Elasticity theory connection rules for epitaxial interfaces

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Elasticity theory provides an accurate description of the long-wavelength vibrational dynamics of homogeneous crystalline solids, and with supplemental boundary conditions on the displacement field can also be applied to abrupt heterojunctions and interfaces. The conventional interface boundary conditions, often referred to as ''connection rules,'' require that the displacement field and its associated stress field be continuous through the interface. We argue, however, that these boundary conditions are generally incorrect for epitaxial interfaces, and we give the general procedure for deriving the correct conditions, which depend essentially on the detailed microscopic structure of the interface. As a simple application of our theory we analyze in detail a one-dimensional model of an inhomogeneous crystal, a chain of harmonic oscillators with an abrupt change in mass and spring-stiffness parameters. Our results have implications for phonon dynamics in nanostructures such as superlattices and nanoparticles, as well as for the thermal boundary resistance at epitaxial interfaces.

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I. INTRODUCTION

Continuum elasticity theory was developed in the 18th and 19th centuries—prior to the wide acceptance of the atomic view of matter—to describe the mechanics of elastic solids.[1] Modern applications of elasticity theory abound throughout science and engineering, from providing a long-wavelength description of the dynamics of crystalline lattices, to the inversion of seismological data to image the three-dimensional structure of the Earth's interior.

The fundamental degree of freedom in a nonpolar elastic medium is the displacement field $\mathbf{u}(\mathbf{r})$, the deviation of the medium at point $\mathbf{r}$ from its position in mechanical equilibrium. When applied to composite media consisting of layers or regions of different materials, characterized by different elastic parameters, a question naturally arises: What boundary conditions should be imposed on the displacement field at the interfaces?

An example of such a composite system is shown schematically in Fig. 1. Alternating layers of type *A* and *B* materials, each characterized by different elastic constants and mass densities, are separated by abrupt interfaces. Within each region the displacement field satisfies an appropriate equation of motion. For an isotropic continuum with mass density ρ, the field equation is

$$\partial_t^2\mathbf{u}=v_\mathrm{l}^2\boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\mathbf{u})-v_\mathrm{t}^2\boldsymbol{\nabla}\times\boldsymbol{\nabla}\times\mathbf{u}, \tag{1}$$

where $v_\mathrm{l}\equiv\sqrt{(\lambda+2\mu)/\rho}$ and $v_\mathrm{t}\equiv\sqrt{\mu/\rho}$ are the longitudinal and transverse bulk sound velocities, respectively, determined by the Lamé coefficients λ and μ. The solution of the set of second-order equations of the form (1), or their generalization to anisotropic media, requires boundary conditions on $\mathbf{u}$ and $(\mathbf{n}\cdot\boldsymbol{\nabla})\mathbf{u}$, where $\mathbf{n}$ is a unit vector normal to the interface.

The conventional boundary conditions applied in this situation (assuming fully bonded materials) are as follows.[2,3] First, the displacement field is assumed to be continuous across an interface

$$\mathbf{u}_A=\mathbf{u}_B. \tag{2}$$

The condition (2) implies that the two materials are attached and do not separate. The second condition follows from momentum conservation and requires that the force density be continuous,

$$T_A^{ij}\ n^j=T_B^{ij}n^j. \tag{3}$$

Here T^{ij} is the stress tensor, defined by the continuity equation

$$\partial_t\Pi^i+\partial_jT^{ij}=0 \tag{4}$$

for momentum density $\boldsymbol{\Pi}\equiv\rho\partial_t\mathbf{u}$, and $\mathbf{n}$ is the unit normal.[4] In an isotropic elastic medium, it follows from Eq. (1) that the stress tensor is given by

$$T^{ij}=-\lambda(\boldsymbol{\nabla}\cdot\mathbf{u})\delta_{ij}-2\mu u_{ij} \tag{5}$$

$$=-c_{ijkl}u_{kl}, \tag{6}$$

where

$$c_{ijkl}=\lambda\delta_{ij}\delta_{kl}+\mu(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}) \tag{7}$$

is the elastic tensor for a linear isotropic solid, and where

$$u_{ij}\equiv(\partial_iu_j+\partial_ju_i)/2 \tag{8}$$

is the strain tensor.

