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Elastic study on singularities interacting with interfaces using alternating technique Part I. Anisotropic trimaterial

S.T. Choi, Y.Y. Earmme *

Department of Mechanical Engineering, Korea Advanced Institute of Science and Technology, Science Town, Daejon 305-701, South Korea

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Abstract

Schwarz–Neumann's alternating technique is applied to singularity problems in an anisotropic 'trimaterial', which denotes an infinite body composed of three dissimilar materials bonded along two parallel interfaces. Linear elastic materials under general plane deformations are assumed, in which the plane of deformation is perpendicular to the two parallel interface planes.

It is well known that if the solution is known for singularities in a homogeneous anisotropic medium, the solution for the same singularities in an anisotropic bimaterial can be constructed by the method of analytic continuation. It is shown here that the solution for singularities in a homogeneous medium may also be used as a base of the solution for the same singularities in a trimaterial. The alternating technique is applied to derive the trimaterial solution in a series form, whose convergence is guaranteed. The solution procedure is universal in the sense that no specific information about the singularity is needed. The energetic forces exerted on a dislocation due to interfaces are also evaluated from the trimaterial solution. The trimaterial solution studied here can be applied to a variety of problems, e.g. a bimaterial (including a half-plane problem), a finite thin film on semi-infinite substrate, and a finite strip of thin film, etc. Some examples are presented to verify the usefulness of the obtained solutions. © 2002 Elsevier Science Ltd. All rights reserved.

1. Introduction

Thin film and layered structures are technologically important in electronics and opto-electronics. Defects like dislocations in these structures are inevitable and affect the performance of the systems. For example, misfit dislocations are generated to relax misfit strain in lattice-mismatched structures, and the dislocations in the relaxed film can have a strong adverse effect on charge transport (Tu et al., 1992). Critical thickness at which a misfit dislocation is generated, strain relaxation due to the array of misfit dislocations, and work hardening caused by the saturation of misfit dislocations have been major issues for

* Corresponding author. Tel.: +82-42-869-3013; fax: +82-42-869-3210.
E-mail address: yyearmme@kaist.ac.kr (Y.Y. Earmme).

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development of strained-layer semiconductor materials. From the mechanical point of view, these dislocations are treated as singularities and the analysis of the elastic field near the singularity plays an important role in understanding the behavior of the structures. In addition to the intrinsic physical significance, they can serve as kernel functions of singular integral equations, to simulate cracks by continuous distributions of dislocations. Therefore, structural failure, such as film debonding, subinterface crack, and channeling crack, which may arise during fabrication and operation of integrated circuits, can be analyzed with the aid of the singularity solutions (Hutchinson and Suo, 1992).

Eshelby et al. (1953) and Stroh (1958) developed the theory of anisotropic elasticity for a generalized two-dimensional deformation and examined dislocations in an infinite homogeneous medium. Following their works, studies on singularities in anisotropic infinite space, half-space, and bimaterial have attracted numerous researchers, as can be found in the references cited in Ting (1996). In particular, using the method of analytic continuation, Suo (1990) expressed the solution for a singularity in an anisotropic bimaterial in terms of that for the same singularity in a homogeneous medium. The elastic fields of dislocations or point forces in an anisotropic strip (i.e. homogeneous material) or film/substrate structure (i.e. bimaterial), which are special cases of a trimaterial, are studied by using the Stroh formalism in conjunction with the Fourier integral transform by many researchers (Alshits and Kirchner, 1995a,b; Blanco et al., 1995; Wu and Chiu, 1995; Zhang, 1995; Chiu and Wu, 1998). Especially, Alshits and Kirchner (1995a) generalized the Stroh formalism for layered media, which were treated as materials with a variation of elastic constants with respect to the direction normal to the layer interfaces, and applied the Fourier integral transform technique. Various geometries, such as strips, coatings, and sandwiches, are dealt with as the applications of the developed theory (Alshits and Kirchner, 1995b). However, their method needs the inverse Fourier transform, which is somewhat cumbersome and difficult to carry out for numerical implementation. It will be shown later that the above works can be dealt with as special cases of the present study, which makes this straightforward method versatile, as evidenced by various examples.

Schwarz–Neumann's alternating technique (Sokolnikoff, 1956) and the method of analytic continuation (Suo, 1990) were applied by Choi and Earmme (1996) to solve subinterface crack problems in an anisotropic bimaterial, in which the corresponding solution for a homogeneous medium is required. Chao and Kao (1997) analyzed an isotropic trimaterial under an anti-plane concentrated force through iterations of Möbius transformation. Their method is similar to the alternating technique and their solution can be derived from the result of the present study. When it is difficult to find out a solution satisfying all the governing equations and boundary conditions, the alternating technique may be used to look for a series solution by successive approximations, which resembles the method of images in potential theory arranging an infinite number of image singularities.

In this study, we employ the alternating technique and the method of analytic continuation, instead of the complicated integral transform, to solve the singularity problems in an anisotropic trimaterial, in which the homogeneous solution for the same singularities is used as a base. In Section 2, we briefly study the theory of anisotropic elasticity, and then, Sections 3–5 are devoted to singularities in a homogeneous medium, a bimaterial, and a trimaterial, respectively. The convergence of the trimaterial solution, the energetic forces on a dislocation, and some examples are presented in Section 6. Finally, Section 7 concludes this article.

2. Anisotropic elasticity

We begin with the brief review of anisotropic elasticity by considering a generalized two-dimensional deformation, in which the displacements u_j depend only on x_1 and x_2. The constitutive equations for a linear elastic material are

$$\sigma_{ij} = C_{ijkm}\frac{\partial u_k}{\partial x_m}, \quad (i, j = 1, 2, 3), \tag{1}$$

in which σ_{ij} are the stresses and C_{ijkm} the elastic constants. The convention of summation over a repeated subscript is used. The equations of equilibrium are

$$C_{ijkm}\frac{\partial^2 u_k}{\partial x_j \partial x_m} = 0. \tag{2}$$

A general solution for the displacement satisfying Eq. (2) and the corresponding stresses may be written as (Eshelby et al., 1953; Stroh, 1958)

$$u_i = 2\,\mathrm{Re}\lfloor A_{ij} f_j(z_{\underline{j}})\rfloor, \tag{3}$$

$$\sigma_{1i} = -2\,\mathrm{Re}\lfloor L_{ij}\mu_{\underline{j}} f_j'(z_{\underline{j}})\rfloor, \tag{4}$$

$$\sigma_{2i} = 2\,\mathrm{Re}\lfloor L_{ij} f_j'(z_{\underline{j}})\rfloor. \tag{5}$$

Here Re denotes the real part and the prime $(\ )'$ implies the derivative with respect to the associated argument. And it should be pointed out that the index with underlined bar does not imply summation, that is, $A_{ij}f_j(z_{\underline{j}}) = A_{i1}f_1(z_1) + A_{i2}f_2(z_2) + A_{i3}f_3(z_3)$ but $f_j(z_{\underline{j}}) \neq f_1(z_1) + f_2(z_2) + f_3(z_3)$. The functions $f_j(z_{\underline{j}})$ are analytic functions of complex variable $z_j = x_1 + \mu_j x_2$. Each column of **A** and each of μ_j are the eigenvector and the eigenvalue with positive imaginary part, respectively, of the sextic equation

$$\lfloor C_{i1k1} + \mu_{\underline{j}}(C_{i1k2} + C_{i2k1}) + \mu_{\underline{j}}^2 C_{i2k2}\rfloor A_{kj} = 0. \tag{6}$$

The matrix **L** is given by

$$L_{ij} = (C_{i2k1} + \mu_{\underline{j}} C_{i2k2})A_{kj}. \tag{7}$$

Explicit expressions of the matrices **A** and **L** in terms of elastic compliances are given in Eqs. (2.3)–(2.8) of Suo (1990). If Eq. (6) has three distinct pairs of complex roots on which we are concentrating, the matrices **A** and **L** are non-singular and may be used to define

$$\mathbf{B} \equiv \mathrm{i}\mathbf{A}\mathbf{L}^{-1}, \tag{8}$$

which is a positive definite Hermitian matrix (Stroh, 1958). Here, $\mathrm{i} = \sqrt{-1}$ and $(\ )^{-1}$ stands for an inverse of the matrix.

