Nanomechanics of a screw dislocation in a functionally graded material using the theory of gradient elasticity

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Abstract

The modest aim of this short article is to provide some new results for a screw dislocation in a functionally graded material within the theory of gradient elasticity. These results, based on a displacement formulation and the Fourier transform technique, completes earlier findings obtained with the stress function method and extends them to the case of the second strain gradient elasticity. Rigorous and easy-to-use analytical expressions for the displacements, the strains and the stresses are obtained which are free from singularities at the dislocation line.

keywords: Screw dislocation; Functionally graded material; Second strain gradient elasticity

1 Introduction

In an earlier paper published a few years ago [1], the stress function technique was employed to derive stress and strain fields for a screw dislocation in a functionally graded material by using the theory of first gradient elasticity. Analytical non-singular expressions were derived for the strains and the (first order) stresses, but the double stresses remained singular. Such results are derived here by using the Fourier transform technique which, in addition, provides exact analytical expressions for the displacement field. Moreover, the problem is reconsidered within the framework of "second strain gradient elasticity" which eliminates the singularities from the double stress expressions as well. Recent work on gradient elasticity [2,3] has revealed the need of using higher order gradients of strain in the stress-strain relation in order ro interpret experimental results pertaining to dislocation density tensor and more accurately describe the details of the relevant stress/strain fields near the core of dislocations contained in small volumes. This is the case in particular, for dislocations contained in functionally graded materials (FGMs), the use of which has advocated since mid 80's in relation to ultra high temperature and ultra high weight requirements for aircraft, space vehicles and other applications. Generally FGMs refer to heterogeneous composite materials, in which mechanical properties are intentionally made to vary smoothly and continuously from point to point. This is controlled by the variation of the volume fraction of the constituent materials. Ceramic/ceramic and metal/ceramic are typical examples of FGMs ([4,5] and references quoted therein). Although several aspects of FGMs have been reviewed comprehensively ([6-8] and references quoted therein) only few investigations have been made to assess the role of the dislocations in FGMs.

With the exception of [1], the classic theory of linear elasticity was routinely utilized to calculate the elastic fields produced by defects (dislocations and disclinations) in FGMs. However, classic continuum theories are scale invariant in which no intrinsic length appears and so fails

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when one attempts to explain the nano-scale phenomena near defects. As a result, elastic singularities are present in these solutions and size effects which dominate in small volumes cannot be captured. These undesirable features are removed within the second strain gradient elasticity formulation presented in this paper. The solutions obtained herein by using the Fourier transform technique and a displacement formulation are reduced to the corresponding expressions of classic elasticity and first gradient elasticity as, for example, were obtained in [1] through the use of the stress function approach. As a result, analytical expressions for the displacement field (in addition to those for the stresses and strains) are derived. The extra dividend is the derivation of non-singular expressions for the double stresses which diverge near the dislocation core in the first order strain gradient theory.

2 classic Solution

We consider a screw dislocation with Burgers vector $\mathbf{b} = (0, 0, b_z)$ in an infinite medium with a varying shear modulus $\mu = \mu(y) = \mu_0 e^{2ay}$ $(a \geq 0)$ in the framework of classic elasticity. This is a problem of anti-plane shear with the only non-vanishing component of displacement $u_z^0(x, y)$ satisfying the displacement equilibrium equation

$$\left(\nabla^2 - 2a \frac{\partial}{\partial y} \right) u_z^0 = 0, \tag{1}$$

where ∇^2 denotes the Laplacian. Using the substitution $u_z^0 = w^0 e^{-ay}$, we obtain

$$\left(\nabla^2 - a^2 \right) w^0 = 0, \tag{2}$$

which by means of the Fourier transform

$$\tilde{f}(s) = \mathfrak{F}\{ f(x); x \to s \} = \int_{-\infty}^{\infty} f(x) e^{-\mathrm{i}sx} dx,$$

where $\mathrm{i} = \sqrt{-1}$, is reduced to the following ordinary differential equation

$$\left(-s^2 - a^2 + \frac{d^2}{dy^2} \right) \tilde{w} = 0. \tag{3}$$

Since u_z^0 is finite everywhere, we arrive at

$$\tilde{u}_z^0 = e^{-ay} \begin{cases} A(s) e^{-y\sqrt{s^2 + a^2}} & (y > 0), \\ B(s) e^{y\sqrt{s^2 + a^2}} & (y < 0), \end{cases} \tag{4}$$

