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A model to calculate surface acoustic waves of a superlattice

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Abstract. A new model to calculate surface acoustic waves of superlattices is proposed. This model may be derived by expanding the exact expression of the amplitudes of the elastic waves up to second order with respect to the wave vector. It can be shown that the effective elastic constant (EEC) model (Grimsditch M 1985 *Phys. Rev.* B **31** 6818) corresponds to the first order expansion approximation. The present model surely reproduces with excellent accuracy the numerical results obtained from the exact calculation for Cu/Al and Cu/Ag systems.

1. Introduction

In our previous paper [1] which we hereafter refer to as reference 1, we have derived the exact dispersion equation [2] for the evaluation of surface acoustic waves of sagittal modes in a metallic superlattice of thickness $LN \cdot D$ in contact with a substrate of thickness d_s; D is the period of the superlattice and LN is the total periodic number. Here the superlattice has been assumed to be prepared by means of sputtering or evaporation [3] and have a strong tendency to form a 'pencil-type texture', i.e., one in which the grains have a common orientation normal to the film but are randomly oriented within the (111) film plane [4]. Our dispersion equation [2] is the ultimate expression to evaluate the surface acoustic waves in various types of superlattices: a bulk, semi-infinite and finite one with or without a substrate.

Many theoretical studies of the acoustic waves of superlattices have been done for more than 15 years and this subject is considered to be well established [5–10]. Superlattices are assumed to be infinite or semi-infinite periodically layered media in these theoretical treatments. For an infinite superlattice, we can apply the Bloch theorem along the axis perpendicular to the layers. Applying the Bloch theorem and the transfer matrix technique one can derive the dispersion equation for the acoustic waves. In a semi-infinite superlattice, one can construct surface waves, each of which is a linear combination of the acoustic waves obtained as solutions of the above dispersion equation and attenuates far from the surface [6, 8]. When the period D is sufficiently small compared to the acoustic wavelengths, the superlattice behaves as a homogeneous medium with symmetry lower than that of the constitutive layers and can be characterized by effective elastic constants (EECs). The EECs for a periodically laminated structure with orthorhombic symmetry have been derived by Grimsditch [11, 12]. Obviously the acoustic waves are non-dispersive within this limit. Thus, the modern theoretical work dealing with periodically layered media has avoided the use of this effective medium approximation [8]. We have demonstrated in our previous paper how the Rayleigh surface wave velocity of a superlattice, which is finite in thickness and contacts with a glass substrate, approaches the one obtained from the effective elastic constant (EEC) model with a increasing periodic number by solving the exact dispersion equation [2]; the surface wave velocity in the EEC model corresponds to that of a superlattice with the infinitesimal period.

Both the EEC model and our dispersion equation give the same results in the limit of zero period, though these approaches appear to be quite different. This fact suggests that both approaches should have a possible corresponding relationship at the limit of zero period. From this corresponding relationship we could derive the EECs and furthermore expect to find out a model to reproduce the surface wave velocity which is dependent on the superlattice period; this model is a modified EEC model with the dispersion relation. A derivation of the EECs for an infinite superlattice has been reported without presenting the actual derivation expressions [7]. In the present work, we will deal with two types of superlattice on a substrate; type I consists of LN alternating m_1 and m_2 layers of materials 1 and 2 as shown in figure 1(a), and type II consists of type I with an additional m_1 layer as shown in figure 2(a).

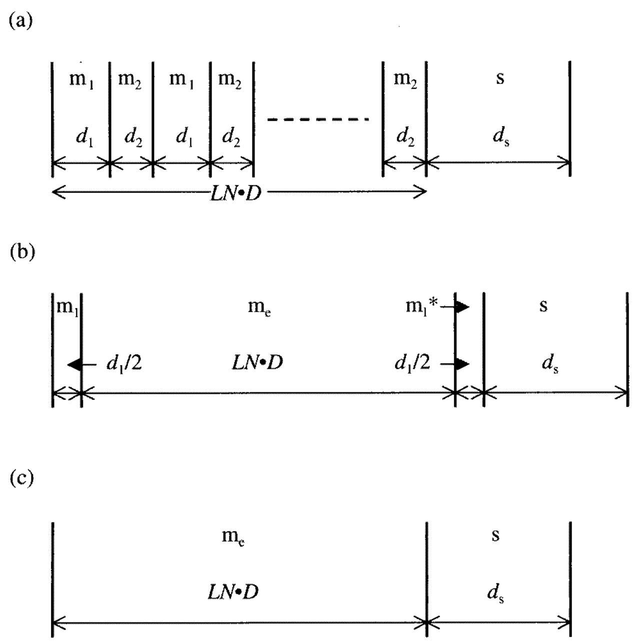

Figure 1. (a) Type I superlattice consisting of LN alternating m_1 and m_2 layers of thickness d_1 of constituent 1 and thickness d_2 of constituent 2 on a substrate s of thickness d_s. A unit spatial period is $D = d_1 + d_2$. (b) A model structure of the type I superlattice based on the extended EEC model. This structure consists of four layers labelled by m_1, m_e, m_1^* and s. The first layer is the constituent 1 of $d_1/2$ thickness, the second layer is the effective medium e of thickness $LN \cdot D$, the third layer is the virtual constituent 1 of $d_1/2$ thickness and the fourth layer is the substrate s of thickness d_s. (c) The EEC model for the type I superlattice. The superlattice structure is replaced by a layer of the effective medium e.

2. Elastic waves in a superlattice

We consider a superlattice occupying a space $0 \geqslant z \geqslant -z_L$ with its top surface at $z = 0$ and a substrate occupying a space $-z_L \geqslant z \geqslant -z_L - d_s$. The superlattice consists of alternating m_1 and m_2 layers of thickness d_1 of constituent 1 and thickness d_2 of constituent 2. A unit

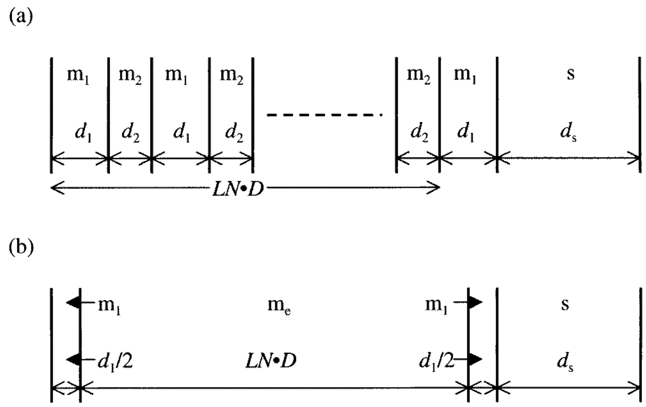

Figure 2. (a) Type II superlattice consisting of type I with an additional m_1 layer of thickness d_1 of constituent 1. (b) A model structure of the type II superlattice based on the extended EEC model. This structure consists of four layers (m_1, m_e, m_1 and s layers) of thickness $d_1/2$ of constituent 1, thickness $LN \cdot D$ of effective medium e, thickness $d_1/2$ of constituent 1 and thickness d_s of substrate s.

spatial period is $D = d_1 + d_2$. We will consider that z_L is $LN \cdot D$ as shown in figure 1(a) or $LN \cdot D + d_1$ as shown in figure 2(a). Each layer is a (111) film plane consisting of numerous grains randomly oriented within the film plane, which ensures elastic isotropy in the plane. We can discuss the layer elastic waves and treat the superlattice elastic waves by connecting the layer elastic waves using the proper boundary conditions.