Now we define a dimensionless bimaterial matrix $\mathbf{T}^{\mathrm{ab}}$ as follows:

$$\mathbf{T}^{\mathrm{ab}} \equiv (\mathbf{B}^{\mathrm{a}} + \overline{\mathbf{B}}^{\mathrm{b}})^{-1}(\mathbf{B}^{\mathrm{b}} - \mathbf{B}^{\mathrm{a}}), \tag{9}$$

in which the indices a and b stand for materials a and b, respectively, and $(\overline{\ })$ the complex conjugate. We note the following properties for subsequent discussion. If material a is rigid, $\mathbf{B}^{\mathrm{a}} = \mathbf{0}$ and therefore, $\mathbf{T}^{\mathrm{ab}} = (\overline{\mathbf{B}}^{\mathrm{b}})^{-1}\mathbf{B}^{\mathrm{b}}$. On the other hand if material a does not exist (i.e. material b with free surface), $\mathbf{T}^{\mathrm{ab}} = -\mathbf{I}$, where **I** is 3×3 identity matrix. In general, $\mathbf{T}^{\mathrm{ab}}$ is not equal to $-\mathbf{T}^{\mathrm{ba}}$. However, if $\mathbf{B}^{\mathrm{a}} + \overline{\mathbf{B}}^{\mathrm{b}}$ is real, $\mathbf{T}^{\mathrm{ab}} = -\mathbf{T}^{\mathrm{ba}}$ (and also real), and an interfacial crack between material a and b has non-oscillatory characteristics (Ting, 1986). The usefulness and properties of $\mathbf{T}^{\mathrm{ab}}$ will be discussed in connection with an anisotropic trimaterial in Section 6. For mathematical simplicity, we define two more bimaterial matrices as follows:

$$\mathbf{U}^{\mathrm{ab}} \equiv (\mathbf{L}^{\mathrm{a}})^{-1}(\mathbf{I} + \mathbf{T}^{\mathrm{ab}})\mathbf{L}^{\mathrm{b}}, \tag{10}$$

$$\mathbf{V}^{\mathrm{ab}} \equiv (\overline{\mathbf{L}}^{\mathrm{b}})^{-1}\mathbf{T}^{\mathrm{ab}}\mathbf{L}^{\mathrm{b}}. \tag{11}$$

Of particular importance is that the following derivatives of displacements and tractions must be continuous across the perfectly bonded interface $x_2 = 0$:

$$\frac{\partial u_i}{\partial x_1}(x_1) = A_{ij} f_j'(x_1) + \overline{A}_{ij} \overline{f}_j'(x_1), \tag{12}$$

$$\sigma_{2i}(x_1) = L_{ij} f_j'(x_1) + \overline{L}_{ij} \overline{f}_j'(x_1). \tag{13}$$

Eq. (12) is equivalent to the continuity of displacements. It is obvious that a function $g(z)$ is an analytic function of $z = x_1 + \mu x_2$ for $x_2 > 0$ (or $x_2 < 0$) for any μ if it is analytic for $x_2 > 0$ (or $x_2 < 0$) for one μ, where μ is any complex number with positive imaginary part (Suo, 1990). Consequently, one can refer to $f_j(z)$ instead of $f_j(z_{\underline{j}})$ and, if necessary, he may reinterpret z by $z_{\underline{j}}$.

3. A singularity in a homogeneous medium

In the previous section, it was shown that a general solution of a generalized two-dimensional deformation in anisotropic elasticity can be expressed by analytic functions $f_j(z)$. Now we examine the solution $f_j^0(z)$ of a singularity in a homogeneous medium. We take the solution form for line force or dislocation at (x_1^0, x_2^0) in an infinite homogeneous medium as (Stroh, 1958; Suo, 1990)

$$f_j^0(z_{\underline{j}}) = q_j \ln(z_{\underline{j}} - s_{\underline{j}}), \tag{14}$$

where $s_j = x_1^0 + \mu_j x_2^0$ and $\mathbf{q} = \{q_j\}$ is related to the Burgers vector $\mathbf{b}$ and the force per unit length $\mathbf{p}$ as

$$\mathbf{q} = \frac{1}{2\pi}\mathbf{L}^{-1}(\mathbf{B} + \overline{\mathbf{B}})^{-1}\mathbf{b} - \frac{1}{2\pi}\mathbf{A}^{-1}(\mathbf{B}^{-1} + \overline{\mathbf{B}}^{-1})^{-1}\mathbf{p}. \tag{15}$$

4. A singularity in a bimaterial and the method of analytic continuation

Consider an anisotropic bimaterial bonded along x_1-axis. Our objective is to construct a bimaterial solution for a singularity as shown in Fig. 1 in terms of the homogeneous one for the same singularity by

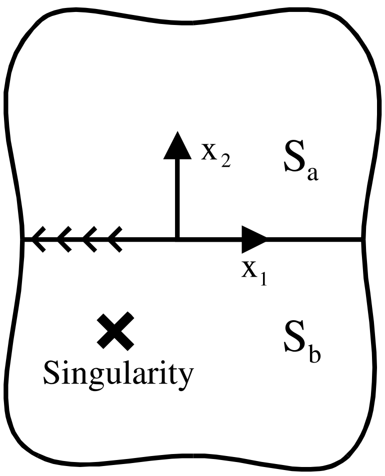

Fig. 1. A singularity in a bimaterial.

using the method of analytic continuation (Suo, 1990). First, a singularity located in lower half space is treated, in which the elastic constants of material b are implied in $f_j^0(z)$. Suo (1990) introduced $f_j^{\mathrm{a}}(z)$ and $f_j^{\mathrm{b}}(z)$ satisfying the continuity of displacements and tractions along the interface as

$$f_i(z_{\underline{i}}) = \begin{cases} f_i^{\mathrm{a}}(z_{\underline{i}}^{\mathrm{a}}), & \text{in } S_{\mathrm{a}}, \\ f_i^{\mathrm{b}}(z_{\underline{i}}^{\mathrm{b}}) + f_i^0(z_{\underline{i}}^{\mathrm{b}}), & \text{in } S_{\mathrm{b}}, \end{cases} \tag{16}$$

where S_{a}, the upper half-space, and S_{b}, the lower half space, are occupied by material a and b, respectively. In order to express $f_j^{\mathrm{a}}(z)$ and $f_j^{\mathrm{b}}(z)$ analytic in S_{a} and S_{b}, respectively, in terms of $f_j^0(z)$, the continuity of tractions across the interface with Eq. (13), by analytic continuation arguments, is used to yield

$$L_{ij}^{\mathrm{a}} f_j^{\mathrm{a}}(z) - \overline{L}_{ij}^{\mathrm{b}} \bar{f}_j^{\mathrm{b}}(z) - L_{ij}^{\mathrm{b}} f_j^0(z) = 0, \quad \text{in } S_{\mathrm{a}}. \tag{17}$$

