Line-integral representations for the elastic displacements, stresses and interaction energy of arbitrary dislocation loops in transversely isotropic bimaterials

J.H. Yuan, E. Pan, W.Q. Chen

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Abstract
The elastic displacements, stresses and interaction energy of arbitrarily shaped dislocation loops with general Burgers vectors in transversely isotropic bimaterials (i.e. joined half-spaces) are expressed in terms of simple line integrals for the first time. These expressions are very similar to their isotropic full-space counterparts in the literature and can be easily incorporated into three-dimensional (3D) dislocation dynamics (DD) simulations for hexagonal crystals with interfaces/surfaces. All possible degenerate cases, e.g. isotropic bimaterials and isotropic half-space, are considered in detail. The singularities intrinsic to the classical continuum theory of dislocations are removed by spreading the Burgers vector anisotropically around every point on the dislocation line according to three particular spreading functions. This non-singular treatment guarantees the equivalence among different versions of the energy formulae and consistency with the stress formula presented in this paper. Several numerical examples are provided as verification of the derived dislocation solutions, which further show significant influence of material anisotropy and bimaterial interface on the elastic fields and interaction energy of dislocation loops.

1. Introduction

It has been known for a long time that dislocations are the fundamental carriers of plastic deformation and are also responsible for the mechanical strength of crystalline solids (Taylor, 1934). As a powerful tool in mesoscale simulation, three-dimensional (3D) dislocation dynamics (DD) aims mainly at predicting macroscopic properties of crystals by directly simulating the interaction and evolution of large groups of discrete dislocation lines within crystals in response to external loads (Arsenlis et al., 2007; Cai et al., 2004; Devincre and Condat, 1992; Ghoniem and Sun, 1999; Ghoniem et al., 2000; Kubin et al., 1992; Kubin and Canova, 1992; Kubin, 1993; Rhee et al., 1998; Schwarz, 1999; Verdier et al., 1998; Wang et al., 2006; Zbib et al., 2000; Zbib et al., 1998). In 3D-DD simulations, dislocation lines are discretized into a set of straight or curved dislocation segments, and the most time-consuming computational task is to evaluate the interactions among all these dislocation segments with arbitrary orientations and general Burgers vectors. For the sake of computational simplicity and time efficiency, when dealing with such dislocation interactions, nearly all 3D-DD simulations assume linear-elastic isotropy (with the exception of Capolungo et al., 2010; Han et al., 2003; Rhee et al., 2001) in spite of the fact that most crystalline materials exhibit elastic anisotropy. For dislocations in isotropic bulk crystals which are far away from any external or internal interfaces (e.g. free surface, grain or phase boundary), simple analytical solutions for infinite solids can be utilized to compute the dislocation interactions efficiently (Blin, 1955; Cai et al., 2006; Devincre, 1995; de-Wit, 1960; Hills et al., 1996; Hirth and Lothe, 1982; Paynter et al., 2007; Peach and Koehler, 1950). When the dislocation lines are close to an interface, however, some special numerical methods are generally required to account for the influence of the interface on the elastic stress field and interaction energy of dislocations (Bulatov et al., 2000; Han et al., 2006).

Obviously, it would be very desirable to derive 3D analytical solutions as simple as those in infinite isotropic solids, which meanwhile take into consideration the effects of material anisotropy and crystal interface. The related issue has received a great deal of attention in recent years. Gosling and Willis (1994) deduced...
a line-integral representation for the stress field due to an arbitrarily shaped dislocation loop in an isotropic half-space via the Fourier transform. By virtue of Rongved’s solution (Rongved, 1955), Tan and Sun (2006) obtained a line-integral representation for the stress field due to a piecewise planar glide dislocation loop in isotropic bimaterials. Employing a general solution due to Walpole (1996) and Akarapu and Zbib (2009) derived line-integral solutions for the displacement and stress fields of an arbitrarily shaped dislocation loop in isotropic bimaterials. (Chu et al., 2012a,b) presented a line-integral expression for the elastic fields due to a dislocation loop of triangular shape in anisotropic bimaterials (or a half-space) using the Fourier transform technique. By introducing the hexagonal stress vector, Yu et al. (1995) derived analytical displacement solutions due to an infinitesimal dislocation loop of arbitrary orientation in transversely isotropic bimaterials. In 3D-DD simulations, another challenge originates from the requirement for accurate evaluations of the self-stress and self-energy of dislocations. According to the classical continuum theory of dislocations, there exist several different but equivalent versions of the energy formulae for infinite isotropic media (Blin, 1955; de Wit, 1960). These energy formulae are consistent with the stress formula of dislocations (de Wit, 1960; Hirth and Lothe, 1982) in the sense that the negative derivative of the energy with respect to the dislocation position is equal to the force produced by the stress through the Peach–Koehler formula (Peach and Koehler, 1950). However, the classical self-stress and self-energy expressions contain singularities due to the unrealistic assumption that the Burgers vector distribution is a delta function. Several attempts were made to remove such singularities since 1960s (Brown, 1964; Gavazza and Barnett, 1976; Hirth and Lothe, 1982; Lothe, 1992). Recently, Cai et al. (2006) proposed a non-singular, self-consistent continuum theory for computing the stress field and the elastic energy of dislocations in infinite isotropic media by spreading the Burgers vector isotropically around every point on the dislocation line according to a spreading function characterized by the spreading radius.

To the best of the authors’ knowledge, for arbitrarily shaped dislocation loops with general Burgers vectors in transversely isotropic bimaterials, explicit line-integral representations of the elastic displacements, stresses and interaction energy are still unavailable in the literature. As an extension to our recent work (Yuan et al., 2013), we attempt to fill this gap via the potential theory of linear elasticity and solve (i) the displacement and stress fields due to an arbitrarily shaped dislocation loop, and (ii) the interaction energy between two arbitrarily shaped dislocation loops in transversely isotropic bimaterials. The bimaterial considered in this paper consists of two dissimilar semi-infinite transversely isotropic solids either perfectly bonded together or in frictionless contact with each other at a planar interface which is parallel to the plane of isotropy of both solids. The expressions presented here are very similar to their isotropic full-space counterparts, and therefore can be easily incorporated into 3D-DD simulations for hexagonal crystals. Following Cai’s approach (Cai et al., 2006), we also develop a self-consistent method to remove the singularities of the self-stress and self-energy of dislocation loops in transversely isotropic media.

The present paper is organized as follows. In Section 2, the Green’s tensor for the non-degenerate or degenerate transversely isotropic bimaterials is expressed in a new, simple and unified form so that it is very suitable for later derivations of the dislocation solutions. In Section 3, based upon the obtained Green’s tensor, we derive line-integral expressions for the displacement and stress fields of an arbitrarily shaped dislocation loop and the interaction energy between two arbitrarily shaped dislocation loops in transversely isotropic bimaterials. In Section 4, we propose a non-singular, self-consistent approach for calculating the self-stress and self-energy of dislocations in transversely isotropic media. In Section 5, several numerical examples are provided to verify the formulations presented in this paper, and to reveal further the considerable influence of material anisotropy and bimaterial interface on the elastic field and interaction energy of dislocation loops. Concluding remarks are drawn in Section 6.

2. Green’s tensor for transversely isotropic bimaterials

In this paper, summation with respect to a repeated (or multi-repeated) index is assumed unless this index occurs on both sides of an equation. Also, the range of values of Roman indices (i,j,k etc.) is 1, 2, 3, and that of Greek ones (\(\alpha, \beta, \gamma\) etc.) is 1, 2, unless otherwise specified. For example, in the equation

\[ D_{ij} = A_{i}B_{j}C_{i,j}(l = 1,2,3) \]

is a free index without summation because it occurs on both sides of this equation, while \(\alpha\) is a dummy index which should be summed from 1 to 2 because it occurs only on the right-hand side of this equation and repeats itself three times. The single index \(j(=1,2,3)\) on the left-hand side of the above equation is also a free one which indicates that \(D_{11} = D_{22} = D_{33}\).

In Cartesian coordinates \((x_1, x_2, x_3)\), as shown in Fig. 1a, the bimaterial consists of two joined elastic half-spaces, one \((x_3 > 0)\) occupied by transversely isotropic material 1 and the other \((x_3 < 0)\) occupied by transversely isotropic material 2. These two half-spaces are either perfectly bonded together or in frictionless contact with each other at the planar interface \((x_3 = 0)\). The perfectly-bonded interface indicates the continuity of the displacement \(u\), the stresses \(\sigma_{ij}\), and the vanishing shear stresses \(\tau_{ij}\) at \(x_3 = 0\).

We suppose that the plane of isotropy of both materials is parallel to the bimaterial interface \((x_3 = 0)\). Then the elastic stiffness tensor of material \(\mu\) can be expressed as

\[
\begin{align*}
\mathbf{C}_{ij}^{(\mu)} &= A_{i}B_{j}C_{i,j}^{(\mu)} + A_{i}B_{j}C_{i,k}^{(\mu)}C_{k,j}^{(\mu)} + A_{i}B_{j}C_{i,l}^{(\mu)}C_{l,k}^{(\mu)}C_{k,j}^{(\mu)} + A_{i}B_{j}C_{i,k}^{(\mu)}C_{k,l}^{(\mu)}C_{l,j}^{(\mu)} \\
&\quad + A_{i}B_{j}C_{i,l}^{(\mu)}C_{l,k}^{(\mu)}C_{k,j}^{(\mu)} + A_{i}B_{j}C_{i,l}^{(\mu)}C_{l,k}^{(\mu)}C_{k,j}^{(\mu)} + A_{i}B_{j}C_{i,l}^{(\mu)}C_{l,k}^{(\mu)}C_{k,j}^{(\mu)} \\
&\quad + A_{i}B_{j}C_{i,l}^{(\mu)}C_{l,k}^{(\mu)}C_{k,j}^{(\mu)}
\end{align*}
\]

where \(\delta_{ij}\) is the Kronecker delta, and \(\alpha \Omega^{(\mu)} \quad (n = 1, 2, 3, 4, 5)\) is related to the contracted elastic stiffness constants as

\[
\begin{align*}
\alpha^{(2)} &= \alpha^{(1)} - 2\alpha^{(66)} , & \alpha^{(2)} &= \alpha^{(66)} \\
\alpha^{(3)} &= \alpha^{(1)} + \alpha^{(33)} - 2\alpha^{(13)} - 4\alpha^{(44)} \\
\alpha^{(4)} &= \alpha^{(1)} - \alpha^{(33)} + 2\alpha^{(13)} + 2\alpha^{(44)} , & \alpha^{(4)} &= \alpha^{(44)} - \alpha^{(66)}
\end{align*}
\]
For the sake of convenience, we first introduce some basic constants in terms of the contracted elastic stiffness constants (Ding et al., 2006; Fabrikant, 2004), i.e.,

\[
m_{ij}^{(0)} = -1 + \frac{c_{ij}^{(0)} c_{kl}^{(0)} - (c_{ij}^{(0)})^2}{2c_{kk}^{(0)} (c_{ij}^{(0)})^2} (3a)
\]

and

\[
\gamma_{ij}^{(0)} = \frac{1}{s_{ij}^{(0)}} = \frac{m_{ij}^{(0)} c_{kl}^{(0)} (c_{ij}^{(0)})^2}{m_{kj}^{(0)} c_{kl}^{(0)} + (c_{ij}^{(0)})^2}
\]

A transversely isotropic material is said to be non-degenerate if \(\gamma_{ij}^{(0)} \neq \gamma_{ij}^{(0,2)},\) i.e. \(m_{ij}^{(0)} \neq m_{ij}^{(2)};\) otherwise it is degenerate. Two useful relations among these basic constants are shown as follows (Fabrikant, 2004)

\[
m_{ij}^{(1)} = 1/m_{ij}^{(2)}
\]

\[
m_{ij}^{(1)} = m_{ij}^{(2)} = \Theta^{(i)} (\gamma_{ij}^{(0)} - \gamma_{ij}^{(0,2)}), \quad \Theta^{(i)} = c_{ij}^{(0)} (1 + \gamma_{ij}^{(0)} + \gamma_{ij}^{(0,2)}) / (c_{ij}^{(0)} + c_{kl}^{(0)})
\]

(4)

As is well-known, there exist many different but equivalent forms of the Green’s tensor for transversely isotropic bimaterials in the literature (Ding and Chen, 1997; Ding et al., 2006; Pan and Chou, 1979). However, for the sake of convenience in later derivations, it is necessary to express the Green’s tensor in an alternative way, as will be shown below.