Since the constituents and the substrate are elastically isotropic in the (x, y) plane, it is enough to restrict the elastic waves propagating in the (x, z) plane with the wave vector $\boldsymbol{q} = (q_x, 0, q_z)$. In addition, we can assume common q_x and frequency ω for the constituents and the substrate because the boundary conditions depend only on the z axis [1, 13]. For a common set of (q_x, ω), there exist three types of solution for q_z in each layer and the substrate. They are a pure transverse wave and two sagittal waves (a quasi-transverse wave and a quasi-longitudinal wave) [7, 8].

For the wave with wave vector $\boldsymbol{q}^{(i)} = q_x(1, 0, Q_i)$ and frequency ω, we will express its displacement at the point (x, y, z) and time t as

$$u_\alpha^{(i)} = U_\alpha^{(i)} \exp\{i q_x(x + Q_i z) - \mathrm{i}\omega t\} = \tilde{U}_\alpha^{(i)} \exp(\mathrm{i} q_x Q_i z) \qquad (\alpha = x, y, z) \tag{1}$$

where i denotes one of the constituents or the substrate ($i = 1$, 2 or s). Using this expression, we can write the wave equations as

$$\rho_1\omega^2 \begin{pmatrix} \tilde{U}_x^{(i)} \\ \tilde{U}_z^{(i)} \\ \tilde{U}_y^{(i)} \end{pmatrix} = q_x^2 \begin{pmatrix} C_{11}^{(i)} + C_{44}^{(i)} Q_i^2 & (C_{13}^{(i)} + C_{44}^{(i)}) Q_i & 0 \\ (C_{13}^{(i)} + C_{44}^{(i)}) Q_i & C_{44}^{(i)} + C_{33}^{(i)} Q_i^2 & 0 \\ 0 & 0 & C_{66}^{(i)} + C_{44}^{(i)} Q_i^2 \end{pmatrix} \begin{pmatrix} \tilde{U}_x^{(i)} \\ \tilde{U}_z^{(i)} \\ \tilde{U}_y^{(i)} \end{pmatrix}. \tag{2}$$

Here $C_{kl}^{(i)}$, which is expressed as $\overline{C}_{kl}^{(i)}$ in reference 1, and ρ_i denote the elastic constant tensor component and the density of the medium i. The first and second equations in matrix equation (2) can be rewritten as

$$U_i (= \tilde{U}_z^{(i)} / \tilde{U}_x^{(i)}) = -\frac{C_{44}^{(i)} Q_i^2 + C_{11}^{(i)} - C_{44}^{(i)} \xi_i^2}{(C_{13}^{(i)} + C_{44}^{(i)}) Q_i} = -\frac{(C_{13}^{(i)} + C_{44}^{(i)}) Q_i}{C_{33}^{(i)} Q_i^2 + C_{44}^{(i)} - C_{44}^{(i)} \xi_i^2}. \tag{3}$$

with

$$\xi_i^2 = \rho_i \omega^2 / (C_{44}^{(i)} q_x^2). \tag{4}$$

From equation (4), we have

$$Q_i^4 + \{A_i - (1 + B_i)\xi_i^2\}Q_i^2 + (1 - \xi_i^2)(C_i - B_i\xi_i^2) = 0 \tag{5}$$

where A_i, B_i and C_i are given by equation (11) in reference 1. Equation (5), a quadratic equation of Q_i^2, gives two solutions Q_{i1}^2 and Q_{i2}^2 ($|Q_{i1}^2| \leqslant |Q_{i2}^2|$) for a given set of q_x and ω, where Q_{i1}^2 and Q_{i2}^2 are related to a quasi-transverse wave and a quasi-longitudinal wave, respectively. The sagittal waves are forward- and backward- travelling quasi-transverse and quasi-longitudinal waves, which are characterized by (U_{i1}, Q_{i1}), $(-U_{i1}, -Q_{i1})$, (U_{i2}, Q_{i2}) and $(-U_{i2}, -Q_{i2})$, respectively. The elastic waves in the medium i are a superposition of these waves.

We can express the location of the medium i ($i = 1, 2$ or s) as $-z_{i1} \geqslant z \geqslant -z_{il} - d_i$ with $z_{1l} = (l-1)D$, $z_{2l} = z_{1l}+d_1$, $z_{sl} = z_L$ and $l = 1, 2, \ldots, LN$ (or $LN+1$ for the last constituent 1 in figure 2(a)). We will write the amplitudes $\tilde{U}_x^{(i)}$ of the elastic wave displacements at the top of the medium i of the lth period at $z = -z_{il}$ as a_{il}^+, b_{il}^+, c_{il}^+ and d_{il}^+ (and those at the bottom at $z = -z_{il} - d_i$ as a_{il}^-, b_{il}^-, c_{il}^- and d_{il}^-) for the above four waves, (U_{i1}, Q_{i1}), $(-U_{i1}, -Q_{i1})$, (U_{i2}, Q_{i2}) and $(-U_{i2}, -Q_{i2})$, respectively. The displacement vector $(u_x^{(i)}, 0, u_z^{(i)})$ for the elastic waves in the medium i can be written as

$$\begin{aligned}\begin{pmatrix} u_x^{(i)} \\ u_z^{(i)} \end{pmatrix} &= \begin{pmatrix} 1 & 1 & 1 & 1 \\ U_{i1} & -U_{i1} & U_{i2} & -U_{i2} \end{pmatrix} P_i(z + z_{il})|u_{i,l}^+\rangle \\ &= \begin{pmatrix} 1 & 1 & 1 & 1 \\ U_{i1} & -U_{i1} & U_{i2} & -U_{i2} \end{pmatrix} P_i(z + z_{il} + d_i)|u_{i,l}^-\rangle \end{aligned} \tag{6}$$

where are used the definitions

$$P_i(z) = \begin{pmatrix} f_{i1}(z) & 0 & 0 & 0 \\ 0 & f_{i1}(-z) & 0 & 0 \\ 0 & 0 & f_{i2}(z) & 0 \\ 0 & 0 & 0 & f_{i2}(-z) \end{pmatrix} \tag{7}$$

with $f_{ij}(z) = \exp(\mathrm{i}q_x Q_{ij} z)$ and

$$|u_{i,l}^\pm\rangle = \begin{pmatrix} a_{il}^\pm \\ b_{il}^\pm \\ c_{il}^\pm \\ d_{il}^\pm \end{pmatrix}. \tag{8}$$

For the substrate we use the variables $u_s^\pm$, z_s, $a_s^\pm$, $b_s^\pm$, $c_s^\pm$ and $d_s^\pm$.