The continuity of displacements with Eq. (12), by the same arguments, results in

$$A_{ij}^{\mathrm{a}} f_j^{\mathrm{a}}(z) - \bar{A}_{ij}^{\mathrm{b}} \bar{f}_j^{\mathrm{b}}(z) - A_{ij}^{\mathrm{b}} f_j^0(z) = 0, \quad \text{in } S_{\mathrm{a}}. \tag{18}$$

From Eqs. (17) and (18), we have

$$\begin{cases} f_i^{\mathrm{a}}(z) = U_{ij}^{\mathrm{ab}} f_j^0(z), & \text{in } S_{\mathrm{a}}, \\ f_i^{\mathrm{b}}(z) = \overline{V}_{ij}^{\mathrm{ab}} \bar{f}_j^0(z), & \text{in } S_{\mathrm{b}}, \end{cases} \tag{19}$$

where $\mathbf{U}^{\mathrm{ab}}$ and $\mathbf{V}^{\mathrm{ab}}$ are as defined in Eqs. (10) and (11). Substitution of Eq. (19) into Eq. (16) yields the solution. This procedure, though slightly different notations are used, was employed by Suo (1990). Even if the material a is rigid or non-existent, the solution still remains valid. For the former case, $\mathbf{T}^{\mathrm{ab}} = \overline{\mathbf{B}}^{\mathrm{b}-1}\mathbf{B}^{\mathrm{b}}$ and therefore

$$f_i(z_{\underline{i}}^{\mathrm{b}}) = f_i^0(z_{\underline{i}}^{\mathrm{b}}) - A_{ij}^{-1} \bar{A}_{jk} \bar{f}_k^0(z_{\underline{i}}^{\mathrm{b}}), \quad \text{in } S_{\mathrm{b}}, \tag{20}$$

while for the latter case, $\mathbf{T}^{\mathrm{ab}} = -\mathbf{I}$ and therefore

$$f_i(z_{\underline{i}}^{\mathrm{b}}) = f_i^0(z_{\underline{i}}^{\mathrm{b}}) - L_{ij}^{-1} \overline{L}_{jk} \bar{f}_k^0(z_{\underline{i}}^{\mathrm{b}}), \quad \text{in } S_{\mathrm{b}}. \tag{21}$$

For a singularity located in the upper half-space, the solution is assumed to be

$$f_i(z_{\underline{i}}) = \begin{cases} f_i^{\mathrm{a}}(z_{\underline{i}}^{\mathrm{a}}) + f_i^0(z_{\underline{i}}^{\mathrm{a}}), & \text{in } S_{\mathrm{a}}, \\ f_i^{\mathrm{b}}(z_{\underline{i}}^{\mathrm{b}}), & \text{in } S_{\mathrm{b}}, \end{cases} \tag{22}$$

and one finds, by the similar procedure,

$$\begin{cases} f_i^{\mathrm{a}}(z) = \overline{V}_{ij}^{\mathrm{ba}} \bar{f}_j^0(z), & \text{in } S_{\mathrm{a}}, \\ f_i^{\mathrm{b}}(z) = U_{ij}^{\mathrm{ba}} f_j^0(z), & \text{in } S_{\mathrm{b}}, \end{cases} \tag{23}$$

where the elastic constants involved in $f_i^0(z)$ are for material a.

5. A singularity in a trimaterial and the alternating technique

The alternating technique together with the results of Sections 3 and 4 can be employed to analyze a singularity in a trimaterial with two parallel interfaces as shown in Fig. 2. Since it is difficult to satisfy the continuity conditions along two interfaces at the same time, the method of analytic continuation should be applied to two interfaces alternatively. A coordinate translation is described as below in order to apply the alternating technique to the case of the trimaterial in Fig. 2.

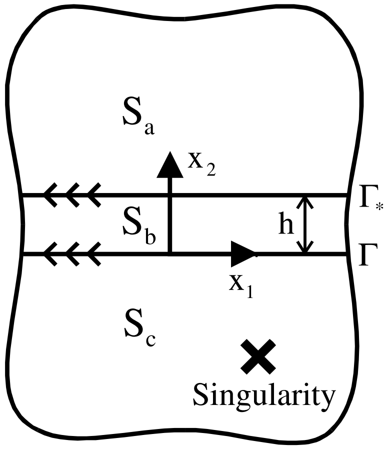

Fig. 2. A singularity in a trimaterial.

5.1. A coordinate translation

Assume that regions $S_a : x_2 \geqslant h$ and $S_b : x_2 \leqslant h$ occupied by material a and b, respectively, are perfectly bonded along the interface $x_2 = h$ (see Fig. 2 with material c = material b). With $x_1 x_2$ coordinate system lying off the interface, let us reformulate the bimaterial solution obtained in the previous section. The solution is also assumed as Eq. (16), in which $f_j^a(z)$ and $f_j^b(z)$ are introduced to satisfy the continuity of displacements and tractions along the interface $x_2 = h$. By applying the same arguments used in Eqs. (17) and (18) to the interface $x_2 = h$, one finds, instead of Eq. (19),

$$\begin{cases} f_i^a(z) = U_{ij}^{ab} f_j^0(z - \mu_{\underline{i}}^a h + \mu_{\underline{j}}^b h), & x_2 \geqslant h, \\ f_i^b(z) = \overline{V}_{ij}^{ab} \bar{f}_j^0(z - \mu_{\underline{i}}^b h + \bar{\mu}_{\underline{j}}^b h), & x_2 \leqslant h. \end{cases} \tag{24}$$

Substitution of Eq. (24) into Eq. (16) gives a singularity solution in a bimaterial bonded along $x_2 = h$.

5.2. Case I: A singularity embedded in S_c

Returning to a trimaterial as shown in Fig. 2, material a, b, and c occupying regions $S_a : x_2 \geqslant h$, $S_b : h \geqslant x_2 \geqslant 0$, and $S_c : x_2 \leqslant 0$, respectively, are perfectly bonded along two parallel interfaces $\Gamma : x_2 = 0$ and $\Gamma_* : x_2 = h$. Assume a series solution for the case of the singularity located in S_c as

$$f_i(z_{\underline{i}}) = \begin{cases} \sum_{n=1}^{\infty} f_i^{an}(z_{\underline{i}}^a), & \text{in } S_a, \\ \sum_{n=1}^{\infty} f_i^{n}(z_{\underline{i}}^b) + \sum_{n=1}^{\infty} f_i^{bn}(z_{\underline{i}}^b), & \text{in } S_b, \\ f_i^0(z_{\underline{i}}^c) + f_i^{c0}(z_{\underline{i}}^c) + \sum_{n=1}^{\infty} f_i^{cn}(z_{\underline{i}}^c), & \text{in } S_c. \end{cases} \tag{25}$$

