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Elastic interface acoustic waves in twinned crystals

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Abstract

A new type of interface acoustic waves (IAW) is presented, for single-crystal orthotropic twins bonded symmetrically along a plane containing only one common crystallographic axis. The effective boundary conditions show that the waves are linearly polarized at the interface, either transversally or longitudinally. Then the secular equation is obtained in full analytical form using new relationships for the displacement–traction quadrivector at the interface. For gallium arsenide and for silicon, it is found that the IAWs with transverse (resp. longitudinal) polarization at the interface are of the Stoneley (resp. leaky) type.

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1. Introduction

The possibilities of existence of Stoneley waves propagating at the interface of two welded half-spaces are quite restricted, especially when the semi-infinite bodies are made of *dissimilar* crystals. For example, Owen (1964) famously studied 900 combinations of isotropic materials and found only 31 pairs supporting Stoneley waves. Similar conclusions are also reached when the materials are anisotropic. In general, the existence of an interfacial Stoneley wave is highly sensitive to the differences in material parameters for each medium, in particular to the difference in shear wave speeds (Chadwick and Currie, 1974).

The situation is somewhat more favorable when the half-spaces are made of misoriented but *identical* crystals. For instance, Stoneley waves were found to exist for any angle of misorientation and for propagation along the twist-angle bisectrix in the case of some hypothetical crystal by Lim and Musgrave (1970), copper by Thölén (1984), gallium arsenide by Barnett et al. (1985), or silicon by Mozhaev et al. (1998); they also exist for 180° domain boundaries of barium titanate or quartz (Mozhaev and Weihnacht, 1996, 1997), for propagation in any direction in the interface plane. In these articles, the interface is normal to a crystallographic axis which is itself common to each half-space.

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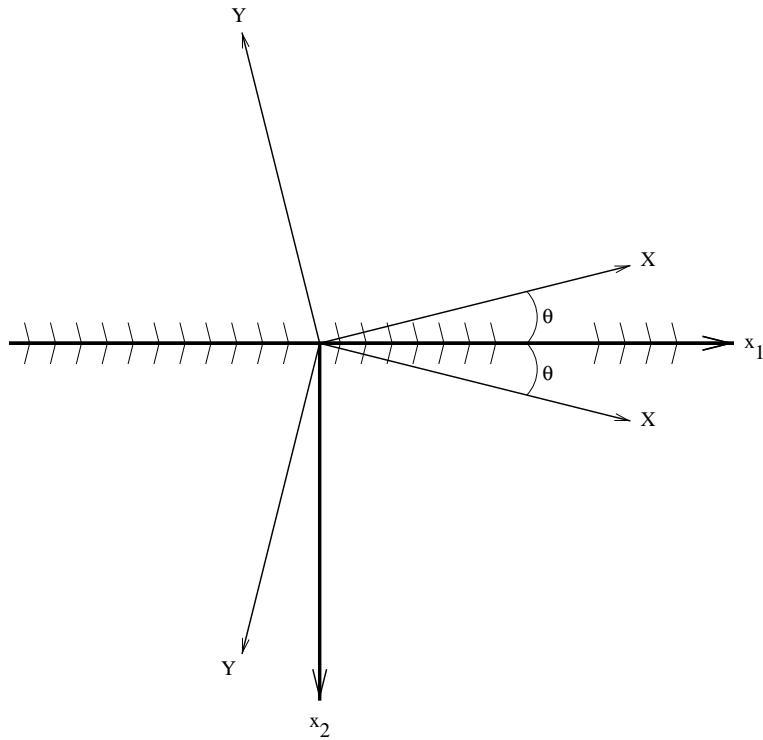


Fig. 1. Twinned crystal.

