The fundamentals of non-singular dislocations in the theory of gradient elasticity: Dislocation loops and straight dislocations

Markus Lazar *

Heisenberg Research Group, Department of Physics, Darmstadt University of Technology, Hochschulstr. 6, D-64289 Darmstadt, Germany
Department of Physics, Michigan Technological University, Houghton, MI 49931, USA

A R T I C L E   I N F O

Article history:
Received 25 April 2012
Received in revised form 13 August 2012
Available online 25 September 2012

Keywords:
Dislocations
Dislocation loops
Gradient elasticity
Size effects
Green tensor

A B S T R A C T

The fundamental problem of non-singular dislocations in the framework of the theory of gradient elasticity is presented in this work. Gradient elasticity of Helmholtz type and bi-Helmholtz type are used. A general theory of non-singular dislocations is developed for linearly elastic, infinitely extended, homogeneous, and isotropic media. Dislocation loops and straight dislocations are investigated. Using the theory of gradient elasticity, the non-singular fields which are produced by arbitrary dislocation loops are given. Modified Mura, Peach–Koehler, and Burgers formulae are presented in the framework of gradient elasticity theory. These formulae are given in terms of an elementary function, which regularizes the classical expressions, obtained from the Green tensor of the Helmholtz–Navier equation and bi-Helmholtz–Navier equation. Using the mathematical method of Green’s functions and the Fourier transform, exact, analytical, and non-singular solutions were found. The obtained dislocation fields are non-singular due to the regularization of the classical singular fields.

© 2012 Elsevier Ltd. All rights reserved.

1. Introduction

Dislocations play an important role in the understanding of many phenomena in solid state physics, materials science, and engineering. They are the primary carriers of crystal plasticity. Dislocations are line defects which can be straight or curved lines. The internal geometry of generally curved dislocations, in deformed crystals is very complex. In the classical theory of dislocation loops in isotropic materials (DeWit, 1960; Lardner, 1974; Hirth and Lothe, 1982) two key equations are the Burgers formula (Burgers, in isotropic materials (DeWit, 1960; Lardner, 1974; Hirth and Koehler, 1950) for the stress. These equations are very important for the interaction between complex arrays of dislocations. The classical description of the elastic fields produced by dislocations is based on the theory of harmonic functions. There is the problem of mathematical singularities at the dislocation core, and an arbitrary core-cutoff radius which must be introduced to avoid divergence. In the classical continuum theory of dislocations (Kröner, 1958; DeWit, 1960; Nabarro, 1967; Lardner, 1974; Mura, 1987; Teodosiu, 1982; Li and Wang, 2008) the concept of Volterra dislocations is used, and the dislocation core is described by a Dirac delta function. This unsatisfactory situation can only be remedied, when the fact that physical dislocations have a finite core region and no singularities exist are taken into account. As already pointed out by Kröner (1958) and Lothe (1992) the divergence can be avoided when dislocation distributions other than the delta function are used. Lothe (1992) considered a standard core model with constant density of dislocations in a planar strip with width d. However, the value of d remains undetermined and the expressions for the elastic fields are more complicated than their singular counterparts and difficult to use for generally curved dislocations. Moreover, for non-planar configurations the theory becomes much more complex. In order to remove the singularities of dislocations and to model the dislocation core more realistically, continuum theories of generalized elasticity may be used. A very promising candidate of such a theory is the so-called gradient elasticity theory. The theory of gradient elasticity was originally proposed by Mindlin (1964); Mindlin (1965); and Mindlin and Eshel (1968) (see also Eshel and Rosenfeld, 1970). The correspondence between the strain gradient theory and the atomic structure of materials with the nearest and next nearest interatomic interactions was exhibited by Toupin and Grazis (1964). The original Mindlin theory possesses too many new material parameters. For isotropic materials, Mindlin's theory of first strain gradient elasticity (Mindlin, 1964; Mindlin and Eshel, 1968) involves two characteristic lengths, and Mindlin's theory of second strain gradient elasticity (Mindlin, 1965) possesses four characteristic lengths. The discrete nature of materials is inherently incorporated in the formulations through the characteristic
lengths. The capability of strain gradient theories in capturing size effects is a direct manifestation of the involvement of characteristic lengths. Simplified versions, which are particular cases of Mindlin’s theories, were proposed and used for dislocation modelling. Such simplified gradient elasticity theories are known as gradient elasticity of Helmholtz type (Lazar and Maugin, 2005), with only one material length scale parameter and gradient elasticity of bimaterial systems (Lazar and Maugin, 2006a; Lazar et al., 2006a) which involves two material length scale parameters as new material coefficients. Gradient elasticity is a continuum model of dislocations with core spreading. Non-singular fields of straight dislocations were obtained in the framework of gradient elasticity of Helmholtz type by Gutkin and Afantis (1999); Lazar and Maugin (2005); Lazar and Maugin (2006a); Lazar et al. (2005) and Gutkin (2000); Gutkin (2006) (see also, Gutkin and Ovid’ko, 2004). Surprisingly enough up until now, not a single work has been done in the direction of non-singular dislocation loops using strain gradient elasticity theory. The reason may be in the expected mathematical complexity of the problem. Such non-singular solutions of arbitrary dislocation loops could be very useful for the so-called discrete dislocation dynamics (e.g. Li and Wang, 2008; Gholami et al., 1999).

The aim of this paper is to present non-singular solutions of arbitrary dislocation loops, by using simplified gradient elasticity theories. We present the key-formulae of dislocations loops valid in the framework of gradient elasticity, and also reemphasize straight dislocations in gradient elasticity. The technique of Green functions for the key-formulae is used, and analytical closed-form solutions for the dislocation fields are derived.

The paper is organized as follows. In Section 2, the fundamentals of gradient elasticity of Helmholtz type are given. Dislocation loops and straight dislocations are investigated. In Section 3, the theory of gradient elasticity of bimaterial systems is considered. Dislocation loops and straight dislocations will be examined in this framework. In Section 4, the conclusions are given. All the mathematical and technical details are given in the Appendices.

2. Gradient elasticity of Helmholtz type

A straightforward framework to obtain non-singular fields of dislocations is the so-called theory of gradient elasticity. A simplified theory of strain gradient elasticity is called gradient elasticity of Helmholtz type (Lazar and Maugin, 2005; Lazar and Maugin, 2006a). This gradient elasticity of Helmholtz type is a particular gradient elasticity theory evolving from Mindlin’s general gradient elasticity theory (Mindlin, 1964; Mindlin and Eshel, 1968). This theory is also known as dipolar gradient elasticity theory (Georgiadis, 2003), simplified strain gradient elasticity theory (Gao and Ma, 2010a; Gao and Ma, 2010b) and special gradient elasticity theory (Altan and Afantis, 1997). The theory of gradient elasticity of Helmholtz type is the gradient version of Eringen’s theory of non-local elasticity of Helmholtz type (Eringen, 1983; Eringen, 2002) which is well-established.

The strain energy density of such a simplified gradient elasticity theory for an isotropic, linearly elastic material has the form (Lazar and Maugin, 2005; Gao and Ma, 2010a)\[ W = \frac{1}{2} C_{ijkl} \epsilon_{ij} \epsilon_{kl} + \frac{1}{2} \epsilon^2 C_{ijkl} \partial_m \epsilon_{ij} \partial_m \epsilon_{kl}, \]where \( C_{ijkl} \) is the tensor of elastic moduli with the symmetry properties\[ C_{ijkl} = C_{ikjl} = C_{jikl} = C_{jilk} \]and it reads for an isotropic material\[ C_{ijkl} = \mu (\delta_{ik} \delta_{jl} + \delta_{ij} \delta_{kl}) + \lambda \delta_{il} \delta_{jk}, \]where \( \mu \) and \( \lambda \) are the Lamé moduli, \( \beta_j \) denotes the elastic distortion tensor. If the elastic distortion tensor is incompatible, it can be decomposed as follows\[ \beta_j = \partial_i u_i - \beta^0_j, \]where \( u \) and \( \beta^0_j \) denote the displacement vector and the plastic distortion tensor, respectively. In addition, \( \epsilon \) is the material length scale parameter of gradient elasticity of Helmholtz type. For dislocations, \( \epsilon \) is related to the dislocation core radius and is proportional to a lattice parameter. Due to the symmetry of \( C_{ijkl} \), Eq. (1) is equivalent to\[ W = \frac{1}{2} C_{ijkl} \epsilon_{ij} \epsilon_{kl} + \frac{1}{2} \epsilon^2 C_{ijkl} \partial_m \epsilon_{ij} \partial_m \epsilon_{kl}, \]where \( \epsilon \) is the elastic strain tensor. The condition for non-negative strain energy density, \( W \geq 0 \), gives\[ (2 \mu + 3 \lambda) \geq 0, \quad \mu \geq 0, \quad \epsilon^2 \geq 0. \]

The reason that the elastic and plastic distortion tensors are incompatible can be the presence of dislocations. Dislocations cause self-stresses that means stresses caused without the presence of body forces. The dislocation density tensor is defined in terms of the elastic and plastic distortion tensors as follows (e.g. Kröner, 1958)\[ \sigma_{ij} = C_{ijkl} \partial_k \beta_l, \]and it fulfills the Bianchi identity of dislocations\[ \partial_i \sigma_{ij} = 0, \]which means that dislocations do not end inside the body. Eq. (9) is a ‘conservation’ law and shows that dislocations are source-free fields.