where the two unknown functions, $A(s)$ and $B(s)$, are constants with respect to y. In view of the present dislocation configuration, we have

$$u_z^0(x, 0^+) - u_z^0(x, 0^-) = b_z H(-x), \tag{5}$$

$$\varepsilon_{zy}^0(x, 0^+) = \varepsilon_{zy}^0(x, 0^-) \Leftrightarrow \frac{\partial u_z^0}{\partial y}(x, 0^+) = \frac{\partial u_z^0}{\partial y}(x, 0^-),$$

where ε_{zy}^0 is the classic strain, and $H(-x)$ is the Heaviside step function. Taking the Fourier transform of the above conditions, we have

$$\tilde{u}_z^0(x, 0^+) - \tilde{u}_z^0(x, 0^-) = b_z \left(\pi \delta(s) + \frac{\mathrm{i}}{s} \right); \quad \frac{\partial \tilde{u}_z^0}{\partial y}(s, 0^+) = \frac{\partial \tilde{u}_z^0}{\partial y}(s, 0^-), \tag{6}$$

and, thus, the unknown functions $A(s)$ and $B(s)$ are determined as

$$A(s) = \frac{-\mathrm{i}a}{2s\sqrt{s^2 + a^2}} + \frac{\mathrm{i}}{2s}, \quad B(s) = \frac{-\mathrm{i}a}{2s\sqrt{s^2 + a^2}} - \frac{\mathrm{i}}{2s} - \pi \delta(s). \tag{7}$$

It follows that

$$\tilde{u}_z^0 = b_z e^{-ay} \left[\frac{-\mathrm{i}a}{2s\sqrt{s^2 + a^2}} e^{-|y|\sqrt{s^2 + a^2}} + \mathrm{sgn}(y) \frac{\mathrm{i}}{2s} e^{-|y|\sqrt{s^2 + a^2}} - \pi \delta(s) H(-y) e^{ay} \right]. \tag{8}$$

and by taking the inverse Fourier transform, i.e.

$$u_z^0(x, y) = \mathfrak{F}^{-1}\{\tilde{u}_z^0(s, y); s \to x\} = \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{u}_z^0(s, y) e^{isx} ds,$$

we obtain (in view of the symmetry of the integral) the final expression

$$u_z^0 = \frac{b_z}{2\pi} e^{-ay} \int_0^{\infty} \frac{a \sin(sx)}{s\sqrt{s^2 + a^2}} e^{-|y|\sqrt{s^2+a^2}} ds \tag{9}$$
$$- \text{sgn}(y) \frac{b_z}{2\pi} e^{-ay} \int_0^{\infty} \frac{\sin(sx)}{s} e^{-|y|\sqrt{s^2+a^2}} ds - \frac{b_z}{2} H(-y).$$

Next we note that in small strain theory the (compatible) total strain ε_{ij}^T may be written as

$$\varepsilon_{ij}^T = (1/2)(u_{i,j} + u_{j,i}) = \varepsilon_{ij} + \varepsilon_{ij}^P,$$

where ε_{ij} and ε_{ij}^P denote the usual (incompatible) elastic and plastic strains, respectively. It follows that

$$\varepsilon_{zx}^{0T} = \frac{1}{2} \frac{\partial u_z^0}{\partial x} = \frac{b_z}{4\pi} e^{-ay} \int_0^{\infty} \frac{a \cos(sx)}{\sqrt{s^2 + a^2}} e^{-|y|\sqrt{s^2+a^2}} ds \tag{10}$$
$$- \text{sgn}(y) \frac{b_z}{4\pi} e^{-ay} \int_0^{\infty} \cos(sx) e^{-|y|\sqrt{s^2+a^2}} ds,$$
$$\varepsilon_{zy}^{0T} = \frac{1}{2} \frac{\partial u_z^0}{\partial y} = \frac{b_z}{4\pi} e^{-ay} \int_0^{\infty} \frac{s \sin(sx)}{\sqrt{s^2 + a^2}} e^{-|y|\sqrt{s^2+a^2}} ds$$
$$- \frac{b_z}{2\pi} \delta(y) \int_0^{\infty} \frac{\sin(sx)}{s} ds + \frac{b_z}{4} \delta(y).$$