The purpose of this paper is to point out that these boundary conditions (2) and (3), while quite appropriate for the

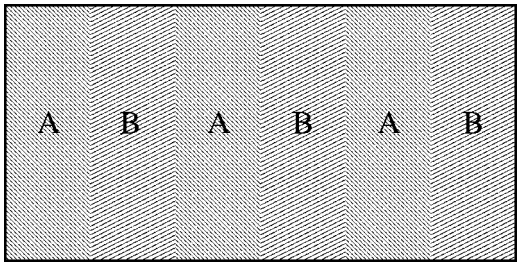

FIG. 1. Superlattice consisting of layers of dissimilar elastic media *A* and *B*.

geophysical application mentioned above, are generally incorrect when applied to long-wavelength vibrational dynamics in crystals with abrupt, epitaxial (crystalline) interfaces. The reason is because in the latter application, elasticity theory is only an approximate long-wavelength description for the underlying microscopic lattice dynamics—which necessarily depends on the detailed atomic structure of the interface—whereas Eqs. (2) and (3) make no reference to that microscopic structure. For example, the correct boundary conditions must depend on the effective force constants between type *A* and *B* atoms in Fig. 1, as well as that between atoms of the same type.

There are numerous applications of elasticity theory to solid state systems with heterostructures, where the use of the conventional boundary conditions would lead to quantitatively incorrect results. Examples include phonons in nanostructures such as quantum dots,[5] quantum wells,[6] superlattices,[7,8] surfaces with overlayers,[9] and nanoparticles embedded in host materials.[10–12] A correct use of boundary conditions might be especially important for nanometer-scale elastic media such as *phononic* band-gap materials.[13] Also, the thermal resistance of a heterojunction is determined by phonon scattering at the interface and is therefore sensitive to the connection rules or *S* matrix.[14]

Finally, we would like to point out a strong analogy between this work and the problem of determining the appropriate interface boundary conditions for the envelope functions in effective mass theory.[15] In this case, effective mass theory serves as the appropriate long-wavelength approximation to the full Schrödinger equation that contains the microscopic periodic potential of the crystalline lattice, and connection rules are required to join envelope functions through an interface between crystals with different effective mass. The microscopic theory of these connection rules was first developed by Kroemer and Zhu,[16,17] and our work may be regarded as an elasticity theory analog of Refs. 16 and 17. In their seminal work on phonons in heterostructures, Akera and Ando[18] analyzed the vibrational connection-rule problem from this point of view, and the boundary conditions we derive are consistent with those of Ref. 18. However, these authors did not realize that the small off-diagonal elements in the connection matrix [defined below in Eq. (10)] do in fact change the boundary conditions from the conventional ones.[19] We will show very clearly that using the conventional boundary conditions can give an incorrect vibrational spectrum.

In the next section we give a detailed derivation of the connection rules for the case of a simple one-dimensional model of an inhomogeneous crystal, a chain of harmonic oscillators with an abrupt change in mass and spring stiffness parameters, and in Sec. III we compare the results of using both our connection rules and the conventional connection rules to exact results obtained by numerical diagonalization. In Sec. IV we relate the connection rule problem to that of calculating the *S* matrix for plane-wave scattering from the interface. The problem of determining the interface boundary conditions between three-dimensional solids is discussed in Sec. V, and our conclusions are summarized in Sec. VI.

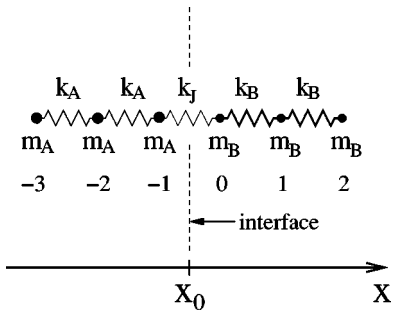

FIG. 2. Model of an atomically sharp interface in a one-dimensional crystal.

II. CONNECTION RULES IN ONE DIMENSION

We turn now to an analysis of the one-dimensional case, where a chain of atoms with nearest-neighbor bonds are constrained to move on a line. The vibrations in this case are purely longitudinal.

An abrupt interface is introduced at position x_0. To the left of x_0 the mass of each atom is m_A, and the effective spring constant of the nearest-neighbor bonds is k_A; the corresponding parameters on the right side are m_B and k_B. The strength of the bond connecting the type *A* and *B* atoms, which is generally different from k_A and k_B, is denoted by k_J. The lattice constant on both sides is equal to *a*. The model we consider is illustrated in Fig. 2.

According to elasticity theory, which is valid for vibrational wavelengths large compared with *a*, the regions to the left and right of the interface are described by the wave equations

$$(\partial_t^2 - v_I^2 \partial_x^2) u_I = 0, \quad v_I \equiv a\sqrt{k_I/m_I}, \quad I = A,B. \tag{9}$$

The elasticity theory description of a homogeneous chain is reviewed in the Appendix. To proceed, the wave equations (9) must be supplemented with boundary conditions on $u(x_0)$ and $u'(x_0)$.