Now, it is required to solve for $f_i^{c0}(z)$, $f_i^{an}(z)$, $f_i^{bn}(z)$, $f_i^{cn}(z)$ and $f_i^n(z)$ $(n = 1, 2, 3, \ldots)$ analytic in their respective regions in terms of $f_i^0(z)$. The details and the physical interpretations of each term in connection with the alternating technique are described in Appendix A. Insertion of the results of Appendix A into Eq. (25) leads to

$$f_i(z_{\underline{i}}) = \begin{cases} U_{ij}^{\mathrm{ab}} \sum_{n=1}^{\infty} f_j^n(z_{\underline{i}}^{\mathrm{a}} - \mu_{\underline{i}}^{\mathrm{a}} h + \mu_{\underline{j}}^{\mathrm{b}} h), & \text{in } S_{\mathrm{a}}, \\ \sum_{n=1}^{\infty} \left[f_i^n(z_{\underline{i}}^{\mathrm{b}}) + \overline{V}_{ij}^{\mathrm{ab}} \bar{f}_j^n(z_{\underline{i}}^{\mathrm{b}} - \mu_{\underline{i}}^{\mathrm{b}} h + \bar{\mu}_{\underline{j}}^{\mathrm{b}} h) \right], & \text{in } S_{\mathrm{b}}, \\ f_i^0(z_{\underline{i}}^{\mathrm{c}}) + \overline{V}_{ij}^{\mathrm{bc}} \bar{f}_j^0(z_{\underline{i}}^{\mathrm{c}}) + U_{ij}^{\mathrm{cb}} \overline{V}_{jk}^{\mathrm{ab}} \sum_{n=1}^{\infty} \bar{f}_k^n(z_{\underline{i}}^{\mathrm{c}} - \mu_{\underline{j}}^{\mathrm{b}} h + \bar{\mu}_{\underline{k}}^{\mathrm{b}} h), & \text{in } S_{\mathrm{c}}, \end{cases} \tag{26}$$

where the recurrence formula for $f_i^n(z)$ is

$$f_i^{n+1}(z) = \begin{cases} U_{ij}^{\mathrm{bc}} f_j^0(z), & \text{if } n = 0, \\ \overline{V}_{ij}^{\mathrm{cb}} V_{jk}^{\mathrm{ab}} f_k^n(z - \bar{\mu}_{\underline{j}}^{\mathrm{b}} h + \mu_{\underline{k}}^{\mathrm{b}} h), & \text{if } n = 1, 2, 3, \ldots \end{cases} \tag{27}$$

Here the elastic constants of material c are implied in $f_i^0(z)$. Eq. (26) with Eq. (27) gives the complete solution for the singularity located in region S_{c}.

5.3. Case II: A singularity embedded in S_b

Using the same procedure as case I, the other case in which the singularity is located in region S_{b} has the following solution:

$$f_i(z_{\underline{i}}) = \begin{cases} U_{ij}^{\mathrm{ab}} \sum_{n=1}^{\infty} f_j^n(z_{\underline{i}}^{\mathrm{a}} - \mu_{\underline{i}}^{\mathrm{a}} h + \mu_{\underline{j}}^{\mathrm{b}} h), & \text{in } S_{\mathrm{a}}, \\ \sum_{n=1}^{\infty} \left[f_i^n(z_{\underline{i}}^{\mathrm{b}}) + \overline{V}_{ij}^{\mathrm{ab}} \bar{f}_j^n(z_{\underline{i}}^{\mathrm{b}} - \mu_{\underline{i}}^{\mathrm{b}} h + \bar{\mu}_{\underline{j}}^{\mathrm{b}} h) \right], & \text{in } S_{\mathrm{b}}, \\ U_{ij}^{\mathrm{cb}} f_j^0(z_{\underline{i}}^{\mathrm{c}}) + U_{ij}^{\mathrm{cb}} \overline{V}_{jk}^{\mathrm{ab}} \sum_{n=1}^{\infty} \bar{f}_k^n(z_{\underline{i}}^{\mathrm{c}} - \mu_{\underline{j}}^{\mathrm{b}} h + \bar{\mu}_{\underline{k}}^{\mathrm{b}} h), & \text{in } S_{\mathrm{c}}, \end{cases} \tag{28}$$

in which the recurrence formula for $f_i^n(z)$ is

$$f_i^{n+1}(z) = \begin{cases} f_i^0(z) + \overline{V}_{ij}^{\mathrm{cb}} \bar{f}_j^0(z), & \text{if } n = 0, \\ \overline{V}_{ij}^{\mathrm{cb}} V_{jk}^{\mathrm{ab}} f_k^n(z - \bar{\mu}_{\underline{j}}^{\mathrm{b}} h + \mu_{\underline{k}}^{\mathrm{b}} h), & \text{if } n = 1, 2, 3, \ldots \end{cases} \tag{29}$$

Here the elastic constants involved in $f_i^0(z)$ are for material b.

The procedure used to derive the trimaterial solutions (26)–(29) is independent of the physical nature of the singularities. Instead of Eq. (14), any homogeneous solutions for other singularities, e.g. a dipole of line forces or dislocations, may be put into Eqs. (26)–(29) in order to obtain the corresponding trimaterial solutions.

6. Discussion

6.1. Convergence of the series solutions

Although it is known that a series solution obtained via the alternating technique converges to a true solution for isotropic elastic materials (Sokolnikoff, 1956), we review and prove directly the convergence of the series solutions (26)–(29) before we extensively make use of the solutions. It is worth pointing out that Eqs. (26) and (28) are expressed in terms of $\mathbf{f}^n(z)$ $(n = 0, 1, 2, \ldots)$, which may be calculated from a homogeneous solution $\mathbf{f}^0(z)$ by the recurrence formulae (27) and (29). Since we are primarily interested in the evaluation of the stresses, which are expressed in terms of $\mathbf{f}'(z)$, instead of $\mathbf{f}(z)$ (see Eqs. (4) and (5)), we will deal with the convergence of $\mathbf{f}'(z)$. Noting that μ's have positive imaginary parts, one can get $|\mathbf{f}'^n(z - \bar{\mu}h + \mu h)| < |\mathbf{f}'^n(z)|$ for z in $S_{\mathrm{a}} \cup S_{\mathrm{b}}$ and $|\bar{\mathbf{f}}'^n(z - \mu h + \bar{\mu}h)| < |\bar{\mathbf{f}}'^n(z)|$ for z in $S_{\mathrm{b}} \cup S_{\mathrm{c}}$, in which $|\cdot|$ stands for the magnitude of a vector. Then, from the inequality, $|\mathbf{a} = \mathbf{Bc}| \leqslant \|\mathbf{B}\||\mathbf{c}|$ for a matrix $\mathbf{B}$ and a vector $\mathbf{c}$, it is easy to show

$$\begin{aligned} |\mathbf{f}'^{n+1}(z)| &\leqslant \|\overline{\mathbf{V}}^{cb}\mathbf{V}^{ab}\||\mathbf{f}'^{n}(z-\bar{\mu}h+\mu h)| < \|\mathbf{T}^{ab}\|\|\mathbf{T}^{cb}\||\mathbf{f}'^{n}(z)|, \quad \text{for } z \text{ in } S_a \cup S_b, \\ |\bar{\mathbf{f}}'^{n+1}(z)| &\leqslant \|\overline{\mathbf{V}}^{cb}\mathbf{V}^{ab}\||\bar{\mathbf{f}}'^{n}(z-\bar{\mu}h+\mu h)| < \|\mathbf{T}^{ab}\|\|\mathbf{T}^{cb}\||\bar{\mathbf{f}}'^{n}(z)|, \quad \text{for } z \text{ in } S_b \cup S_c, \end{aligned} \tag{30}$$