Denote the Green’s tensor for transversely isotropic bimaterials by \(U_{ij}^{(3)}(y;x),\) which means the \(i\)-th component of the displacement vector at \(y\) \((y_1, y_2, y_3)\) in material \(\mu\), due to a unit force in the \(j\)-th direction applied at \(x\) \((x_1, x_2, x_3)\) in material \(\nu\). Using the image method, the Green’s tensor for transversely isotropic bimaterials can be expressed in terms of simple superposition of two individual parts as

\[
U_{ij}^{(3)}(y;x) = \delta_{ij} U_{ij}^{(0)}(y;x) + U_{ij}^{(3)}(y;x)
\]

(5)

where \(U_{ij}^{(0)}(y;x)\) is the Green’s tensor for a transversely isotropic full space occupied by material \(\mu\), while \(U_{ij}^{(3)}(y;x)\) accounts for contribution of the image sources due to the presence of bimaterial interface. According to the reciprocity theorem in linear elasticity, the following relations should be satisfied, i.e.

\[
U_{ij}^{(0)}(y;x) = U_{ij}^{(0)}(x;y) = U_{ij}^{(3)}(x;y)
\]

(6)

As a key advance in the bimaterial Green’s tensor, we express the two parts in Eq. (5) in a new, simple and unified way as

\[
\left\{ \begin{array}{l}
U_{ij}^{(0)}(y;x) \\
U_{ij}^{(0)}(x;y) \\
U_{ij}^{(3)}(y;x) \\
U_{ij}^{(3)}(x;y)
\end{array} \right\} = \frac{1}{4\pi c_{kl}^{(0)}} \frac{\partial^2}{\partial y^j \partial x^k} \left\{ \begin{array}{l}
\Psi_{ij}^{(0)}(y;x) \\
\Phi_{ij}^{(0)}(y;x) \\
\Psi_{ij}^{(3)}(y;x) \\
\Phi_{ij}^{(3)}(y;x)
\end{array} \right\}
\]

(7)

where

\[
\left\{ \Psi_{ij}^{(0)}(y;x) \right\} = \left\{ \begin{array}{l}
\psi_{ij}^{(0)}(y;x) - \psi_{ij}^{(0)}(y;x) \\
\psi_{ij}^{(0)}(y;x) - \psi_{ij}^{(0)}(y;x)
\end{array} \right\}
\]

\[
\left\{ \Psi_{ij}^{(3)}(y;x) \right\} = \left\{ \begin{array}{l}
\psi_{ij}^{(3)}(y;x) \\
\psi_{ij}^{(3)}(y;x)
\end{array} \right\}
\]

\[
\left\{ \Phi_{ij}^{(0)}(y;x) \right\} = \left\{ \begin{array}{l}
\phi_{ij}^{(0)}(y;x) - \phi_{ij}^{(0)}(y;x) \\
\phi_{ij}^{(0)}(y;x) - \phi_{ij}^{(0)}(y;x)
\end{array} \right\}
\]

\[
\left\{ \Phi_{ij}^{(3)}(y;x) \right\} = \left\{ \begin{array}{l}
\phi_{ij}^{(3)}(y;x) \\
\phi_{ij}^{(3)}(y;x)
\end{array} \right\}
\]

(8a)

\[
\left\{ \Phi_{ij}^{(0)}(y;x) \right\} = \left\{ \begin{array}{l}
\phi_{ij}^{(0)}(y;x) \\
\phi_{ij}^{(0)}(y;x)
\end{array} \right\}
\]

(8b)

\[
\{ \Phi_{ij}^{(0)}(y;x) \} \subseteq \{ \phi_{ij}^{(0)}(y;x) \} = H^{(0y)} \left\{ \begin{array}{l}
\phi_{ij}^{(0)}(y;x) \\
\phi_{ij}^{(0)}(y;x)
\end{array} \right\}
\]

(9a)

\[
\{ \Psi_{ij}^{(0)}(y;x) \} = \left\{ \psi_{ij}^{(0)}(y;x) - \psi_{ij}^{(0)}(y;x) \right\}
\]

(9b)

We emphasize that Eq. (7) is the main result in this section.

For the non-degenerate case of transversely isotropic bimaterials, we have (Ding et al., 2006)

\[
\left\{ \psi_{ij}^{(0)}(y;x) \right\} = \left\{ \psi_{ij}^{(0)}(y;x) - \psi_{ij}^{(0)}(y;x) \right\} = H^{(0y)} \left\{ \begin{array}{l}
\phi_{ij}^{(0)}(y;x) \\
\phi_{ij}^{(0)}(y;x)
\end{array} \right\}
\]

(10)

The symbol \(\psi_{ij}^{(0)}\) in Eqs. (9a,b) means that, without confusion, \(\psi_{ij}^{(0)}(y;x)\) and \(\psi_{ij}^{(0)}(y;x)\) can be written, respectively, as \(\psi_{ij}^{(0)}\) and \(\psi_{ij}^{(0)}\) for short, where \(n = 0, 1, 2, 3, 4\). Note that Eq. (10) suggests a simple relationship between the horizontal and vertical point force solutions for transversely isotropic bimaterials, and this has never appeared explicitly in the literature to the best of the authors’ knowledge.

The other unknown coefficients in Eqs. (9a,b) are determined by (Ding et al., 2006)

\[
H^{(0y)} = \gamma^{(0)}_{13} \quad H^{(0y)} = \frac{(-1)^{n+1}}{m_{ij}^{(2)} (m_{ij}^{(0)} - m_{ij}^{(2)})}
\]

(11)

and

\[
\left\{ \begin{array}{l}
p_{ij}^{(3)}(y;x) \\
p_{ij}^{(3)}(x;y)
\end{array} \right\} \subseteq \left\{ \begin{array}{l}
\psi_{ij}^{(3)}(y;x) - \psi_{ij}^{(3)}(y;x) \\
\psi_{ij}^{(3)}(y;x) - \psi_{ij}^{(3)}(y;x)
\end{array} \right\}
\]

(12a)

\[
\left\{ \begin{array}{l}
p_{ij}^{(3)}(y;x) \\
p_{ij}^{(3)}(x;y)
\end{array} \right\} \subseteq \left\{ \begin{array}{l}
p_{ij}^{(3)}(y;x) - \psi_{ij}^{(3)}(y;x) \\
p_{ij}^{(3)}(y;x) - \psi_{ij}^{(3)}(y;x)
\end{array} \right\}
\]

(12b)

for the perfectly-bonded interface, and

\[
p_{ij}^{(3)}(y;x) = 1, \quad p_{ij}^{(3)}(y;x) = 0
\]

(13a)
for the interface in frictionless contact, where

\[
\rho^{(i)}_{p} = \frac{\rho^{(i)}}{C_0}, \quad \rho^{(i)}_{p} = m^{(i)} \rho^{(i)}_{p}, \quad \rho^{(i)}_p = (m^{(i)} + 1) \rho^{(i)}_{p}, \quad \rho^{(i)}_p = m^{(i)} + 1
\]  

Also in Eqs. (9a,b), the so-called potential functions are defined as (Ding et al., 2006; Fabrikant, 2004)

\[
\chi^{(i)}_p(y, x) = \left\{ \begin{array}{ll}
+z^{(i)}_p \ln (R^{(i)}_y + z^{(i)}_y) - R^{(i)}_y & \text{if } R^{(i)}_y + z^{(i)}_y 
eq 0 \\
-z^{(i)}_p \ln (R^{(i)}_y - z^{(i)}_y) - R^{(i)}_y & \text{if } R^{(i)}_y - z^{(i)}_y 
eq 0 \\
0 & \text{otherwise}
\end{array} \right.
\]  

or

\[
\chi^{(i)}_p(y, x) = \left\{ \begin{array}{ll}
+z^{(i)}_p \ln (R^{(i)}_y + z^{(i)}_y) - R^{(i)}_y & \text{if } R^{(i)}_y + z^{(i)}_y 
eq 0 \\
-z^{(i)}_p \ln (R^{(i)}_y - z^{(i)}_y) - R^{(i)}_y & \text{if } R^{(i)}_y - z^{(i)}_y 
eq 0 \\
0 & \text{otherwise}
\end{array} \right.
\]

where

\[
R^{(i)}_y = (y - x)^2 + (y - x)^2 + (z^{(i)}_y)^2
\]

\[
R^{(i)}_y = (y - x)^2 + (y - x)^2 + (z^{(i)}_y)^2
\]

and

\[
\zeta^{(i)}_y = \zeta^{(i)}_y(y, x) = \zeta^{(i)}_y(x, y)
\]

\[
\zeta^{(i)}_y = \zeta^{(i)}_y(y, x) = \zeta^{(i)}_y(x, y)
\]

The potential functions shown in Eq. (15) are quasi-harmonic and satisfy the following basic relations

\[
\gamma^{(i)}_{y} = \frac{\partial^2}{\partial y^2} \chi^{(i)}_p = -\frac{\partial^2}{\partial y^2} \chi^{(i)}_p = \frac{1}{R^{(i)}_y}
\]

\[
\gamma^{(i)}_{y} = \frac{\partial^2}{\partial y^2} \chi^{(i)}_p = -\frac{\partial^2}{\partial y^2} \chi^{(i)}_p = \frac{1}{R^{(i)}_y}
\]

and

\[
\frac{\partial}{\partial y} \chi^{(i)}_p = -\frac{\partial}{\partial y} \chi^{(i)}_p, \quad \frac{\partial^2}{\partial y^2} \chi^{(i)}_p = \frac{\partial^2}{\partial y^2} \chi^{(i)}_p
\]

\[
\frac{\partial}{\partial y} \chi^{(i)}_p = -\frac{\partial}{\partial y} \chi^{(i)}_p, \quad \frac{\partial^2}{\partial y^2} \chi^{(i)}_p = \frac{\partial^2}{\partial y^2} \chi^{(i)}_p
\]

Note that the double indices \(ij\) in Eqs. (15)–(18b) only take the combinations \(12\) or \(23\).

We emphasize that, throughout this paper, multi-valued functions \(lnz\) and \(\gamma^z\) take values in their own single-valued analytic branches which satisfy, respectively, \(-\pi < lnz < \pi\) and \(-\pi < \arg z < \pi\), where “Re” or “Im” denotes the real or imaginary part of a complex number, and “arg” means its argument.

For future applications, we now write Eq. (9b) in another way.

With aid of Eqs. (4) and (14), we can solve Eqs. (12b) and (13b) by Cramer’s rule as

\[
P^{(i)}_{23} = \frac{1}{\Lambda^{(i)}} \left( \begin{array}{c}
1 - \frac{1}{\gamma_1^{(i)}}
\end{array} \right)
\]

in which

\[
\Lambda^{(i)} = \left| \begin{array}{ccc}
\rho^{(i)}_1 & 1 & 0 \\
0 & \rho^{(i)}_2 & 0 \\
0 & 0 & \rho^{(i)}_p
\end{array} \right|
\]

\[
\Lambda^{(i)} = \left| \begin{array}{ccc}
\rho^{(i)}_1 & 1 & 0 \\
0 & \rho^{(i)}_2 & 0 \\
0 & 0 & \rho^{(i)}_p
\end{array} \right|
\]  

(20a)

\[
P^{(i)}_{23} = \left( \begin{array}{c}
1 - \frac{1}{\gamma_1^{(i)}}
\end{array} \right)
\]

(20b)

for the perfectly-bonded interface, and

\[
P^{(i)}_{23} = \left( \begin{array}{c}
1 - \frac{1}{\gamma_1^{(i)}}
\end{array} \right)
\]

(21b)

for the interface in frictionless contact.