The displacements and the stress components must be continuous at the boundary $z = -z_{il} - d_i$. By application of these boundary conditions the amplitudes of the elastic waves on the top surface of the superlattice at $z = 0$ ($|u_{1,l}^+\rangle$) can be related to those on the bottom surface of the substrate at $z = -z_L - d_s$ ($|u_s^-\rangle$) through

$$|u_s^-\rangle = T_s^{-1}(T_s P_s T_s^{-1})(T_1 P_1 T_1^{-1})^n[(T_2 P_2 T_2^{-1})(T_1 P_1 T^{-1})]^{LN} T_1|u_{1,1}^+\rangle. \tag{9}$$

Here $n = 0$ stands for the case shown in figure 1(a) and $n = 1$ for the case shown in figure 2(a), and the matrix T_i ($i = 1, 2$ or s) is defined as

$$T_i = \begin{pmatrix} 1 & 1 & 1 & 1 \\ U_{i1} & -U_{i1} & U_{i2} & -U_{i2} \\ \alpha_{i1} & \alpha_{i1} & \alpha_{i2} & \alpha_{i2} \\ \beta_{i1} & -\beta_{i1} & \beta_{i2} & -\beta_{i2} \end{pmatrix} \tag{10}$$

with

$$\alpha_{ij} = C_{13}^{(i)} + C_{33}^{(i)} U_{ij} Q_{ij} \text{ and } \beta_{ij} = C_{44}^{(i)}(U_{ij} + Q_{ij}) \tag{11}$$

and the matrix P_i ($i = 1, 2$ or s) is defined in equation (7) for $z = -d_i$.

The last equation in matrix equation (2) can be rewritten using equation (4) as

$$Q_i^2 = \xi_i^2 - C_{66}^{(i)}/C_{44}^{(i)}. \tag{12}$$

We will represent this solution as Q_{i3}^2. For this solution we have a forward wave ($+Q_{i3}$) and a backward wave ($-Q_{i3}$). We can derive a relation for the amplitudes of the present waves, which we denote by $|v_{1,1}^+\rangle$ and $|v_s^-\rangle$, at the top surface of the superlattice and the bottom surface of the substrate as

$$|v_s^-\rangle = t_s^{-1}(t_s p_s t_s^{-1})(t_1 p_1 t_1^{-1})^n[(t_2 p_2 t_2^{-1})(t_1 p_1 t^{-1})]^{LN} t_1 |v_{1,1}^+\rangle \tag{13}$$

where the meaning of n is the same as in equation (9). Here the matrices t_i and p_i ($i = 1$, 2 or s) are given by

$$t_i = \begin{pmatrix} 1 & 1 \\ C_{44}^{(i)} Q_{i3} & -C_{44}^{(i)} Q_{i3} \end{pmatrix} \tag{14}$$

and

$$p_i = \begin{pmatrix} f_{i3}(-d_i) & 0 \\ 0 & f_{i3}(d_i) \end{pmatrix} \tag{15}$$

with $f_{i3}(d) = \exp(\mathrm{i} q_x Q_{i3} d)$.

3. Expansion of phase transfer matrices and the effective elastic constants

In reference 1, we have demonstrated that the Rayleigh wave velocity obtained from our dispersion equation [2], which is essentially derived from equation (9), approaches the velocity given by the EEC model and that both velocities coincide with each other in the limit of the zero period. This fact suggests that the transfer matrices in equations (9) and (13) may be replaced by the corresponding transfer matrices of the EEC model in the zero period limit. In order to elucidate the relationship between our dispersion equation and the EEC model as well as gaining insight into modifying the EEC model, we will expand these transfer matrices with respect to the period D.

The amplitudes of the sagittal elastic waves and the pure transverse waves on the top of the lth layer at $z = -z_{il}$ and those on the top of the $(l+1)$th layer at $z = -z_{il+1}$ are related by the transfer matrices $T_2 P_2 T_2^{-1} T_1 P_1 T_1^{-1}$ and $t_2 p_2 t_2^{-1} t_1 p_1 t_1^{-1}$ as

$$T_1 |u_{1,l+1}^+\rangle = T_2 P_2 T_2^{-1} T_1 P_1 T_1^{-1} \cdot T_1 |u_{1,l}^+\rangle \tag{16}$$

and

$$t_1 |v_{1,l+1}^+\rangle = t_2 p_2 t_2^{-1} t_1 p_1 t_1^{-1} \cdot t_1 |v_{1,l}^+\rangle. \tag{17}$$

These transfer matrices $T_2 P_2 T_2^{-1} T_1 P_1 T_1^{-1}$ and $t_2 p_2 t_2^{-1} t_1 p_1 t_1^{-1}$ look different from the standard ones [6–8]. The transformation from the present forms to the standard forms is given in appendix A.

Now we expand the phase matrix P_i or p_i in terms of phase variable $q_x Q_{ij} d_i$. For example the matrix $T_i P_i T_i^{-1}$ ($i = 1$ or 2) can be written as

$$T_i P_i T_i^{-1} = \mathbf{1} - \mathrm{i} q_x d_i (T_i \tilde{Q}_i T_i^{-1}) + \tfrac{1}{2}(-\mathrm{i} q_x d_i)^2 (T_i \tilde{Q}_i T_i^{-1})^2 + \cdots \tag{18}$$

with

$$\tilde{Q}_i = \begin{pmatrix} Q_{i1} & 0 & 0 & 0 \\ 0 & -Q_{i1} & 0 & 0 \\ 0 & 0 & Q_{i2} & 0 \\ 0 & 0 & 0 & -Q_{i2} \end{pmatrix}. \tag{19}$$

We obtain the same result for $t_i p_i t_i^{-1}$ ($i = 1$ or 2) simply replacing T_i and $\tilde{Q}_i$ by t_i and $\tilde{q}_i = \begin{pmatrix} Q_{i3} & 0 \\ 0 & -Q_{i3} \end{pmatrix}$, respectively.