From Eq. (1) it follows that the constitutive equations are\[ \sigma_{ij} = \frac{\partial W}{\partial \beta_{ij}} = \frac{\partial W}{\partial \epsilon_{ij}} = C_{ijkl} \beta_{kl} = C_{ijkl} \epsilon_{kl}, \]were \( \epsilon_{ij} \) are the components of the Cauchy stress tensor, \( \sigma_{ij} \) are the components of the so-called double stress tensor. It can be seen that \( \epsilon \) is the characteristic length scale for double stresses. Using Eqs. (10) and (11), Eq. (5) can also be written as (Lazar and Maugin, 2005)\[ W = \frac{1}{2} \sigma_{ij} \epsilon_{ij} + \frac{1}{2} \epsilon^2 \partial_k \sigma_{ij} \partial_k \epsilon_{ij}. \]

The strain energy density (12) exhibits the symmetry both in \( \sigma_{ij} \) and \( \epsilon_{ij} \) and in \( \partial_k \sigma_{ij} \) and \( \partial_k \epsilon_{ij} \).

The total stress tensor is given as a combination of the Cauchy stress tensor and the divergence of the double stress tensor\[ \sigma^0_{ij} = \sigma_{ij} - \partial_k \tau_{ijk} = (1 - \epsilon^2 \Delta) \sigma_{ij}, \]and it fulfills the equilibrium condition for vanishing body forces\[ \partial_i \sigma^0_{ij} = \partial_i (\sigma_{ij} - \partial_k \tau_{ijk}) = 0. \]

The stress tensor \( \sigma^0_{ij} \) is called in the notation of Jaumann (1967) the polarization of the Cauchy stress \( \sigma_{ij} \). Due to gradient elasticity of Helmholtz type, Eq. (13) reduces to an inhomogeneous Helmholtz equation where the total stress tensor is the inhomogeneous piece. As pointed out by Lazar and Maugin (2005); Lazar and Maugin (2006a), the total stress tensor may be identified with the singular classical stress tensor. This identifies that the inhomogeneous Helmholtz equation (13) is in full agreement with the equation

As shown by Lazar and Maugin (2005); Lazar and Maugin (2006a) the following governing equations for the displacement vector, the elastic distortion tensor, the dislocation density tensor, and the plastic distortion tensor can be derived in the framework of gradient elasticity of Helmholtz type

\[ Lu_i = u_i^0, \]
\[ L\beta_{ij} = \beta_{ij}^0, \]
\[ L\lambda = \lambda_0, \]
\[ L\lambda_0 = \lambda_0^0, \]
\[ L\beta_{ij}^0 = \beta_{ij}^0, \]
\[ \lambda_0^0 = \lambda_0^0, \]

where

\[ L = 1 - \ell^2 \Delta \]

is the Helmholtz operator. The singular fields \( u_i^0, \beta_{ij}^0, \lambda_0^0 \) and \( \beta_{ij}^0 \) are the sources of the inhomogeneous Helmholtz Equation (15)-(18). The Helmholtz Equation (15) and (16) can be further reduced to Helmholtz–Navier equations

\[ LL_k u_k = C_{ijkl} \partial_j \beta_{kl}^0, \]
\[ LL_k \lambda_{km} = -C_{ijkl} \partial_j A_{kl}^0, \]

where \( L_k = C_{ijkl} \partial_j \partial_i \) is the differential operator of the Green function of the Helmholtz–Navier equation.

Thus, \( A(R) \) is the Green function of Eq. (30) which is a Helmholtz-Laplace equation.

Using Eqs. (A.3) and (A.4) for the differentiation of Eq. (24), the explicit form of the three-dimensional Green tensor of the Helmholtz–Navier equation is obtained

\[ G_0(R) = \frac{1}{16\pi \mu(1 - \nu)} \left[ \frac{\delta_0}{R} \left( 3 - 4\nu \right) \left( 1 - e^{-R/\ell} \right) \right. \]
\[ + \frac{1}{R^2} \left( 2e^2 - R^2 + 2R + 2e^2 \right) \left( e^{-R/\ell} \right) \]
\[ \left. + \frac{RR_0}{R^2} \left( 1 - e^2 + 2 + e^2 \right) \left( e^{-R/\ell} \right) \right], \]

which is non-singular. It is worth noting as a check, that Eq. (33) is in agreement with the corresponding expressions derived by Polyzos et al. (2003) and Gao and Ma (2009) using slightly different approaches.

The Green tensor (33) gives the non-singular displacement field, \( u_i = G_0 \delta_0 \) (\( \delta_0 \) is the constant value of the magnitude of the point force acting at the arbitrary position \( x \) in an infinite body), of the Kelvin point force problem (e.g. Gurtin, 1972; Mura, 1987; Hetnarski and Ignaczuk, 2004) in the framework of gradient elasticity of Helmholtz type. The original solution of a concentrated force in an infinite body in the context of the classical continuum theory of elasticity was given by Kelvin (1882).

2.1. Dislocation loops

In this subsection, the characteristic fields of dislocation loops in the framework of gradient elasticity theory of Helmholtz type are calculated.

For a general (non-planar or planar) dislocation loop \( L \), the classical dislocation density and the plastic distortion tensors are (e.g. DeWit, 1973a; Kossecka, 1974)

\[ \beta_{ij}^p = \beta_{ij}(L) = b_j \int_L \delta(x - x') \, dl', \]
\[ \beta_{ij}^0 = -b_j \delta_0(S) = -b_j \int_S \delta(x - x') \, ds', \]

where \( b_j \) is the Burgers vector of the dislocation line element \( dl' \) at \( x \) and \( ds' \) is the dislocation loop area. The surface \( S \) is the dislocation surface, which is a cap of the dislocation line \( L \). \( \delta_0(S) \) is the Dirac delta function for a closed curve \( L \) and \( \delta_0(S) \) is the Dirac delta function for a surface \( S \) with boundary \( L \).

The solution of Eq. (17) can be written as the following convolution integral

\[ x_0 = G * \beta_{ij}^0 = b_j \int_L G(R) \, dl', \]

where \( G(R) \) denotes the three-dimensional Green function of the Helmholtz equation given by Eq. (28). The explicit solution of the dislocation density tensor for a dislocation loop in gradient elasticity is calculated as

\[ x_0(x) = \frac{b_j}{4\pi \ell^2} \int_L e^{-R/\ell} \, dl', \]

describing a spreading dislocation core distribution. The plastic distortion tensor of a dislocation loop, which is the solution of Eq. (18), is given by the convolution integral

\[ \beta_{ij}^p = G * \beta_{ij}^0 = -b_j \int_S G(R) \, ds', \]

It reads as...
\[
\rho_0^k(\mathbf{x}) = -\frac{b_k}{4\pi r^2} \int_0^r \frac{e^{-r/\mathbf{R}}}{\mathbf{R}} \, dS', \quad (39)
\]
Substituting Eq. (39) in Eq. (8) and using the Stokes theorem, we obtain formula (37).