in which the matrix norm $\|\cdot\|$ is defined as the largest magnitude of its eigenvalues. Therefore, a sufficient condition for the convergence of the series solutions that $|\mathbf{f}'^{n+1}(z)| < |\mathbf{f}'^{n}(z)|$ $(n \geqslant 1)$ for z in $S_a \cup S_b$ and $|\bar{\mathbf{f}}'^{n+1}(z)| < |\bar{\mathbf{f}}'^{n}(z)| (n \geqslant 1)$ for z in $S_b \cup S_c$ is satisfied if the norm of $\mathbf{T}^{ab}$ (and also $\mathbf{T}^{cb}$) is $\leqslant 1$, which is proved in Appendix B by considering the eigenvalue equation of $\mathbf{T}^{ab}$. The rate of the convergence depends on the bimaterial matrices $\mathbf{T}^{ab}$ and $\mathbf{T}^{cb}$ representing the mismatch of elastic constants of two constituent materials. The smaller the difference of elastic constants of two adjacent materials a and b (or c and b) is, the less the norm of $\mathbf{T}^{ab}$ (or $\mathbf{T}^{cb}$) is, which is obvious from the definition of $\mathbf{T}^{ab}$, Eq. (9). Consequently, the convergence rate becomes more rapid. The thickness h of material b also affects the rate of convergence in such a way that as h gets larger, the series solution is more rapidly convergent, because the ordinates of the image singularities are linearly proportional to h. It is found that the sum of the first three or four terms provides a good approximation for most combinations of materials (Choi and Earmme, 1999).

Even if materials a and/or c are rigid or non-existent, the solutions still remain valid. For these limiting cases, we replace $\mathbf{T}^{ab}$ and/or $\mathbf{T}^{cb}$ in the solutions (26)–(29) by those indicated in Table 1 for the four special combinations of three dissimilar materials. All the combinations illustrated in Table 1 are meaningful for a singularity located in S_b, while only the combination 4 has the meaning for a singularity located in S_c. For another limiting case in which two adjacent materials, say materials a and b, are identical, the series solution for a trimaterial reduces to the bimaterial one. Furthermore, if material b is rigid or non-existent, the trimaterial solution (26) with solution (27) reduces to the solution (20) or solution (21), respectively.

6.2. The energetic forces exerted on a dislocation

The elastic force on a dislocation segment is given by (Peach and Koehler, 1950)

$$\mathrm{d}\boldsymbol{f} = (\sigma \cdot \mathbf{b}) \times \mathrm{d}\mathbf{l}, \tag{31}$$

for the stress field σ, the Burgers vector $\mathbf{b}$ and the line segment $\mathrm{d}\mathbf{l}$. The stress field may originate not only from the image field required to satisfy the boundary conditions, but also from external sources such as the other dislocations, residual stresses, applied forces, etc. Note that the trimaterial solution for a dislocation consists of a singular term and the other regular terms corresponding to the image singularities. Therefore, combining Eqs. (26) or (28), (4), (5) and (31), the image forces in x_2 direction per unit length of a dislocation due to two parallel interfaces in a trimaterial are given by

$$f_2 = 2b_i \mathrm{Re}\left\{ L^b_{ij}\mu^b_{\underline{j}} \left[\overline{V}^{cb}_{jk}\bar{f}'^0_k(s^b_{\underline{j}}) + \sum_{n=2}^{\infty} f'^n_j(s^b_{\underline{j}}) + \overline{V}^{ab}_{jk} \sum_{n=1}^{\infty} \bar{f}'^n_k(s^b_{\underline{j}} - \mu^b_{\underline{j}}h + \bar{\mu}^b_{\underline{k}}h) \right] \right\}, \tag{32}$$

Table 1
Special combinations of three dissimilar materials forming a trimaterial

Combination	1	2	3	4
Material a	Empty	Empty	Rigid	Empty
Material b	Elastic	Elastic	Elastic	Elastic
Material c	Empty	Rigid	Rigid	Elastic
$\mathbf{T}^{ab}$	$-\mathbf{I}$	$-\mathbf{I}$	$\overline{\mathbf{B}}^{b-1}\mathbf{B}^b$	$-\mathbf{I}$
$\mathbf{T}^{cb}$	$-\mathbf{I}$	$\overline{\mathbf{B}}^{b-1}\mathbf{B}^b$	$\overline{\mathbf{B}}^{b-1}\mathbf{B}^b$	$\mathbf{T}^{cb}$

$$f_2 = 2b_i \mathrm{Re}\left\{ L^{\mathrm{c}}_{ij}\mu^{\mathrm{c}}_{\underline{j}} \left[\overline{V}^{\mathrm{bc}}_{jk} \bar{f}'^{0}_{k}(s^{\mathrm{c}}_{\underline{j}}) + U^{\mathrm{cb}}_{jk} \overline{V}^{\mathrm{ab}}_{km} \sum_{n=1}^{\infty} \bar{f}'^{n}_{m}(s^{\mathrm{c}}_{\underline{j}} - \mu^{\mathrm{b}}_{\underline{k}} h + \bar{\mu}^{\mathrm{b}}_{\underline{m}} h) \right] \right\}, \tag{33}$$

for a dislocation in material b or c, respectively. It is straightforward that the image force f_1 in the x_1 direction is equal to zero. One may also evaluate the image forces due to the other external agencies in the same way.

6.3. Some examples

Here exemplified is the structure of a Ge_xSi_{1-x} epitaxial layer on a Si substrate as shown in Fig. 3. Zhang (1995) solved the problem of the same geometry and materials, focusing on the evaluation of the critical film thickness, in which the Fourier transform technique is used. The elastic constants of Ge, Si, and Ge_xSi_{1-x} with respect to the crystallographic axes, where x represents the fraction of lattice sites occupied by Ge atoms, are given in Table 2 (Zhang, 1995; Jain et al., 1997). A Ge_xSi_{1-x} epitaxial film on the {1 0 0} or {1 1 0} plane of Si substrate is chosen with the so-called "60° dislocation" (Zhang, 1995) on {1 1 1} glide plane. For the {1 0 0} plane epitaxy, the coordinates x_1 and x_2 coincide with the crystallographic directions $[10\bar{1}]$ and [0 1 0], respectively, with $x_3 = [101]$. Burgers vector $\mathbf{b}$ of the 60° dislocation is $\mathbf{b} = b[1/\sqrt{2}, -1/\sqrt{2}, 0]$ in crystallographic notation and $\mathbf{b} = (b_1, b_2, b_3) = b(1/2, -1/\sqrt{2}, 1/2)$ in (x_1, x_2, x_3) coordinate system. The dislocation tangent vector is along the x_3-axis, with the normal to the slip plane $\mathbf{n} = [11\bar{1}]$ in crystallographic notation and $\mathbf{n} = (n_1, n_2, n_3) = (\sqrt{2}/\sqrt{3}, 1/\sqrt{3}, 0)$ in (x_1, x_2, x_3) coordinate system. Notice both the edge and the screw components. For the {1 1 0} plane epitaxy, the coordinate directions x_1 and x_2 coincide with the crystallographic directions [0 1 0] and [1 0 1], respectively, with $x_3 = [10\bar{1}]$. Burgers vector $\mathbf{b}$ of the 60° dislocation is $\mathbf{b} = b[1/\sqrt{2}, -1/\sqrt{2}, 0]$ in crystallographic notation and $\mathbf{b} = (b_1, b_2, b_3) = b(-1/\sqrt{2}, 1/2, 1/2)$ in (x_1, x_2, x_3) coordinate system. The dislocation tangent vector is along the x_3-axis, with the normal to the slip plane $\mathbf{n} = [111]$ in crystallographic notation and $\mathbf{n} = (n_1, n_2, n_3) = (1/\sqrt{3}, \sqrt{2}/\sqrt{3}, 0)$ in (x_1, x_2, x_3) coordinate system. Also there are both the edge and the

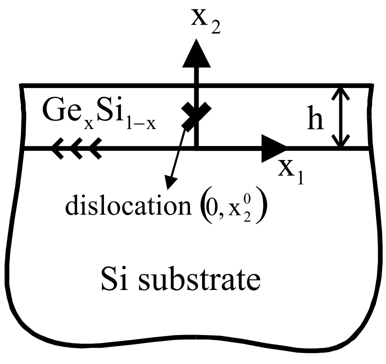

Fig. 3. A dislocation in a Ge_xSi_{1-x} epilayer on a Si substrate.