The unknown constants in Eqs. (20a)–(21b) are defined as

\[
\frac{\rho^{(i)}_1 - \rho^{(i)}_2}{\rho^{(i)}_1 - \rho^{(i)}_2} = E^{(i)}(\gamma_1^{(i)} - \gamma_2^{(i)}), \quad E^{(i)} = \frac{\gamma_1^{(i)}(\gamma_1^{(i)} - \gamma_2^{(i)})}{\gamma_1^{(i)} - \gamma_2^{(i)}}
\]

\[
\omega^{(i)}_1 - \omega^{(i)}_2 = W^{(i)}(\gamma_1^{(i)} - \gamma_2^{(i)}), \quad W^{(i)} = \frac{\gamma_1^{(i)}(\gamma_1^{(i)} - \gamma_2^{(i)})}{\gamma_1^{(i)} - \gamma_2^{(i)}}
\]

(22)

After substitution of Eqs. (10), (11) and (19) into Eq. (9b), we thus obtain

\[
\psi^{(i)}_1 = \frac{1}{\Lambda^{(i)}} \left( \begin{array}{c}
\gamma_1^{(i)} - \gamma_2^{(i)}
\end{array} \right)
\]

\[
\psi^{(i)}_1 = \frac{1}{\Lambda^{(i)}} \left( \begin{array}{c}
\gamma_1^{(i)} - \gamma_2^{(i)}
\end{array} \right)
\]

\[
(q = 1, 2, 3, 4)
\]

in which

\[
T^{(i)}_{1,2} = \frac{\gamma_1^{(i)}}{m^{(i)}}, \quad T^{(i)}_{1,2} = \frac{\gamma_1^{(i)}}{m^{(i)}}, \quad T^{(i)}_{1,2} = \frac{\gamma_1^{(i)}}{m^{(i)}}, \quad T^{(i)}_{1,2} = \frac{\gamma_1^{(i)}}{m^{(i)}}, \quad T^{(i)}_{1,2} = \frac{\gamma_1^{(i)}}{m^{(i)}}
\]

(23)

While Eq. (23) is obtained based on the assumption of non-degenerate property of transversely isotropic bimatrices, it is actually valid for all possible degenerate cases after proper limiting processes. The main steps as well as the final result are shown in Appendix A. In other words, no matter if the transversely isotropic bimaternal is non-degenerate or not, the Green’s tensor has exactly the same structure as given in Eqs. (5), (7) and (8a,b). This will lead to a simple and unified derivation of the dislocation solutions in the next section.
3. Line-integral representations for the elastic fields and interaction energy of arbitrary dislocation loops in transversely isotropic bimaterials

3.1. Displacement field of an arbitrarily shaped dislocation loop

According to the theory of dislocations, the elastic displacement field induced by a dislocation loop C of arbitrary shape, which bounds some curved surface A in transversely isotropic bimaterials (Fig. 1b), can be expressed as (Hirth and Lothe, 1982)

\[ u_{m}^{ij}(\mathbf{x}) = -\int_{A} d\mathbf{A}_{k}b\varepsilon_{ik}^{(j)} \frac{\partial}{\partial y_{l}} u_{m}^{ij}(\mathbf{y}; \mathbf{x}) \]  

(25)

where \( u_{m}^{ij}(\mathbf{x}) \) is the mth component of the displacement vector at \( \mathbf{x} = (x_1, x_2, x_3) \) in material \( \mu \) due to a dislocation loop located completely within material \( \lambda \). \( \varepsilon_{ik}^{(j)} \) is the jth component of the Burgers vector \( \mathbf{b} \), and \( d\mathbf{A}_{k} \) at \( \mathbf{y} = (y_1, y_2, y_3) \) is the ith component of the vector area element \( d\mathbf{A} \). The positive normal of \( d\mathbf{A} \) is associated with the positive direction of the dislocation curve according to the right-hand rule (Fig. 1b).

Substituting Eqs. (1), (5), (7) and (8a,b) into Eq. (25) and utilizing the Stokes’ theorem (Mura, 1987)

\[ \int_{A} (\varepsilon_{ik}^{(j)} \frac{\partial}{\partial y_{l}} u_{m}^{ij}(\mathbf{y}; \mathbf{x}) - \frac{\partial}{\partial y_{l}} (\varepsilon_{ik}^{(j)} u_{m}^{ij}(\mathbf{y}; \mathbf{x}) d\mathbf{A}_{k} = \int_{C} \varepsilon_{ik}^{(j)} d\mathbf{A}_{k} \frac{\partial}{\partial y_{l}} \phi(\mathbf{y}) d\mathbf{y}_{k} \]  

(26)

we finally obtain the elastic displacement field of an arbitrarily shaped dislocation loop with a general Burgers vector as

\[ u_{m}^{ij}(\mathbf{x}) = \delta_{ij}U_{m}^{ij}(\mathbf{x}) + U_{m}^{ij}(\mathbf{x}) \]  

(27)

where \( U_{m}^{ij}(\mathbf{x}) \) denotes the displacement field of an arbitrarily shaped dislocation loop in a transversely isotropic full space occupied by material \( \lambda \), while \( U_{m}^{ij}(\mathbf{x}) \) accounts for contributions of the image sources due to the presence of a bimaterial interface. Both of them can be expressed in terms of line integrals as

\[ \begin{align*}
U_{m}^{ij}(\mathbf{x}) &= -\frac{1}{4\pi} \int_{\Gamma} \frac{\varepsilon_{ik}^{(j)} u_{m}^{ij}(\mathbf{y}; \mathbf{x})}{(\gamma_{ij})^2} d\mathbf{A}_{k} \frac{\partial}{\partial y_{l}} \psi_{0}(\mathbf{y}) \left( \begin{array}{c}
\psi_{0}^{i} \\
\psi_{0}^{j}
\end{array} \right) \\
U_{m}^{ij}(\mathbf{x}) &= -\frac{1}{4\pi} \int_{\Gamma} \frac{\varepsilon_{ik}^{(j)} u_{m}^{ij}(\mathbf{y}; \mathbf{x})}{(\gamma_{ij})^2} d\mathbf{A}_{k} \frac{\partial}{\partial y_{l}} \psi_{0}(\mathbf{y}) \left( \begin{array}{c}
\psi_{0}^{i} \\
\psi_{0}^{j}
\end{array} \right)
\end{align*} \]  

(28)

where \( \varepsilon_{ik} \) is the permutation tensor, and

\[ \begin{align*}
\Omega_{m}^{ij}(\mathbf{x}) &= \int_{A} d\mathbf{A}_{k} \frac{\partial}{\partial y_{l}} \psi_{0}(\mathbf{y}) \left( \begin{array}{c}
\frac{\partial}{\partial y_{l}} \gamma_{ij}^{(k)} \\
\frac{\partial}{\partial y_{l}} \gamma_{ij}^{(m)}
\end{array} \right) \\
\Omega_{m}^{ij}(\mathbf{x}) &= \int_{A} d\mathbf{A}_{k} \frac{\partial}{\partial y_{l}} \psi_{0}(\mathbf{y}) \left( \begin{array}{c}
\frac{\partial}{\partial y_{l}} \gamma_{ij}^{(k)} \\
\frac{\partial}{\partial y_{l}} \gamma_{ij}^{(m)}
\end{array} \right)
\end{align*} \]  

(29a)

and

\[ \begin{align*}
\left\{ \begin{array}{c}
U_{m}^{ij}(\mathbf{y}; \mathbf{x}) \\
U_{m}^{ij}(\mathbf{y}; \mathbf{x})
\end{array} \right\} &= \left( \frac{\partial}{\partial y_{l}} \right) \left( \begin{array}{c}
\psi_{0}^{i} \\
\psi_{0}^{j}
\end{array} \right) \\
\left\{ \begin{array}{c}
\frac{\partial}{\partial y_{l}} \psi_{0}^{i} \\
\frac{\partial}{\partial y_{l}} \psi_{0}^{j}
\end{array} \right\}
\end{align*} \]

(29b)

Note that the line integrals in Eq. (28) are integrated along the positive direction of the closed dislocation loop. The area integral \( \Omega_{m}^{ij}(\mathbf{x}) \) shown in Eq. (29a) is the quasi-solid angle subtended by the cut surface of the dislocation loop in material \( \lambda \) at point \( \mathbf{x} \), which can also be transformed into a line integral (For further details, see Yuan et al., 2013.)

In the above derivation, use has been made of both the quasi-harmonic property and spatial symmetry of potential functions as given in Eqs. (18a,b), respectively, and the variants of Eq. (3b) as follows

\[ \begin{align*}
(a_{2}^{(k)} + a_{3}^{(k)})m_{j}^{(k)}(\gamma_{j}^{(k)})^2 + (a_{1}^{(k)} + a_{2}^{(k)} + a_{4}^{(k)})m_{j}^{(k)}(\gamma_{j}^{(k)})^2 &= (a_{1}^{(k)} + 2a_{2}^{(k)} + a_{3}^{(k)} + 2a_{4}^{(k)} + 4a_{5}^{(k)})m_{j}^{(k)}; \\
(a_{2}^{(k)} + a_{4}^{(k)}) + (a_{1}^{(k)} + a_{2}^{(k)} + a_{4}^{(k)} + a_{5}^{(k)})m_{j}^{(k)} &= (a_{1}^{(k)} + 2a_{2}^{(k)})(\gamma_{j}^{(k)})^2; \\
(a_{2}^{(k)} + a_{3}^{(k)}) &= a_{2}^{(k)}(\gamma_{j}^{(k)})^2
\end{align*} \]  

(30)

As verification, in the special case of an isotropic full-space, Eq. (28) reduced to the well-known Burgers’ formula (Burgers, 1939; Hirth and Lothe, 1982) due to the fact that

\[ \Omega_{m}^{ij}(\mathbf{x}) \rightarrow \Omega_{m}^{ij}(\mathbf{x}); \quad U_{m}^{ij}(\mathbf{y}; \mathbf{x}) \rightarrow \frac{R}{2(1-\nu^{2})} \]  

(31)

where \( \Omega_{m}^{ij}(\mathbf{x}) \) is the classical solid angle, \( R(=R(\mathbf{y}; \mathbf{x})) \) is the distance between two points \( \mathbf{y} \) and \( \mathbf{x} \), and \( \nu^{2} \) is the Poisson’s ratio of material \( \lambda \).

3.2. Stress field of an arbitrarily shaped dislocation loop

Let \( \sigma_{ij}^{(p)(k)}(\mathbf{x}) \) denote the stress tensor at \( \mathbf{x} = (x_1, x_2, x_3) \) in material \( \mu \) due to an arbitrarily shaped dislocation loop located completely within material \( \lambda \). Using the stress–strain relation, we can derive from Eq. (27) that

\[ \sigma_{ij}^{(p)(k)}(\mathbf{x}) = \delta_{ij}S_{ij}^{(k)}(\mathbf{x}) + S_{ij}^{(p)(k)}(\mathbf{x}) \]  

(32)

where

\[ S_{ij}^{(k)}(\mathbf{x}) = \varepsilon_{ij}^{(k)} \frac{\partial}{\partial y_{l}} U_{k}^{(ij)}(\mathbf{x}) \]  

(33)

In Eq. (33), \( S_{ij}^{(k)}(\mathbf{x}) \) denotes the stress field of an arbitrarily shaped dislocation loop in a transversely isotropic full space occupied by material \( \lambda \), while \( S_{ij}^{(p)(k)}(\mathbf{x}) \) accounts for the contribution of the image sources due to the presence of the bimaterial interface. By virtue of Eq. (28), both of them can be expressed in terms of line integrals as
functions as given in Eqs. (18a,b), and the identity/relation as

\[(34)\]

\[\begin{align*}
S_{p,q}^{(i)}(\mathbf{x}) &= -\frac{G_{0}}{4\pi} \int_{C} b_{i} e_{i p q} dy_{p} + e_{i p q} dy_{p} \left\{ \frac{\partial}{\partial y_{j}} S_{p,q}^{(i)}(\mathbf{y}; \mathbf{x}) \right\} \\
&\quad - \frac{G_{0}}{4\pi} \int_{C} b_{i} e_{i p q} dy_{p} \left\{ \frac{\partial^{2}}{\partial x_{i} \partial y_{j}} S_{p,q}^{(i)}(\mathbf{y}; \mathbf{x}) \right\} \\
&\quad + \frac{G_{0}}{4\pi} \int_{C} b_{i} e_{i p q} dy_{p} \frac{\partial^{2}}{\partial x_{i} \partial y_{j}} S_{p,q}^{(i)}(\mathbf{y}; \mathbf{x}) \\
&\quad + \frac{\partial^{2}}{\partial x_{j}^{2}} \left\{ \frac{\partial}{\partial y_{j}} \frac{1}{R} S_{p,q}^{(i)}(\mathbf{y}; \mathbf{x}) \right\} + \frac{\partial}{\partial y_{j}} \frac{1}{R} S_{p,q}^{(i)}(\mathbf{y}; \mathbf{x}) \\
&\quad - \frac{1}{R} S_{p,q}^{(i)}(\mathbf{y}; \mathbf{x}) \to \frac{1}{R}, \quad \frac{\partial}{\partial y_{j}} \frac{1}{R} S_{p,q}^{(i)}(\mathbf{y}; \mathbf{x}) \to \frac{R}{1 - \nu^{(i)}}, \quad \text{when } \frac{1}{R} \to 1 (39)
\end{align*}\]

where \(R \) and \( \nu^{(i)} \) are defined the same as those in Eq. (31), and \( G^{(i)} \) is the shear modulus of material \( i \).