With the help of the identities

$$\int_0^{\infty} \frac{\sin(sx)}{s} ds = \frac{\pi}{2} \text{sgn}(x), \quad \int_0^{\infty} \frac{\cos(sx)}{\sqrt{s^2 + a^2}} e^{-|y|\sqrt{s^2+a^2}} ds = K_0(ar),$$

where $r = \sqrt{x^2 + y^2}$ and K_n denotes the modified Bessel function of the second kind and of order n, the integrals appearing in Eq. (10) can readily be evaluated to give

$$\varepsilon_{zx}^{0T} = \frac{b_z}{4\pi} e^{-ay} \left[a K_0(ar) - \frac{ay}{r} K_1(ar) \right], \quad \varepsilon_{zy}^{0T} = \frac{b_z}{4\pi} e^{-ay} \frac{ax}{r} K_1(ar) + \frac{b_z}{2} \delta(y) H(-x). \tag{11}$$

The last term in Eq. (11)$_2$ which is singular on the half-plane $y = 0$ and $x \le 0$, corresponds to the plastic strain $\varepsilon_{zy}^{0P} = b_z \delta(y) H(-x)/2$. The other term on the right hand side of Eq. (11)$_2$ may thus be regarded as the elastic strain. Using the constitutive law, $\sigma_{zi}^0 = 2\mu\varepsilon_{zi}^0$ ($i = x, y$), the stresses read

$$\sigma_{zx}^0 = \frac{b_z \mu_0}{2\pi} e^{ay} \left[a K_0(ar) - \frac{ay}{r} K_1(ar) \right], \quad \sigma_{zy}^0 = \frac{b_z \mu_0}{2\pi} e^{ay} \frac{ax}{r} K_1(ar). \tag{12}$$

which are the same as those earlier obtained in [1] by the stress function approach, and which are singular at the dislocation line.

3 Strain gradient elasticity solution

Within a simplified theory of linearized anisotropic theory of the second strain gradient elasticity proposed in [9] (for a corresponding form of the first strain gradient elasticity and a robust method for the solutions of the corresponding boundary value problems, the reader may consult [10,11]), the strain energy density has the form

$$W = \frac{1}{2} C_{ijkl}\varepsilon_{ij}\varepsilon_{kl} + \frac{1}{2} \ell^2 C_{ijmn}\varepsilon_{mn,k}\varepsilon_{ij,k} + \frac{1}{2} \ell'^4 C_{ijmn}\varepsilon_{mn,kl}\varepsilon_{ij,kl}, \tag{13}$$

3

where ε_{ij} is the elastic strain tensor, ℓ and ℓ' are internal lengths, and C_{ijkl} is the stiffness tensor of the form

$$C_{ijkl} = \lambda(\boldsymbol{x})\delta_{ij}\delta_{kl} + \mu(\boldsymbol{x})\left(\delta_{ik}\delta_{jl} + \delta_{jk}\delta_{il}\right),$$

with the Lamé constants $\lambda(\boldsymbol{x})$ and $\mu(\boldsymbol{x})$ being given functions of the spatial coordinates. The corresponding expressions for the elastic-like first order stress (σ_{ij}^E) and the higher-order double (τ_{ijk}) and triple (τ_{ijkl}) stresses are given by

$$\sigma_{ij}^E := \frac{\partial W}{\partial \varepsilon_{ij}} = C_{ijkl}\varepsilon_{kl}, \quad \tau_{ijk} := \frac{\partial W}{\partial \varepsilon_{ij,k}} = \ell^2 C_{ijmn}\varepsilon_{mn,k}, \quad \tau_{ijkl} := \frac{\partial W}{\partial \varepsilon_{ij,kl}} = \ell'^4 C_{ijmn}\varepsilon_{mn,kl}.$$

while the Cauchy stress σ_{ij} (note that in the notation of [1] this was denoted by σ_{ij}^0 and termed total stress) satisfies, in the absence of body forces, the usual equilibrium equation

$$\sigma_{ij,j} = \sigma_{ij,j}^E - \tau_{ijk,kj} + \tau_{ijkl,klj} = 0. \tag{14}$$

The Cauchy stress σ_{ij} can be identified with the classic stress tensor. For the present case of anti-plane shear we have

$$\sigma_{zj}^E = 2\mu\epsilon_{zj}, \quad \tau_{zjk} = 2\ell^2\mu\epsilon_{zj,k}, \quad \tau_{zjkl} = 2\ell'^4\mu\epsilon_{zj,kl}; \qquad (j,k,l = x,y).$$