Table 2
Elastic constants of Ge, Si, and Ge_xSi_{1-x} in unit of GPa (Zhang, 1995; Jian et al., 1997) with respect to crystallographic directions

Crystal	c_{11}	c_{12}	c_{44}
Ge	128.9	48.3	67.1
Si	165.7	63.9	79.6
Ge_xSi_{1-x}	$128.9x + 165.7(1-x)$	$48.3x + 63.9(1-x)$	$67.1x + 79.6(1-x)$

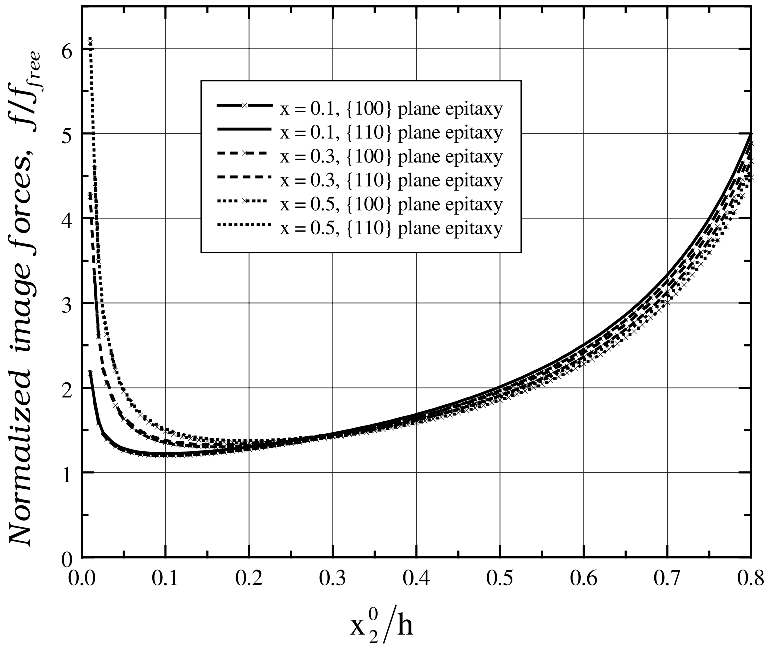

Fig. 4. Normalized image forces vs. the position of a dislocation.

screw components. Elastic constants given in Table 2 are transformed to yield the elastic constants with respect to the (x_1, x_2, x_3) coordinate system. The image forces f_2/f_{free} exerted on the 60° dislocation are plotted for $x = 0.1$, 0.3, and 0.5 respectively in Fig. 4, in which the curves are evaluated with terms up to $n = 3$ in Eq. (32), and the normalizing constant f_{free} is the image force on the dislocation at a distance h from the $\{1\,0\,0\}$ free surface in Si half space. It is found that the contributions of terms with $n = 2$, 3, and 4 to the image forces are about 3.4%, 0.15%, and 0.0075%, respectively, for $x = 0.5$ signifying that $|\mathbf{f}'^{n+1}(z)|/|\mathbf{f}'^{n}(z)|$ is about 0.05, which is less than $\|\mathbf{T}^{\text{cb}}\| = 0.08424$. Therefore, it can be seen that the error of the approximations with terms up to $n = 3$ is <0.01%. Furthermore, the approximations are more accurate for $x = 0.3$ and 0.1 than for $x = 0.5$, because $\|\mathbf{T}^{\text{cb}}\| = 0.05129$ and 0.01736 for $x = 0.3$ and 0.1, respectively. As can be seen in Fig. 4, the crystallographic orientation rarely affects the image force on the dislocation. Near the Ge_xSi_{1-x}/Si interface, the image force increases as the mismatch of elastic constants increases, and is proportional to 1/(distance from the dislocation to the interface) as shown in the work of Barnett and Lothe (1974).

Next, as an extreme example with the slowest rate of convergence, we revisit an edge dislocation in an anisotropic potassium strip (Wu and Chiu, 1995), that is, a trimaterial whose region S_{b} is composed of potassium and regions S_{a} and S_{c} are non-existent or rigid as shown in Fig. 5, therefore $\|\mathbf{T}^{\text{ab}}\| = \|\mathbf{T}^{\text{cb}}\| = 1$. Potassium has body-centered cubic structure and three independent elastic constants $c_{11} = 4.57$ GPa, $c_{12} = 3.74$ GPa, and $c_{44} = 2.63$ GPa (Wu and Chiu, 1995) with respect to the cubic axes. In order to compare the results, we choose the same Burgers vector, dislocation tangent vector, etc as those by Wu and Chiu (1995), i.e., Burgers vector is $(b/\sqrt{3})[1\,1\,1]$ and the slip plane is $(3\,\bar{2}\,\bar{1})$ in crystallographic notation. We choose (x_1, x_2, x_3) coordinate system as follows: The x_3-axis is in the direction of $[1\,4\,\bar{5}]$, while x_1- and x_2-axes are chosen in such a way that $\mathbf{b} = (b/\sqrt{3})[1\,1\,1]$ in crystallographic notation has the components $\mathbf{b} = b(\cos\psi, \sin\psi, 0)$ in (x_1, x_2, x_3) coordinate system. Accordingly, the dislocation has the edge component only and the normal to the slip plane is $\mathbf{n} = (-\sin\psi, \cos\psi, 0)$ in (x_1, x_2, x_3) system. The slip plane of the edge

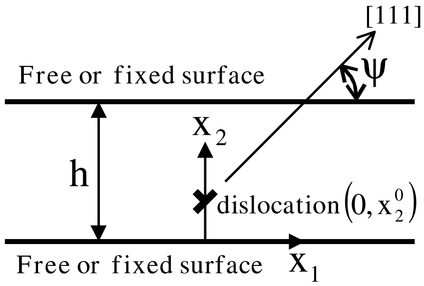

Fig. 5. A dislocation in an infinite strip.

dislocation is therefore inclined at an angle ψ with respect to the x_1x_3 plane of the strip (see Fig. 5). The image forces exerted on the dislocation whose slip plane is inclined at $\psi = 0°$, 45°, and 90° are computed when regions S_a and S_c are rigid (Fig. 6) or non-existent (Fig. 7). The curve f_2 vs. x_2^0 in Fig. 6 is obtained by adding the terms up to $n = 6$ while in Fig. 7, the terms up to $n = 15$ are included in Eq. (32). The normalizing constant f_{fix} (or f_{free}) is the image force on a dislocation at a distance h from fixed (or free) surface in K half space. It is a well-known fact that a dislocation is attracted to the free surface and repelled by the fixed surface. For the strip with fixed surfaces (Fig. 6), the image force exerted on a dislocation is toward the center of the strip $x_2^0/h = 0.5$, which is a stable equilibrium position, and the magnitude of the image force at a given position decreases with the slip plane inclination ψ. Present result (Fig. 6) agrees well with the Fig. 5 of Wu and Chiu (1995). It is interesting that for the strip with free surfaces (Fig. 7), the center of the