### 3.3. Interaction energy between two arbitrarily shaped dislocation loops

Suppose that \( C \) is an arbitrarily shaped dislocation loop with Burgers vector \( \mathbf{b} \) which is located completely within material \( \lambda \) and bounds some curved surface \( \Lambda \), whilst \( \tilde{C} \) is another arbitrarily shaped dislocation loop with Burgers vector \( \mathbf{b} \) which is located completely within material \( \mu \) and bounds some curved surface \( \Lambda \). According to the theory of dislocations (Hirth and Lothe, 1982), if a second loop \( \tilde{C} \) is created while the first loop \( C \) is present, then the interaction energy between these two dislocation loops can be expressed as

\[W_{I}^{(i)(i)}(\tilde{C}, C) = \delta_{i\mu} W_{I}^{(i)(\tilde{C}, C)} + W_{I}^{(i)(i)}(\tilde{C}, C)
\]

in which

\[W_{I}^{(i)(i)}(\tilde{C}, C) = \int_{\Lambda} dA_{\tilde{C}} b_{i} S_{p,q}^{(i)}(\mathbf{x}), \quad W_{I}^{(i)(i)}(\tilde{C}, C) = \int_{\Lambda} dA_{\tilde{C}} b_{i} S_{p,q}^{(i)}(\mathbf{x})
\]

where \( S_{p,q}^{(i)}(\mathbf{x}) \) and \( S_{p,q}^{(i)}(\mathbf{x}) \) are the stress field of loop \( C \), as given in Eq. (34).

In Eq. (41), \( W_{I}^{(i)(i)}(\tilde{C}, C) \) denotes the interaction energy between two arbitrarily shaped dislocation loops \( \tilde{C} \) and \( C \) in a transversely isotropic full-space occupied by material \( \lambda \), while \( W_{I}^{(i)(i)}(\tilde{C}, C) \) accounts for the contribution of the image sources due to the presence of bimaterial interface. According to the reciprocity theorem in linear elasticity, the following relations should be satisfied, i.e.

\[W_{I}^{(i)(i)}(\tilde{C}, C) = W_{I}^{(i)(i)}(C, \tilde{C}), \quad W_{I}^{(i)(i)}(\tilde{C}, C) = W_{I}^{(i)(i)}(C, \tilde{C})
\]

Substituting Eq. (34) into Eq. (41) and utilizing the Stokes’ theorem given in Eq. (26), we finally obtain the interaction energy in terms of double line integrals as

\[\begin{align*}
W_{I}^{(i)(i)}(\tilde{C}, C) &= \left\{ \frac{S_{p,q}^{(i)}(\mathbf{x})}{W_{I}^{(i)(i)}(\tilde{C}, C)} \right\} = \left\{ \frac{W_{I}^{(i)}(\mathbf{x})}{W_{I}^{(i)(i)}(\tilde{C}, C)} \right\} \\
&\quad - \frac{G_{0}}{4\pi} \int_{C} b_{i} e_{i p q} \left\{ \frac{\partial}{\partial y_{j}} S_{p,q}^{(i)(i)}(\mathbf{x}) \right\} \\
&\quad - \frac{G_{0}}{4\pi} \int_{C} b_{i} e_{i p q} \left\{ \frac{\partial^{2}}{\partial x_{i} \partial y_{j}} S_{p,q}^{(i)(i)}(\mathbf{x}) \right\} \\
&\quad + \frac{G_{0}}{4\pi} \int_{C} b_{i} e_{i p q} \frac{\partial^{2}}{\partial x_{i} \partial y_{j}} S_{p,q}^{(i)(i)}(\mathbf{x})
\end{align*}\]

in which

\[\begin{align*}
\left\{ \begin{array}{l}
W_{I}^{(i)}(\mathbf{x}) \\
W_{I}^{(i)(i)}(\mathbf{x})
\end{array} \right\} = \left\{ \begin{array}{l}
W_{I}^{(i)}(\mathbf{x}) \\
W_{I}^{(i)(i)}(\mathbf{x})
\end{array} \right\} \\
\left\{ \begin{array}{l}
W_{I}^{(i)}(\mathbf{x}) \\
W_{I}^{(i)(i)}(\mathbf{x})
\end{array} \right\} = \left\{ \begin{array}{l}
W_{I}^{(i)}(\mathbf{x}) \\
W_{I}^{(i)(i)}(\mathbf{x})
\end{array} \right\}
\end{align*}\]

In the above derivation, use has been made of both the quasi-harmonic property and spatial symmetry of the potential functions as given in Eqs. (18a,b), and the identity/relation as follows

\[\delta_{\lambda\mu} e_{i p q} - \delta_{\lambda\mu} e_{i p q} = \delta_{\lambda\mu} e_{i p q}
\]

\[\int_{C} e_{i p q} dy_{p} \left\{ \frac{\partial}{\partial y_{j}} S_{p,q}^{(i)(i)}(\mathbf{x}) \right\} = \int_{C} e_{i p q} dy_{p} \left\{ \frac{\partial}{\partial y_{j}} S_{p,q}^{(i)(i)}(\mathbf{x}) \right\} + \int_{C} e_{i p q} dy_{p} \left\{ \frac{\partial}{\partial y_{j}} S_{p,q}^{(i)(i)}(\mathbf{x}) \right\}
\]

Eq. (37) can be easily proved by using the Stokes’ theorem given in Eq. (26).

As verification, in the special case of an isotropic full-space, Eq. (34) reduced to the classical stress formula as follows (deWit, 1960; Hirth and Lothe, 1982)

\[S_{p,q}^{(i)}(\mathbf{x}) = \frac{G_{0}}{4\pi} \int_{C} b_{i} e_{i p q} dy_{p} + e_{i p q} dy_{p} \left\{ \frac{\partial}{\partial y_{j}} S_{p,q}^{(i)}(\mathbf{y}; \mathbf{x}) \right\} \\
\times \int_{C} b_{i} e_{i p q} dy_{p} \left\{ \frac{\partial^{2}}{\partial y_{j} \partial y_{k}} S_{p,q}^{(i)}(\mathbf{y}; \mathbf{x}) \right\}
\]

due to the fact that

\[\int_{C} e_{i p q} dy_{p} \left\{ \frac{\partial}{\partial y_{j}} S_{p,q}^{(i)}(\mathbf{x}) \right\} = \int_{C} d\theta_{i p q} \left\{ \frac{\partial}{\partial y_{j}} \psi_{i p q}(\mathbf{x}) \right\} = \left\{ 0 \right\}
\]
Noting that $S_{y3}^{(j)}(y; x) = S_{x3}^{(j)}(y; x)$ due to the relation $\psi^{(j)} = \psi^{(j)}$ as indicated in Eq. (24), we can thus derive another useful version of the interaction energy from Eq. (43) for a transversely isotropic full-space, i.e.

$$W_{ij}^{(j)}(\bar{C}, C) = -\frac{\epsilon_{ij}}{4\pi} \int_C \int_C dy \nabla_y \nabla_x \psi^{(j)} - \frac{C_{ij}}{4\pi} \int_C \int_C dy \nabla_y \nabla_x \psi^{(j)} - \frac{C_{ij}}{4\pi} \int_C \int_C dy \nabla_y \nabla_x \psi^{(j)}$$

(47)

where

$$W_{ij}^{(j)}(y; x) = S_{y3}^{(j)}(y; x), \quad W_{ij}^{(j)}(y; x) = S_{x3}^{(j)}(y; x)$$

(48)

$$W_{ij}^{(j)}(y; x) = S_{y3}^{(j)}(y; x), \quad W_{ij}^{(j)}(y; x) = S_{x3}^{(j)}(y; x)$$

In the above derivation, use has also been made of Eq. (45), and the spatial symmetry of potential functions as given in Eq. (18b) for a transversely isotropic full-space, and the following relations

$$\int_C e_{ij} \nabla_x \nabla_y \psi^{(j)} = \int_C \nabla_x \nabla_y S_{y3}^{(j)}(y; x) + \int_C \nabla_x \nabla_y S_{x3}^{(j)}(y; x)$$

(49)

$$\int_C e_{ij} dy \nabla_x \nabla_y S_{y3}^{(j)}(y; x) + \int_C e_{ij} dy \nabla_x \nabla_y S_{x3}^{(j)}(y; x) = 0$$

(50)

Eq. (49) can be easily proved by using the Stokes’ theorem given in Eq. (26).

As verification, in the special case of an isotropic full-space, by virtue of Eq. (39) the energy formulæ in Eq. (43) and Eq. (47) reduced to the following well-known Blin’s formula and deWit’s formula, respectively (Blin, 1955; deWit, 1960; Hirth and Lothe, 1982).

$$W_{ij}^{(j)}(\bar{C}, C) = -\frac{G^{(j)}}{2\pi} b_j b_i \int_C \int_C dy \nabla_y S_{x3}^{(j)}(y; x) + \frac{G^{(j)}}{2\pi} b_j b_i \int_C \int_C dy \nabla_y S_{y3}^{(j)}(y; x)$$

(51)

$$W_{ij}^{(j)}(\bar{C}, C) = -\frac{G^{(j)}}{4\pi} b_j b_i \int_C \int_C dy \nabla_y S_{x3}^{(j)}(y; x) + \frac{G^{(j)}}{4\pi} b_j b_i \int_C \int_C dy \nabla_y S_{y3}^{(j)}(y; x)$$

(52)

where $R, G^{(j)}$ and $\psi^{(j)}$ are the same as those in Eq. (38).

According to Hirth and Lothe (1982), the self-energy of an arbitrarily shaped dislocation loop $C$ in material $\lambda$ of a transversely isotropic bimaterial can be expressed in terms of the associated interaction energy as

$$W_{ij}^{(j)}(C) = W_{ij}^{(j)}(C) + W_{ij}^{(j)}(C)$$

(53)

where

$$W_{ij}^{(j)}(C) = \frac{1}{2} W_{ij}^{(j)}(C), \quad W_{ij}^{(j)}(C) = \frac{1}{2} W_{ij}^{(j)}(C, C)$$

(54)

with $W_{ij}^{(j)}(C, C)$ and $W_{ij}^{(j)}(C, C)$ being defined in Eq. (41).

In Eq. (54), $W_{ij}^{(j)}$ denotes the self-energy of an arbitrarily shaped dislocation loop $C$ in a transversely isotropic full-space occupied by material $\lambda$, while $W_{ij}^{(j)}$ is the image self-energy which accounts for contributions of the image sources due to the presence of bimaterial interface.

As presented in Eqs. (28), (34), (43) and (47), we have obtained the line-integral representations for the elastic displacements, stresses and interaction energy due to arbitrarily shaped dislocation loops in transversely isotropic bimaterials. These expressions are the main results of this paper, and they are valid for both non-degenerate and degenerate cases of transversely isotropic bimaterials (See Appendix A).