For an exponentially graded material in the y-direction, i.e. $\mu = \mu(y) = \mu_0\,e^{2ay}$, it follows from the above relations that Eq. (14) can be written as

$$\left[1 - c_1^2\left(\nabla^2 - 2a\frac{\partial}{\partial y}\right)\right]\left[1 - c_2^2\left(\nabla^2 - 2a\frac{\partial}{\partial y}\right)\right]\sigma_{zj}^E = \sigma_{zj}, \qquad (j = x,y) \tag{15}$$

where $c_1^2 + c_2^2 = \ell^2$ and $c_1^2 c_2^2 = \ell'^4$. By expressing the stresses in terms of the displacement field in both sides, we have

$$\left[1 - c_1^2\left(\nabla^2 - 2a\frac{\partial}{\partial y}\right)\right]\left[1 - c_2^2\left(\nabla^2 - 2a\frac{\partial}{\partial y}\right)\right]\left(\frac{1}{2}\frac{\partial u_z}{\partial x_j} + \varepsilon_{zj}^P\right) = \left(\frac{1}{2}\frac{\partial u_z^0}{\partial x_j} + \varepsilon_{zj}^{0P}\right), \tag{16}$$

where u_z and u_z^0 are, respectively, the displacement components calculated for gradient and classic elasticity, while ε_{zj}^P and ε_{zj}^{0P} denote the gradient and classic plastic strains. If we assume that the relationship

$$\left[1 - c_1^2\left(\nabla^2 - 2a\frac{\partial}{\partial y}\right)\right]\left[1 - c_2^2\left(\nabla^2 - 2a\frac{\partial}{\partial y}\right)\right]\varepsilon_{zj}^P = \varepsilon_{zj}^{0P}, \tag{17}$$

is fulfilled, we will immediately find that the displacement satisfies the following governing differential equation

$$\left[1 - c_1^2\left(\nabla^2 - 2a\frac{\partial}{\partial y}\right)\right]\left[1 - c_2^2\left(\nabla^2 - 2a\frac{\partial}{\partial y}\right)\right]u_z = u_z^0. \tag{18}$$

As before, by the substitution $u_z = w\,e^{-ay}$, we obtain

$$\left[1 - c_1^2\left(\nabla^2 - a^2\right)\right]\left[1 - c_2^2\left(\nabla^2 - a^2\right)\right]w = w^0 \tag{19}$$

where w^0 is given in Section 2. Use of the two dimensional Fourier transform yields the algebraic equation

$$\left[1 + c_1^2\left(s^2 + t^2 + a^2\right)\right]\left[1 + c_2^2\left(s^2 + t^2 + a^2\right)\right]\widetilde{w} = \widetilde{w}^0, \tag{20}$$

where

$$\widetilde{w} = \mathfrak{F}\{\mathfrak{F}\{w; x \to s\}; y \to t\} = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} w(x,y)\,e^{-i(sx+ty)}\,ds\,dt,$$

and

$$\widetilde{w}^0 = \mathfrak{F}\{\tilde{w}^0; y \to t\} = \frac{-ia}{s\left(\omega^2 + a^2\right)} + \frac{t}{s\left(\omega^2 + a^2\right)} - \frac{\pi\delta(s)}{a - it}; \quad \omega^2 = s^2 + t^2. \tag{21}$$

4

Then the inverse Fourier transform gives

$$w = \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} \left\{ \left(\frac{-\mathrm{i}a}{s} + \frac{t}{s} \right) \frac{e^{\mathrm{i}(sx+ty)}}{\omega^2 + a^2} \right\} ds\, dt \tag{22}$$

$$+ \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} \left\{ -\frac{c_1^2}{c_1^2 - c_2^2} \frac{-\mathrm{i}a}{s(\omega^2 + \kappa_1^2)} + \frac{c_2^2}{c_1^2 - c_2^2} \frac{-\mathrm{i}a}{s(\omega^2 + \kappa^2)} \right\} e^{\mathrm{i}(sx+ty)} ds\, dt$$

$$+ \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} \left\{ -\frac{c_1^2}{c_1^2 - c_2^2} \frac{t}{s(\omega^2 + \kappa_1^2)} + \frac{c_2^2}{c_1^2 - c_2^2} \frac{t}{s(\omega^2 + \kappa_2^2)} \right\} e^{\mathrm{i}(sx+ty)} ds\, dt$$

$$- \frac{\pi}{(2\pi)^2} \int_{-\infty}^{\infty} \left\{ \frac{\mathrm{i}}{\mathrm{i}a + t} - \frac{c_1^2}{c_1^2 - c_2^2} \frac{a + \mathrm{i}t}{t^2 + \kappa_1^2} + \frac{c_2^2}{c_1^2 - c_2^2} \frac{a + \mathrm{i}t}{t^2 + \kappa_2^2} \right\} e^{\mathrm{i}ty} dt,$$

where $\kappa_j = \sqrt{a^2 + 1/c_j^2}$. If we integrate out the variable s, and use the integral relations