After complicated but straightforward calculations, we obtain

$$T_i \tilde{Q}_i T_i^{-1} = \begin{pmatrix} 0 & -1 & 0 & 1/C_{44}^{(i)} \\ -C_{13}^{(i)}/C_{33}^{(i)} & 0 & 1/C_{33}^{(i)} & 0 \\ 0 & C_{44}^{(i)}\xi_i^2 & 0 & -1 \\ \eta_i & 0 & -C_{13}^{(i)}/C_{33}^{(i)} & 0 \end{pmatrix}$$
$$\left(\eta_i = C_{44}^{(i)}\xi_i^2 - C_{11}^{(i)} + \frac{C_{13}^{(i)^2}}{C_{33}^{(i)}}\right) \tag{20}$$

the derivation of which is given in appendix B, and

$$t_i \tilde{q}_i t_i^{-1} = \begin{pmatrix} 0 & 1/C_{44}^{(i)} \\ C_{44}^{(i)} Q_{i3}^2 & 0 \end{pmatrix}. \tag{21}$$

Since the matrices with capital symbols and small letter symbols give the same results by replacing the symbols, we will in principle present only the results for the capital symbol matrices. Utilizing the expansion form (18), we can expand the transfer matrix in equation (16) as

$$\begin{aligned} T_2 P_2 T_2^{-1} T_1 P_1 T_1^{-1} = \mathbf{1} &- \mathrm{i} q_x D[f_1(T_1\tilde{Q}_1 T_1^{-1}) + f_2(T_2\tilde{Q}_2 T_2^{-1})] \\ &+ \tfrac{1}{2}(-\mathrm{i} q_x D)^2[f_1^2(T_1\tilde{Q}_1 T_1^{-1})^2 + 2 f_1 f_2 (T_2\tilde{Q}_2 T_2^{-1})(T_1\tilde{Q}_1 T_1^{-1}) \\ &+ f_2^2(T_2\tilde{Q}_2 T_2^{-1})^2] + \cdots \end{aligned} \tag{22}$$

with $f_i = d_i/D$ ($i = 1$ or 2).

We will replace the lth layer, which consists of two constituents 1 and 2 of thickness d_1 and d_2, by a medium of thickness D with EECs. Then the above discussions and relations can be applied for the effective medium by suitable replacements of variables. We will omit the suffix i ($i = e$) for the effective medium. Then the corresponding relations to equations (16) and (17) are given as

$$T|u_{1,l+1}^+\rangle = TPT^{-1} \cdot T|u_{1,l}^+\rangle \tag{23}$$

and

$$t|v_{1,l+1}^+\rangle = tpt^{-1} \cdot t|v_{1,l}^+\rangle. \tag{24}$$

It is easy to write down the matrices T and t for the effective medium from the matrices (10) and (14). The matrices P and p are defined in equations (7) with $z = -D$ and (15) with $d_i = D$ for $i = e$.

The transfer matrix TPT^{-1} is expanded with respect to the phase factor $q_x Q_j D$ as

$$TPT^{-1} = \mathbf{1} - \mathrm{i} q_x D(T\tilde{Q}T^{-1}) + \tfrac{1}{2}(-\mathrm{i} q_x D)^2 (T\tilde{Q}T^{-1})^2 + \cdots \tag{25}$$

where the matrix product $T\tilde{Q}T^{-1}$ can be readily obtained from the matrix (20).

We expect that the transfer matrices in equations (16) and (17) are equivalent to the ones in equations (23) and (24) in the vicinity of zero period ($D \to 0$). Then the expansions of these transfer matrices with respect to $q_x D$, which are represented in equations (22) and (25), must be equal at least in the first order terms:

$$T\tilde{Q}T^{-1} = f_1(T_1\tilde{Q}_1 T_1^{-1}) + f_2(T_2\tilde{Q}_2 T_2^{-1}). \tag{26}$$

From equations (20) and (26) one can readily derive the following relations.

$$f_1 + f_2 = 1 \tag{27}$$

$$\frac{1}{C_{44}} = \frac{f_1}{C_{44}^{(1)}} + \frac{f_2}{C_{44}^{(2)}} \tag{28}$$

$$\frac{1}{C_{33}} = \frac{f_1}{C_{33}^{(1)}} + \frac{f_2}{C_{33}^{(2)}} \tag{29}$$

$$\frac{C_{13}}{C_{33}} = f_1\frac{C_{13}^{(1)}}{C_{33}^{(1)}} + f_2\frac{C_{13}^{(2)}}{C_{33}^{(2)}} \tag{30}$$

$$C_{44}\xi^2 = f_1 C_{44}^{(1)}\xi_1^2 + f_2 C_{44}^{(2)}\xi_2^2 \tag{31}$$

and

$$C_{11} - \frac{C_{13}^2}{C_{33}} = f_1\left[C_{11}^{(1)} - \frac{C_{13}^{(1)^2}}{C_{33}^{(1)}}\right] + f_2\left[C_{11}^{(2)} - \frac{C_{13}^{(2)^2}}{C_{33}^{(2)}}\right]. \tag{32}$$

Equations (4) and (31) yield $\rho = f_1\rho_1 + f_2\rho_2$, which indicates that the density of the effective medium is the mean density of two constituents. Equations (21) and $t\tilde{q}t^{-1} = f_1(t_1\tilde{q}_1 t_1^{-1}) + f_2(t_2\tilde{q}_2 t_2^{-1})$ give

$$C_{44}Q_3^2 = f_1 C_{44}^{(1)} Q_{13}^2 + f_2 C_{44}^{(2)} Q_{23}^2. \tag{33}$$

From equations (12), (31) and (33), we obtain

$$C_{66} = f_1 C_{66}^{(1)} + f_2 C_{66}^{(2)}. \tag{34}$$

Equations (28), (29), (30), (32) and (34) are the same expressions for the superlattice EECs as derived by Grimsditch [11].

The expansions (22) and (25) are not equivalent in the second order terms. The second order term in expansion (25) is given by

$$\begin{aligned}[f_1(T_1\tilde{Q}_1T_1^{-1}) + f_2(T_2\tilde{Q}_2T_2^{-1})]^2 &= f_1^2(T_1\tilde{Q}_1T_1^{-1})^2 + f_2^2(T_2\tilde{Q}_2T_2^{-1})^2 \\ &\quad + f_1 f_2[(T_1\tilde{Q}_1T_1^{-1})(T_2\tilde{Q}_2T_2^{-1}) + (T_2\tilde{Q}_2T_2^{-1})(T_1\tilde{Q}_1T_1^{-1})]\end{aligned} \tag{35}$$

using the relation (26). This expression is symmetric in terms of two transfer matrices $T_1\tilde{Q}_1T_1^{-1}$ and $T_2\tilde{Q}_2T_2^{-1}$, while the second order term in expansion (22) lacks this symmetry. This fact results from the symmetry difference between a layer consisting of two constituents and an effective medium layer with respect to the inversion or mirror symmetry. Here we notice that we obtain the EEC model if we neglect this symmetry difference and assume the expansions of $T_2P_2T_2^{-1}T_1P_1T_1^{-1}$ and $t_2p_2t_2^{-1}t_1p_1t_1^{-1}$ are completely expressed in terms of the first order terms of their expansion, which we will call the first order expansion approximation. This is an essential defect of the EEC model. Next we will introduce the modified EEC model which is derived from devising that both the transfer matrices may be adjusted to coincide with each other up to the order of $(q_x D)^2$ in their expansions.