Using the Green tensor (24), and after a straightforward calculation all the generalizations of the Mura, Peach–Koehler, and Burgers formulae towards gradient elasticity can be obtained. Starting with the elastic distortion tensor of a dislocation loop, the solution of Eq. (21) gives the representation as the following convolution integral
\[
\rho_{im}(\mathbf{x}) = \int_{-\infty}^{\infty} \epsilon_{mm} \mathcal{G}_{khk}(R) \rho_0^k(\mathbf{x}) \, dV', \quad (40)
\]
where \( \mathcal{G}_{khk} = \partial_k G_k \). Substituting the classical dislocation density tensor of a dislocation loop (34) and carrying out the integration of the delta function, we find the modified Mura formula valid in gradient elasticity
\[
\rho_{im}(\mathbf{x}) = \int_{\mathbb{R}^3} \epsilon_{mm} b_k \mathcal{G}_{khk}(R) \, dS', \quad (41)
\]
Substitute Eqs. (3) and (24) into Eq. (41) and obtain after rearranging terms
\[
\rho_{ij}(\mathbf{x}) = \frac{1}{8\pi} \int_{\mathbb{R}^3} \epsilon_{mm} \left[(b_i \partial_j - b_j \partial_i) \Delta + \frac{1}{2} (b_i \partial_j - b_j \partial_i) \Delta \right] (R) \, dS', \quad (42)
\]
Using the identity
\[
\epsilon_{mm} (b_i \partial_j - b_j \partial_i) = \epsilon_{mm} \epsilon_{kln} \varepsilon_{i} \varepsilon_{j} b_l \partial_k \partial_l = (\delta_{il} \partial_j - \delta_{lj} \partial_i) \epsilon_{kln} b_l \partial_k = \epsilon_{il} \partial_j - \epsilon_{lj} \partial_i = (\epsilon_{kl} \partial_j - \epsilon_{jl} \partial_k) b_l \partial_k \partial_l, \quad (43)
\]
and the relation
\[
\int_{\mathbb{R}^3} \epsilon_{mm} (b_i \partial_j - b_j \partial_i) \partial_l A(R) \, dS' = \frac{b_k}{8\pi} \int_{\mathbb{R}^3} \left((\delta_{ik} \partial_j - \delta_{ij} \partial_k) \partial_l (R) \right) \, dS' = \frac{b_k}{8\pi} \int_{\mathbb{R}^3} \left((\delta_{ik} \partial_j - \delta_{ij} \partial_k) \partial_l (R) \right) \, dS', \quad (52)
\]
Except the first term of Eq. (52), we apply the Stokes theorem in order to obtain line integrals with
\[
\int_{\partial V} (\delta_{lj} \partial_i - \delta_{ij} \partial_l) (\partial A(R)) \, dS' = -\int_{V} \epsilon_{mm} (\delta_{lj} \partial_i - \delta_{ij} \partial_l) (\partial A(R)) \, dS', \quad (53)
\]
and
\[
\int_{\partial V} (\delta_{lj} \partial_i - \delta_{ij} \partial_l) (\partial A(R)) \, dS' = -\int_{V} \epsilon_{mm} (\delta_{lj} \partial_i - \delta_{ij} \partial_l) (\partial A(R)) \, dS', \quad (54)
\]
In this way, the key-formula for the non-singular displacement vector in gradient elasticity is found
\[
u_l(\mathbf{x}) = \frac{b_k}{8\pi} \int_{\partial V} \left(\delta_{lj} \partial_i - \delta_{ij} \partial_l - \delta_{ij} \partial_l \right) (\partial A(R)) \, dS', \quad (55)
\]
which is the Burgers formula in the framework of gradient elasticity of Helmholtz type. Eq. (55) determines the displacement field of a single dislocation loop. The Eqs. (45)–(55) are straightforward, simple, and closely resemble the singular solutions of classical elasticity theory. In the limit \( \; t \rightarrow 0 \), the classical expressions are recovered in Eqs. (45)–(55). The expressions (45), (49), and (55) retain most of the analytic structure of the classical Mura, Peach–Koehler, and Burgers formulae. The expressions (45)–(55) are given in terms of the elementary function \( A(R) \) given in Eqs. (A.2)–(A.6). It is important to note that Eqs. (45)–(55) are non-singular due to the regularization of the classical singular expressions (see Appendix A). As an example, we substitute Eqs. (A.5) and (A.6) into Eq. (49) and obtain the explicit expression for the stress tensor
\[
\sigma_{ij}(\mathbf{x}) = \frac{\mu b_k}{8\pi} \int_{\mathbb{R}^3} \left((\epsilon_{ijl} \partial_r + \epsilon_{ilr} \partial_j) \partial_l \right) (R) \, dS', \quad (49)
\]
The elastic rotation vector is defined as the skew-symmetric part of the elastic distortion tensor \( \omega_{l} = \frac{1}{2} \epsilon_{lj} \delta_{jk} \) and reads
\[
\omega_{l}(\mathbf{x}) = \frac{b_k}{8\pi} \int_{\mathbb{R}^3} \left(\delta_{lj} \partial_r - \delta_{rj} \partial_l - \delta_{lj} \partial_r \right) \Delta \, (R) \, dS', \quad (48)
\]
\[ \sigma_{ij}(x) = \frac{-\mu b}{8\pi \ell} \int_{S} \left[ \rho_{ij} \delta_{ij} \partial_{n} \partial_{n} - \frac{2}{1 - \nu} \rho_{ij} \partial_{n} \partial_{n} \right] \frac{2R}{R^2} \left( 1 - \left( \frac{R}{\ell} \right)^2 \right) e^{R \cdot r} \] 
\[ + \frac{2}{1 - \nu} \int_{S} \left\{ \frac{\partial_{n} \partial_{n} \delta_{ij} - \frac{2}{1 - \nu} \rho_{ij} \partial_{n} \partial_{n}}{R^2} \left( 1 - e^{-R \cdot r} \right) + \left( 4 + \frac{10\ell}{R^2} + \frac{2R}{R^2} \right) e^{R \cdot r} \right\} dL'. \]  

(56)

To give the expression (55) more explicitly, using Eq. (A.6) we introduce a generalized solid angle valid in gradient elasticity of Helmholtz type

\[ \Omega(\ell, \ell) = -\frac{1}{2} \int_{S} \Delta \partial_{n} A(\ell) dS_{r} = \frac{R_{i} R_{j}}{R_{r} \left( 1 - \left( \frac{R}{\ell} \right)^2 \right)} dL'. \]  

(57)

Eq. (57) is non-singular and depends on the length scale \( \ell \). In the limit \( \ell \to 0 \), the usual solid angle (e.g. Li and Wang, 2008) is recovered. Thus, using Eq. (57) and carrying out some differentiations with Eqs. (A.2) and (A.4), we obtain from Eq. (55) the explicit gradient elastic-ity version of the Burgers formula

\[ u_{i}(x) = -\frac{b_{i}}{4\pi} \Omega(\ell, \ell) = -\frac{b_{i}}{4\pi} \int_{S} \frac{R_{i}}{R_{r} \left( 1 - \left( \frac{R}{\ell} \right)^2 \right)} dL' - \frac{b_{i}}{8\pi (1 - \nu)} \int_{S} \frac{2\ell \delta_{ij} - 2\ell R_{i} R_{j} - 2\ell R_{i} R_{j}}{\left( 1 - \left( \frac{R}{\ell} \right)^2 \right) e^{-R \cdot r}} dL'. \]  

(58)

The simplicity of our results is based on the use of gradient elasticity theory of Helmholtz type. Our results can be used in computer simulations of dislocation cores at nano-scale and in numerics as fast numerical sums of the relevant elastic fields as it is used for the classical equations (e.g. Ghoniem et al., 1999).

### 2.2. Straight dislocations

In this subsection, using the modified Mura equation of gradient elasticity of Helmholtz type (40), the non-singular elastic distortion fields of straight dislocations as a check of our general approach are calculated.