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{e^{\mathrm{i}sx}}{s(s^2 + k^2)} ds = \frac{\mathrm{i}}{2k^2} \left(1 - e^{-|kx|} \right) \mathrm{sgn}(x), \quad \int_0^{\infty} \frac{t \sin(ty)}{t^2 + k^2} dt = \frac{\pi}{2} \mathrm{sgn}(y) e^{-|ky|},$$

$$\int_0^{\infty} \frac{\cos(ty)}{t^2 + k^2} dt = \frac{\pi}{2|k|} e^{-|ky|},$$

as well as the symmetry properties of these integrals, u_z can finally be expressed in terms of sine and cosine integrals as follows

$$u_z = u_z^0 - \frac{c_1^2}{c_1^2 - c_2^2} \frac{b_z e^{-ay}}{2\pi} \int_0^{\infty} \frac{t \sin(ty)}{t^2 + \kappa_1^2} \left[\mathrm{sgn}(x) e^{-\sqrt{t^2 + \kappa_1^2}|x|} + 2H(-x) \right] dt \tag{23}$$

$$+ \frac{c_2^2}{c_1^2 - c_2^2} \frac{b_z e^{-ay}}{2\pi} \int_0^{\infty} \frac{t \sin(ty)}{t^2 + \kappa_2^2} \left[\mathrm{sgn}(x) e^{-\sqrt{t^2 + \kappa_2^2}|x|} + 2H(-x) \right] dt$$

$$+ \frac{c_1^2}{c_1^2 - c_2^2} \frac{b_z e^{-ay}}{2\pi} \int_0^{\infty} \frac{a \cos(ty)}{t^2 + \kappa_1^2} \left[\mathrm{sgn}(x) e^{-\sqrt{t^2 + \kappa_1^2}|x|} + 2H(-x) \right] dt$$

$$- \frac{c_2^2}{c_1^2 - c_2^2} \frac{b_z e^{-ay}}{2\pi} \int_0^{\infty} \frac{a \cos(ty)}{t^2 + \kappa_2^2} \left[\mathrm{sgn}(x) e^{-\sqrt{t^2 + \kappa_2^2}|x|} + 2H(-x) \right] dt,$$

where u_z^0 is the classic solution given by Eq. (9).

It is easily seen that this expression for $a \to 0$ coincides with earlier results obtained by the third author and co-workers for homogeneous media and amended in [12]. Since Mura [13] neglected the last term of Eq. (21) when $a = 0$, and Lazar and Maugin [12] used Mura's calculations, their intermediate calculations are inaccurate, while the final solution is precise. It also turns out that for $\ell = 0$ and $\ell' = 0$ the result reduces to Eq.(9). When $x \to 0$, the displacement field can be expressed in an explicit form

$$u_z(0, y) = \frac{b_z}{2} H(-y) + \frac{b_z}{4} \frac{e^{-ay}}{c_1^2 - c_2^2} \left[-c_1^2 \mathrm{sgn}(y) e^{-\kappa_1|y|} + c_2^2 \mathrm{sgn}(y) e^{-\kappa_2|y|} \right.$$

$$\left. + c_1^2 \frac{a}{\kappa_1} e^{-\kappa_1|y|} - c_2^2 \frac{a}{\kappa_2} e^{-\kappa_2|y|} \right]. \tag{24}$$

It is worth noting that the classic displacement $u_z^0(0, y)$ has an abrupt jump at the dislocation line $y = 0$, while the gradient solution of Eq. (24), is smooth there (Fig. 1a,b). For a fixed value of a, the larger the ratio c_2/c_1 is, the smoother the solution becomes, Fig. 1a. The case of $c_2 = 0$ represents the first gradient solution. The gradient solution tends to the classic displacement when $y \to \pm\infty$, as expected.