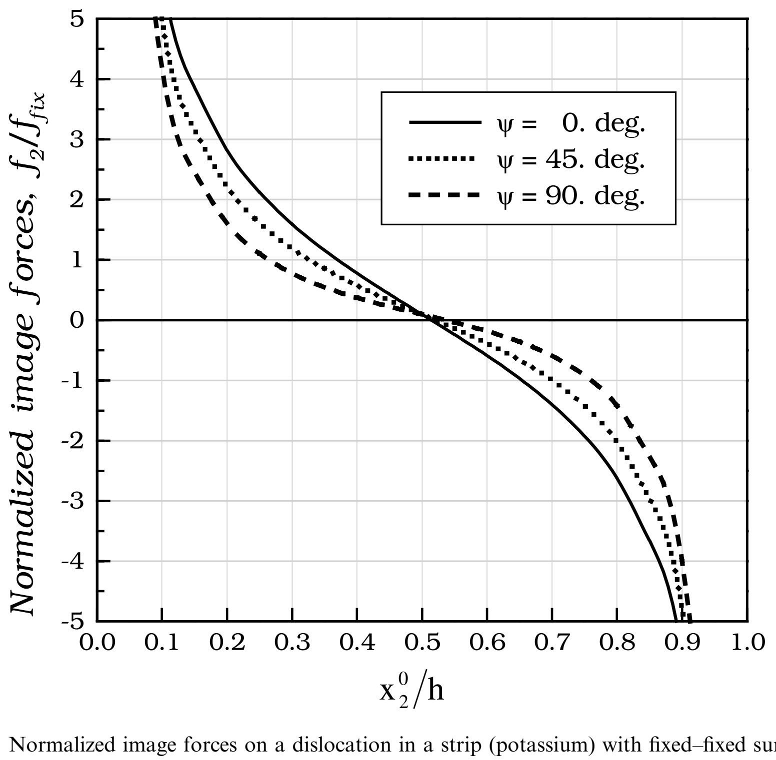

Fig. 6. Normalized image forces on a dislocation in a strip (potassium) with fixed–fixed surfaces.

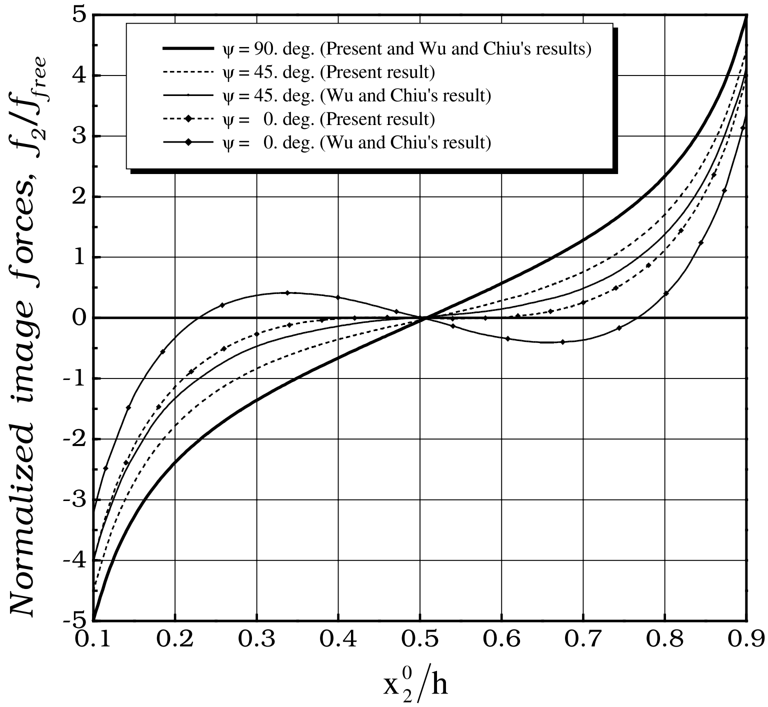

Fig. 7. Normalized image forces on a dislocation in a strip (potassium) with free–free surfaces.

strip $x_2^0/h = 0.5$ is a stable equilibrium for a dislocation with $\psi = 0°$, but not for a dislocation with $\psi = 45°$ or 90°. Present result (Fig. 7) is slightly different from the Fig. 3 of Wu and Chiu (1995) for $\psi = 0°$ and 45°, which is reproduced in Fig. 7 by scanning their original figure. The difference is believed to be due to the error of approximation in present result, even though in Fig. 7 the terms up to $n = 15$ in Eq. (32) are added (in Fig. 6, it was found that the terms up to $n = 6$ yield satisfactory results). It is found that the rate of convergence for an infinite strip, i.e., an extreme case of trimaterial, is dependent on the type of singularity and boundary conditions (Choi and Earmme, in preparation). A strip with free surfaces has the slowest rate of convergence for a dislocation with $\psi = 0°$.

7. Conclusion

The alternating technique and the method of analytic continuation are employed to study the singularities in an anisotropic trimaterial. It is shown here that a homogeneous solution for singularities serves as a base to derive the trimaterial solution for the same singularities in a series form. As the solution of a singularity in a bimaterial is interpreted with the concept of image singularities, the solution of a singularity in a trimaterial can also be explained as the arrangement of an infinite number of image singularities. We prove that the norm of the dimensionless bimaterial matrix $\mathbf{T}^{ab}$ is $\leqslant 1$, which guarantees the convergence of the trimaterial solution. The convergence rate of the series solution depends on the material combinations and the thickness of middle material. The smaller the mismatch of elastic constants of adjacent materials is, the more rapid the convergence rate is. The solution procedure is universal in the sense that it is completely independent of the physical nature of the singularities. In the limiting cases, in which one material (or even two materials) in an anisotropic trimaterial is rigid or non-existent, the solution still remains valid. Furthermore, as two adjacent materials degenerates to be a homogeneous one, the trimaterial solution reduces to the bimaterial one. Consequently, the trimaterial solution studied here can be applied to a variety of problems, e.g. a bimaterial (including a half-plane problem), a finite thin film on semi-infinite substrate, and a finite strip of thin film, etc. In fact, the merit of this trimaterial solution is its wide applicability to bimaterial problems in addition to the trimaterial problem per se. The energetic forces exerted on a dislocation due to interfaces are also estimated in a series form, which play an important role in the motion of dislocation.

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Appendix A. Four steps to solve the problem of a singularity embedded in S_c

Illustrated here is the procedure to solve the problem shown in Fig. 2.

A.1. Step 1. Analytic continuation across the interface Γ

First, we regard regions S_a and S_b composed of the same material b and region S_c of material c. As in Eq. (16), if $f_i^0(z)$ is taken to be a homogeneous solution and $f_i^1(z)$ and $f_i^{c0}(z)$ are introduced to satisfy the continuity of displacements and tractions across the interface Γ, Eq. (19) leads to

$$\begin{cases} f_i^1(z) = U_{ij}^{bc} f_j^0(z), & \text{in } S_a \cup S_b, \\ f_i^{c0}(z) = \overline{V}_{ij}^{bc} \bar{f}_j^0(z), & \text{in } S_c. \end{cases} \tag{A.1}$$

Since this result is based on the assumption that region S_a is made up of material b, the fields produced by $f_i^1(z)$ cannot satisfy the continuity conditions at the interface Γ_*, which lies between material a and b.