3.4. Further reductions of the elastic fields and interaction energy

Introduction of the potential functions defined in Eq. (15) is just an intermediate step which largely simplifies the derivation of our dislocation solutions. Substituting these potential functions into Eqs. (28), (34), (43) and (47), we find that the elastic fields and interaction energy can be expressed in terms of the kernel integrals below (Yuan et al., 2013).

$$I_{NM,ijkl}(x_1, x_2, x_3) = \int_C \frac{(y_1 - y_2)(x_1 - x_2)(x_3 - x_4)}{R} dy$$

(55a)

$$I_{NM,ijkl}(x_1, x_2, x_3) = \int_C \frac{(y_1 - y_2)(x_1 - x_2)(x_3 - x_4)}{R} dy$$

(55b)

where $N$ is even (or zero), $M$ is odd (or zero), and

$$r_{pm} = \sqrt{(y_1 - x_1)^2 + (y_2 - x_2)^2}, \quad x_{ij} = (-1)^{j+i+1}x^{(j)}_i x^{(j)}_j$$

(56)

Note that the above reduction is independent of the specific form of the potential functions $\psi^{(j)}$ defined in Eq. (15), and thus independent of the specific configuration of the cut face of a dislocation loop due to the following relations, i.e.

$$\psi^{(j)}_0 - \psi^{(j)} = -\frac{1}{2} \frac{1}{R} \nabla \cdot \nabla \phi^{(j)}$$

(57)

$$\psi^{(j)}_0 + \psi^{(j)}_2 - \psi^{(j)}_0 - \frac{1}{2} \frac{1}{R} \nabla \cdot \nabla \phi^{(j)}$$

and

$$I_{NM,ijkl}^{(j)}(x_1, x_2, x_3) = 0, \quad g_{ij}^{(j)}(x_1, x_2, x_3) = 0, \quad h_{ij}^{(j)}(x_1, x_2, x_3) = 0$$

(58)

in which

$$\left\{ \begin{array}{l} I_{ij}^{(j)}(x_1, x_2, x_3) \\ I_{ij}^{(j)}(x_1, x_2, x_3) \\ I_{ij}^{(j)}(x_1, x_2, x_3) \end{array} \right\} = \left\{ \begin{array}{l} m^{(j)}_1 - m^{(j)}_2, m^{(j)}_1 - m^{(j)}_2, 1 \\ m^{(j)}_1 + 1, m^{(j)}_1 + 1, -m^{(j)}_1 - m^{(j)}_2, 1 \\ m^{(j)}_1 + m^{(j)}_2 + 2, m^{(j)}_1 + m^{(j)}_2 + 2 \end{array} \right\}$$

(59)
We also point out that, for a dislocation loop \( C \) which is approximated by a set of straight dislocation segments, the kernel integrals defined in Eqs. (55a,b) can be solved analytically (Yuan et al., 2013). Moreover, the elastic displacements, stresses and interaction energy as given in Eqs. (28), (34), (43) and (47) can be further simplified with the aid of Eqs. (18a,b) and (26) if one is interested in analytical dislocation solutions (Yuan et al., 2013). There are two minor errors in Yuan et al. (2013) and we correct them here for future reference:

(i) The correct expression of Eq. (39) in Yuan et al. (2013) should be

\[
\tilde{\Phi}(x) = \text{sgn}(S(x_1, x_2)) \left[ \arctan \left( \frac{2x_1 - x_2}{2x_1 + x_2} \right) - \arctan \left( \frac{2x_1 - x_2}{2x_1 + x_2} \right) \right]
\]

(ii) \((x_{ba} - x_{sa})\) in Eq. (61) of Yuan et al. (2013) should be replaced by \((x_{ba} - x_{sb})\).

It is obvious that in numerical computation (e.g. Ghoniem and Sun, 1999), the integrands of the kernel integrals in Eqs. (55a,b) become unbounded once \( \beta_{\text{pi}} = 0 \). Fortunately, this singular behavior can be circumvented by expressing Eqs. (28), (34), (43) and (47) in terms of another type of integrals as follows

\[
J_{\text{NM}}^{(3,s)}(x, C) = \int_C \left( \frac{y_i - x_i}{(R_i^{(s)} + z_i^{(s)})^{2}} \right) \cdots \frac{y_i - x_i}{(R_i^{(s)} + z_i^{(s)})^{2}} \, dy_k \quad (R_i^{(s)} + z_i^{(s)} \neq 0 \text{ on } C)
\]

\[
K_{\text{NM}}^{(3,s)}(x, C) = \int_C \left( \frac{y_i - x_i}{(R_i^{(s)} - z_i^{(s)})^{2}} \right) \cdots \frac{y_i - x_i}{(R_i^{(s)} - z_i^{(s)})^{2}} \, dy_k \quad (R_i^{(s)} - z_i^{(s)} \neq 0 \text{ on } C)
\]

\[
J_{\text{NM}}^{(3,s)}(x, C) = \int_C \left( \frac{y_i - x_i}{(R_i^{(s)} + z_i^{(s)})^{2}} \right) \cdots \frac{y_i - x_i}{(R_i^{(s)} + z_i^{(s)})^{2}} \, dy_k
\]

where \( N \) and \( M \) are non-negative integers, and \( C \) is a certain segment of loop \( C \). However, there exists another singularity due to \( R_i^{(s)} = 0 \) in Eqs. (55a) and (60a) which is intrinsic to the classical continuum theory of dislocations. This issue is discussed in the next section.

4. A self-consistent approach for removing the singularities

As is well-known, the self-energy \( W_s^{(s)} \) defined in Eq. (54) always diverges due to the presence of singularity when \( R_i^{(s)} \to 0 \). Following Cai’s approach (Cai et al., 2006), we now propose a self-consistent method to remove such singularities for infinite transversely isotropic media.

To facilitate our discussion, let us first denote the stress field in Eq. (34) and the interaction energy in Eq. (43) or (47) as

\[
S_{\text{pi}}^{(s)}(x) \sim F_{\text{pi}}(\hat{\psi}_n^{(s)}) \quad W_i^{(s)}(\hat{C}, C) \sim G(\hat{\psi}_n^{(s)}) \quad n = 0, 1, 2, 3, 4
\]

which means that \( S_{\text{pi}}^{(s)} \) and \( W_i^{(s)} \) are expressed in terms of \( \hat{\psi}_n^{(s)} \) \((n = 0,1,2,3,4)\).

Then, similar to Cai et al. (2006), we introduce a Burgers vector density function that removes the dislocation singularity by spreading its Burgers vector around every point on the dislocation line as follows

\[
b_n = b_m \int \rho(\mathbf{x}) d^3 \mathbf{x}, \quad \hat{b}_n = b_m \int \hat{\rho}(\mathbf{x}) d^3 \mathbf{x}
\]

For dislocation loops whose Burgers vector spread out according to Eq. (62), the local stress field and the interaction energy originally given in Eq. (61) become

\[
\hat{S}_{\text{pi}}^{(s)}(x) \sim F_{\text{pi}}(\hat{\psi}_n^{(s)}) \quad \hat{W}_i^{(s)}(\hat{C}, C) \sim G(\hat{\psi}_n^{(s)}) \quad n = 0, 1, 2, 3, 4
\]

where

\[
\hat{\psi}_n^{(s)}(y; \mathbf{x}) = \rho(\mathbf{y}) \ast \psi_n^{(s)}(y; \mathbf{x}) \quad \hat{\psi}_n^{(s)}(y; \mathbf{x}) = \rho(\mathbf{y}) \ast \psi_n^{(s)}(y; \mathbf{x}) \ast \hat{\rho}(\mathbf{x})
\]

which satisfy the spatial symmetry as follows

\[
\frac{\partial}{\partial \psi_n^{(s)}} \hat{\psi}_n^{(s)} = -\frac{\partial}{\partial \psi_n^{(s)}} \hat{\psi}_n^{(s)} \quad \frac{\partial}{\partial \psi_n^{(s)}} \hat{\psi}_n^{(s)} = -\frac{\partial}{\partial \psi_n^{(s)}} \hat{\psi}_n^{(s)}
\]

In Eq. (64), the star “∗” means the convolution operator defined by

\[
f(\mathbf{x}) \ast g(\mathbf{x}) = \int f(\mathbf{x} - \mathbf{x'}) g(\mathbf{x'}) d^3 \mathbf{x'} = \int f(\mathbf{x}) g(\mathbf{x} - \mathbf{x'}) d^3 \mathbf{x'}
\]

As is indicated in Section 3, when deriving the interaction energy expression in Eq. (43) from the stress field in Eq. (34) and then

---

**Fig. 2.** Variation of \( \sigma_{13} \) with \( x_3 / b = 5, x_3 / b = 0 \) due to a circular prismatic dislocation loop in isotropic Cu/Ni bimaterials with a perfectly-bonded interface.
transforming it into another form as given in Eq. (47), we only make use of the spatial symmetry and the single-valued property of the potential functions as shown in Eq. (18b) and Eqs. (46) and (50), respectively, without using the quasi-harmonic property of the potential functions as shown in Eq. (18a). Therefore, if we introduce a relevant measure of the local stress field as

\[
\tilde{S}_{pq}^{(i)}(\mathbf{x}) = \hat{S}_{pq}^{(i)}(\mathbf{x}) + \hat{\rho}^{(i)}(\mathbf{x}) \sim F_{pq} \hat{\psi}_{n}^{(i)}, \quad n = 0, 1, 2, 3, 4
\]  

(67)

then \(\tilde{W}_{i}^{(i)}\) in Eq. (63) can be derived from \(\tilde{S}_{pq}^{(i)}\) in Eq. (67) due to the fact that \(\hat{\psi}_{n}^{(i)}\) defined in Eq. (64) sustains both the spatial symmetry and the single-valued property of \(\psi_{n}^{(i)}\) \((n = 0,1,2,3,4)\). In other words, \(S_{pq}^{(i)}\) is consistent with \(W_{i}^{(i)}\), and the equivalence is also established between two different versions of \(W_{i}^{(i)}\) corresponding to Eq. (43) and Eq. (47), respectively.

However, it seems difficult to find a Burgers vector density function such as in Eq. (62) which leads to simple analytical formulations for the stress field and interaction energy. Alternatively, we assume that the Burgers vector density function is associated with the material constants \(\gamma_{i}^{(i)}\) in Eq. (3b), i.e.

\[
b_{m} = b_{m} \int \rho_{i}^{(i)}(\mathbf{x}) d^{3}x, \quad b_{m} = b_{m} \int \hat{\rho}_{i}^{(i)}(\mathbf{x}) d^{3}x \quad \text{corresponding to} \quad \gamma_{i}^{(i)}
\]  

(68)

This assumption is reasonable from the physical point of view because the deviation of \(\gamma_{i}^{(i)}\) from unity can be considered as a measure of the degree of anisotropy. In so doing, Eqs. (63) and (67) are changed to

\[
\tilde{W}_{i}^{(i)}(\mathbf{C}, C) \sim \psi_{0}^{(i)}\tilde{S}_{pq}^{(i)}(\mathbf{x}) \sim S_{pq}^{(i)}\hat{\chi}_{i}^{(i)} \quad i = 1, 2, 3
\]  

(69)

where

\[
\hat{\chi}_{i}^{(i)} = \hat{\chi}_{i}^{(i)}(\mathbf{y}, \mathbf{x}) = \rho_{i}^{(i)}(\mathbf{y}) * \hat{\rho}_{i}^{(i)}(\mathbf{x})
\]  

(70)

Obviously, the expressions in Eq. (69) are still consistent with each other.