Using the definition of strain field, the total strains read

$$\varepsilon_{zx}^T = \varepsilon_{zx}^0 + \frac{b_z}{4\pi} \frac{e^{-ay}}{c_1^2 - c_2^2} \left[-c_1^2 a K_0(\kappa_1 r) + c_2^2 a K_0(\kappa_2 r) + c_1^2 \frac{\kappa_1 y}{r} K_1(\kappa_1 r) \right.$$

$$\left. - c_2^2 \frac{\kappa_2 y}{r} K_1(\kappa_2 r) \right], \tag{25}$$

$$\varepsilon_{zy}^T = \varepsilon_{zy}^0 + \frac{b_z}{4\pi} \frac{e^{-ay}}{c_1^2 - c_2^2} \frac{x}{r} \left[-c_1^2 \kappa_1 K_1(\kappa_1 r) + c_2^2 \kappa_2 K_1(\kappa_2 r) \right]$$

$$+ \frac{b_z}{4\pi} \frac{e^{-ay} c_1^2}{c_1^2 - c_2^2} \int_0^\infty \frac{\cos(ty)}{1 + c_1^2 (t^2 + a^2)} \left[\text{sgn}(x) e^{-|x|\sqrt{t^2 + \kappa_1^2}} + 2H(-x) \right] dt$$

$$- \frac{b_z}{4\pi} \frac{e^{-ay} c_2^2}{c_1^2 - c_2^2} \int_0^\infty \frac{\cos(ty)}{1 + c_2^2 (t^2 + a^2)} \left[\text{sgn}(x) e^{-|x|\sqrt{t^2 + \kappa_2^2}} + 2H(-x) \right] dt. \qquad (26)$$

where ε_{zx}^0 and ε_{zy}^0 are the classic (elastic) strains given in Section 2. It is seen that ε_{zx}^T does not contain a plastic part, while ε_{zy}^T is decomposed into the elastic and plastic strains, i.e. $\varepsilon_{zx} = \varepsilon_{zx}^T$; $\varepsilon_{zx}^P = 0$, and

$$\varepsilon_{zy} = \varepsilon_{zy}^0 + \frac{b_z}{4\pi} \frac{e^{-ay}}{c_1^2 - c_2^2} \frac{x}{r} \left[-c_1^2 \kappa_1 K_1(\kappa_1 r) + c_2^2 \kappa_2 K_1(\kappa_2 r) \right], \quad \varepsilon_{zy}^P = \varepsilon_{zy}^T - \varepsilon_{zy}.$$

It is also follows that the expression for the plastic strain $\varepsilon_{zy}^P(0, y)$ is given by the simple formula

$$\varepsilon_{zy}^P(0, y) = \frac{b_z}{8} \frac{e^{-ay}}{c_1^2 - c_2^2} \left[\frac{e^{-\kappa_1|y|}}{\kappa_1} - \frac{e^{-\kappa_2|y|}}{\kappa_2} \right].$$

The maximum value of $\varepsilon_{zy}^P(0, y)$ decreases as c_2/c_1 or a increases, Fig. 2.

The lower-order elastic-like stresses stresses are given by the expressions:

$$\sigma_{zx}^E = \sigma_{zx}^0 + \frac{b_z \mu_0 e^{ay}}{2\pi (c_1^2 - c_2^2)} \left[-c_1^2 a K_0(\kappa_1 r) + c_2^2 a K_0(\kappa_2 r) + c_1^2 \frac{\kappa_1 y}{r} K_1(\kappa_1 r) - c_2^2 \frac{\kappa_2 y}{r} K_1(\kappa_2 r) \right]$$

$$\sigma_{zy}^E = \sigma_{zy}^0 + \frac{b_z \mu_0 e^{ay}}{2\pi (c_1^2 - c_2^2)} \frac{x}{r} \left[-c_1^2 \kappa_1 K_1(\kappa_1 r) + c_2^2 \kappa_2 K_1(\kappa_2 r) \right], \qquad (27)$$

where σ_{zx}^0 and σ_{zy}^0 are the classic stresses given by Eqs. (12). It is seen from the above expressions that σ_{zx}^E is still symmetric with respect to the plane $x = 0$, while σ_{zy}^E has lost symmetry with respect to plane $y = 0$. Higher order stresses, τ_{ijk} and τ_{ijkl}, can be calculated easily using the fact that

$$\frac{d}{dz} K_n(z) = \frac{n}{2} K_n(z) - K_{n+1}(z).$$

Fig. 4 and Fig. 5 show how double stresses and triple stresses vary, respectively, when $c_2/c_1 = 0.5$. It is worth mentioning that within the second strain gradient theory $\tau_{(zx)x} \neq -\tau_{(zy)y}$ in contrast to homogeneous medium. Because

$$K_0(z) \sim -\log(z/2), \text{ as } z \to 0,$$

$$K_n(z) \sim \frac{1}{2}(n-1)! \left(\frac{z}{2} \right)^{-n}, \text{ as } z \to 0,$$

it can be easily shown that neither double stresses nor triple stresses are singular anymore within the second strain gradient theory, in contrast to the first strain gradient in which some components of double stress field remain singular, Fig 6. More details and for this problem their physical implications to possible improvements of designing FGMs and the expressions for higher stresses will be given in a forthcoming publication.