4. A new model to calculate surface elastic waves

As already discussed in section 2, the amplitudes of the quasi-transverse and longitudinal waves in a substrated superlattice on the top surface are related to the ones on the bottom surface of the substrate through equation (9). For the pure transverse waves we derived equation (13) and these waves form the surface waves known as the Love waves. We will discuss first the surface elastic waves known as the Rayleigh waves and the Sezawa waves, which are related to equation (9).

The transfer matrix $T_1 P_i T_i^{-1}$ ($i = 1$ or 2) in equation (9) can be rewritten as $T_i P_i T_i^{-1} = T_i P_i^{1/2} T_i^{-1} T_i P_i^{1/2} T_i^{-1}$, because of a trivial relation $(P_i^{1/2})^2 = P_i$. Using this expression we can rewrite the quantity $[(T_2 P_2 T_2^{-1})(T_1 P_1 T_1^{-1})]^{LN}$ as

$$[(T_2 P_2 T_2^{-1})(T_1 P_1 T_1^{-1})]^{LN} = (T_1 P_1^{1/2} T_1^{-1})^{-1}[(T_1 P_1^{1/2} T_1^{-1} T_2 P_2^{1/2} T_2^{-1}) \times (T_2 P_2^{1/2} T_2^{-1} T_1 P_1^{1/2} T_1^{-1})]^{LN} (T_1 P_1^{1/2} T_1^{-1}). \tag{36}$$

Here we can easily derive a following expansion relation by referring the expansion (22) to equation (26):

$$(T_1 P_1^{1/2} T_1^{-1} T_2 P_2^{1/2} T_2^{-1})(T_2 P_2^{1/2} T_2^{-1} T_1 P_1^{1/2} T_1^{-1}) = \mathbf{1} - \mathrm{i}q_x D(T\tilde{Q}T^{-1}) + \tfrac{1}{2}(-\mathrm{i}q_x D)^2 (T\tilde{Q}T^{-1})^2 + \cdots. \tag{37}$$

Equation (37) suggests that the matrix $(T_1 P_1^{1/2} T_1^{-1} T_2 P_2^{1/2} T_2^{-1})(T_2 P_2^{1/2} T_2^{-1} T_1 P_1^{1/2} T_1^{-1})$, which is also a transfer matrix, can be replaced by the transfer matrix TPT^{-1} for the effective medium in a pretty good approximation. Note that both of the transfer matrices have inversion symmetry. This is the reason why the expansions of these transfer matrices with respect to the phase factor are identical up to the second order. Thus we have

$$[(T_2 P_2 T_2^{-1})(T_1 P_1 T_1^{-1})]^{LN} \cong (T_1 P_1^{1/2} T_1^{-1})^{-1}[TP(-LN \cdot D)T^{-1}](T_1 P_1^{1/2} T_1^{-1}) \tag{38}$$

in the second order approximation. Substitution of the approximation (38) in equation (9) gives

$$T_s|u_s^-\rangle = (T_s P_s T_s^{-1})(T_1 P_1^{k/2} T_1^{-1})[TP(-LN \cdot D)T^{-1}](T_1 P_1^{1/2} T_1^{-1}) T_1 |u_{1,1}^+\rangle \tag{39}$$

in which $k = 2n - 1$ ($= -1$ or 1) and $(P_1^{1/2})^{-1} = P^{-1/2}$. In equation (39) the case of $k = -1$ corresponds to the four layered structure labelled by m_1, m_e, m_1^* and s in figure 1(b), instead of the original structure shown in figure 1(a); the first layer is the constituent 1 with thickness $d_1/2$, the second layer an effective medium e with thickness $LN \cdot D$, the third layer the virtual constituent 1 with thickness $d_1/2$ and the last layer is a substrate with thickness d_s, respectively. Note that the traveling direction of the elastic waves is reversed in the third layer. The case of $k = 1$ is illustrated in figure 2(b).

The elastic waves should satisfy the stress free conditions $\sigma_{zz}^{(i)} = 0$ and $\sigma_{zx}^{(i)} = 0$ ($i = 1$ or s) at the top surface, $z = 0$, and the bottom surface, $z = -z_L - z_s$, of a substrated superlattice. These conditions are summarized as

$$A_1|u_{1,1}^+\rangle = 0 \text{ and } A_s|u_s^-\rangle = 0 \tag{40}$$

using the matrix A_i ($i = 1$ or s) defined by

$$A_i = (\hat{0} \quad \hat{1})T_i \qquad \text{with } \hat{0} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \text{ and } \hat{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{41}$$

The stress-free boundary conditions (40) together with the amplitude equation (9) yield an exact dispersion equation [2] to calculate the surface elastic waves for a substrated superlattice illustrated in figure 1(a) or 2(a) [1]. By using the approximate equation (39) instead of the exact equation (9) we obtain

$$\begin{pmatrix} (\hat{0} \quad \hat{1}) \\ (\hat{0} \quad \hat{1})(T_s P_s T_s^{-1})(T_1 P_1^{k/2} T_1^{-1})[TP(-LN \cdot D)T^{-1}](T_1 P_1^{1/2} T_1^{-1}) \end{pmatrix} T_1|u_{1,1}^+\rangle = 0. \tag{42}$$

Equation (42) has non-trivial solutions, when the determinant of the 2×2 matrix included in the above equation becomes zero:

$$\det\left\{(\hat{0} \quad \hat{1})(T_s P_s T_s^{-1})(T_1 P_1^{k/2} T_1^{-1})[TP(-LN \cdot D)T^{-1}](T_1 P_1^{1/2} T_1^{-1})\begin{pmatrix} \hat{1} \\ \hat{0} \end{pmatrix}\right\} = 0. \tag{43}$$

Here the case of $k = -1$ corresponds to the superlattice shown in figure 1(b) and $k = 1$ to the one shown in figure 2(b), respectively.

We obtain a similar dispersion equation for the pure transverse waves:

$$(\,0 \quad 1\,)(t_s p_s t_s^{-1})(t_1 p_1^{k/2} t_1^{-1})[tp(-LN \cdot D)t^{-1}](t_1 p_1^{1/2} t_1^{-1}) \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 0 \tag{44}$$

with the case of $k = -1$ for the model illustrated by figure 1(b) and $k = 1$ for the model of figure 2(b). Here $(p_1^{1/2})^2 = p_1$, $p(-LN \cdot D) = p^{LN}$ and the stress free conditions $\sigma_{zy}^{(i)} = 0$ ($i = 1$ or s) on the top and bottom surfaces are given by

$$(\,0 \quad 1\,)t_1|v_{1,1}^+\rangle = 0 \text{ and } (\,0 \quad 1\,)t_s|v_s^-\rangle = 0. \tag{45}$$

5. Results and discussions

We have considered two types of substrated superlattice; type I consists of LN alternating m_1 and m_2 layers as shown in figure 1(a) and type II consists of the type I superlattice with an additional m_1 layer as shown in figure 2(a). Our substrated superlattice must not be confused with the capped semi-infinite superlattice [10]. Our superlattice has a finite thickness and its bottom surface contacts with a substrate of an arbitrary thickness d_s, while the capped one is semi-infinite in thickness and its top surface is covered with a thin layer. The distinction between the finite thickness and the semi-infinite thickness is significant. While our approach starts with the elastic waves in a finite superlattice, the conventional theories [6–10] consider elastic waves in an infinite superlattice.