A general linear homogeneous interface boundary condition may be expressed in the form

$$\begin{bmatrix} u(x_0) \\ u'(x_0) \end{bmatrix}_B = M \begin{bmatrix} u(x_0) \\ u'(x_0) \end{bmatrix}_A, \tag{10}$$

where M is a 2×2 matrix. The connection rule matrix implied by the boundary conditions (2) and (3) is

$$M = \begin{pmatrix} 1 & 0 \\ 0 & k_A/k_B \end{pmatrix}. \tag{11}$$

A common application of Eq. (11) is to an elastic string with an abrupt change in mass density, but no change in elasticity;[20,21] in this case Eq. (11) reduces to the identity matrix.[22]

It is simple to demonstrate that (11) is the only matrix consistent with conditions (2) and (3): First, continuity requires that $M_{11}=1$ and $M_{12}=0$. To find the other elements, we note that in one dimension the *xx* component of the stress tensor of Eq. (5) is $T^{xx} = -\rho v^2 \partial_x u$. The stress immediately

to the left of the interface is therefore $T_A^{xx}=-k_A u_A'(x_0)$, and that to the immediate right is $T_B^{xx}=-k_B u_B'(x_0)$. Now, Eq. (10) requires that

$$k_B u_B'(x_0)=k_B[M_{21}\,u_A(x_0)+M_{22}\,u_A'(x_0)], \tag{12}$$

which implies

$$T_B^{xx}=-M_{21}\;k_B u_A(x_0)+M_{22}(k_B/k_A)T_A^{xx}. \tag{13}$$

Therefore, the condition (3) requires that $M_{21}=0$ and $M_{22}=k_A/k_B$.

We now proceed with our derivation of the correct boundary condition matrix M for the model shown in Fig. 2. The coordinates $x_n(t)$ of the atoms are written as

$$x_n(t)=x_n^0+\xi_n(t), \quad x_n^0\equiv na. \tag{14}$$

The equation of motion for atom n is

$$m_n\ddot{\xi}_n=k_r(\xi_{n+1}-\xi_n)-k_l(\xi_n-\xi_{n-1}), \tag{15}$$

where k_r is the stiffness of the spring to the right of mass m_n, and k_l is that to the left. Assuming harmonic time dependence we have, for the atoms immediately to the left ($n=-1$) and right ($n=0$) of the interface

$$-\omega^2 m_A\xi_{-1}=k_J(\xi_0-\xi_{-1})-k_A(\xi_{-1}-\xi_{-2}) \tag{16}$$

and

$$-\omega^2 m_B\xi_0=k_B(\xi_1-\xi_0)-k_J(\xi_0-\xi_{-1}). \tag{17}$$

Next we introduce the displacement field $u(x)$ as a smooth interpolating function between the ξ_n, such that

$$u(x_n^0)=\xi_n, \tag{18}$$

and use the following relations:

$$\xi_{-2}=u_A\left(x_0-\frac{3}{2}a\right)\approx u_A(x_0)-\frac{3}{2}a u_A'(x_0), \tag{19}$$

$$\xi_{-1}=u_A\left(x_0-\frac{1}{2}a\right)\approx u_A(x_0)-\frac{1}{2}a u_A'(x_0), \tag{20}$$

$$\xi_0=u_B\left(x_0+\frac{1}{2}a\right)\approx u_B(x_0)+\frac{1}{2}a u_B'(x_0), \tag{21}$$

$$\xi_1=u_B\left(x_0+\frac{3}{2}a\right)\approx u_B(x_0)+\frac{3}{2}a u_B'(x_0). \tag{22}$$

Because the interface boundary conditions involve the displacement field and its first derivative only, second and higher-order gradients are neglected here. Furthermore, as the frequency ω is formally of the order of a gradient (recall the bulk dispersion relation $\omega=v|k|$), for consistency we also neglect the terms proportional to ω^2 in Eqs. (16) and (17).[23]