Now consider the interface described in Fig. 1, where the upper and lower half-spaces are made of the same crystal with at least rhombic symmetry and with misoriented crystallographic axes X and Y (represented on the figure making an angle $\pm\theta$ with the interface and its normal) and common crystallographic axis Z (normal to the plane of the figure). This geometry of chevron or "herringbone" pattern might be encountered in crystals subjected to a gliding twinning plane, or to the formation of conjugate kink bands through compression. Hussain and Ogden (2000) recently proposed a theoretical simulation of the plastic deformation associated with the twinning of crystals, with a possible exploitation in non-destructive testing of materials. Another way of producing such twins would be the following. Consider an infinite crystal with orthotropic or higher symmetry; cut it in two halves so that the plane interface contains one crystallographic axis (say x_3) and makes an angle θ with another crystallographic axis (say x_1), see Fig. 2(a); then rotate one half-space by 180° about the normal to the interface, see Fig. 2(b); finally rebond the half-spaces, see Fig. 2(c). A thorough review article by Gösele and Tong (1998) presents several experimental procedures of wafer bonding (also known as direct bonding or fusion bonding or "gluing without glue") and its numerous applications, not only for silicon-based sensors and actuators but also in microsystem technologies, non-linear optics, light-emitting diodes, etc. using gallium arsenide, quartz, or sapphire.

When the boundary conditions take the symmetries of the problem into consideration then the interface wave is found to be linearly polarized at the interface, either longitudinally or transversally. Once these effective boundary conditions are established in Section 2 (and Appendix A), two corresponding secular equations are derived explicitly in Section 3 as cubics in the squared wave speed. The results are illustrated graphically for gallium arsenide and for silicon. For these materials, it turns out that one of the secular equations corresponds to a non-physical supersonic leaky interface wave, and that the other corre-

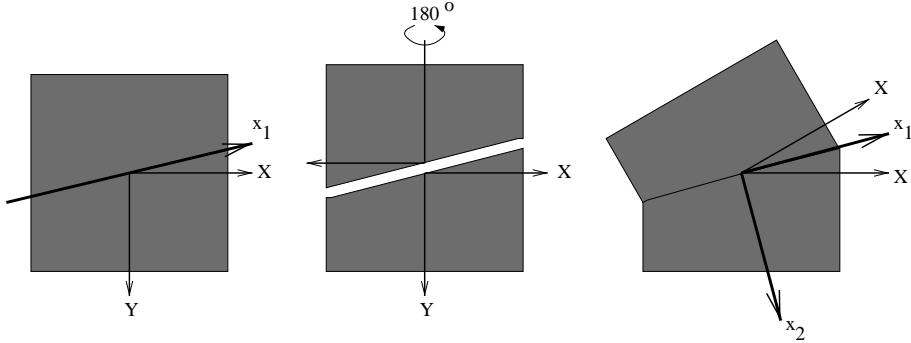


Fig. 2. Cutting, rotating, and bonding of a rhombic crystal.

sponds to a subsonic interface acoustic wave (IAW) having the characteristics of a Stoneley wave: decay with increasing distance from the interface, speed larger than that of the corresponding surface Rayleigh wave.

2. Effective boundary conditions

Consider Stoneley waves traveling with speed v and wave number k at the interface of a bimaterial made of two perfectly bonded orthotropic media. Both half-spaces are made of the same crystal (mass density ρ , non-zero reduced compliances $s'_{11}, s'_{22}, s'_{12}, s'_{44}, s'_{55}, s'_{66}$). However, the normal to the interface Ox_2 and the direction of propagation Ox_1 are inclined at an angle θ to the crystallographic axes Oy and Ox of the lower ($x_2 > 0$) half-space and at an angle $-\theta$ for the upper ($x_2 < 0$) half-space.

In the lower half-space, the strain–stress relation is $\epsilon_{ij} = s_{ik}\sigma_{ik}$ where the reduced compliances s_{ik} are given by (see for instance Ting, 2000 or Destrade, 2003),

$$\begin{aligned}
 s_{11} &= s'_{11} \cos^4 \theta + (2s'_{12} + s'_{66}) \cos^2 \theta \sin^2 \theta + s'_{22} \sin^4 \theta, \\
 s_{22} &= s'_{22} \cos^4 \theta + (2s'_{12} + s'_{66}) \cos^2 \theta \sin^2 \theta + s'_{11} \sin^4 \theta, \\
 s_{12} &= s'_{12} + (s'_{11} + s'_{22} - 2s'_{12} - s'_{66}) \cos^2 \theta \sin^2 \theta, \\
 s_{66} &= s'_{66} + 4(s'_{11} + s'_{22} - 2s'_{12} - s'_{66}) \cos^2 \theta \sin^2 \theta, \\
 s_{16} &= [2s'_{22} \sin^2 \theta - 2s'_{11} \cos^2 \theta + (2s'_{12} + s'_{66})(\cos^2 \theta - \sin^2 \theta)] \cos \theta \sin \theta, \\
 s_{26} &= [2s'_{22} \cos^2 \theta - 2s'_{11} \sin^2 \theta - (2s'_{12} + s'_{66})(\cos^2 \theta - \sin^2 \theta)] \cos \theta \sin \theta.
 \end{aligned} \tag{2.1}$$