![Fig. 3. Variation of stress components with \(x_{3}\) \((x_{1} = 50 \text{ nm}, x_{2} = 50 \text{ nm})\) due to an inclined, circular glide dislocation loop in isotropic GaAs/Si bimaterials with a perfectly-bonded interface.](image-url)
Suppose now that we find a Burgers vector density function such that
\[ 
\tilde{\gamma}_i^{(j)}(y, x) = +z_i^{(j)} \ln \left( \tilde{R}_i^{(j)} + z_i^{(j)} \right) - \tilde{R}_i^{(j)} 
\]
or
\[ 
- z_i^{(j)} \ln \left( \tilde{R}_i^{(j)} - z_i^{(j)} \right) - \tilde{R}_i^{(j)} 
\]
(71)
in which
\[ 
\tilde{R}_i^{(j)} = \tilde{R}_i^{(j)}(y, x) = \sqrt{(y_1 - x_1)^2 + (y_2 - x_2)^2 + (z_i^{(j)})^2 + \varepsilon^2} 
\]
(72)
with \( \varepsilon \) being an arbitrary real constant. Then, from Eq. (70), we can obtain that
\[ 
\left[ \frac{\partial^2}{\partial y_1 \partial y_1} + (\gamma_i^{(j)})^2 \frac{\partial^2}{\partial y_2 \partial y_2} \right] \tilde{\gamma}_i^{(j)}(y, x) 
= \rho_i^{(j)}(y) \left\{ \left[ \frac{\partial^2}{\partial y_1 \partial y_1} + (\gamma_i^{(j)})^2 \frac{\partial^2}{\partial y_2 \partial y_2} \right] \tilde{\gamma}_i^{(j)}(y, x) \right\} - \tilde{\rho}_i^{(j)}(x) 
\]
(73)
which leads to
\[ 
\rho_i^{(j)}(y - x) * \tilde{\rho}_i^{(j)}(x) = \frac{1}{4\pi\gamma_i^{(j)}} \frac{3\varepsilon^2}{(R_i^{(j)})^5} 
\]
(74)
due to the fact that
\[ 
\left[ \frac{\partial^2}{\partial y_1 \partial y_1} + (\gamma_i^{(j)})^2 \frac{\partial^2}{\partial y_2 \partial y_2} \right] \tilde{\gamma}_i^{(j)}(y, x) = -4\pi\gamma_i^{(j)} \delta^3(y - x) 
\]
(75)
where \( \delta^3(x) \) is the 3D Dirac delta function. The Burgers vector density functions can be determined by Eq. (74) in combination with the following normalization conditions as indicated in Eq. (68), i.e.,
\[ 
\int \rho_i^{(j)}(y - x) d^3x = 1, \quad \int \tilde{\rho}_i^{(j)}(x) d^3x = 1 
\]
(76)
In summary, by introducing three particular spreading functions characterized by the spreading radius \( \varepsilon \) as shown in Eqs. (68), (74) and (76), we thus obtain the non-singular stress field and interaction energy which are consistent with each other. In other words, the singularity can be removed if we replace the function \( R_i^{(j)} \) involved in the potential functions of Eqs. (34), (43), and (47) simply by \( \tilde{R}_i^{(j)} \) as given in Eq. (72). The treatment to the self-energy of a dislocation loop is exactly the same \( \langle \tilde{\gamma}_i^{(j)}(x) \rangle = \gamma_i^{(j)}(x) \) in this case) due to the fact that the self-energy is in terms of the interaction energy according to Eq. (54). We also remark that the spreading radius \( \varepsilon \) should be so chosen that the non-singular solution matches the atomistic simulation (Cai et al., 2006).

In the special case of infinite isotropic media, it is verified that the singularity can be removed if we replace \( R \) in Eqs. (38), (51) and (52) simply by \( \tilde{R} \) defined as
\[ 
\tilde{R} = \tilde{R}(y, x) = \sqrt{(y_1 - x_1)^2 + (y_2 - x_2)^2 + (y_3 - x_3)^2 + \varepsilon^2} 
\]
(77)
Note that this reduction leads to slightly different expressions from those of Cai et al. (2006). In terms of the expressions by Cai et al. (2006), the function \( 1/R \) in our Eqs. (38), (51) and (52) would need to be replaced by \( \nabla^2 R/2 \), with \( \nabla^2 \) being the 3D Laplacian operator.

As an immediate application of our non-singular expressions, we now calculate the self-energy of dislocation loops with simple configurations.

For a circular glide dislocation loop of radius \( R \) located in the plane of isotropy with a Burgers vector \( (b, 0, 0) \), the non-singular solution for the self-energy can be obtained from Eqs. (54), (69) and (71) as
\[ 
W_s^{(j)} = 2\pi R \frac{c_s^{(j)} b^2}{8\pi} \frac{1}{(\gamma_x^{(j)})^2} \left( \ln \frac{R}{\varepsilon} - 2 \right) + \mathcal{O}\left( \frac{\varepsilon^2}{R^2} \right) 
\]
(78a)
Similarly, for a circular prismatic dislocation loop of radius \( R \) located in the plane of isotropy with a Burgers vector \( (0, 0, b) \), the non-singular self-energy is
In Eqs. (78a,b), $K(\kappa)$ and $E(\kappa)$ are the complete elliptic integrals of the first and second kinds with modulus $\kappa$ defined as

$$\kappa = \frac{2R}{\sqrt{4R^2 + \varepsilon^2}}$$

(79)

We remark that the asymptotic solutions in Eqs. (78a,b) agree well with those in Chou and Eshelby (1962), except that the number “1” in our Eq. (78b) would be “2” in Chou and Eshelby (1962). This discrepancy can be reconciled by properly choosing the spreading radius $\varepsilon$.

For a screw dislocation dipole which is located within the plane of isotropy and is parallel to the $x_1$-axis with a Burgers vector $(b_1, 0, 0)$, the non-singular solution of the self-energy per unit length can be obtained from Eqs. (54), (69) and (71) as

$$W_S^{(j)} = 2\pi R \frac{c_{44}^{(j)} b_1^2}{8\pi} \frac{4R}{\sqrt{4R^2 + \varepsilon^2}} \left( \frac{\ln \frac{R}{\varepsilon} - 1}{\varepsilon} \right) + O\left( \frac{\varepsilon^2}{R^2} \right)$$

(80a)

where $D$ is the distance between the two dislocations of the dipole (Cai et al., 2006).

Similarly, for an edge dislocation dipole which is located within the plane of isotropy and is parallel to the $x_1$-axis with a Burgers vector $(0, b_2, 0)$ or $(0, 0, b_3)$, the respective non-singular self-energy per unit length is

![Fig. 5. Variation of $u_3$ with $x_3$ ($x_1/a = 0.5, x_2/a = 0.5$) due to hexagonal glide dislocation loop C in (a) GaN/InN bimaterial with a perfectly-bonded interface (i.e. perfect interface); and in (b) GaN/InN bimaterial with an interface in frictionless contact (i.e. smooth interface). T.I. means transverse isotropy, and Iso. indicates isotropy of Voigt average.](image-url)
\[ W(k) = \frac{C_0}{c(k)} \left( b_0 \right) \]

or

\[ W(k) = \frac{C_0}{c(k)} \left( b_0 \right) \]

5. Numerical examples and discussions

In this section, our solutions in Section 3 are applied to a couple of dislocation cases to verify our formulations while illustrating certain interesting features due to the presence of material anisotropy and bimaterial interface.

**Example 1.** Stress field of a circular prismatic dislocation loop in isotropic bimaterials with a perfectly-bonded interface.

This example was suggested by Akarapu and Zbib (2009). The bimaterial system consists of Cu (material 1, \( x_3 > 0 \)) and Ni (material 2, \( x_3 < 0 \)) which are perfectly bonded together at the planar interface \( x_3 = 0 \). The material parameters (i.e. shear modulus and Poisson's ratio) used here are listed as follows: \( G^{(1)} = 54.6 \) GPa, \( \nu^{(1)} = 0.324 \) for Cu, and \( G^{(2)} = 94.7 \) GPa, \( \nu^{(2)} = 0.276 \) for Ni. Within Cu, there exists a circular prismatic dislocation loop of radius \( r_0 = 50b \) with a Burgers vector \((0, 0, b)\). The loop is parallel to the bimaterial interface with its center being at \((0, 0, 5b)\). We approximate this circle with an inscribed regular 25-side polygon. As verification, our numerical results are compared with those of certain interesting features due to the presence of material anisotropy and bimaterial interface.
It can be observed from Fig. 2 that the shear stress $\sigma_{13}$ along the line parallel to $x_3$-axis in both materials ($\mu = 1.2$) agrees very well with each other.

**Example 2.** Stress field of an inclined, circular glide dislocation loop in isotropic bimaterials with a perfectly-bonded interface.

This example was suggested by Tan and Sun (2006). The bimaterial system consists of GaAs (material 1, $x_3 > 0$) and Si (material 2, $x_3 < 0$) which are perfectly bonded together at the planar interface $x_3 = 0$. The material parameters (i.e. Young’s modulus and Poisson’s ratio) used here are listed as follows: $E^{(1)} = 85.5$ GPa, $\nu^{(1)} = 0.31$ for GaAs, and $E^{(2)} = 165.5$ GPa, $\nu^{(2)} = 0.25$ for Si. The circular glide dislocation loop of radius $r_0(=25\text{ nm})$ is located in GaAs with its center being at the point $(0, 0, 50\text{ nm})$ and lies on the slip plane with positive normal ($\cos30^\circ,0,\cos60^\circ$). The Burgers vector is $(\cos60^\circ,0,\cos150^\circ) \times 0.384\text{ nm}$. We approximate this circle with an inscribed regular 32-side polygon. As verification, our numerical results are compared with those of Tan and Sun (2006). It can be seen from Fig. 3 that all the stress components along the line parallel to $x_3$-axis in both materials ($\mu = 1.2$) agree very well with each other. We should point out, however, that the discrete data in Fig. 3 are 0.01 times the raw-data extracted directly from the figures in Tan and Sun (2006). Moreover, due to possible misprints, the stress components in Tan and Sun (2006) should be normalized by the shear modulus instead of the Young’s modulus of GaAs.

**Example 3.** Interaction energy between two hexagonal prismatic dislocation loops in a transversely isotropic full-space.
This example was suggested by Willis (1965). We first introduce a hexagonal prismatic dislocation loop \( C \) of side-length \( a \) with a Burgers vector \((0,0,0)\) lying in the basal plane of an infinite hexagonal crystal (magnesium or zinc in this example). In the Cartesian coordinates, the center of this loop is fixed at the origin \((0,0,0)\) while its six vertices are located at \((a,0,0)\), \((a/2,\sqrt{3}a/2,0)\), \((-a/2,\sqrt{3}a/2,0)\), \((-a,0,0)\), \((-a/2,-\sqrt{3}a/2,0)\) and \((a/2,-\sqrt{3}a/2,0)\), respectively. We now bring in the second prismatic dislocation loop \( \bar{C} \) with a Burgers vector \((0,0,0)\) by simple translation of the first loop \( C \), with its center being confined in the \( x_1-x_3 \) plane. Denoting the center of the second loop as \( (X_1,0,X_3) \), the contours of the interaction energy in the \( X_1-X_3 \) plane between these two dislocation loops in (a) magnesium and (b) zinc are shown in Fig. 4, where the symbol \( E \) denotes the non-dimensional interaction energy normalized by \( \epsilon_{\text{dd}} \), i.e. \( E = W/(C,C)/\epsilon_{\text{dd}} \). It can be seen from these figures that the slopes of the asymptotic line (i.e. \( E = 0 \)) are the same as those of infinitesimal loops in Willis (1965). When the second loop is far away from the first one, the contours coincide with those in Willis (1965) for the infinitesimal loop case. However, when these two loops become close to each other, the contours show significant deviation from those of Willis (1965). Comparison of Fig. 4(a) with Fig. 4(b) also indicates that the degree of material anisotropy can significantly influence the contour shapes. The material parameters used here are: \( c_{11} = 59.7 \), \( c_{33} = 61.7 \), \( c_{44} = 16.4 \), \( c_{13} = 21.7 \), \( c_{66} = 16.75 \) (GPa) for magnesium, and \( c_{11} = 158.35 \), \( c_{33} = 61.6 \), \( c_{44} = 40.0 \), \( c_{13} = 47.44 \), \( c_{66} = 63.42 \) (GPa) for zinc.

**Example 4.** Displacements, stresses, interaction energy and image self-energy of glide dislocation loops in transversely isotropic bimaterials.