The resulting coupled equations can be put in the form

$$\begin{pmatrix} k_J & \frac{1}{2}ak_J \\ -k_J & a\left(k_B-\frac{1}{2}k_J\right)\end{pmatrix}\begin{bmatrix} u(x_0) \\ u'(x_0)\end{bmatrix}_B = \begin{pmatrix} k_J & a\left(k_A-\frac{1}{2}k_J\right) \\ -k_J & \frac{1}{2}ak_J\end{pmatrix}\begin{bmatrix} u(x_0) \\ u'(x_0)\end{bmatrix}_A, \tag{23}$$

which, upon comparison with Eq. (10), identifies

$$\begin{pmatrix} k_J & \frac{1}{2}ak_J \\ -k_J & a\left(k_B-\frac{1}{2}k_J\right)\end{pmatrix}^{-1}\begin{pmatrix} k_J & a\left(k_A-\frac{1}{2}k_J\right) \\ -k_J & \frac{1}{2}ak_J\end{pmatrix} \tag{24}$$

as the connection rule matrix. Therefore we obtain, for the model shown in Fig. 2, the connection rules

$$M=\begin{pmatrix} 1 & a\left[k_Ak_B-\frac{1}{2}k_J(k_A+k_B)\right]/k_Jk_B \\ 0 & k_A/k_B\end{pmatrix}. \tag{25}$$

Several remarks are in order. First, the correct connection rules clearly depend on the microscopic structure of the interface, including the stiffness k_J of the interface bond, which is generally different than k_A and k_B. The boundary conditions cannot be deduced by conservation laws that do not make reference to the microscopic structure. Second, the matrix (25) is generally off diagonal, implying a connection between the displacement field u on one side of the interface, with the strain u', as well as the displacement, on the other. Third, the displacement field is generally *not* continuous through the interface, in contrast with the conventional assumption.[24] This discontinuity, however, does not imply that the two sides are separated. It simply means that the atomic displacements ξ_n, when extrapolated from each side to the ''mathematical interface'' at x_0, do not meet. Fourth, we note that in the limit $a\to 0$ the boundary conditions (11) and (25) agree. However, this limit is not meaningful in a real crystal. Fifth, Eqs. (11) and (25) also become equivalent in the event that k_J has the special value k_J^* given by

$$\frac{1}{k_J^*}=\frac{1}{2}\left(\frac{1}{k_A}+\frac{1}{k_B}\right). \tag{26}$$

Sixth, although we have assumed that the lattice structure is the same at the interface as in the bulk, the method we used would apply to a relaxed interface as well, once that relaxed structure is known. And finally, although the connection rules themselves may depend on the arbitrary choice of interface position x_0, observable quantities do not. For example, if the interface position is moved from x_0 to x_0' and the vibrational spectrum is computed with the shifted connection rules *and* the new interface position, the spectrum remains unchanged

(within the accuracy of elasticity theory). We have therefore chosen the simplest interface position.

III. NUMERICAL STUDIES OF VIBRATIONAL SPECTRA

When k_J differs from k_J^*, the influence of the off-diagonal element in Eq. (25) can become substantial. To demonstrate this we use elasticity theory with both Eqs. (11) and (25) to predict the normal-mode frequencies of a one-dimensional inhomogeneous crystal of finite length L, and compare both with the exact spectrum obtained numerically. The interface is placed at $x_0 = L/2$.

The elasticity theory spectrum is obtained by (numerically) searching for frequencies such that the three conditions $u(0)=0$, $u(L)=0$, and Eq. (10), are satisfied. The appropriate solution of the wave equation to the left of the interface, on the interval $0 \leqslant x \leqslant x_0$, is

$$u_A(x) = \sin(\omega x/v_A), \tag{27}$$

and to the right $(x_0 \leqslant x \leqslant L)$ is

$$u_B(x) = \alpha\cos(\omega x/v_B) + \beta\sin(\omega x/v_B). \tag{28}$$

α and β are uniquely determined (at each frequency) by the requirement that Eq. (10) be satisfied. This leads to

$$\begin{bmatrix} u(x_0) \\ u'(x_0) \end{bmatrix}_B = C\begin{bmatrix} \alpha \\ \beta \end{bmatrix} = M\begin{bmatrix} u(x_0) \\ u'(x_0) \end{bmatrix}_A, \tag{29}$$

where

$$C \equiv \begin{pmatrix} \cos(\omega L/2v_B) & \sin(\omega L/2v_B) \\ -(\omega/v_B)\sin(\omega L/2v_B) & (\omega/v_B)\cos(\omega L/2v_B) \end{pmatrix}. \tag{30}$$

From Eq. (29) we obtain $\alpha(\omega)$ and $\beta(\omega)$ as

$$\begin{bmatrix} \alpha \\ \beta \end{bmatrix} = C^{-1}M\begin{bmatrix} \sin(\omega L/2v_A) \\ (\omega/v_A)\cos(\omega L/2v_A) \end{bmatrix}, \tag{31}$$

and the normal mode frequencies follow from the remaining boundary condition $u_B(L)=0$.