When the mechanical displacement $\mathbf{u}(x_1, x_2, x_3, t)$ is modelled as a linear combination of the partial modes $e^{ik(x_1+px_2-vt)}\mathbf{U}$ (say), then the in-plane strain decouples from the anti-plane strain, and so does in-plane stress from anti-plane stress (Stroh, 1962); also, p is a root of the characteristic polynomial,

$$\omega_4 p^4 - 2\omega_3 p^3 + \omega_2 p^2 - 2\omega_1 p + \omega_0 = 0, \tag{2.2}$$

where the (real) coefficients ω_i are given in terms of the reduced compliances and of $X = \rho v^2$ by (Destrade, 2003),

$$\begin{aligned}
\omega_4 &= s_{11}, \quad \omega_3 = s_{16}, \\
\omega_2 &= s_{66} + 2s_{12} - [s_{11}(s_{22} + s_{66}) - s_{12}^2 - s_{16}^2]X, \\
\omega_1 &= s_{26} + [s_{16}(s_{22} - s_{12}) + s_{26}(s_{11} - s_{12})]X, \\
\omega_0 &= s_{22} - [s_{22}(s_{11} + s_{66}) - s_{12}^2 - s_{26}^2]X + \begin{vmatrix} s_{11} & s_{12} & s_{16} \\ s_{12} & s_{22} & s_{26} \\ s_{16} & s_{26} & s_{66} \end{vmatrix} X^2.
\end{aligned} \tag{2.3}$$

In the upper half-space, θ is changed to its opposite so that by (2.1), s_{11} , s_{22} , s_{12} , s_{66} remain unchanged whilst s_{16} and s_{26} change signs. Consequently, by (2.3) the characteristic polynomial in the upper half-space is

$$\omega_4 p^4 + 2\omega_3 p^3 + \omega_2 p^2 + 2\omega_1 p + \omega_0 = 0. \tag{2.4}$$

It follows that if p is a root of the characteristic polynomial (2.2) for the lower half-space, then $-p$ is a root of the characteristic polynomial (2.4) for the upper half-space.

As a consequence of these properties (change of sign across the interface for s_{16} , s_{26} , and for the p 's), the following effective boundary conditions apply at $x_2 = 0$ (see Appendix A),

$$u_1 = \sigma_{22} = 0, \quad \text{or} \quad u_2 = \sigma_{12} = 0. \tag{2.5}$$

Following Mozhaev et al. (1998), interface acoustic waves satisfying the first condition (2.5)₁ are denoted IAW1, and those satisfying the second condition (2.5)₂ are denoted IAW2. The polarization of the waves at the interface is linear: transverse for IAW1 and longitudinal for IAW2. Note that Mozhaev and collaborators obtained similar effective boundary conditions for other types of twin boundaries (180° ferroelectric domain boundary in tetragonal single-crystals with crystallographic propagation direction (Mozhaev and Weihnacht, 1995, 1996); Dauphiné twins in quartz with boundary coincident with the YZ mirror plane and propagation along the Y direction (Mozhaev and Weihnacht, 1997); twisted single-crystal cubic wafers with basal plane boundary and propagation along the twist-angle bisectrix (Mozhaev and Tokmakova, 1994; Mozhaev et al., 1998)).