4 Conclusions

In this work, a screw dislocation in a material exponentially graded in one direction is studied. The displacement field approach and the Fourier transform technique are used to find the displacement and strain fields, and consequently the stress field, in the framework of classic and strain gradient theories. While the classic displacement field has a discontinuity on an arbitrary branch-cut, the displacement field within the gradient theory is smooth everywhere. Accordingly, strain and stress fields in classic continuum theory which are singular at the dislocation line, become regular in the gradient theory. In the framework of the first strain gradient, some double

stresses are singular at the dislocation line; however, within the second strain gradient theory, not only all double stresses, but also triple stresses are regular, similar to the case of a homogeneous medium. When a or c_2/c_1 increases, the fields become smoother.

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FIGURE CAPTIONS

Fig. 1. The profile of $u_z(0, y)$ in units of $b_z/4$ when (a) $a = 0.1$ for $c_2/c_1 =$ 0, 0.5, 1 and 2 (b) $c_2 = c_1$ and $a =$ 0, 0.1, and 0.5. The long-dashed curves in (a) and (b) are pertinent to the classic solutions.
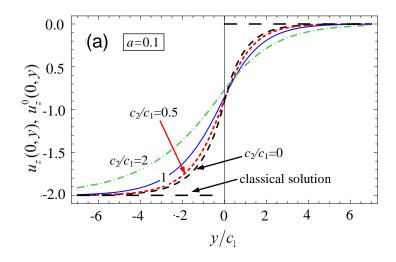
Fig. 2. The elastic strain components (a) ε_{zx} (b) ε_{zy} of a screw dislocation in an FGM when $a = 0.5$ and $c_2/c_1 = 0.5$ within the second strain gradient elasticity. The strain values are given in units of $b/(4\pi c_1)$.
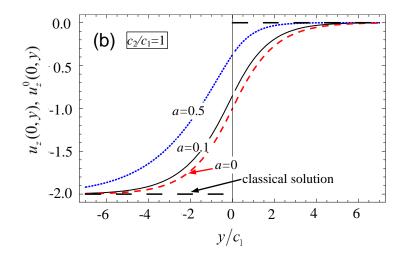
Fig. 3. The profile of plastic strain $\varepsilon_{zy}^P(0, y)$ of a screw dislocation in an FGM within the second strain gradient elasticity (a) when $a = 0.5$ and $c_2/c_1 =$ 0, 0.5, 1 and 2 (b) when $c_2/c_1 = 1$ and $a =$ 0, 0.5 and 1. The strain values are given in units of $\mu_0 b/(2\pi c_1)$.

Fig. 4. Double stresses of a straight screw dislocation in an FGM within second strain gradient when $a = 0.5$ and $c_2/c_1 = 0.5$. Double stresses are given in units of $\mu_0 b/(4\pi)$.

Fig. 5. Triple stresses of a straight screw dislocation in an FGM within second strain gradient when $a = 0.5$ and $c_2/c_1 = 0.5$. Double stresses are given in units of $\mu_0 b c_1/(4\pi)$.