The exact spectrum is obtained by expressing the coupled equations of motion (15) for a chain of N atoms, with the first and last atoms held fixed, as a nonsymmetric eigenvalue problem. The system size is then given by $L=Na$. For the results presented below, we use $N=101$.

Representative results are shown in Figs. 3–5. In each case the angular frequency ω of mode n is given in units of $\pi v_A/L$. Figures 3 and 4 the show vibrational spectra of two inhomogeneous chains, both with $k_B = 5.0\ k_A$. The curves in these figures are independent of the masses m_A and m_B; the only mass dependence is in the energy scale $\pi v_A/L$. In each case the solid line is the exact spectrum, the dotted line is the elasticity theory spectrum calculated with the conventional connection rules (11), and the dashed line is the elasticity theory spectrum calculated with the connection rules (25). In Fig. 3, $k_J = 0.20\ k_A$, and the three spectra are similar. In Fig. 4, where $k_J = 0.05\ k_A$, the two sides are only weakly bonded together, and the spectrum calculated with Eq. (25) agrees with the exact spectrum, whereas the spectrum calculated with Eq. (11) does not. At higher frequencies both elasticity theory spectra deviate from the exact spectrum because the wavelength becomes shorter.

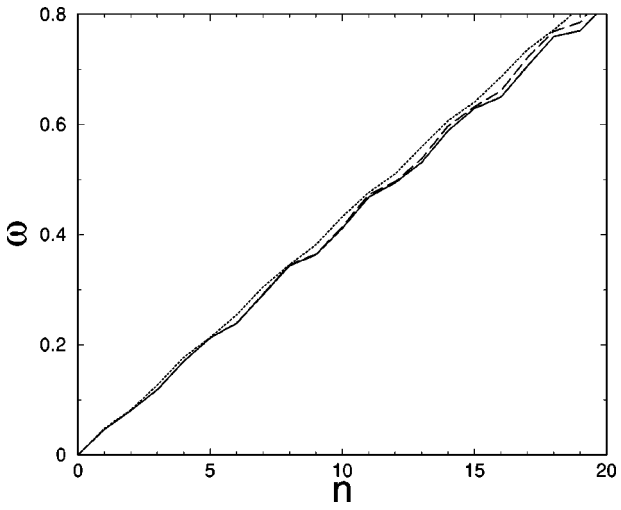

FIG. 3. Vibrational spectrum with $k_B/k_A = 5.0$ and $k_J/k_A = 0.20$.

The final set of spectra we present, shown in Fig. 5, corresponds to a homogeneous chain $k_B = k_A$, with a weakly bonded interface $k_J = 0.20\ k_A$. The spectrum calculated with Eq. (25) agrees well with the exact spectrum. The elasticity theory spectrum calculated with Eq. (11) misses the fine structure present in the exact spectrum because Eq. (11) makes no reference to the value of k_J.

These examples are meant demonstrate our point that the conventional boundary conditions are, as a matter of principle, incorrect. However, a particular heterojunction may turn out to have boundary conditions close to the conventional ones.

IV. *S* MATRIX

An alternative but physically equivalent way of expressing the interface boundary conditions is through an *S* matrix.

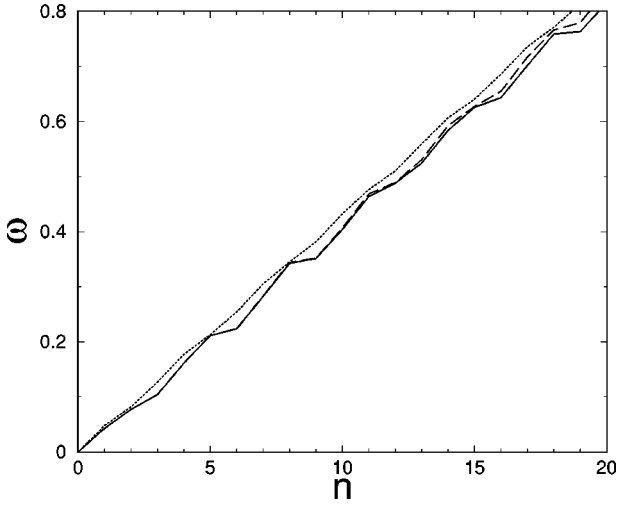

FIG. 4. Vibrational spectrum with $k_B/k_A = 5.0$ and $k_J/k_A = 0.05$.