In Cartesian coordinates, we consider a transversely isotropic bimaterial which is composed of GaN (material 1, \( x_3 > 0 \)) and InN (material 2, \( x_3 < 0 \)), with the basal plane of both materials being parallel to the bimaterial interface (i.e. \( x_3 = 0 \)). The material parameters used are: \( c_{11} = 390 \), \( c_{33} = 398 \), \( c_{44} = 105 \), \( c_{13} = 106 \), \( c_{66} = 122.5 \) (GPa) for GaN, and \( c_{11} = 223 \), \( c_{33} = 224 \), \( c_{44} = 48 \), \( c_{13} = 92 \), \( c_{66} = 54 \) (GPa) for InN. There are two hexagonal glide dislocation loops in this bimaterial. The first loop \( C \) of side-length \( a \) with a Burgers vector \((b,0,0)\) is located in GaN and is parallel to the bimaterial interface. The center of loop \( C \) is fixed at \((0,0,H)\) where \( H = a/4 \), and its six vertices are fixed at \((a,0,H)\), \((a/2,\sqrt{3}a/2,H)\), \((-a/2,\sqrt{3}a/2,H)\), \((-a,0,H)\), \((-a/2,-\sqrt{3}a/2,H)\) and \((a/2,-\sqrt{3}a/2,H)\), respectively. The second loop \( \bar{C} \) with a Burgers vector \((b,0,0)\) is introduced by superpositions of the following operations: (i) simple translation of the first loop \( C \) with its center being confined in the \( x_1-x_3 \) plane, and (ii) pure rotation of the first loop \( C \) about a rotation-axis which is parallel to the \( x_1 \)-axis while passing through the center of \( C \). The center of loop \( \bar{C} \) is thus denoted as \((X_1,0,X_3)\), and the orientation of loop \( \bar{C} \) is described by the rotation angle \( \theta \), i.e. the inclined angle between the two dislocation planes.

Shown in Figs. 5 and 6 are, respectively, the displacement component \( u_3 \) and stress component \( \sigma_{22} \) in GaN/InN bimaterials under both perfect and smooth interface conditions, induced by the first dislocation loop \( C \) only. It can be observed from these figures that material anisotropy can have a considerable influence on the displacement and stress fields at some field points (i.e. with different \( x_1 \)). We point out that the corresponding isotropic Lamé constants used here are \( \lambda = 29.4 \), \( \mu = 121.2 \) (GPa) for GaN and \( \lambda = 104.4 \), \( \mu = 54.7 \) (GPa) for InN, which are determined by the Voigt average (Hirth and Lothe, 1982).

Shown in Fig. 7 are the contours of the interaction energy between the two dislocation loops \( C \) and \( \bar{C} \) in the \( X_1-x_3 \) plane (with \( \theta = 0^\circ \)), where the symbol \( E \) denotes the non-dimensional interaction energy normalized by \( \epsilon_{\text{dd}} \), with \( \epsilon_{\text{dd}} \) being the modulus of GaN. Obviously, the presence of bimaterial interface causes the asymmetry of the contours about \( x_1/a = 0.25 \) in Figs. 7(b) and (c) in comparison with Fig. 7(a) for the GaN full-space case. Different types of interfaces (perfect or smooth interface in this case) can also substantially influence the contour shapes (Figs. 7(b) vs. (c)). Moreover, the contour shape for glide loops is quite different from that for prismatic loops as shown in Example 3 (Figs. 7(a) vs. 4(a,b)).

Fig. 8 shows the influence of the orientation of loop \( \bar{C} \) on the interaction energy between two dislocation loops, where the
symbol $E$ also denotes the non-dimensional interaction energy normalized by $(c_{44} b b a)$, with $c_{44}$ being the modulus of GaN. It can be seen from Fig. 8 that there exist two extreme points ($\theta = 0^\circ$ and $\theta = 60^\circ$) at which the slope of $E$ with respect to $\theta$ becomes zero. We further notice that $\theta = 0^\circ$ is stable if $b b > 0$ whilst $\theta = 60^\circ$ is stable if $b b < 0$.

Fig. 9 shows the influence of the distance from the loop center to the bimaterial interface on the image self-energy of a dislocation loop, where the symbol $E_{\text{image}}^{(\text{loop})}$ denotes the non-dimensional image self-energy normalized by $(c_{44} b b a)$, with $c_{44}$ being the modulus of GaN. It can be observed from Fig. 9 that the smooth interface always imposes an attractive force upon the glide dislocation loop, no matter whether this loop is located within GaN or within InN. However, the perfect interface imposes an attractive force upon the glide dislocation loop if it is located within GaN which has a relatively large shear modulus, and imposes a repulsive force upon this loop if it is located within InN which has a relatively small shear modulus.

6. Conclusions

In this paper, we have obtained simple line-integral representations for the elastic displacements, stresses, self-energy and interaction energy of arbitrarily shaped dislocation loops with general Burgers vectors in either non-degenerate or degenerate transversely isotropic bimaterials. These expressions are very similar to their isotropic full-space counterparts (e.g. Burgers’ formula, de-Wit’s formula, Blin’s formula) and therefore can be easily applied to 3D-DD simulations for hexagonal or isotropic crystals with interfaces/surfaces. We have also proposed a non-singular and self-consistent approach to evaluate the self-stress and self-energy of a dislocation loop in transversely isotropic media efficiently. Our numerical examples show clearly the significant influence of material anisotropy and bimaterial interface on the elastic fields and interaction energy of dislocation loops.

Our line-integral expressions for the elastic displacements, stresses and interaction energy are also applicable to the important case of a transversely isotropic (or isotropic) half-space with free surface, provided that we slightly modify the associated coefficients of the Green’s tensor for bimaterials, as discussed in Appendix B.

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Appendix A. Explicit expressions of the functions $\psi_q^{(\mu)}$ and $\psi_q^{(\mu)(\nu)}$ ($q = 1, 2, 3, 4$) for all possible degenerate cases of transversely isotropic bimaterials

It can be easily observed from Eq. (23) that, when $\gamma_1^{(\mu)} = \gamma_2^{(\mu)} = \gamma_0^{(\mu)}$ (i.e. $m_1^{(\mu)} = m_2^{(\mu)} = m_0^{(\mu)} = 1$) or $\gamma_1^{(\mu)} = \gamma_2^{(\mu)}$ (i.e. $m_1^{(\mu)} = m_2^{(\mu)} = 1$), the functions $\psi_q^{(\mu)}$ and $\psi_q^{(\mu)(\nu)}$ ($q = 1, 2, 3, 4$) are ill-defined. However, we will show below that they become well-defined after a proper limiting process. In the following discussion, the symbol ‘$\sim$’ indicates that there is no index in the given position.

We now deal with $\psi_q^{(\mu)}$ first. Using the method of undetermined coefficients, the first of Eq. (23) can be expressed as

$$\psi_q^{(\mu)} = \left(-K_q^{(\mu)} \chi^{(\mu)} + Q_q^{(\mu)} \chi_1^{(\mu)} \right) / \Theta^{(\mu)} \quad (A1)$$

in which

$$\chi^{(\mu)} = \frac{1}{\gamma_2^{(\mu)}} \frac{\gamma_1^{(\mu)} - \gamma_0^{(\mu)} \gamma_2^{(\mu)}}{\gamma_1^{(\mu)} - \gamma_2^{(\mu)}} \quad (A2)$$

and

$$K_q^{(\mu)} = \frac{T_1^{(\mu)}}{\gamma_2^{(\mu)}} \quad Q_q^{(\mu)} = \frac{T_2^{(\mu)}}{\gamma_2^{(\mu)}} - \frac{T_1^{(\mu)} - T_2^{(\mu)}}{\gamma_1^{(\mu)} - \gamma_2^{(\mu)}} \quad (A3)$$

Fig. 9. Variations of the image self-energy of the second hexagonal glide dislocation loop vs. the center coordinate $X_i$ of this loop. Other fixed parameters are $X_1 = 0, X_3 = 0$, and $\theta = 45^\circ$. 
When $\gamma_{1}^{(p)} - \gamma_{q}^{(p)} \leq \gamma_{1}^{(p)}$, it can be verified that

$$
\lim_{\gamma_{1}^{(p)} \rightarrow \gamma_{1}^{(p)} - \gamma_{0}^{(p)}} \Delta_{C}^{(p)} \approx -R_{C}^{(p)}
$$

where $R_{C}^{(p)}$ and $T_{q}^{(p)}$ are defined the same as in Eq. (16) and Eq. (24), respectively, provided that we replace the corresponding index by “0”, and

$$
\Delta_{C}^{(p)} = -\gamma_{1}^{(p)} E^{(p)}, \quad T_{q}^{(p)} = \gamma_{1}^{(p)} = 1, \quad T_{q}^{(p)} = (\gamma_{0}^{(p)})^{2} E^{(p)} + 2
$$

In obtaining Eq. (A5), use has been made of Eqs. (4) and (22).

Making use of Eq. (A4), we thus obtain the limit expression of Eq. (A1) as

$$
\psi_{q}^{(f)} = \frac{1}{\Lambda_{q}^{(f)} \Theta_{q}^{(f)}} \left[ T_{q}^{(f)} R_{q}^{(f)} + \left( T_{q}^{(f)} - \gamma_{1}^{(p)} T_{q}^{(p)} \right) \Delta_{q}^{(f)} \right]
$$

where $\Delta_{q}^{(f)}$ is defined the same as in Eq. (15), provided that we replace the corresponding index by “0”.

As the next step, we deal with $\psi_{q}^{(f)}(q = 1, 2, 3, 4)$ as follows. (i) $\gamma_{1}^{(p)} \rightarrow \gamma_{2}^{(p)} = \gamma_{0}^{(p)}$ only; or (ii) $\gamma_{1}^{(p)} \rightarrow \gamma_{2}^{(p)} = \gamma_{0}^{(f)}$ only.

Using the method of undetermined coefficients, the second of Eq. (23) can be expressed as

$$
\psi_{q}^{(f)} = \frac{1}{\Lambda_{q}^{(f)} \Theta_{q}^{(f)}} \left[ \gamma_{2}^{(f)} R_{q}^{(f)} - \gamma_{1}^{(f)} \Delta_{q}^{(f)} \right]
$$

or

$$
\psi_{q}^{(f)} = \frac{1}{\Lambda_{q}^{(f)} \Theta_{q}^{(f)}} \left[ \gamma_{2}^{(f)} R_{q}^{(f)} - \gamma_{1}^{(f)} \Delta_{q}^{(f)} \right]
$$

in which

$$
\Delta_{q}^{(f)} = \frac{\gamma_{2}^{(f)} R_{q}^{(f)} - \gamma_{1}^{(f)} \Delta_{q}^{(f)}}{\gamma_{1}^{(f)} - \gamma_{0}^{(f)}} = \frac{\gamma_{2}^{(f)} R_{q}^{(f)} - \gamma_{1}^{(f)} \Delta_{q}^{(f)}}{\gamma_{1}^{(f)} - \gamma_{0}^{(f)}}
$$

and

$$
\Delta_{q}^{(f)} = \frac{\gamma_{2}^{(f)} R_{q}^{(f)} - \gamma_{1}^{(f)} \Delta_{q}^{(f)}}{\gamma_{1}^{(f)} - \gamma_{0}^{(f)}} = \frac{\gamma_{2}^{(f)} R_{q}^{(f)} - \gamma_{1}^{(f)} \Delta_{q}^{(f)}}{\gamma_{1}^{(f)} - \gamma_{0}^{(f)}}
$$