#### 2.2.1. Screw dislocation

A screw dislocation corresponds to the anti-plane strain problem. The Green function of the anti-plane strain problem in gradient elasticity of Helmholtz type is nothing but the Green function of the two-dimensional Helmholtz–Laplace equation and it reads (see Eq. (B.21))

\[ G(R) = -\frac{1}{2\pi \ell \mu} \left( \gamma_{x} + \ln R + K_{0}(R/\ell) \right). \]  

(59)

where \( R = \sqrt{(x - x')^2 + (y - y')^2} \), \( \gamma_{x} \) is the Euler constant and \( K_{0} \) is the modified Bessel function of order \( n \). The Green function (59) is non-singular. The gradient of the Green function (59) is obtained as

\[ G_{i22}(R) = -\frac{1}{2\pi \ell \mu R} \left( \frac{R_{i}}{\ell} K_{0}(R/\ell) \right). \]  

(60)

Next, substituting Eq. (60) and the dislocation density of a screw dislocation \( \delta_{x} = b_{i} \delta(x) \delta(y) \) into Eq. (40), the elastic distortion produced by a screw dislocation is obtained. For an infinite screw dislocation along the \( z \)-axis with Burgers vector \( b_{z} \), the non-singular components for the elastic distortion are calculated as

\[ \beta_{xx} = \frac{b_{x}}{2\pi \ell \mu} \frac{y}{r^2} \left( 1 - r^2 K_{1}(r/\ell) \right), \]  

(61)

\[ \beta_{yy} = \frac{b_{x}}{2\pi \ell \mu} \frac{x}{r^2} \left( 1 - r^2 K_{1}(r/\ell) \right), \]  

(62)

where \( r = \sqrt{x^2 + y^2} \). The expressions obtained earlier by Lazar (2003) and Lazar and Maugin (2006a) are recovered. In the limit \( \ell \to 0 \), the classical expressions given by DeWit (1973b) are recovered in Eqs. (61) and (62).

The Green function (59) gives the non-singular displacement field \( u_{i} = -G_{i22} \) of a line force with the magnitude \( f_{i} \) calculated by Lazar and Maugin (2006b) in the framework of gradient elasticity.

#### 2.2.2. Edge dislocation

Now the plane strain problem of an edge dislocation is investigated. The Green tensor of the plane strain problem in gradient elasticity of Helmholtz type is derived as (see Eq. (B.17))

\[ G_{0}(R) = -\frac{1}{2\pi \ell \mu} \left( \frac{3 - 4\nu}{1 - \nu} \frac{R_{0}}{R_{r}} - \frac{\partial_{k} R_{i} R_{j} - \partial_{k} R_{i} R_{j}}{R_{r}^2} + \frac{2 R_{i} R_{j} R_{k}}{R_{r}^4} K_{1}(R/\ell) \right) \]  

(63)

It is obvious that the terms proportional to the Euler constant do not contribute to the elastic distortion fields. The two-dimensional Green tensor (63) is non-singular. In the limit \( \ell \to 0 \), the two-dimensional Green tensor of classical elasticity (Mura, 1987; Li and Wang, 2008) is recovered in Eq. (63). The gradient of the Green tensor (63) is given by

\[ G_{0,i}(R) = -\frac{1}{8\pi \mu \ell \left( 1 - \nu \right)} \left( 3 - 4\nu \frac{R_{0}}{R_{r}} - \frac{\partial_{k} R_{i} R_{j} - \partial_{k} R_{i} R_{j}}{R_{r}^2} + 2 \frac{R_{i} R_{j} R_{k}}{R_{r}^4} K_{1}(R/\ell) \right) \]  

(64)

Substituting Eq. (64) and the dislocation density of an edge dislocation along \( z \) axis with Burgers vector \( b_{x} \), \( \delta_{x} = b_{i} \delta(x) \delta(y) \), into Eq. (40), the elastic distortion of an edge dislocation is obtained. Eventually, the non-vanishing components of the elastic distortion of an edge dislocation are calculated as

\[ \beta_{xx} = -\frac{b_{x}}{4\pi \ell \mu \left( 1 - \nu \right)} \frac{y}{r^2} \left( 1 - 2r^2 + \frac{2x^2}{r^2} + \frac{4y^2}{r^2} \right) \]  

(65)

\[ \beta_{xy} = \frac{b_{x}}{4\pi \ell \mu \left( 1 - \nu \right)} \frac{x}{r^2} \left( 3 - 2x^2 - 2y^2 - \frac{4r^2}{r^2} \right) \]  

(66)

\[ \beta_{yx} = -\frac{b_{x}}{4\pi \ell \mu \left( 1 - \nu \right)} \frac{x}{r^2} \left( 1 - 2y^2 + \frac{2x^2}{r^2} + \frac{4y^2}{r^2} \right) \]  

(67)

\[ \beta_{yy} = -\frac{b_{x}}{4\pi \ell \mu \left( 1 - \nu \right)} \frac{y}{r^2} \left( 1 - 2y^2 + \frac{2x^2}{r^2} + \frac{4y^2}{r^2} \right) \]  

(68)

which are non-singular and agree with the formulae given by Lazar (2003) and Lazar and Maugin (2006a). In the limit \( \ell \to 0 \), we obtain in Eqs. (65)–(68) the classical expressions given by DeWit (1973b). As discussed by Lazar et al. (2006a), the dislocation core radius can be defined straightforwardly in the framework of gradient elasticity.
as \( R_c \approx 6 \ell \). If \( \ell \approx 0.4a \), where \( a \) denotes the lattice parameter, it is adopted as proposed by Eringen (1983), the dislocation core radius is \( R_c \approx 2.5a \). Using \( \ell \approx 0.4a \), the internal length reduces to \( \ell \approx 1.97 \text{ Å} \) for lead (Pb) with \( a = 4.95 \text{ Å} \).

Note that the two-dimensional Green function (63) gives the non-singular displacement field, \( u_i = -C_{ij}f_j \), of a line force with magnitude \( f_j \) calculated by Lazar and Maugin (2006b) in the framework of gradient elasticity.

3. Gradient elasticity of bi-Helmholtz type

In this section, gradient elasticity theory of higher order is considered. Gradient elasticity theory of higher order was originally introduced by Mindlin (1965); Mindlin (1972) (see also, Jauzemis, 1967; Wu, 1992; Agiasofitou and Lazar, 2009). Mindlin’s theory of second strain gradient elasticity involves for isotropic materials, in addition to the two Lamé constants, sixteen additional material constants. These constants produce four characteristic length scales.

A simple and robust gradient elasticity of higher order which is called gradient elasticity theory of bi-Helmholtz type was introduced by Lazar et al. (2006a) and Lazar and Maugin (2006a) and successfully applied to the problems of straight dislocations (Lazar et al., 2006a; Lazar and Maugin, 2006a), straight disclinations (Deng et al., 2007) and point defects (Zhang et al., 2006). Lazar et al., 2006a and Lazar and Maugin, 2006a have shown that all state quantities are non-singular. By means of this second order gradient theory it is possible to eliminate not only the singularities of the strain and stress tensors, but also the singularities of the double and triple stress tensors and of the dislocation density tensors of straight dislocations at the dislocation line. In general, all fields calculated in the theory of gradient elasticity of bi-Helmholtz type are smoother than those calculated by gradient elasticity theory of bi-Helmholtz type. In general, there are two main motivations for the use of gradient elasticity of bi-Helmholtz type: a consistent regularization of all state quantities, and a more realistic modelling of dispersion relations. A simple higher-order gradient theory in order to investigate dislocation loops should be used. The theory of gradient elasticity of bi-Helmholtz type is the gradient version of nonlocal elasticity of bi-Helmholtz type (Lazar et al., 2006b).