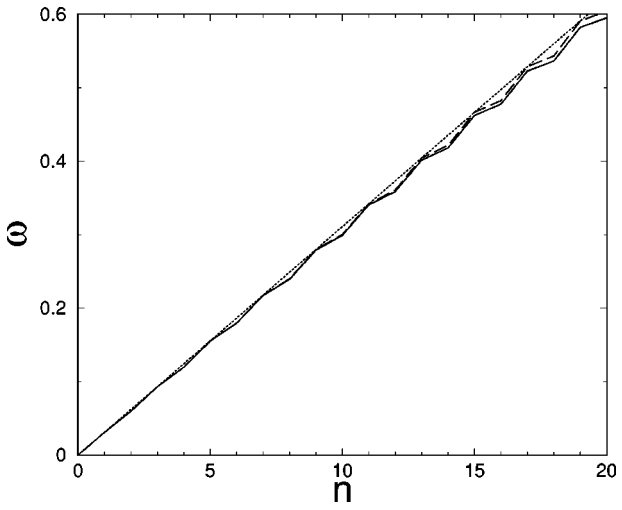

FIG. 5. Vibrational spectrum with $k_A = k_B$ and $k_J/k_A = 0.20$.

Whereas the matrix M gives the linear relation between the displacement field $u(x_0)$ and its derivative $u'(x_0)$ on side A to that on side B, the S matrix relates the amplitudes of waves incident on the interface, from both sides, to the corresponding outgoing waves. In this case we take x_0 to be at the origin and we write the elasticity theory solutions as[25]

$$u_A(x) = A_+ \ e^{i\omega x/v_A} + A_- e^{-i\omega x/v_A} \tag{32}$$

and

$$u_B(x) = B_+ e^{i\omega x/v_B} + B_- e^{-i\omega x/v_B}, \tag{33}$$

where $A_\pm$ and $B_\pm$ are complex coefficients giving the amplitudes of the plane waves shown in Fig. 6.

The S matrix relates the coefficients in Eqs. (32) and (33), and is defined by

$$\begin{bmatrix} A_- \\ B_+ \end{bmatrix} = S \begin{bmatrix} A_+ \\ B_- \end{bmatrix}. \tag{34}$$

From Eq. (10) we obtain

$$\begin{bmatrix} B_+ \\ B_- \end{bmatrix} = \mathcal{M} \begin{bmatrix} A_+ \\ A_- \end{bmatrix} \tag{35}$$

and therefore

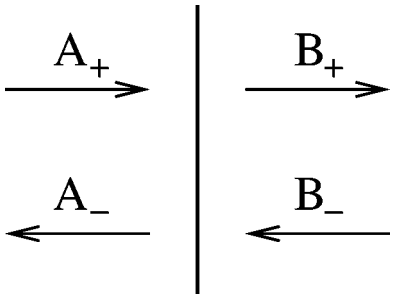

FIG. 6. Incoming and outgoing waves related by the S matrix. The interface is at $x = 0$.

$$S = \frac{1}{\mathcal{M}_{22}} \begin{pmatrix} -\mathcal{M}_{21} & 1 \\ \det\mathcal{M} & \mathcal{M}_{12} \end{pmatrix}, \tag{36}$$

where

$$\mathcal{M} \equiv \begin{pmatrix} 1 & 1 \\ i\omega/v_B & -i\omega/v_B \end{pmatrix}^{-1} M \begin{pmatrix} 1 & 1 \\ i\omega/v_A & -i\omega/v_A \end{pmatrix}. \tag{37}$$

Here $\det\mathcal{M}$ is the determinant of $\mathcal{M}$. A useful expression for $\mathcal{M}$ may be obtained by combining Eqs. (11) and (25) as

$$M = \begin{pmatrix} 1 & M_{12} \\ 0 & k_A/k_B \end{pmatrix}, \tag{38}$$

where M_{12} is either equal to zero or to the off-diagonal element $a[k_A k_B - \frac{1}{2} k_J(k_A + k_B)]/k_J k_B$ in Eq. (25). Using this representation for M we obtain

$$\mathcal{M} = \frac{1}{2} \begin{pmatrix} 1 + \dfrac{k_A v_B}{k_B v_A} + iM_{12}\dfrac{\omega}{v_A} & 1 - \dfrac{k_A v_B}{k_B v_A} - iM_{12}\dfrac{\omega}{v_A} \\ 1 - \dfrac{k_A v_B}{k_B v_A} + iM_{12}\dfrac{\omega}{v_A} & 1 + \dfrac{k_A v_B}{k_B v_A} - iM_{12}\dfrac{\omega}{v_A} \end{pmatrix} \tag{39}$$

and

$$\det\mathcal{M} = k_A v_B / k_B v_A . \tag{40}$$

Note that the complex terms in the S matrix come from the off-diagonal element in Eq. (25).