When $\gamma_{1}^{(p)} \rightarrow \gamma_{2}^{(p)} = \gamma_{0}^{(p)}$ or $\gamma_{1}^{(p)} \rightarrow \gamma_{2}^{(p)} = \gamma_{0}^{(f)}$, it can be verified that

$$
\lim_{\gamma_{1}^{(p)} \rightarrow \gamma_{1}^{(p)} - \gamma_{0}^{(p)}} \Delta_{q}^{(p)} = \frac{R_{q}^{(p)}}{\gamma_{1}^{(p)} - \gamma_{0}^{(p)}}
$$

and

$$
\lim_{\gamma_{1}^{(p)} \rightarrow \gamma_{1}^{(p)} - \gamma_{0}^{(p)}} \Delta_{q}^{(p)} = \frac{R_{q}^{(p)}}{\gamma_{1}^{(p)} - \gamma_{0}^{(p)}}
$$

$$
\lim_{\gamma_{1}^{(p)} \rightarrow \gamma_{1}^{(p)} - \gamma_{0}^{(p)}} \Delta_{q}^{(p)} = \frac{R_{q}^{(p)}}{\gamma_{1}^{(p)} - \gamma_{0}^{(p)}}
$$

$$
\lim_{\gamma_{1}^{(p)} \rightarrow \gamma_{1}^{(p)} - \gamma_{0}^{(p)}} \Delta_{q}^{(p)} = \frac{R_{q}^{(p)}}{\gamma_{1}^{(p)} - \gamma_{0}^{(p)}}
$$

in which $R_{q}^{(p)}(R_{q}^{(p)}) =\frac{R_{q}^{(p)}}{\gamma_{1}^{(p)} - \gamma_{0}^{(p)}}$ and $R_{q}^{(p)}(R_{q}^{(p)}) =\frac{R_{q}^{(p)}}{\gamma_{1}^{(p)} - \gamma_{0}^{(p)}}$ are defined the same as in Eq. (16), Eq. (17), Eq. (24) and Eq. (20b) or (21b), respectively, provided that we replace the corresponding index by “0”. and $P_{q}^{(p)}$ is defined the same as in Eq. (20b) or (21b), provided that we replace the corresponding index by “3”, and

$$
\tilde{P}_{2}^{(p)} = \begin{pmatrix}
0 & 0 & 1 & 0
\end{pmatrix}
$$

for the perfectly-bonded interface.

$$
\tilde{P}_{2}^{(p)} = \begin{pmatrix}
0 & 0 & 1 & 0
\end{pmatrix}
$$

for the interface in frictionless contact, and

$$
\tilde{T}_{2}^{(p)} = \begin{pmatrix}
-\gamma_{2}^{(p)} E^{(p)}, T_{q}^{(p)} = \gamma_{2}^{(p)} = 1, T_{q}^{(p)} = (\gamma_{0}^{(p)})^{2} E^{(p)} + 2
\end{pmatrix}
$$

We remark that use has also been made of Eqs. (4) and (22) in obtaining Eqs. (A12a) and (A13).

Making use of Eqs. (A10) and (A11), we thus obtain the limit expression of Eq. (A7a) or (A7b) as

$$
\psi_{q}^{(f)} = \frac{1}{\Lambda_{q}^{(f)} \Theta_{q}^{(f)}} \left[ \gamma_{2}^{(f)} R_{q}^{(f)} - \gamma_{1}^{(f)} \Delta_{q}^{(f)} \right]
$$

or

$$
\psi_{q}^{(f)} = \frac{1}{\Lambda_{q}^{(f)} \Theta_{q}^{(f)}} \left[ \gamma_{2}^{(f)} R_{q}^{(f)} - \gamma_{1}^{(f)} \Delta_{q}^{(f)} \right]
$$

(ii) $\gamma_{1}^{(p)} \rightarrow \gamma_{2}^{(p)} = \gamma_{0}^{(p)}$ and $\gamma_{1}^{(p)} \rightarrow \gamma_{2}^{(p)} = \gamma_{0}^{(f)}$ simultaneously.

In this case, we only need to follow a similar limiting process once more based on Eq. (A14a) or Eq. (A14b). The final result is given as follows

$$
\Lambda_{q}^{(f)} \Theta_{q}^{(f)} \psi_{q}^{(f)} = -\sum_{\psi_{q}^{(f)}} \lambda_{q}^{(f)}
$$

$$
-\left( \Xi_{q}^{(i)} - \Xi_{q}^{(i)} - \Xi_{q}^{(i)} + \Xi_{q}^{(i)} \right) \lambda_{q}^{(i)}
$$

$$
+ \left( \Xi_{q}^{(i)} - \Xi_{q}^{(i)} \right) \lambda_{q}^{(i)}
$$

$$
+ \left( \Xi_{q}^{(i)} - \Xi_{q}^{(i)} \right) \lambda_{q}^{(i)}
$$

(A14c)
where \( \hat{Z}^{(i)}_{20} \) and \( \hat{Z}^{(i)}_{21} \) are defined the same as in Eq. (A10), provided that we replace the corresponding index by “0”, and

\[
\begin{align*}
\hat{Z}^{(i)}_{20} &= \lim_{z \to 0^+} \left[ \frac{\hat{T}^{(i)}_{20}}{\gamma} - \frac{\hat{T}^{(i)}_{21}}{\gamma} \right] \\
\hat{Z}^{(i)}_{21} &= \lim_{z \to 0^+} \left[ \frac{\hat{T}^{(i)}_{20}}{\gamma} - \frac{\hat{T}^{(i)}_{21}}{\gamma} \right] \\
(1) &= (1) \times \frac{x_3 y_3}{\gamma_0^0} - \frac{1}{\gamma_0^0} - \frac{R_{00}^0}{\gamma_0^0} \\
&= (1) \times \frac{1}{R_{00}^0} - \frac{R_{00}^0}{\gamma_0^0},
\end{align*}
\]

and

\[
\begin{align*}
\hat{Z}^{(i)}_{00} &= \frac{\hat{P}^{(i)}_{00}}{\gamma_0^0} \\
\hat{Z}^{(i)}_{01} &= \left( \frac{\hat{P}^{(i)}_{00}}{\gamma_0^0} + \frac{\hat{P}^{(i)}_{01}}{\gamma_0^0} \right) \gamma_0^0 \\
\hat{Z}^{(i)}_{02} &= \left( \frac{\hat{P}^{(i)}_{00}}{\gamma_0^0} + \frac{\hat{P}^{(i)}_{01}}{\gamma_0^0} \gamma_0^0 \right) \gamma_0^0 \\
\hat{Z}^{(i)}_{03} &= \left( \frac{\hat{P}^{(i)}_{00}}{\gamma_0^0} + \frac{\hat{P}^{(i)}_{01}}{\gamma_0^0} \gamma_0^0 \right) \gamma_0^0
\end{align*}
\]

in which \( \hat{Z}^{(i)}_{00} \), \( \hat{Z}^{(i)}_{01} \), and \( \hat{Z}^{(i)}_{02} \) as in Eqs. (A24), Eq. (A13) and Eqs. (A12a,b), respectively. We also replace the corresponding index by “0”, and \( \hat{P}^{(i)}_{00} \) is defined the same as in Eqs. (A12a,b), provided that we replace the corresponding index by “3” and “0”, and \( \hat{P}^{(i)}_{00} \) is defined the same as in Eq. (20b) or (21b), provided that we replace the corresponding indices by “3” and “0”, and

\[
\hat{P}^{(i)}_{00} = \begin{bmatrix}
E^{(i)} & E^{(i)} & E^{(i)} & E^{(i)} \\
E^{(i)} & E^{(i)} & E^{(i)} & E^{(i)} \\
E^{(i)} & E^{(i)} & E^{(i)} & E^{(i)} \\
E^{(i)} & E^{(i)} & E^{(i)} & E^{(i)} \\
\end{bmatrix}
\]

(A17a)

for the perfectly-bonded interface, and

\[
\hat{P}^{(i)}_{00} = - \begin{bmatrix}
0 & [1 - (1 - i^{(i)}_{j}) W_{20} / 2] & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
\end{bmatrix}
\]

(A17b)

for the interface in frictionless contact, and

\[
\begin{align*}
\hat{Z}^{(i)}_{10} &= 0; \quad \hat{Z}^{(i)}_{11} = (1) \times \frac{1}{\gamma_0^0}, \\
\hat{Z}^{(i)}_{12} &= 0; \quad \hat{Z}^{(i)}_{13} = (1) \times \gamma_0^0
\end{align*}
\]

(A18)

In obtaining Eqs. (A17a,b) and (A18), use has also been made of Eqs. (4) and (22).

As a special case, the solution for an isotropic bimaterial can be achieved by simply setting

\[
\begin{align*}
\gamma_1 &= 1, \quad m_0 = 1, \quad \theta_0 = 2, \quad \phi_0 = 1, \quad \alpha_0 = 2 \\
\hat{G}^{(i)} &\equiv G^{(i)}, \quad \theta^{(i)} = 4(1 - i^{(i)}), \quad E^{(i)} = 3 - 4 \nu^{(i)},
\end{align*}
\]

(A19)

\[
W^{(i)} = 2(1 - 2 \nu^{(i)}),
\]

where \( G^{(i)} \) and \( \nu^{(i)} \) are the shear modulus and Poisson’s ratio of the isotropic material \( \xi \), respectively.

**Appendix B. Dislocation loops in a transversely isotropic half-space with free surface (assuming that the plane of isotropy is parallel to the free surface)**

The whole treatment to transversely isotropic bimaterials is also suitable for a transversely isotropic half-space \( x_3 > 0 (\lambda = \mu = 1) \) or \( x_3 < 0 (\lambda = \mu = 2) \) with free surface (i.e. \( \sigma_{33} = 0 \) at \( x_3 = 0 \)), provided that we make some slight modifications to Eqs. (12a)–(13b), (20a)–(21b), (A12a,b) and (A17a,b) correspondingly, i.e.

\[
\begin{align*}
\hat{P}^{(i)}_{23} &= \begin{cases} 1 & \text{if } x_3 > 0 (\lambda = \mu = 1) \\
0 & \text{if } x_3 < 0 (\lambda = \mu = 2)
\end{cases} \\
\end{align*}
\]

(B1a)

\[
\begin{align*}
\begin{bmatrix}
\theta^{(i)}_1 & \theta^{(i)}_2 & \theta^{(i)}_3 & -\theta^{(i)}_4
\end{bmatrix}^{-1}
\end{align*}
\]

(B1b)

\[
\begin{align*}
\Lambda^{(i)} &= \begin{bmatrix}
\omega^{(i)}_1 & \omega^{(i)}_2 & \omega^{(i)}_3 & -\omega^{(i)}_4
\end{bmatrix}
\end{align*}
\]

(B2a)

\[
\begin{align*}
\begin{bmatrix}
\phi^{(i)}_1 & \phi^{(i)}_2 & \phi^{(i)}_3 & -\phi^{(i)}_4
\end{bmatrix}
\end{align*}
\]

(B2b)

\[
\begin{align*}
\begin{bmatrix}
\omega^{(i)}_1 & \omega^{(i)}_2 & \omega^{(i)}_3 & -\omega^{(i)}_4
\end{bmatrix}
\end{align*}
\]

(B3)

\[
\begin{align*}
\begin{bmatrix}
\omega^{(i)}_1 & \omega^{(i)}_2 & \omega^{(i)}_3 & -\omega^{(i)}_4
\end{bmatrix}
\end{align*}
\]

(B4)

Here use has been made of Eqs. (4) and (22) in obtaining Eqs. (B3) and (B4).

Obviously, for the specific problem of dislocation loops in a transversely isotropic half-space, there is no need for us to calculate any quantity with double material-indices \((\lambda, \mu)\) where \( \lambda \neq \mu \).

For the special case of an isotropic half-space, the associated potential functions can be significantly simplified and the final results are listed below for future reference.

\[
\begin{align*}
\psi^{(i)}_1 - \psi^{(i)}_0 &= \psi^{(i)}_2 - \psi^{(i)}_3 = \psi^{(i)}_4 + \psi^{(i)}_5 = \frac{R}{4(1 - \nu^{(i)})}, \\
\end{align*}
\]

(B5)

\[
\begin{align*}
\begin{bmatrix}
\omega^{(i)}_1 & \omega^{(i)}_2 & \omega^{(i)}_3 & -\omega^{(i)}_4
\end{bmatrix}
\end{align*}
\]

(B6)

\[
\begin{align*}
\begin{bmatrix}
\phi^{(i)}_1 & \phi^{(i)}_2 & \phi^{(i)}_3 & -\phi^{(i)}_4
\end{bmatrix}
\end{align*}
\]

(B7)

\[
\begin{align*}
\begin{bmatrix}
\omega^{(i)}_1 & \omega^{(i)}_2 & \omega^{(i)}_3 & -\omega^{(i)}_4
\end{bmatrix}
\end{align*}
\]

(B8)