligned}\hat{\sigma}_{zy}^{(1)}(x=0, s) &= \hat{\sigma}_{zy}^{(2)}(x=0, s), \\ \frac{\partial \hat{\sigma}_{zy}^{(1)}}{\partial x}(x=0, s) &= \frac{\partial \hat{\sigma}_{zy}^{(2)}}{\partial x}(x=0, s),\end{aligned}\quad (16)$$

where $\hat{\sigma}_{zy}^{(j)}(x, s) = F\{\sigma_{zy}^{(j)}(x, y); y \rightarrow s\}$. After some simplifications, the final results turn out

$$\begin{aligned}\sigma_{zy}^{(1)} &= \sigma_{zy}^{0(1)} - \frac{x-x_0}{l_1 r_1} K_1\left(\frac{r_1}{l_1}\right) \\ &+ \int_0^\infty \frac{\lambda_2 \cos(sy)}{\lambda_1 + \lambda_2} e^{-x\lambda_1} \left[\frac{\lambda_1 - \lambda_2}{\lambda_2} e^{-x_0\lambda_1} - 2\gamma e^{-x_0s} \right] ds, \\ \sigma_{zy}^{(2)} &= \sigma_{zy}^{0(2)} + 2 \int_0^\infty \frac{\lambda_1 \cos(sy)}{\lambda_1 + \lambda_2} e^{x\lambda_2} [e^{-x_0\lambda_1} + \gamma e^{-x_0s}] ds.\end{aligned}\quad (17)$$

Figure 3 shows that while the gradient term for the zy -component of the stress field is continuous and smooth across the interface, the value of the classical stress jumps on the interface.

Figure 3: The profile of $\sigma_{zy}(x, y=0)$ when $\mu_2/\mu_1 = 10$, $l_2/l_1 = 2$, and the dislocation is placed at different locations x_0/l_1 . Solid and dashed curves are pertinent to the gradient and classical solutions, respectively. The stress values are given in units of $\mu_1 b / (2\pi l_1)$.

4 Size effect

An advantage of the gradient solution as compared to the classical solution is that one can investigate the effect of

the inner structure of both regions on the maximum stress magnitude, $\max |\sigma_{zy}|$. In the case that materials 1 and 2 have different shear moduli, but the same gradient coefficients, numerical evaluation of $\max |\sigma_{zy}|$ shows that when the material 1 is elastically softer than material 2 (when $x_0 \geq 0$), $\max |\sigma_{zy}|$ increases when the dislocation is shifted towards the interface. In this case, the peak value of stress is obtained when the dislocation is situated on the interface. If material 2 is elastically harder, the value of $\max |\sigma_{zy}|$ starts increasing when the dislocation is shifted toward the interface and starts decreasing when the dislocation is closer than $\approx 3l$. These facts are shown in Fig. 4.

Figure 4: Dependence of $\max |\sigma_{zy}|$ on the normalized dislocation position x/l for $l_1 = l_2 = l$ and different values of μ_2/μ_1 . The stress values are given in units of $\mu_1 b / (2\pi l_1)$.

If the regions have the same elastic constants, but different gradient coefficients, when $l_2/l_1 < 1$, $\max |\sigma_{zy}|$ increases with the decreasing ratio and when $l_2/l_1 > 1$, this trend reverses. These results agree with what Davoudi et al. [11, 33] have obtained for a screw dislocation inside or outside a circular inhomogeneity.

5 Image force

Now, let us consider the image force (Peach-Koehler force) F_x per unit length of the dislocation imposed by the inter-

Figure 5: Dependence of $\max |\sigma_{zy}|$ on the normalized dislocation position x/l_1 for $\mu_1 = \mu_2$ and different values of l_2/l_1 . The stress values are given in units of $\mu_1 b/(2\pi l_1)$.

face. The gradient solution (in units of $\mu_1 b^2/2\pi$) reads

$$F_x = b \sigma_{zy}^{(1)}(x = x_0, y = 0) = \frac{\gamma}{2 x_0} + \int_0^\infty \frac{\lambda_2}{\lambda_1 + \lambda_2} \left[\frac{\lambda_1 - \lambda_2}{\lambda_2} e^{-2x_0\lambda_1} - 2\gamma e^{-x_0(s+\lambda_1)} \right] ds, \quad (18)$$

in which the first term on the right-hand side forms the classical solution and the integral term comes from the gradient solution. It is evident that the classical image force becomes infinite as the dislocation nears the interface ($x_0 \rightarrow 0$).