The S matrix provides a simple and direct way to obtain transmission and reflection amplitudes t and r for scattering from the interface. From Eq. (36) we observe that the transmission and reflection amplitudes for a wave of unit amplitude incident from the left ($A_+ = 1$ and $B_- = 0$) are

$$\mathsf{t} = \frac{\det\mathcal{M}}{\mathcal{M}_{22}} = \frac{2k_A v_B}{k_A v_B + k_B v_A - iM_{12}\omega k_B} \tag{41}$$

and

$$\mathsf{r} = -\frac{\mathcal{M}_{21}}{\mathcal{M}_{22}} = \frac{k_A v_B - k_B v_A - iM_{12}\omega k_B}{k_A v_B + k_B v_A - iM_{12}\omega k_B}. \tag{42}$$

In the limit $k_A = k_B = k_J$, where the mass density is discontinuous but the elasticity is continuous, these amplitudes reduce to

$$\mathsf{t} \to \frac{2v_B}{v_B + v_A} \quad \text{and} \quad \mathsf{r} \to \frac{v_B - v_A}{v_B + v_A}, \tag{43}$$

the well-known results for scattering from a mass discontinuity.[21] It can be shown that the transmission and reflection coefficients T and R defined as the fraction of transmitted and reflected energy flux, are determined from Eqs. (41) and (42) according to

$$\mathsf{T} = \frac{v_A k_B}{v_B k_A} \ |\mathsf{t}|^2 \quad \text{and} \quad \mathsf{R} = |\mathsf{r}|^2. \tag{44}$$

In addition to relating the connection rule matrix M to observable quantities, this scattering theory formulation serves to reemphasize the main thesis of this paper, that the connection rules must depend on the microscopic structure of the heterojunction and cannot be determined by ''far field'' information alone.

V. BEYOND ONE DIMENSION

In this section we give a brief discussion of the generalization of our method to three-dimensional epitaxial heterojunctions. To allow for both longitudinal and transverse elastic waves one must work with a 6×6 connection matrix M_{3D} satisfying

$$\begin{bmatrix} u_x(x_0) \\ u_y(x_0) \\ u_z(x_0) \\ u_x'(x_0) \\ u_y'(x_0) \\ u_z'(x_0) \end{bmatrix}_B = M_{3D} \begin{bmatrix} u_x(x_0) \\ u_y(x_0) \\ u_z(x_0) \\ u_x'(x_0) \\ u_y'(x_0) \\ u_z'(x_0) \end{bmatrix}_A . \tag{45}$$

Here $u_i' \equiv \mathbf{n}\cdot\boldsymbol{\nabla} u_i$, with $\mathbf{n}$ a unit vector normal to the interface, and $i=x,y,z$. The procedure for obtaining M_{3D} is identical to that described in Sec. II; however, in general it will be necessary to include atomic bonds beyond those connecting nearest-neighbor atoms.

To obtain quantitatively accurate connection rules one would need to determine the atomic structure of the particular interface and the required force constants. This can be accomplished using first-principles electronic structure calculation methods (for example, those based on density functional theory), although a full treatment of a three-dimensional heterojunction would be very demanding computationally.

VI. DISCUSSION

We have shown that the conventional interface boundary conditions used in elasticity theory, requiring that the displacement field and its associated stress field be continuous, are generally incorrect for epitaxial interfaces. The correct boundary conditions are nonuniversal and depend on the detailed microscopic structure of the heterojunction.

The conventional boundary conditions are incorrect because the displacement field $\mathbf{u}(\mathbf{r})$ is generally discontinuous. However, this discontinuity does *not* imply that the two sides separate. In the elasticity theory description of crystalline lattice dynamics

$$\mathbf{u}(\mathbf{r}_0) = \mathbf{r}_n - \mathbf{r}_n^0 \tag{46}$$

is simply a function giving the displacement of atom n at each equilibrium lattice point $\mathbf{r}_n^0$. A discontinuity in $\mathbf{u}(\mathbf{r})$ at a ''mathematical'' interface between layers of atoms implies that the atomic displacements $\mathbf{r}_n - \mathbf{r}_n^0$ on each side of an interface do not meet when smoothly interpolated to that interface. In contrast, the condition that the stress be continuous follows from momentum conservation and is always correct.[26]

It is tempting to approach the interface boundary condition problem by using elasticity equations generalized to the case of a compositionally graded crystal, characterized by a position-dependent mass density and elastic parameters, and then take the limit of an abrupt composition change. But this too is incorrect, for elasticity theory is intrinsically a long-wavelength description and can be formulated only for slowly graded systems, making the required limit invalid.