The strain energy density of gradient elasticity theory of bi-Helmholtz type for an isotropic, linear elastic material has the form (Lazar et al., 2006a)

\[
W = \frac{1}{2} C_{ijkl} \varepsilon_{ij} \varepsilon_{kl} + \frac{1}{2} \ell_2^2 C_{ijkl} \partial_i \varepsilon_{jkl} \partial_j \varepsilon_{kl} + \frac{1}{2} \ell_4^2 C_{ijkl} \partial_i \varepsilon_{jkl} \partial_j \varepsilon_{kl} \partial_k \varepsilon_{kl},
\]

where \( \ell_1, \ell_2, \) and \( \ell_4 \) are another characteristic length scale and \( C_{ijkl} \) is given in (3). Due to the symmetry of \( C_{ijkl} \), Eq. (69) is equivalent to

\[
W = \frac{1}{2} C_{ijkl} \varepsilon_{ij} \varepsilon_{kl} + \frac{1}{2} \ell_2^2 C_{ijkl} \partial_i \varepsilon_{jkl} \partial_j \varepsilon_{kl} + \frac{1}{2} \ell_4^2 C_{ijkl} \partial_i \varepsilon_{jkl} \partial_j \varepsilon_{kl} \partial_k \varepsilon_{kl},
\]

In addition to the constitutive Eqs. (10) and (11) another one is present in such a higher-order gradient theory,

\[
\tau_{ijkl} = \frac{\partial W}{\partial h_i h_j} = \frac{\partial W}{\partial \varepsilon_i \varepsilon_j} = \ell_3^2 C_{ijkl} \partial_i \varepsilon_{jkl} \partial_j \varepsilon_{kl} = \ell_3^2 \partial_i \varepsilon_{jkl} \partial_j \varepsilon_{kl},
\]

where \( \tau_{ijkl} \) is called the triple stress tensor. It can be seen that \( \ell_3 \) is the characteristic length scale for double stresses. On the other hand, \( \ell_1 \) is the characteristic length scale for double stresses. Using Eqs. (10), (11), and (71), Eq. (70) can also be written as (Lazar et al., 2006a)

\[
W = \frac{1}{2} \sigma_{ij} \varepsilon_{ij} + \frac{1}{2} \ell_2^2 \partial_i \sigma_{ij} \partial_j \varepsilon_{ij} + \frac{1}{2} \ell_4^2 \partial_i \sigma_{ij} \partial_j \varepsilon_{ij}.
\]

The strain energy density (72) exhibits the symmetry in \( \sigma_{ij} \) and \( \varepsilon_{ij} \), in \( \partial_i \sigma_{ij} \) and \( \partial_i \varepsilon_{ij} \), and in \( \partial_i \partial_j \sigma_{ij} \) and \( \partial_i \partial_j \varepsilon_{ij} \). The condition for non-negative strain energy density, \( W \geq 0 \), gives

\[
\ell_1^2 \geq 0, \quad \ell_2^2 \geq 0, \quad \ell_4^2 \geq 0.
\]

In addition to \((3\mu + 2\lambda) \geq 0\) and \( \mu \geq 0 \).

The total stress tensor reads now

\[
\sigma_{ij}^0 = \sigma_{ij} - \partial_i \tau_{ijk} + \partial_j \partial_k \tau_{ijk}.
\]

In absence of body forces, the equation of equilibrium has the following form

\[
\partial_i \sigma_{ij}^0 = \partial_i (\sigma_{ij} - \partial_k \tau_{ijk} + \partial_k \partial_l \tau_{ikl}) = 0.
\]

Using Eqs. (11) and (71), the total stress tensor (74) can be written

\[
\sigma_{ij}^0 = L \sigma_{ij},
\]

where the differential operator \( L \) is given by

\[
L = (1 - \ell_1^2 \Delta + \ell_2^2 \Delta^2) (1 - \ell_1^2 \Delta) (1 - \ell_1^2 \Delta^2)
\]

with

\[
\ell_1^2 = \frac{c_1^2}{2} \left( 1 + \sqrt{1 - 4 \frac{c_2^4}{c_1^4}} \right),
\]

\[
\ell_2^2 = \frac{c_2^2}{2} \left( 1 - \sqrt{1 - 4 \frac{c_1^4}{c_2^4}} \right),
\]

and

\[
\ell_4^2 = c_1^2 c_2^2.
\]

Due to its structure as a product of two Helmholtz operators, the differential operator (77) is called bi-Helmholtz operator.

An important point is, the question concerning the mathematical character of the length scales \( c_1 \) and \( c_2 \). Mindlin, 1965 (see also, Mindlin, 1972; Wu, 1992) pointed out that the conditions for non-negative \( W \) supply no indications of the character, real or complex, of the characteristic lengths. Mindlin (1965) and Wu (1992) have treated the characteristic lengths as if they were real and positive. They also pointed out that a complex character of the lengths is equally admissible. The character, real or complex, of the lengths dictates the behaviour of the field variables. In the theory of gradient elasticity of bi-Helmholtz type the condition for the character, real or complex, of the lengths scales \( c_1 \) and \( c_2 \) can be obtained from the condition if the argument of the square root in Eqs. (78) and (79) is positive or negative. Thus, \( c_1 \) and \( c_2 \) are real if

\[
\ell_1^2 - 4 \frac{c_1^4}{c_2^4} \geq 0,
\]

and \( c_1 \) and \( c_2 \) are complex if

\[
\ell_1^2 - 4 \frac{c_1^4}{c_2^4} < 0.
\]

If the lengths \( c_1 \) and \( c_2 \) are complex, then the behaviour of the solutions of the field quantities would be oscillatory. In this case, the far-field behaviour of the strain and stress fields of dislocations would not agree with the classical behaviour. The limit from gradient elasticity of bi-Helmholtz type to gradient elasticity of Helmholtz type is: \( c_2 \rightarrow 0, c_1 \rightarrow 0 \) and \( c_1 \rightarrow c_1 \). If \( c_1 \) is complex, then also \( \ell_1 \) becomes complex what would be rather strange. Thus, a real character of the length scales \( c_1 \) and \( c_2 \) seems to be more realistic and more physical. In addition, Zhang et al., 2006 determined, in an atomistic calculation, the length scales \( c_1 \) and \( c_2 \) as positive and real for graphene. In what follows, the length scales \( c_1 \) and \( c_2 \) will be treated as if they are real and positive.

The Green tensor of the bi-Helmholtz–Navier equation is calculated as (see Eq. (B.27))

\[
G_u(R) = \frac{1}{16 \pi \mu (1 - v)} \left[ 2(1 - v) \delta_0 \Delta - \partial_i \partial_j \right] A(R),
\]

where...
where the elementary function (25) is changed to
\[ A(R) = R + \frac{2(c_1^2 + c_2^2)}{R} - \frac{2}{c_1^2 - c_2^2} \left( e^{-c_1 R} - e^{-c_2 R} \right). \] (85)

Eq. (85) is the Green function of the three-dimensional bi-Helmholtz–bi-Laplace equation. It is worth noting that the Green tensor (84) with (85) is in agreement with the corresponding expression derived by Zhang et al. (2006). On the other hand, the Green function of the bi-Helmholtz equation is given by (e.g. Lazar et al., 2006b)
\[ G(R) = \frac{1}{4\pi(c_1^2 - c_2^2) R} \left( e^{-c_1 R} - e^{-c_2 R} \right). \] (86)

In the framework of gradient elasticity of bi-Helmholtz, the differential operator of bi-Helmholtz type (77) appears in Eqs. (15)–(18).

If we use Eqs. (A.9) and (A.10) for the differentiation of Eq. (84), we obtain the explicit form of the three-dimensional Green tensor of the bi-Helmholtz–Navier equation
\[ G_{ij}(R) = -\frac{1}{16\pi\mu(1-v)} \left\{ \frac{\delta_{ij}}{R} \left( 3 - 4v \right) \left( 1 - \frac{1}{c_1^2 - c_2^2} \left( c_{11}'e^{-c_1 R} - c_{22}'e^{-c_2 R} \right) \right) \ight. \\
\left. + \frac{2(c_1^2 + c_2^2)}{R^2} \right\} \\
\left. - \frac{1}{c_1^2 - c_2^2} \left( R^2 e^{c_1 R} - c_{11}'e^{-c_1 R} - c_{22}'e^{-c_2 R} \right) \ight. \\
\left. - \frac{2}{c_1^2 - c_2^2} \left( R^2 e^{c_2 R} - c_{22}'e^{-c_2 R} - c_{11}'e^{-c_1 R} \right) \right\} + \frac{R}{R^2} \left( 1 - \frac{6(c_1^2 + c_2^2)}{R^2} \right) \left[ \frac{1}{c_1^2 - c_2^2} \left( c_{11}'e^{-c_1 R} - c_{22}'e^{-c_2 R} \right) \right] \\
\left. + \frac{1}{c_1^2 - c_2^2} \left( c_{22}'e^{-c_1 R} - c_{11}'e^{-c_2 R} \right) \right\}. \] (87)

The Green tensor (87) gives the non-singular displacement field \( u_i = G_{ij} f_j \) of the Kelvin point force problem in the framework of gradient elasticity of bi-Helmholtz type.