3. Equations of motion and explicit secular equations

The equations of motion in the lower half-space are written as a first-order homogeneous differential system for the in-plane displacement–traction vector,

$$\xi(kx_2) = [U_1(kx_2), U_2(kx_2), t_{12}(kx_2), t_{22}(kx_2)]^T, \tag{3.1}$$

where the U_i and t_{i2} are defined by

$$u_i(x_1, x_2, x_3, t) = U_i(kx_2)e^{ik(x_1-vt)}, \quad \sigma_{i2}(x_1, x_2, x_3, t) = ik t_{i2}(kx_2)e^{ik(x_1-vt)}. \tag{3.2}$$

Explicitly, the system is given by (Destrade, 2001),

$$\xi' = i\mathbf{N}\xi, \quad \mathbf{N} = \begin{bmatrix} -r_6 & -1 & n_{66} & n_{26} \\ -r_2 & 0 & n_{26} & n_{22} \\ X - \eta & 0 & -r_6 & -r_2 \\ 0 & X & -1 & 0 \end{bmatrix}, \tag{3.3}$$

where $X = \rho v^2$ and (Ting, 2002)

$$\eta = \frac{1}{s_{11}}, \quad r_i = -\frac{s_{1i}}{s_{11}}, \quad n_{ij} = \frac{1}{s_{11}} \begin{vmatrix} s_{11} & s_{1j} \\ s_{1i} & s_{ij} \end{vmatrix}. \quad (3.4)$$

Note that in passing from the lower half-space to the upper half-space, only r_6 and n_{26} change signs.

Ting (in press) proved that for any positive or negative integer n , the matrix \mathbf{N}^n has the structure,

$$\mathbf{N}^n = \begin{bmatrix} \mathbf{N}_1^{(n)} & \mathbf{N}_2^{(n)} \\ \mathbf{K}^{(n)} & \mathbf{N}_1^{(n)T} \end{bmatrix}, \quad \text{with } \mathbf{K}^{(n)} = \mathbf{K}^{(n)T}, \quad \mathbf{N}_2^{(n)} = \mathbf{N}_2^{(n)T}, \quad (3.5)$$

see also Currie (1979). Hence the following matrix $\mathbf{M}^{(n)}$ is symmetric,

$$\mathbf{M}^{(n)} \equiv \widehat{\mathbf{I}} \mathbf{N}^n, \quad \widehat{\mathbf{I}} = \begin{bmatrix} 0 & \mathbf{1} \\ \mathbf{1} & 0 \end{bmatrix}, \quad \mathbf{1} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}. \quad (3.6)$$

Now premultiply both sides of (3.3)₁ by $-i\bar{\xi}' \widehat{\mathbf{I}} \mathbf{N}^{n-1}$ and add the complex conjugate quantity to obtain $\bar{\xi}' \cdot \mathbf{M}^{(n)} \xi + \bar{\xi} \cdot \mathbf{M}^{(n)} \xi' = 0$. Assuming that the IAWs vanish at great distance from the interface ($\xi(\infty) = \mathbf{0}$), integration between $x_2 = 0$ and $x_2 = \infty$ yields,

$$\bar{\xi}(0) \cdot \mathbf{M}^{(n)} \xi(0) = \bar{\xi}(0) \cdot \widehat{\mathbf{I}} \mathbf{N}^n \xi(0) = 0. \quad (3.7)$$

This relationship is valid for any type of anisotropy. Because of the Cayley–Hamilton theorem, it yields five linearly independent equations for a 6×6 matrix \mathbf{N} , and three equations for a 4×4 matrix \mathbf{N} , as here. Note that for surface wave boundary conditions, the tractions are zero at $x_2 = 0$, and the relationship reduces to (Taziev, 1989): $\bar{\mathbf{u}}(0) \cdot \mathbf{K}^{(n)} \mathbf{u}(0) = 0$. At $n = 1, 2, -1$, the following expressions are found for $\mathbf{M}^{(n)}$,

$$\mathbf{M}^{(1)} = \begin{bmatrix} X - \eta & & & \\ 0 & X & & \\ -r_6 & -1 & n_{66} & \\ -r_2 & 0 & n_{26} & n_{22} \end{bmatrix}, \quad (3.8)$$

$$\mathbf{M}^{(2)} = \begin{bmatrix} 2r_6(\eta - X) & & & \\ \eta - (1 + r_2)X & 0 & & \\ r_2 + r_6^2 - n_{66}(\eta - X) & r_6 + n_{26}X & -2(n_{26} + r_6 n_{66}) & \\ r_2 r_6 - n_{26}(\eta - X) & r_2 + n_{22}X & -n_{22} - r_2 n_{66} - r_6 n_{26} & -2r_2 n_{26} \end{bmatrix}, \quad (3.9)$$