The dispersion equations to evaluate the surface acoustic waves for the sagittal and in-plane transverse modes in a superlattice of thickness $LN \cdot D$ or $LN \cdot D + d_1$ in contact with a substrate of thickness d_s, as shown in figure 1(a) or figure 2(a), are given by

$$\det\left\{(\,\hat{0} \quad \hat{1}\,)(T_s P_s T_s^{-1})(T_1 P_1 T_1^{-1})^n[(T_2 P_2 1 T_2^{-1})(T_1 P_1 T_1^{-1})]^{LN} \begin{pmatrix} \hat{1} \\ \hat{0} \end{pmatrix}\right\} = 0 \tag{46}$$

and

$$(\,0 \quad 1\,)(t_s p_s t_s^{-1})(t_1 p_1 t_1^{-1})^n[(t_2 p_2 t_2^{-1})(t_1 p_1 t_1^{-1})]^{LN} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 0. \tag{47}$$

Here the dispersion equations with the case of $n = 0$ and $n = 1$ correspond to those for the superlattice shown in figure 1(a) and 2(a), respectively.

In reference 1, the dispersion equation (46) with $n = 0$ [2] has been expressed in terms of the 4×4 matrix as equation (26) in reference 1. Using equation (41) one can easily reduce the previous expression [2] to the form of the 2×2 matrix given by equation (46) with $n = 0$.

The thickness of the substrate is considered infinite in the standard Brillouin scattering experiment [1]. For the case of $d_s \to \infty$, the terms $(\,\hat{0} \quad \hat{1}\,)T_s P_s$ in equations (43) and (46) and $(\,0 \quad 1\,)t_s p_s$ in equations (44) and (47) can be replaced by the terms of $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ and $(\,1 \quad 0\,)$, respectively. The validity of these replacements is proved in appendix C.

We have shown in section 3 that the EEC model is equivalent to the first order expansion approximation of the exact dispersion equations (46) and (47) regarding the phase factor $q_x D$. Under this approximation, the $(T_1 P_1 T_1^{-1})^n[(T_2 P_2 T_2^{-1})(T_1 P_1 T_1^{-1})]^{LN}$ and $(t_1 p_1 t_1^{-1})^n[(t_2 p_2 t_2^{-1})(t_1 p_1 t_1^{-1})]^{LN}$ matrices in equations (46) and (47) are replaced by the $TP(-LN \cdot D - nd_1)T^{-1}$ and $tp(-LN \cdot D - nd_1)t^{-1}$ matrices, which are independent of the period D. It is obvious that the EEC model does not provide the dispersion relation as the exact expressions (46) and (47) do.

In section 4, we have derived a new model or approximation which is an extended EEC model and recovers the dispersion relation of interest. That is represented by equations (43) and (44). It is essential to symmetrize the transfer matrices under the inversion operation in this model. This model replaces a real substrated superlattice illustrated by figure 1(a) or figure 2(a) by a virtual four layered structure shown by figure 1(b) or figure 2(b).

We have carried out the exact calculations of the Rayleigh wave velocities in Cu/Al and Cu/Ag superlattices illustrated in figure 1(a) applying our dispersion equation [2] (equation (46) with $n = 0$) for the case of $d_s \to \infty$ or $d_s \geqslant 3.5\lambda_s$ (the wavelength of the surface wave $\lambda_s \cong 3000$ Å in the standard Brillouin scattering experiment) [1]. In our extended EEC model, the corresponding surface wave velocities of the substrated superlattices can be evaluated from equation (43) with $k = -1$.

The corresponding numerical results in our extended EEC model are listed in tables 1 and 2 and compared with exact ones. Here $LD = \lambda_s/D$ (D: the period of the superlattice), and the Rayleigh wave velocity is normalized by the transverse wave velocity of pure Cu metal. We can conclude that our extended EEC model can reproduce the exact dispersion relation of the Rayleigh surface waves of a superlattice with good accuracy.

Table 1. Numerical comparisons between the extended EEC model and the exact calculation of the relative Rayleigh wave velocities in Cu/Al superlattices on glass substrate of infinite thickness ($LN/LD = 1.5$) in two cases; case a: $d_{Cu}/d_{Al} = 1/2$ and case b: $d_{Cu}/d_{Al} = 2/1$. The parameter LD means the number of periods included in the wavelength of the Rayleigh wave ($\lambda_s = 2\pi/q_x$): $LD = \lambda_s/D$ with $D = d_{Cu} + d_{Al}$.

	Case a			Case b		
LD	Exact	Model	RE	Exact	Model	RE
2	1.026 16	1.051 32	−0.024 52	0.981 84	0.987 20	−0.005 46
6	1.090 02	1.090 23	−0.000 19	1.000 28	1.000 50	−0.000 22
12	1.098 88	1.098 26	0.000 56	1.005 58	1.005 28	0.000 30
18	1.100 88	1.100 48	0.000 36	1.006 88	1.006 65	0.000 23
30	1.102 23	1.102 04	0.000 17	1.007 71	1.007 59	0.000 12
54	1.103 03	1.102 96	0.000 06	1.008 16	1.008 12	0.000 04
90	1.103 41	1.103 38	0.000 03	1.008 36	1.008 35	0.000 01
270	1.103 78	1.103 78	0.000 00	1.008 55	1.008 55	0.000 00
∞	1.103 96			1.008 63		

∞: EEC model.
RE: the relative error of the extended EEC model calculation against the exact calculation.

Appendix A

Here we will elucidate the relationships between transfer matrices used in equations (16) and (17) and those used generally in conventional theoretical treatments [6–8].

We have defined $T_2P_2T_2^{-1}T_1P_1T_1^{-1}$ and $t_2p_2t_2^{-1}t_1p_1t_1^{-1}$ as the transfer matrices in equations (16) and (17). These expressions are our device to treat the transfer matrices theoretically without employing the Bloch theorem. Equations (16) and (17) can be rewritten as

$$|u^+_{1,l+1}\rangle = T_1^{-1}T_2P_2T_2^{-1}T_1P_1|u^+_{1,l}\rangle \tag{A1}$$

and

$$|v^+_{1,l+1}\rangle = t_1^{-1}t_2p_2t_2^{-1}t_1p_1|v^+_{1,l}\rangle. \tag{A2}$$

Table 2. Numerical comparisons between the extended EEC model and the exact calculation of the relative Rayleigh wave velocities in Cu/Ag superlattices on glass substrate of infinite thickness ($LN/LD = 1.5$) in two cases; Case a: $d_{Cu}/d_{Ag} = 1/2$ and Case b: $d_{Cu}/d_{Ag} = 2/1$. The meaning of the parameter LD is the same as in table 1.