For example, the generalized wave equation describing the long-wavelength vibrational dynamics in a one-dimensional crystal with lattice constant a, mass density $\rho(x)$, and stiffness $k(x)$, can be shown to be (see the Appendix)

$$[\rho(x)\partial_t^2 - a\,\partial_x k(x)\,\partial_x]u(x,t) = 0. \tag{47}$$

Integration of Eq. (47) shows that $u(x)$ and $k(x)\,u'(x)$ are continuous, consistent with the conventional boundary conditions of Eq. (11). However, Eq. (47), which neglects stiffness gradients higher order than $k'(x)$, is not valid in the abrupt limit.

Having made the case that the conventional interface boundary conditions given in Eqs. (2) and (3) do not apply to epitaxial interfaces, we must emphasize again that we have not provided generally applicable conditions to replace Eqs. (2) and (3). The connection rules in Eq. (25) are only valid for the simple one-dimensional interface model shown in Fig. 2. We also emphasize that for some heterojunctions, the actual boundary conditions may be very close to the conventional ones.

In closing, we would like to speculate about the reason the subject of this paper has been, to the best of our knowledge, overlooked in the solid state physics literature. Historically, elasticity theory was developed as a self-contained branch of mechanics that made no reference to a possible underlying atomic structure, and much of the theory was developed before the general acceptance of the atomic view of matter. The conventional boundary conditions (2) and (3) are certainly correct within elasticity theory proper. However, within solid state physics, elasticity theory is regarded as a long-wavelength description with a well-defined but limited regime of validity, and we believe that the connection rules in question were applied to heterostructures without considering that regime of validity.

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APPENDIX: HOMOGENEOUS CHAIN

Here we record the long-wavelength theory of the homogeneous harmonic oscillator chain with masses m, spring

constants k, and lattice constant a. In this case the equation of motion leads to

$$\partial_t^2 u(x,t) - \frac{k}{m}[u(x+a,t) - 2\ u(x,t) + u(x-a,t)] = 0. \tag{A1}$$

Taylor expanding Eq. (A1) leads to the one-dimensional wave equation

$$(\partial_t^2 - v^2 \partial_x^2) u(x,t) = 0, \tag{A2}$$

with sound velocity

$$v \equiv a\sqrt{k/m}. \tag{A3}$$

Next we derive the momentum conservation condition satisfied by the displacement field u. The momentum density carried by a longitudinal elastic wave in one dimension is $\Pi = \rho \partial_t u$, where ρ is the mass density. In the absence of external forces, Eq. (A2) shows that Π satisfies the continuity equation

$$\partial_t \Pi + \partial_x T = 0, \tag{A4}$$

where

$$T = -\rho v^2 \partial_x u \tag{A5}$$

is the scalar stress. As expected, Eq. (A5) is identical to the xx component of the stress tensor of Eq. (5). Similarly, the energy density $\mathcal{E} = \frac{1}{2}\rho[(\partial_t u)^2 + v^2(\partial_x u)^2]$ satisfies the continuity equation

$$\partial_t \mathcal{E} + \partial_x j_e = 0, \tag{A6}$$

where

$$j_e = -\rho v^2 \partial_x u \partial_t u \tag{A7}$$

is the energy current.

The long-wavelength description of a harmonic oscillator chain with spatially varying masses and spring constants follows from the appropriate gradient expansion of

$$\begin{aligned} m(x)\partial_t^2 u(x,t) &= k\left(x + \frac{a}{2}\right)[u(x+a) - u(x)] \\ &\quad - k\left(x - \frac{a}{2}\right)[u(x) - u(x-a)]. \end{aligned} \tag{A8}$$

Neglecting gradients beyond $k'(x)$ leads to Eq. (47) quoted in Sec. VI.

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[25] The physical displacement fields, which are real, are given in this case by the real parts of $u_A(x)e^{-i\omega t}$ and $u_B(x)e^{-i\omega t}$.

[26] Recall from Eq. (13) that the M_{21} and M_{22} elements are determined by momentum conservation, whereas M_{11} and M_{12} are determined by displacement field continuity.