and

$$\mathbf{M}^{(-1)} = \frac{1}{\Delta} \begin{bmatrix} d & & & \\ X[r_2 r_6 + n_{26}(\eta - X)] & a & & \\ X[r_6 n_{22} - r_2 n_{26}] & b & & \\ e & r_2 r_6 + n_{26}(\eta - X) & r_6 n_{22} - r_2 n_{26} & f \end{bmatrix}, \quad (3.10)$$

with $\Delta = \det \mathbf{N}$ and

$$\begin{aligned} a &= (1 - n_{66}X)(\eta - X) - r_6^2 X, & b &= -r_2 + X(r_2 n_{66} - r_6 n_{26}), \\ c &= -n_{22} + X(n_{22} n_{66} - n_{26}^2), & & \\ d &= -X[r_2^2 + n_{22}(\eta - X)], & e &= -r_2^2 - n_{22}(\eta - X), \\ f &= 2r_2 r_6 n_{26} - r_2^2 n_{66} - r_6^2 n_{22} - (\eta - X)(n_{22} n_{66} - n_{26}^2). \end{aligned} \quad (3.11)$$

Corresponding to the first effective boundary condition (2.5)₁ is the interface acoustic mode IAW1, for which the quadrivector $\xi(0)$ is in the form,

$$\xi(0) = U_2(0)[0, 1, \alpha, 0]^T, \quad (3.12)$$

(say), so that Eqs. (3.7) read

$$M_{22}^{(n)} + M_{23}^{(n)}(\alpha + \bar{\alpha}) + M_{33}^{(n)}\alpha\bar{\alpha} = 0. \quad (3.13)$$

Choosing in turn $n = -1, 1, 2$, an homogeneous linear system of equations follows,

$$\begin{bmatrix} a & b & c \\ X & -1 & n_{66} \\ 0 & r_6 + n_{26}X & -2(n_{26} + r_6 n_{66}) \end{bmatrix} \begin{bmatrix} 1 \\ \alpha + \bar{\alpha} \\ \alpha\bar{\alpha} \end{bmatrix} = \mathbf{0}. \quad (3.14)$$

Similarly, corresponding to the second effective boundary condition (2.5)₂ is the interface acoustic mode IAW2, for which the quadrivector $\xi(0)$ is in the form,

$$\xi(0) = U_1(0)[1, 0, 0, \alpha]^T, \quad (3.15)$$

(say), so that Eq. (3.7) read

$$M_{11}^{(n)} + M_{14}^{(n)}(\alpha + \bar{\alpha}) + M_{44}^{(n)}\alpha\bar{\alpha} = 0. \quad (3.16)$$

Choosing in turn $n = -1, 1, 2$, an homogeneous linear system of equations follows,

$$\begin{bmatrix} d & e & f \\ \eta - X & r_2 & -n_{22} \\ 2r_6(\eta - X) & r_2 r_6 - n_{26}(\eta - X) & -2r_2 n_{26} \end{bmatrix} \begin{bmatrix} 1 \\ \alpha + \bar{\alpha} \\ \alpha\bar{\alpha} \end{bmatrix} = \mathbf{0}. \quad (3.17)$$

The secular equations for IAW1 and IAW2 correspond to the vanishing of the determinant of the 3×3 matrices given in (3.14) and (3.17), respectively. They are both cubics in $X = \rho v^2$. For purposes of com-