Fig. 6. Comparison between double stresses within the first strain gradient (dashed lines) and the second strain gradient (solid lines). It is apparent that τ_{zxy} and τ_{zyx} are singular in first strain gradient.
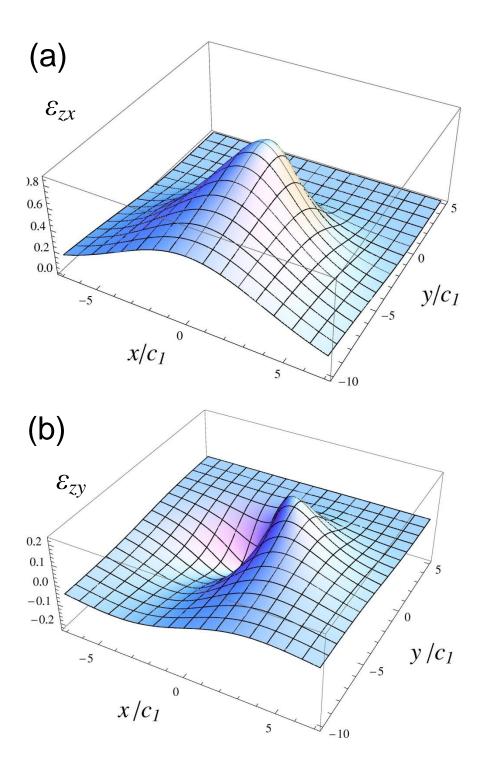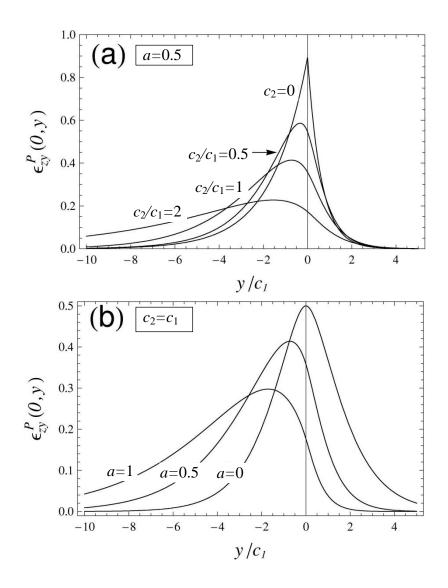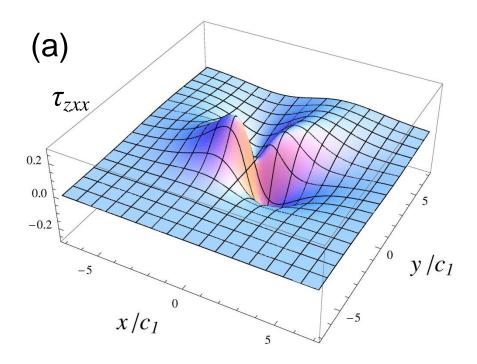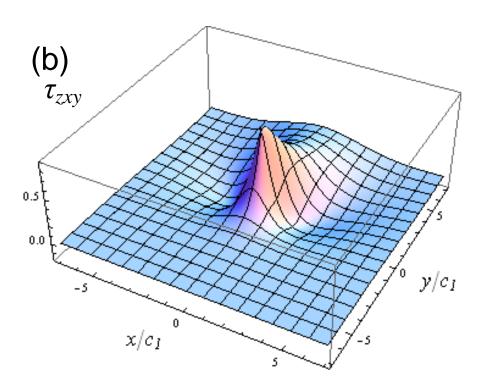
Fig. 1

(a) ε_{zx}

(b) ε_{zy}

Fig. 2

(a) $a=0.5$

$\epsilon_{zy}^{P}(0,y)$

$c_2=0$

$c_2/c_1=0.5$ →

$c_2/c_1=1$

$c_2/c_1=2$

y/c_1

(b) $c_2=c_1$

$\epsilon_{zy}^{P}(0,y)$

$a=1$ $a=0.5$ $a=0$

y/c_1

Fig. 3

(a)

τ_{zxx}

0.2

0.0

−0.2

−5

0

5

x/c_1

5

0

−5

y/c_1

(b)

τ_{zxy}

0.5

0.0

−5

0

5

x/c_1

5

0

−5

y/c_1

Fig. 4a,b

(c) τ_{zyx}

(d) τ_{zyy}

Fig. 4c,d

(a) τ_{zxxx}

x/c_1 y/c_1

(b) τ_{zxxy}

x/c_1 y/c_1

Fig. 5a,b

(c)

τ_{zxyy}

0.4
0.2
0.0
-0.2

y/c_1

2

1

0

-1

-2

-2

-1

0

1

2

x/c_1

(d)

τ_{zyxx}

0.2

0.0

-0.2

y/c_1

1.0

0.5

0.0

-0.5

-1.0

-1.0

-0.5

0.0

0.5

1.0

x/c_1

Fig. 5c,d

(e) τ_{zyxy}

(f) τ_{zyyy}

Fig. 5e,f

(a)

$\tau_{zxx}(x,0)$

x/c_1

(b)

$\tau_{zxy}(x,0)$

y/c_1

(c)

$\tau_{zyx}(0,y)$

y/c_1

Fig. 6a,b,c

Fig. 6d