	Case a			Case b		
LD	Exact	Model	RE	Exact	Model	RE
2	0.795 33	0.791 88	0.004 34	0.888 37	0.884 87	0.003 94
4	0.788 62	0.787 33	0.001 64	0.875 97	0.873 77	0.002 51
6	0.786 76	0.785 66	0.001 40	0.873 09	0.871 94	0.001 32
12	0.784 21	0.783 64	0.000 73	0.870 59	0.870 10	0.000 56
18	0.783 15	0.782 83	0.000 41	0.869 68	0.869 40	0.000 32
30	0.782 24	0.782 11	0.000 17	0.868 89	0.868 77	0.000 14
54	0.781 63	0.781 58	0.000 06	0.868 33	0.868 29	0.000 05
90	0.781 32	0.781 30	0.000 03	0.868 04	0.868 03	0.000 01
136	0.781 16	0.781 15	0.000 01	0.867 90	0.867 89	0.000 01
270	0.781 01	0.781 01	0.000 00	0.867 75	0.867 75	0.000 00
∞	0.780 86			0.867 61		

∞: EEC model.
RE: the relative error of the extended EEC model calculation against the exact calculation.

These expressions will be considered usual rather than ours. On the basis of equations (A1) and (A2), the transfer matrices should be defined as $T_1^{-1}T_2P_2T_2^{-1}T_1P_1$ and $t_1^{-1}t_2p_2t_2^{-1}t_1p_1$. The transformation from the transfer matrices in equations (16) and (17) into the usual ones in equations (A1) and (A2) is obviously a similarity transformation:

$$T_1^{-1}T_2P_2T_2^{-1}T_1P_1 = T_1^{-1}[T_2P_2T_2^{-1}T_1P_1T_1^{-1}]T_1 \tag{A3}$$

$$t_1^{-1}t_2p_2t_2^{-1}t_1p_1 = t_1^{-1}[t_2p_2t_2^{-1}t_1p_1t_1^{-1}]t_1. \tag{A4}$$

In the conventional theoretical treatment [6], one chooses the standard amplitudes of the elastic waves at the middle of each constituent layer, i.e., $z = -z_{il} - d_i/2$. Now we will write these amplitudes as

$$|u_{i,l}\rangle = \begin{pmatrix} a_{il} \\ b_{il} \\ c_{il} \\ d_{il} \end{pmatrix} \tag{A5}$$

for the sagittal modes and $|v_{i,l}\rangle$ for the transverse mode. These amplitudes are related to our amplitudes as follows:

$$|u_{i,l}\rangle = P_i^{1/2}|u_{i,l}^{+}\rangle = P_i^{-1/2}|u_{i,l}^{-}\rangle \tag{A6}$$

and

$$|v_{i,l}\rangle = p_i^{1/2}|v_{i,l}^{+}\rangle = p_i^{-1/2}|v_{i,l}^{-}\rangle. \tag{A7}$$

Here we have $(P_i^{1/2})^2 = P_i$ and $(P_i^{1/2})^{-1} = P_i^{-1/2}$, $(p_i^{1/2})^2 = p_i$ and $(p_i^{1/2})^{-1} = p_i^{-1/2}$.

In the conventional theoretical treatment [6], the exponential terms in P_i and p_i in equations (A1), (A2), (A6) and (A7) are expressed in terms of hyperbolic cosines and sines; we interpret our Q_{ij} as $\mathrm{i}Q_{ij}$ and the axis z as $-z$ in the conventional theory. Accordingly we replace P_i and p_i by $U^{-1}P_iU$ and $\sigma p_i\sigma/2$, where is used the notation

$$U = \begin{pmatrix} \sigma & \hat{0} \\ \hat{0} & \sigma \end{pmatrix} \tag{A8}$$

with $\hat{0} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$, $U^{-1} = U/2$, $\sigma = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$ and $\sigma^{-1} = \sigma/2$.

Equations (A1) and (A2) can be rewritten as

$$U^{-1}|u_{1,l+1}\rangle = (U^{-1}P_1^{1/2}U)(U^{-1}T_1^{-1}T_2U)(U^{-1}P_2U)(U^{-1}T_2^{-1}T_1U)(U^{-1}P_1^{1/2}U)U^{-1}|u_{1,l}\rangle \tag{A9}$$

and

$$\sigma^{-1}|v_{1,l+1}\rangle = (\sigma^{-1}p_1^{1/2}\sigma)(\sigma^{-1}t_1^{-1}t_2\sigma)(\sigma^{-1}p_2\sigma)(\sigma^{-1}t_2^{-1}t_1\sigma)(\sigma^{-1}p_1^{1/2}\sigma)\sigma^{-1}|v_{1,l}\rangle. \tag{A10}$$

We write equations (A9) and (A10) as

$$|\psi_{l+1}\rangle = \tilde{T}|\psi_l\rangle \tag{A11}$$

and

$$|\phi_{l+1}\rangle = \tilde{t}|\phi_l\rangle \tag{A12}$$

with $|\psi_l\rangle = U^{-1}|u_{1,l}\rangle$ and $|\phi_l\rangle = \sigma^{-1}|v_{1,l}\rangle$. Here we have an expression

$$|\psi_l\rangle = \frac{1}{2}\begin{pmatrix} a_{1,l} + b_{1,l} \\ a_{1,l} - b_{1,l} \\ c_{1,l} + d_{1,l} \\ c_{1,l} - d_{1,l} \end{pmatrix} \tag{A13}$$

which appears in the conventional theory [6]. The matrices $\tilde{T}$ and $\tilde{t}$ have been defined as the transfer matrices in the conventional theory [6–8]. Obviously from the above discussion, the transfer matrices $\tilde{T}$ and $\tilde{t}$ in the conventional theory are related to those in equations (16) and (17) by

$$\tilde{T} = U^{-1}P_1^{1/2}T_1^{-1}(T_2P_2T_2^{-1}T_1P_1T_1^{-1})T_1P_1^{-1/2}U \tag{A14}$$

and

$$\tilde{t} = \sigma^{-1}p_1^{1/2}t_1^{-1}(t_2p_2t_2^{-1}t_1p_1t_1^{-1})t_1p_1^{-1/2}\sigma. \tag{A15}$$