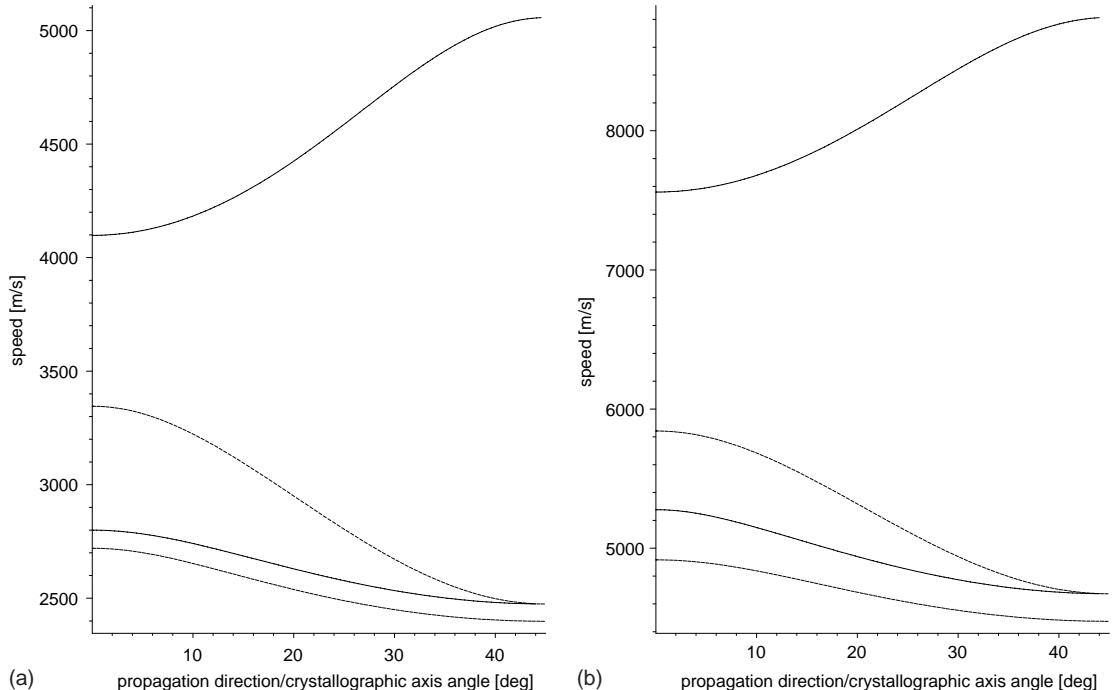


Fig. 3. Interface wave speeds in twinned crystals: leaky wave (upper solid) and Stoneley wave (lower solid); also included: quasi-bulk shear wave (upper dashed) and Rayleigh wave (lower dashed). (a) Gallium arsenide; (b) Silicon.

parison, recall that a homogeneous bulk wave propagates in the Ox_1 direction at a speed v_a such that $X = \rho v_a^2$ is root of the quadratic,

$$\Lambda = \det \mathbf{N} = 0, \quad (3.18)$$

and that a surface Rayleigh wave propagates over either half-space along Ox_1 at a speed v_R such that $X = \rho v_R^2$ is root of the quartic (Currie, 1979; Destrade, 2001; Ting, 2002),

$$\begin{vmatrix} d & a & X[r_2 r_6 + n_{26}(\eta - X)] & 0 \\ X - \eta & X & 0 & \\ 2r_6(\eta - X) & 0 & \eta - (1 + r_2)X & \end{vmatrix} = 0. \quad (3.19)$$

Fig. 3 shows the influence of the twinning angle θ upon the wave speeds, for (a) gallium arsenide and (b) silicon. The respective elastic stiffnesses (10^{10} N/m 2) and mass densities (kg/m 3) are (Royer and Dieulesaint, 1996): $c_{11} = 11.88$, $c_{12} = 5.38$, $c_{66} = 5.94$, $\rho = 5307$, and $c_{11} = 16.56$, $c_{12} = 6.39$, $c_{66} = 7.95$, $\rho = 2329$. Similar comments apply to both crystals. The secular equation (3.17) corresponds to a non-physical leaky wave IAW2 with a speed (upper full curve) which is always supersonic (always above the curve for the speed given by (3.18) of a bulk shear wave (upper dotted curve)). The secular equation (3.14) corresponds to a Stoneley wave IAW1 with a speed (lower full curve) which is always larger than the speed of a Rayleigh wave propagating in either half-space (always above the curve for the speed given by (3.19) (lower dotted curve)).

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Appendix A

Here the effective boundary conditions (2.5) for twinned crystals are derived.