A.2. Step 2. Analytic continuation across the interface Γ_*

Region S_a is composed of material a and regions S_b and S_c are regarded as made up of the same material b. $f_i^1(z)$ in Eq. (A.1) having the singular points in $S_b \cup S_c$ is treated as a homogeneous solution of material b. This is justified, for the method of analytic continuation is completely independent of the physical nature of the singularities. To satisfy the continuity conditions at the interface Γ_*, if $f_i^{a1}(z)$ and $f_i^{b1}(z)$ are introduced as in Eq. (16) and Eq. (24) yields

$$\begin{cases} f_i^{a1}(z) = U_{ij}^{ab} f_j^1(z - \underline{\mu}_i^a h + \underline{\mu}_j^b h), & \text{in } S_a, \\ f_i^{b1}(z) = \overline{V}_{ij}^{ab} \bar{f}_j^1(z - \underline{\mu}_i^b h + \underline{\bar{\mu}}_j^b h), & \text{in } S_b \cup S_c, \end{cases} \tag{A.2}$$

in which $f_i^{a1}(z)$ and $f_i^{b1}(z)$ can be expressed in terms of $f_i^0(z)$ through Eq. (A.1). Here $\bar{f}_j^1(z - \underline{\mu}_i^b h + \underline{\bar{\mu}}_j^b h) = \overline{f_j^1(\bar{z} - \underline{\bar{\mu}}_i^b h + \underline{\mu}_j^b h)}$. Since this result is based on the assumption that region S_c is made up of material b, the fields produced by $f_i^{b1}(z)$ in the above equation does not satisfy the continuity conditions at the interface Γ.

A.3. Step 3. Analytic continuation across the interface Γ

We again regard regions S_a and S_b composed of the same material b and region S_c of material c. As in Eq. (22), $f_i^{b1}(z)$ is taken to be a homogeneous solution of material b, and $f_i^2(z)$ and $f_i^{c1}(z)$ are introduced to satisfy the continuity of displacements and tractions across the interface Γ. Accordingly it can be shown from Eq. (23) that

$$\begin{cases} f_i^2(z) = \overline{V}_{ij}^{cb}\bar{f}_j^{b1}(z) = \overline{V}_{ij}^{cb}V_{jk}^{ab}f_k^1(z - \bar{\mu}_{\underline{j}}^{b}h + \mu_{\underline{k}}^{b}h), & \text{in } S_a \cup S_b, \\ f_i^{c1}(z) = U_{ij}^{cb}f_j^{b1}(z) = U_{ij}^{cb}\overline{V}_{jk}^{ab}\bar{f}_k^1(z - \mu_{\underline{j}}^{b}h + \bar{\mu}_{\underline{k}}^{b}h), & \text{in } S_c, \end{cases} \tag{A.3}$$

where $f_i^2(z)$ and $f_i^{c1}(z)$ can be expressed in terms of $f_i^0(z)$ through Eq. (A.1). The fields produced by $f_i^2(z)$ do not satisfy the continuity conditions at the interface Γ_*.

A.4. Step 4. Repetitions of steps 2 and 3

Steps 2 and 3 are alternatively performed with $f_i^n(z)$, $f_i^{an}(z)$, $f_i^{bn}(z)$, $f_i^{cn}(z)$, and $f_i^{n+1}(z)$ respectively for $n = 2, 3, \ldots$ instead of $f_i^1(z)$, $f_i^{a1}(z)$, $f_i^{b1}(z)$, $f_i^{c1}(z)$, and $f_i^2(z)$ in steps 2 and 3. Consequently, one can express all functions $f_i^{an}(z)$, $f_i^{bn}(z)$, $f_i^{cn}(z)$ and $f_i^{n+1}(z)$ $(n = 1, 2, 3, \ldots)$ in terms of $f_i^0(z)$.

Appendix B. Proof of $\|\mathbf{T}^{ab}\| \leqslant 1$

The bimaterial matrix $\mathbf{T}^{ab}$ defined in Eq. (9) is rewritten as

$$\mathbf{T}^{ab} = 2\mathbf{H}^{-1}\mathbf{S}^{b} - \mathbf{I}, \tag{B.1}$$

where $\mathbf{H} = \mathbf{B}^a + \overline{\mathbf{B}}^b$ is also a positive definite Hermitian matrix and $\mathbf{S}^b = \mathrm{Re}\,\mathbf{B}^b$ a symmetric matrix. The norm of the matrix $\mathbf{T}^{ab}$ is defined as

$$\|\mathbf{T}^{ab}\| \equiv \max(|\lambda_1|, |\lambda_2|, |\lambda_3|), \tag{B.2}$$

in which λ_i $(i = 1, 2, 3)$ are three eigenvalues of the eigenvalue equation

$$\mathbf{T}^{ab}\mathbf{x} = \lambda\mathbf{x}, \tag{B.3}$$

where $\mathbf{x}$ is a complex vector in general. Substituting Eq. (B.1) into Eq. (B.3) yields

$$\mathbf{S}^b\mathbf{x} = \zeta\mathbf{H}\mathbf{x}, \qquad \zeta = \tfrac{1}{2}(\lambda + 1). \tag{B.4}$$

Making use of $\mathbf{x} = \mathbf{a} + \mathrm{i}\mathbf{b}$ and $\mathbf{H} = \mathbf{S}^a + \mathbf{S}^b + \mathrm{i}(\mathbf{W}^a - \mathbf{W}^b)$ the complex equation (B.4) can be written as two real equations:

$$\mathbf{S}^b\mathbf{a} = \zeta(\mathbf{S}^a + \mathbf{S}^b)\mathbf{a} - \zeta(\mathbf{W}^a - \mathbf{W}^b)\mathbf{b}, \tag{B.5}$$

$$\mathbf{S}^b\mathbf{b} = \zeta(\mathbf{S}^a + \mathbf{S}^b)\mathbf{b} + \zeta(\mathbf{W}^a - \mathbf{W}^b)\mathbf{a}. \tag{B.6}$$

If Eqs. (B.5) and (B.6) are pre-multiplied by $\mathbf{a}^T$ and $\mathbf{b}^T$, respectively, and Eq. (B.6) is subtracted from Eq. (B.5), the symmetry of $(\mathbf{S}^a + \mathbf{S}^b)$ and the anti-symmetry of $(\mathbf{W}^a - \mathbf{W}^b)$ result in

$$\mathbf{y}^T\mathbf{S}^b\mathbf{y} = \zeta\mathbf{y}^T(\mathbf{S}^a + \mathbf{S}^b)\mathbf{y}, \tag{B.7}$$

where $\mathbf{y} = \mathbf{a} - \mathbf{b}$. Since real matrices $\mathbf{S}^a$ and $\mathbf{S}^b$ are positive definite, Eq. (B.7) means

$$0 \leqslant \zeta = \frac{\mathbf{y}^T\mathbf{S}^b\mathbf{y}}{\mathbf{y}^T(\mathbf{S}^a + \mathbf{S}^b)\mathbf{y}} \leqslant 1, \tag{B.8}$$

that is, the eigenvalues, λ_i $(= 2\zeta_i - 1)$, of $\mathbf{T}^{ab}$ are real and $|\lambda_i| \leqslant 1$.

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