### 3.1. Dislocation loops

The calculation of the characteristic fields of a dislocation loop in gradient elasticity of bi-Helmholtz type, is analogous to the technique used in gradient elasticity of Helmholtz type. The only difference in the results is that now the Green function (86) and the elementary function (85) of bi-Helmholtz type enter the characteristic fields of a dislocation loop. In gradient elasticity of bi-Helmholtz type, the dislocation density tensor (36) and the plastic distortion tensor (38) are given in terms of the Green function of bi-Helmholtz type (86). Thus, they are calculated as
\[ \gamma_0(x) = \frac{b_i}{4\pi(c_1^2 - c_2^2)} \int \frac{e^{-c_1 R} - e^{-c_2 R}}{R} \, dl, \] (88)
\[ \beta_0(x) = -\frac{b_i}{4\pi(c_1^2 - c_2^2)} \int \frac{e^{-c_1 R} - e^{-c_2 R}}{R} \, ds. \] (89)

In the limit \( R \to 0 \), the integrands of Eqs. (88) and (89) are non-singular at the dislocation line in contrast to the corresponding ones, Eqs. (37) and (39), calculated in gradient elasticity of Helmholtz type. On the other hand, the elastic distortion tensor (45), the elastic strain tensor (46), the elastic dilatation (47), the elastic rotation vector (48), the stress tensor (49), and the displacement vector (55) are given in terms of the elementary function (85) and only (85) has to be substituted in these formulæ. The explicit formulæ are not reproduced. The only difference between the fields of a dislocation loop in gradient elasticity of bi-Helmholtz type, and of Helmholtz type is that the Green function of bi-Helmholtz type (86) and the elementary function (85) have to be substituted instead of the Green function of Helmholtz type (28) and the elementary function (17). For the derivatives of the function (85), Eqs. (A.7)–(A.12) can be substituted into the corresponding formulæ.

The characteristic fields of a dislocation loop in gradient elasticity of bi-Helmholtz type retain all the analytical tensor structure of the corresponding classical formulæ.

The triple stress tensor of a dislocation loop is easily obtained if the stress tensor \( \sigma_{ij} \) is substituted into Eq. (71). In gradient elasticity of bi-Helmholtz type the fields produced by a dislocation loop are smoother than those predicted by gradient elasticity of Helmholtz type.

### 3.2. Straight dislocations

In this subsection, the modified Mura Equation (40) is used for gradient elasticity of bi-Helmholtz type. The technique of Green functions is used in order to determine the non-singular elastic distortion of straight dislocations.

#### 3.2.1. Screw dislocation

The Green function of the anti-plane strain problem in gradient elasticity of bi-Helmholtz type is the Green function of the two-dimensional bi-Helmholtz–Laplace equation and is given by (see Eq. (B.34))
\[ g_{al}(R) = -\frac{1}{2\pi R} \left\{ \frac{\gamma_0 + \ln R + \frac{1}{c_1^2 - c_2^2} [c_1 K_0(R/c_1) - c_2 K_0(R/c_2)]}{R} \right\}. \] (90)

where \( R = \sqrt{(x-x')^2 + (y-y')^2} \). The gradient of the Green function (90) is calculated as
\[ g_{al}(R) = -\frac{1}{2\pi R^2} \left\{ \frac{1}{c_1^2 - c_2^2} \left[ c_1 R K_1(R/c_1) - c_2 R K_1(R/c_2) \right] \right\}. \] (91)

If Eq. (91) and \( x''_{al} = b_i \delta(x) \delta(y) \) are substituted into Eq. (40), the elastic distortion produced by a screw dislocation with Burgers vector \( b_i \) is obtained
\[ \beta_{2x} = \frac{b_i}{2\pi R^2} \left\{ \frac{1}{c_1^2 - c_2^2} [c_1 R K_1(R/c_1) - c_2 R K_1(R/c_2)] \right\}, \] (92)
\[ \beta_{2y} = \frac{b_i}{2\pi R^2} \left\{ \frac{1}{c_1^2 - c_2^2} [c_2 R K_1(R/c_1) - c_1 R K_1(R/c_2)] \right\}, \] (93)

where \( r = \sqrt{x^2 + y^2} \). Eqs. (92) and (93) are in agreement with the expressions obtained by Lazar and Maugin (2006a).

The Green function (90) gives the non-singular displacement field \( u_i = -\varepsilon_{al} f_j \) of a line force with the magnitude \( f_j \) in the framework of gradient elasticity of bi-Helmholtz type.

#### 3.2.2. Edge dislocation

The plane strain problem of an edge dislocation is now investigated. The Green tensor of the plane strain problem in gradient elasticity of bi-Helmholtz type is found as (see Eq. (B.30))
\[ G_{al}(R) = -\frac{1}{2\pi R^2} \left\{ \frac{\gamma_0 + \ln R + \frac{1}{c_1^2 - c_2^2} [c_1 K_0(R/c_1) - c_2 K_0(R/c_2)]}{R} \right\} \\
+ \left\{ \frac{1}{16\pi R^4} R_{ik} \left\{ \frac{\gamma_0 + \ln R + 4(c_1^2 + c_2^2) \gamma_0 + \ln R}{c_1^2 - c_2^2} \right\} \right\}. \] (94)

The gradient of the Green tensor Eq. (94) is calculated as
If Eq. (95) and \( \alpha_2 = b(x)/\delta(y) \) are substituted into Eq. (40), the non-vanishing components of the elastic distortion of an edge dislocation are found as

\[
\beta_{xx} = -\frac{b_t}{4\pi(1-v)R^2} y \left( (1-2v) + \frac{2x^2}{R^2} + \frac{4(c_y^2 + c_z^2)}{R^4} (y^2 - 3x^2) \right)
\]

\[
- \frac{2(y^2 - 3x^2)}{R^2} \left( c_1 r K_1(r/c_1) - c_2 r K_1(r/c_2) \right)
\]

\[
+ \frac{2(x^2 - 3y^2)}{R^2} \left( c_1^2 r K_2(r/c_1) - c_2^2 r K_2(r/c_2) \right)
\]

\[
\beta_{xy} = -\frac{b_t}{4\pi(1-v)R^2} x \left( (3-2v) - \frac{2y^2}{R^2} + \frac{4(c_y^2 + c_z^2)}{R^4} (x^2 - 3y^2) \right)
\]

\[
- \frac{2(y^2 - (1-v)y^2)}{R^2} \left( c_1 r K_1(r/c_1) - c_2 r K_1(r/c_2) \right)
\]

\[
+ \frac{2(x^2 - 3y^2)}{R^2} \left( c_1^2 r K_2(r/c_1) - c_2^2 r K_2(r/c_2) \right)
\]

\[
\beta_{yy} = -\frac{b_t}{4\pi(1-v)R^2} y \left( (1-2v) - \frac{2x^2}{R^2} + \frac{4(c_y^2 + c_z^2)}{R^4} (y^2 - 3x^2) \right)
\]

\[
- \frac{2(y^2 - 3x^2)}{R^2} \left( c_1 r K_1(r/c_1) - c_2 r K_1(r/c_2) \right)
\]

\[
+ \frac{2(x^2 - 3y^2)}{R^2} \left( c_1^2 r K_2(r/c_1) - c_2^2 r K_2(r/c_2) \right)
\]

\[
\beta_{yy} = -\frac{b_t}{4\pi(1-v)R^2} y \left( (1-2v) - \frac{2x^2}{R^2} + \frac{4(c_y^2 + c_z^2)}{R^4} (y^2 - 3x^2) \right)
\]

\[
- \frac{2(y^2 - 3x^2)}{R^2} \left( c_1 r K_1(r/c_1) - c_2 r K_1(r/c_2) \right)
\]

\[
+ \frac{2(x^2 - 3y^2)}{R^2} \left( c_1^2 r K_2(r/c_1) - c_2^2 r K_2(r/c_2) \right)
\]

which are in agreement with the formulae given by Lazar and Maugin (2006a).

The two-dimensional Green function (94) gives the non-singular displacement field, \( u_i = -G_{jij} \), of a line force with magnitude \( f_j \) calculated in the framework of gradient elasticity of bi-Helmholtz type.