The sign of F_x determines whether the dislocation is repelled or attracted toward the interface. Since $x_0 \geq 0$, the positive value of F_x means attraction and the negative value of it indicates repulsion.

For a purely elastic interface ($\mu_1 \neq \mu_2$, $l_1 = l_2$), the formula of the image force, $F_x^{el} = F_x$, is simplified to

$$F_x^{el} = \frac{\gamma}{2 x_0} - \gamma \int_0^\infty e^{-x_0(s+\lambda)} ds, \quad \lambda_1 = \lambda_2 = \lambda. \quad (19)$$

The numerical evaluation of F_x^{el} is depicted in Fig. 6a. It is seen that when $\mu_2 > \mu_1$, F_x^{el} is positive and when $\mu_2 < \mu_1$, F_x^{el} becomes negative. This means that the dislocation is pushed away by the harder medium. The maximum force on the dislocation occurs when the dislocation is at $x_0 \approx l$.

In the case of a purely gradient interface ($\mu_1 = \mu_2$, $l_1 \neq l_2$), the image force, $F_x^{gr} = F_x$ reduces to

$$F_x^{gr} = \int_0^\infty \frac{\lambda_1 - \lambda_2}{\lambda_1 + \lambda_2} e^{-2x_0\lambda_1} ds. \quad (20)$$

In the case of $l_1 > l_2$ or $\lambda_1 < \lambda_2$, the gradient image force is negative and in the case of $l_1 < l_2$ or $\lambda_1 > \lambda_2$, the gradient image force has a positive value (Fig. 6b). In other words, the dislocation is pulled into the medium having a smaller gradient coefficient. This result agrees with what Mikaelyan et. al. [7] obtained for an edge dislocation in a bi-medium. Since Gutkin et. al. [1] made certain miscalculations in obtaining the gradient solution for a screw dislocation in a bi-medium, their results differ from the result obtained by Mikaelyan et. al. [7] for an edge dislocation in a bi-medium; the nature of this difference could not be determined.

Figure 6: Dependence of the image forces (a) F_x^{el} and (b) F_x^{gr} on the normalized positions, (a) x_0/l and (b) x_0/l_1 , of a screw dislocation near (a) a purely elastic interface for $l_1 = l_2 = l$ and = 10, 5, 2, 0.5, 0.1, and 0 (from top to bottom); (b) a purely gradient interface with $\mu_2 = \mu_1$ and $l_2/l_1 = 10, 2, 1.1, 1, 0.9, 0.7$ and 0.5. The force values are given in units of (a) $\mu_1 b^2/(2\pi l)$ and (b) $\mu_1 b^2/(2\pi l_1)$. The dashed curves in (a) correspond to the classical solutions.

6 Conclusions

In this paper, we have employed gradient elasticity theory to calculate the nonsingular stress components are not singular at the dislocation line which also experiences a continuous and smooth transition at the interface. The classi-

cal and gradient stress fields coincide at a distance larger than $\sim 5-7l$ from the dislocation line or the interface.

For a purely elastic interface, when $\mu_2 > \mu_1$, the maximum shear stress in the media, $\max |\sigma_{zy}|$, monotonically increases as the dislocation approaches the interface. When $\mu_2 < \mu_1$, however, $\max |\sigma_{zy}|$ reaches its peak value when the dislocation is a few l 's away from the interface. For a purely gradient interface, $\max |\sigma_{zy}|$ attains its peak value when the dislocation is at the interface.

The force on the dislocation remains finite no matter where the dislocation is, unlike the classical force on the dislocation which approaches infinity as the dislocation approaches the interface. It is shown that the dislocation is pulled into the medium of smaller shear stress for a purely elastic interface and of smaller gradient coefficient for a purely gradient interface.

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