Solutions to the equations of motion (3.3) are in the form $\xi(kx_2) = \xi_0 e^{ipkx_2}$. By substitution, ξ_0 is found from the adjoint matrix to $\mathbf{N} - p\mathbf{1}$ as

$$\xi_0^i = [a_i, b_i, c_i, d_i]^T, \quad (A.1)$$

with

$$\begin{aligned} a_i &= [(1 + r_2)X - \eta]p_i + r_2 r_6 X + n_{26}(\eta - X)X, \\ b_i &= -Xp_i^2 - 2r_6 Xp_i - [1 + r_6^2 + n_{66}(\eta - X)]X + \eta, \\ c_i &= p_i^2 + (r_6 - n_{26}X)p_i - r_2(1 - n_{66}X) - r_6 n_{26}X, \\ d_i &= -p_i^3 - 2r_6 p_i^2 + [r_2 - r_6^2 - n_{66}(\eta - X)]p_i + n_{26}(\eta - X) + r_2 r_6. \end{aligned} \quad (A.2)$$

Here p is a root of the characteristic polynomial $\det(\mathbf{N} - p\mathbf{1}) = 0$, which is given explicitly by (2.2). For the lower half-space, only the roots p_1, p_2 with positive imaginary parts are kept in order to ensure decay away from the interface $x_2 = 0$. Thus the solution for $x_2 > 0$ is

$$\xi(kx_2) = \beta_1 \xi_0^1 e^{ip_1 kx_2} + \beta_2 \xi_0^2 e^{ip_2 kx_2}, \quad (A.3)$$

for some constants β_1 and β_2 .

In the upper half-space $x_2 < 0$, the p 's are changed to their opposite so that the roots of the characteristic polynomial with negative imaginary parts are $-p_1, -p_2$. Moreover, r_6 and n_{26} also change signs, so that the eigenvectors $\hat{\xi}_0$ are in the form,

$$\hat{\xi}_0^i = [-a_i, b_i, c_i, -d_i]^T, \quad (\text{A.4})$$

and the solution for $x_2 < 0$ is

$$\hat{\xi}(kx_2) = \hat{\beta}_1 \hat{\xi}_0^1 e^{-ip_1 kx_2} + \hat{\beta}_2 \hat{\xi}_0^2 e^{-ip_2 kx_2}, \quad (\text{A.5})$$

for some constants $\hat{\beta}_1$ and $\hat{\beta}_2$.

It follows that the continuity of the displacements and of the tractions across the interface $x_2 = 0$ reads

$$\beta_1 \xi_0^1 + \beta_2 \xi_0^2 = \hat{\beta}_1 \hat{\xi}_0^1 + \hat{\beta}_2 \hat{\xi}_0^2. \quad (\text{A.6})$$

This system of equations is re-written as

$$\begin{bmatrix} \mathbf{A} & \mathbf{A} \\ \mathbf{B} & -\mathbf{B} \end{bmatrix} \begin{bmatrix} \boldsymbol{\beta} \\ \hat{\boldsymbol{\beta}} \end{bmatrix} = \mathbf{0}, \quad (\text{A.7})$$

where

$$\mathbf{A} = \begin{bmatrix} a_1 & a_2 \\ d_1 & d_2 \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} b_1 & b_2 \\ c_1 & c_2 \end{bmatrix}, \quad \boldsymbol{\beta} = \begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix}, \quad \hat{\boldsymbol{\beta}} = \begin{bmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \end{bmatrix}. \quad (\text{A.8})$$

The determinant of the 4×4 matrix in (A.7) is $4 \det \mathbf{A} \det \mathbf{B}$. It is zero when either (a) $\det \mathbf{A} = 0$, and then $\mathbf{B}\boldsymbol{\beta} - \mathbf{B}\hat{\boldsymbol{\beta}} = \mathbf{0}$ yields $\hat{\boldsymbol{\beta}} = \boldsymbol{\beta}$; or (b) $\det \mathbf{B} = 0$, and then $\mathbf{A}\boldsymbol{\beta} + \mathbf{A}\hat{\boldsymbol{\beta}} = \mathbf{0}$ yields $\hat{\boldsymbol{\beta}} = -\boldsymbol{\beta}$. In case (a), $\mathbf{A}\boldsymbol{\beta} + \mathbf{A}\hat{\boldsymbol{\beta}} = \mathbf{0}$ means $\mathbf{A}\boldsymbol{\beta} = \mathbf{0}$, that is

$$u_1(0) = t_{22}(0) = 0; \quad (\text{A.9})$$

in case (b), $\mathbf{B}\boldsymbol{\beta} - \mathbf{B}\hat{\boldsymbol{\beta}} = \mathbf{0}$ means $\mathbf{B}\boldsymbol{\beta} = \mathbf{0}$, that is

$$u_2(0) = t_{12}(0) = 0. \quad (\text{A.10})$$

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