4. Conclusions

Non-singular dislocation fields are presented in the framework of gradient elasticity. The technique of Green functions is used. The Green tensors of all relevant partial differential equations of generalized Navier type were calculated. For the first time, the elastic distortion, plastic distortion, stress, displacement, and dislocation density of a closed dislocation loop, using the theories of gradient elasticity of Helmholtz type and of bi-Helmholtz type were calculated. Straight dislocations using Green tensors were revisited. Such generalized continuum theories allow dislocation core spreading in a straightforward manner. In classical dislocation theory the dislocation function is a Dirac delta function, \( \delta(x) \), without core spreading. In the non-singular approaches by Cai et al. (2006) and Lazar, presented in the present paper, the dislocation spreading functions are \( w \) and \( G \), respectively (see Table 1). In the theory of gradient elasticity all formulae are close in contrast to the theory of Cai et al. (2006) where the spreading function \( w \) is determined in a sophisticated way in order to obtain \( R_c = (R^2 + a^2)^{1/2} \). Due to the use of simplified theories of gradient elasticity, the dislocation fields retain most of the analytical structure of the classical expressions for these quantities but remove the singularity at the dislocation core due to the mathematical regularization of the classical singular expressions. In gradient elasticity of Helmholtz type, the characteristic length \( \ell \) takes into account the information from atomistic calculations as discussed in this paper. In a straightforward manner, the length \( \ell \) determines the dislocation core radius. Therefore, in gradient elasticity it is not necessary to introduce an artificial core-cutoff radius. It should be mentioned that the characteristic lengths which arise in first strain gradient elasticity (e.g. Maranganti and Sharma, 2007: Shodja and Tehranchi, 2010) and in second strain gradient elasticity (e.g. Zhang et al., 2006; Shodja et al., 2012) have been recently computed using atomistic approaches.

The obtained results can be used in computer simulations and numerics of dislocation cores, discrete dislocation dynamics, and arbitrary 3D dislocation configurations. The results can be implemented in dislocation dynamics codes (finite element implementation, technique of fast numerical sums), and compared to atomistic models (e.g. Choniem et al., 1999; Li and Wang, 2008).

Acknowledgements

The author gratefully acknowledges the grants from the Deutsche Forschungsgemeinschaft (Grant Nos. La1974/2-1, La1974/3-1). The author also wishes to thank Professor David A. Hills and two anonymous reviewers for their encouragement and comments.

Appendix A. Appendix: A and its derivatives

In gradient elasticity theory, the stress tensor, the elastic distortion tensor, the elastic strain tensor, and the displacement vector of a dislocation loop are given in terms of derivatives of the elementary function \( A \).

A.1. Helmholtz type

For gradient elasticity of Helmholtz type, the elementary function \( A \) is given by

\[
A = R + 2 \frac{\ell^2}{R} (1 - e^{-kR}).
\]

Higher-order derivatives of \( A \) are given by the following set of equations.
The expressions (A.1)–(A.6) are non-singular. For 

\[ A = R + \frac{2(c_1^2 + c_2^2)}{R} - \frac{2}{c_1^2 - c_2^2} \left( c_1^2 e^{-R/c_1} - c_2^2 e^{-R/c_2} \right), \]  

A.2. Bi-Helmholtz type

In gradient elasticity of bi-Helmholtz type, the elementary function \( A \) reads

\[ A = R + \frac{2(c_1^2 + c_2^2)}{R} - \frac{2}{c_1^2 - c_2^2} \left( c_1^2 e^{-R/c_1} - c_2^2 e^{-R/c_2} \right). \]  

The higher-order derivatives of \( A \) are given by

\[ A_i = R \left[ 1 - \frac{2(c_1^2 + c_2^2)}{R^2} + \frac{2}{c_1^2 - c_2^2} \left( c_1^2 e^{-R/c_1} - c_2^2 e^{-R/c_2} \right) \right. \]

and

\[ A_{ijk} = \frac{2R_k}{R^3} \left( -1 + \left( \frac{R}{R} \right) e^{-R/c_1} \right). \]  

The expressions (A.7)–(A.12) are non-singular. In the limit \( c_2 \to 0 \) and \( c_1 = \ell \), Eqs. (A.7)–(A.12) reduce to Eqs. (A.1)–(A.6).

Appendix B. Green tensors of generalized Navier equations

The following notation is used for the \( n \)-dimensional Fourier transform \( \text{Guelfand and Chilov, 1962} \)

\[ \tilde{f}(k) = \mathcal{F}(f(r)) = \int_{-\infty}^{\infty} f(r) e^{ikr} dr, \]

\[ f(r) = \mathcal{F}^{-1}(\tilde{f}(k)) = \frac{1}{(2\pi)^n} \int_{-\infty}^{\infty} \tilde{f}(k) e^{-ikr} dk. \]  

We have \( \text{Wladimirov, 1971; Nowacki, 1986} \)

\[ \mathcal{F}^{-1}\left[ \frac{1}{|k|^2} \right] = -\frac{1}{2\pi} \left( \gamma_0 + \ln \sqrt{x^2 + y^2} \right), \]

\[ \mathcal{F}^{-1}\left[ \frac{1}{|k|^2} \right] = \frac{1}{4\pi} \sqrt{x^2 + y^2 + z^2}, \]

\[ \mathcal{F}^{-1}\left[ \frac{1}{k^4 + \frac{1}{k^2}} \right] = \frac{1}{2\pi} K_0 \left( \sqrt{x^2 + y^2} / c \right), \]

\[ \mathcal{F}^{-1}\left[ \frac{1}{4\pi \sqrt{x^2 + y^2} + z^2} \right] = \exp \left( -\sqrt{x^2 + y^2} / c \right). \]

B.1. Green tensor of the Helmholtz–Navier equation

The Green tensor of the Helmholtz–Navier equation is defined by

\[ (1 - \ell^2 \Delta)(\mu \delta_{ab} \Delta + (\lambda + \mu) \partial_a \partial_b) G_0(r) = -\delta_{ij} \delta(r). \]  

The Fourier transform of Eq. (B.9) reads

\[ (1 + \ell^2 k^2) \left( \mu \delta_{ab} k^2 + (\lambda + \mu) k_k k_l \right) \tilde{G}_0(k) = \delta_{ij}, \]  

where \( \lambda = 2\nu / (1 - 2\nu) \) and \( \nu \) is Poisson’s ratio. The Fourier transformed Green tensor is found as

\[ \tilde{G}_0(k) = \frac{1}{\mu} \frac{\delta_{ij}}{|k|} - \frac{1}{2(1 - \nu)} \frac{k_k k_l}{|k|^2} \frac{1}{1 + \ell^2 k^2}. \]  

Using partial fractions and the inverse Fourier transform, we find

\[ \mathcal{F}^{-1}\left[ \frac{k_k k_l}{k^4 (1 + \ell^2 k^2)} \right] = -\partial_j \partial_i \mathcal{F}^{-1}\left[ \frac{1}{k^4 (1 + \ell^2 k^2)} \right] \]

and

\[ \partial_j \partial_i \mathcal{F}^{-1}\left[ \frac{1}{k^4 \left( k^2 + \frac{\ell^2}{k^2} \right)} \right] = \partial_j \partial_i \mathcal{F}^{-1}\left[ \frac{1}{k^4 \left( k^2 + \frac{\ell^2}{k^2} \right)} \right] \]

\[ = \partial_j \partial_i \left( \frac{r^2}{r} - \frac{2\ell^2}{r^2} e^{-r^2} \right). \]
the two-dimensional Green function is calculated as

$$G_\nu(r) = \frac{1}{16\pi\mu(1-v)} \left[ 2(1-v)\delta_\nu r + \partial_\nu \right] \left[ r + \frac{2r^2}{r}(1 - e^{-r/\ell}) \right],$$

(B.14)

where $r = \sqrt{x^2 + y^2 + z^2}$. On the other hand, using

$$\mathcal{F}^{-1}\left( \frac{k k_j}{k^2(1 + c_j^2 k^2)} \right) = -\partial_\nu \mathcal{F}^{-1}\left( \frac{1}{k^2(1 + c_j^2 k^2)} \right),$$

(B.15)

and

$$\mathcal{F}^{-1}\left( \frac{1}{k^2(1 + c_j^2 k^2)} \right) = \mathcal{F}^{-1}\left( \frac{1}{k^2 + \frac{\ell^2}{r}} \right) = \frac{1}{2\sqrt{\pi}} \left( r^2(\gamma_k + \ln r) + 4\ell^2(\gamma_k + \ln r + K_0(r/\ell)) \right),$$

(B.16)

the two-dimensional Green tensor of the Helmholtz–Navier equation is obtained as

$$G_\nu(r) = -\frac{1}{2\pi\mu} \delta_\nu \{ \gamma_k + \ln r + K_0(r/\ell) \} + \frac{1}{16\pi\mu(1-v)} \partial_\nu \{ r^2(\gamma_k + \ln r) + 4\ell^2(\gamma_k + \ln r + K_0(r/\ell)) \},$$

(B.17)

where $r = \sqrt{x^2 + y^2}$. 

B.2. Green function of the Helmholtz–Laplace equation

For the anti-plane strain problem, the Green tensor of the Navier–Helmholtz–Laplace equation reduces to the Green function of the two-dimensional Helmholtz–Laplace equation which is defined by

$$(1 - \ell^2 \Delta)\Delta G_{zz}(r) = -\frac{1}{\mu} \delta_\nu(r).$$

(B.18)

The Fourier transform of Eq. (B.18) reads

$$(1 + \ell^2 k^2)k^2 \tilde{G}_{zz}(k) = \frac{1}{\mu}$$

(B.19)

The Fourier transformed Green function is

$$\tilde{G}_{zz}(k) = \frac{1}{\mu k^2} \frac{1}{(1 + \ell^2 k^2)}.$$  

(B.20)

Using Eq. (B.16), the two-dimensional Green function is calculated as

$$G_{zz}(r) = -\frac{1}{2\pi\mu} \{ \gamma_k + \ln r + K_0(r/\ell) \}.$$

(B.21)

B.3. Green tensor of the bi-Helmholtz–Navier equation

The Green tensor of the bi-Helmholtz–Navier equation is defined by

$$(1 - c_i^2\Delta)(1 - c_i^2\Delta)(\mu \delta_\nu \Delta + (\lambda + \mu) \partial_\nu \partial_\nu) G_\nu(r) = -\delta_\nu \delta(r).$$

(B.22)

The Fourier transform of Eq. (B.22) reads

$$(1 + c_i^2 k^2)(1 + c_i^2 k^2) \left( \mu \delta_\nu k^2 + (\lambda + \mu) k k_\nu \right) \tilde{G}_\nu(k) = \delta_\nu.$$  

(B.23)

The Fourier space Green tensor is

$$\tilde{G}_\nu(k) = \frac{1}{\mu} \left[ \delta_\nu - \frac{1}{2(1-v)} \frac{k k_\nu}{k^2} \right] \frac{1}{(1 + c_i^2 k^2)(1 + c_i^2 k^2)}.$$  

(B.24)

Using

$$\mathcal{F}^{-1}\left( \frac{k k_\nu}{k^2(1 + c_i^2 k^2)(1 + c_i^2 k^2)} \right) = -\partial_\nu \mathcal{F}^{-1}\left( \frac{1}{k^2(1 + c_i^2 k^2)(1 + c_i^2 k^2)} \right)$$

$$= -\partial_\nu \mathcal{F}^{-1}\left( \frac{1}{k^2(1 + c_i^2 k^2)(1 + c_i^2 k^2)} \right)$$

(B.25)

and

$$\mathcal{F}^{-1}\left( \frac{1}{k^2(1 + c_i^2 k^2)(1 + c_i^2 k^2)} \right) = -\Delta \mathcal{F}^{-1}\left( \frac{1}{k^2(1 + c_i^2 k^2)(1 + c_i^2 k^2)} \right)$$

$$= \frac{\Delta}{8\pi} \left( r^2(\gamma_k + \ln r) + \frac{1}{c_i^2 - c_j^2} \left( c_i^2 k^2 + \frac{1}{k^2} - k^2 + \frac{1}{k^2} \right) \right).$$

(B.26)

the three-dimensional Green tensor of the bi-Helmholtz–Navier equation is found as

$$G_\nu(r) = \frac{1}{16\pi\mu(1-v)} \left[ 2(1-v)\delta_\nu r + \partial_\nu \right] \left[ r + \frac{2(r^2 + c_i^2)(c_i^2 - c_j^2)}{c_i^2 - c_j^2} \right]$$

(B.27)

where $r = \sqrt{x^2 + y^2 + z^2}$.  

In two dimensions, we use the formulae

$$\mathcal{F}^{-1}\left( \frac{1}{k^2(1 + c_i^2 k^2)(1 + c_i^2 k^2)} \right)$$

$$= \mathcal{F}^{-1}\left( \frac{1}{k^2 - c_i^2 k^2} \left( c_i^2 k^2 + \frac{1}{k^2} - k^2 + \frac{1}{k^2} \right) \right)$$

$$= \frac{1}{4\pi} \left( \gamma_k + \ln r + \frac{1}{c_i^2 - c_j^2} \left[ c_i^2 K_0(r/c_i) - c_j^2 K_0(r/c_j) \right] \right)$$

(B.28)

and

$$\mathcal{F}^{-1}\left( \frac{k k_\nu}{k^2(1 + c_i^2 k^2)(1 + c_i^2 k^2)} \right)$$

$$= -\partial_\nu \mathcal{F}^{-1}\left( \frac{1}{k^2(1 + c_i^2 k^2)(1 + c_i^2 k^2)} \right)$$

$$= -\partial_\nu \mathcal{F}^{-1}\left( \frac{1}{k^2 - c_i^2 k^2} \left( c_i^2 k^2 + \frac{1}{k^2} - k^2 + \frac{1}{k^2} \right) \right)$$

$$= \frac{\partial_\nu}{8\pi} \left( r^2(\gamma_k + \ln r) + 4(c_i^2 + c_j^2)(\gamma_k + \ln r) + \frac{4}{c_i^2 - c_j^2} \left[ c_i^2 K_0(r/c_i) - c_j^2 K_0(r/c_j) \right] \right).$$

(B.29)
Eventually, the two-dimensional Green tensor of the bi-Helmholtz–Navier equations is obtained as

\[
G_{0}(r) = \frac{1}{2\pi\mu} \delta_{ij} \left[ \gamma_{ij} + \ln r + \frac{1}{c_{1} - c_{2}} \left( c_{1}^{2}K_{0}(r/c_{1}) - c_{2}^{2}K_{0}(r/c_{2}) \right) \right] + \frac{1}{16\pi\mu(1 - \nu)} \partial_{ij} \left[ R \left( \gamma_{ij} + \ln r \right) + 4\left( c_{1}^{2} + c_{2}^{2} \right) \right] + \frac{4}{c_{1} - c_{2}} \left[ c_{1}^{2}K_{0}(r/c_{1}) - c_{2}^{2}K_{0}(r/c_{2}) \right].
\]  

(B.30)

B.4. Green function of the bi-Helmholtz-Laplace equation

For the anti-plane strain problem, the Green tensor of the Navier–Helmholtz–Laplace equation reduces to the Green function of the two-dimensional bi-Helmholtz-Laplace equation which is defined by

\[
(1 - c_{1}^{2})\Delta(1 - c_{2}^{2})\Delta G_{zz}(r) = -\frac{1}{\mu} \delta_{ij}(x).
\]  

(B.31)

The Fourier transform of Eq. (B.31) reads

\[
(1 + c_{1}^{2}k^{2})^{-1} \left[ 1 + c_{2}^{2}k^{2} \right] k^{2}G_{zz}(k) = \frac{1}{\mu}.
\]  

(B.32)

The Fourier transformed Green function is

\[
\tilde{G}_{zz}(k) = \frac{1}{\mu} k^{2} \left( 1 + c_{1}^{2}k^{2} \right) \left( 1 + c_{2}^{2}k^{2} \right).
\]  

(B.33)

Using Eq. (B.28), the two-dimensional Green function is obtained as

\[
G_{zz}(r) = \frac{1}{2\pi\mu} \left[ \gamma_{zz} + \ln r + \frac{1}{c_{1} - c_{2}} \left( c_{1}^{2}K_{0}(r/c_{1}) - c_{2}^{2}K_{0}(r/c_{2}) \right) \right].
\]  

(B.34)

References