Appendix B

The inverse matrix T_i^{-1} of the matrix T_i defined by equation (10) is given by

$$T_i^{-1} = \frac{1}{2}\begin{pmatrix} -\alpha_{i2}/\overline{\alpha}_i & \beta_{i2}/\overline{U\beta}_i & 1/\overline{\alpha}_i & -U_{i2}/\overline{U\beta}_i \\ -\alpha_{i2}/\overline{\alpha}_i & -\beta_{i2}/\overline{U\beta}_i & 1/\overline{\alpha}_i & U_{i2}/\overline{U\beta}_i \\ -\alpha_{i1}/\overline{\alpha}_i & -\beta_{i1}/\overline{U\beta}_i & -1/\overline{\alpha}_i & U_{i1}/\overline{U\beta}_i \\ -\alpha_{i1}/\overline{\alpha}_i & \beta_{i1}/\overline{U\beta}_i & -1/\overline{\alpha}_i & -U_{i1}/\overline{U\beta}_i \end{pmatrix} \tag{B1}$$

where

$$\overline{\alpha}_i \equiv \alpha_{i1} - \alpha_{i2} = C_{33}^{(i)}(U_{i1}Q_{i1} - U_{i2}Q_{i2}) \tag{B2}$$

and

$$\overline{U\beta}_i \equiv U_{i1}\beta_{i2} - U_{i2}\beta_{i1} = C_{44}^{(i)}(U_{i1}Q_{i2} - U_{i2}Q_{i1}). \tag{B3}$$

By use of matrices (10), (19) and (B1) with the expression (11), one can easily obtain

$$T_i\tilde{Q}_iT_i^{-1} \equiv \tilde{B}^{(i)} = \begin{pmatrix} 0 & -1 & 0 & 1/C_{44}^{(i)} \\ -C_{13}^{(i)}/C_{33}^{(i)} & 0 & 1/C_{33}^{(i)} & 0 \\ 0 & \tilde{B}_{32}^{(i)} & 0 & \tilde{B}_{34}^{(i)} \\ \tilde{B}_{41}^{(i)} & 0 & \tilde{B}_{43}^{(i)} & 0 \end{pmatrix} \tag{B4}$$

with

$$\tilde{B}_{32}^{(i)} = -C_{13}^{(i)} + C_{33}^{(i)} \frac{(U_{i1}Q_{i1})(U_{i2}Q_{i2})(Q_{i1}^2 - Q_{i2}^2) + Q_{i1}^2 Q_{i2}^2 (U_{i1}Q_{i1} - U_{i2}Q_{i2})}{(U_{i1}Q_{i2} - U_{i2}Q_{i1})Q_{i1}Q_{i2}} \tag{B5}$$

$$\tilde{B}_{34}^{(i)} = \frac{C_{13}^{(i)}}{C_{44}^{(i)}} + \frac{C_{33}^{(i)}}{C_{44}^{(i)}} \frac{(U_{i1}Q_{i1})(U_{i2}Q_{i2})(Q_{i2}^2 - Q_{i1}^2)}{(U_{i1}Q_{i2} - U_{i2}Q_{i1})Q_{i1}Q_{i2}} \tag{B6}$$

$$\tilde{B}_{41}^{(i)} = C_{44}^{(i)} \left\{ \frac{C_{13}^{(i)}}{C_{33}^{(i)}} \left(\frac{Q_{i2}^2 - Q_{i1}^2}{U_{i1}Q_{i1} - U_{i2}Q_{i2}} - 1 \right) + \frac{Q_{i1}Q_{i2}(U_{i1}Q_{i2} - U_{i2}Q_{i1})}{U_{i1}Q_{i1} - U_{i2}Q_{i2}} \right\} \tag{B7}$$

and

$$\tilde{B}_{43}^{(i)} = \frac{C_{44}^{(i)}}{C_{33}^{(i)}} \left(1 - \frac{Q_{i2}^2 - Q_{i1}^2}{U_{i1}Q_{i1} - U_{i1}Q_{i2}} \right). \tag{B8}$$

Now we can find the following relations between U_{ij} and Q_{ij}, which are the solutions of equation (3):

$$U_{i2}Q_{i2} - U_{i1}Q_{i1} = -\frac{C_{44}^{(i)}}{C_{13}^{(i)} + C_{44}^{(i)}} (Q_{i2}^2 - Q_{i1}^2) \tag{B9}$$

$$(U_{i2}Q_{i1} - U_{i1}Q_{i2})Q_{i1}Q_{i2} = \frac{C_{11}^{(i)} - C_{44}^{(i)}\xi_i^2}{C_{13}^{(i)} + C_{44}^{(i)}} (Q_{i2}^2 - Q_{i1}^2) \tag{B10}$$

and

$$(U_{i1}Q_{i1})(U_{i2}Q_{i2}) = \frac{C_{11}^{(i)} - C_{44}^{(i)}\xi_i^2}{C_{33}^{(i)}}. \tag{B11}$$

Furthermore, from equation (5) we have

$$Q_{i1}^2 Q_{i2}^2 = \frac{C_{11}^{(i)} - C_{44}^{(i)}\xi_i^2}{C_{33}^{(i)}} (1 - \xi_i^2). \tag{B12}$$

Substituting relations (B9)–(B12) into equations (B5)–(B8), we have

$$\tilde{B}_{32}^{(i)} = C_{44}^{(i)}\xi_i^2 \qquad \tilde{B}_{34}^{(i)} = -1 \qquad \tilde{B}_{41}^{(i)} = C_{44}^{(i)}\xi_i^2 - C_{11}^{(i)} + \frac{C_{13}^{(i)^2}}{C_{33}^{(i)}} \text{ and } \tilde{B}_{43}^{(i)} = -\frac{C_{13}^{(i)}}{C_{33}^{(i)}}. \tag{B13}$$

Thus we can derive the expression (20).

Appendix C

At the top surface of the substrate the boundary conditions, which are included in equations (40) and (45), can be expressed as

$$(\hat{0} \quad \hat{1})T_s P_s |u_s^+\rangle = 0 \text{ and } (0 \quad 1)t_s p_s |v_s^+\rangle = 0. \tag{C1}$$

The surface elastic waves damp as they propagate from the surface into the inside of the superlattice. Thus for the case of $d_s \to \infty$ we have

$$f_{sj}(d_s)/f_{sj}(-d_s) \approx 0 \qquad j = 1, 2 \text{ and } 3 \tag{C2}$$

where $f_{sj}(z)$ is defined in equations (7) and (15). Using (C2) one has

$$(\hat{0} \quad \hat{1})T_s P_s \cong \begin{pmatrix} \alpha_{s1}f_{s1} & 0 & \alpha_{s2}f_{s2} & 0 \\ \beta_{s1}f_{s1} & 0 & \beta_{s2}f_{s2} & 0 \end{pmatrix} = \begin{pmatrix} \alpha_{s1}f_{s1} & \alpha_{s2}f_{s2} \\ \beta_{s1}f_{s1} & \beta_{s2}f_{s2} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} \tag{C3}$$

and

$$(\,0 \quad 1\,)t_s p_s \cong C_{44}^{(s)} Q_{s3} f_{s3} (\,1 \quad 0\,) \tag{C4}$$

where f_{sj} denotes $f_{sj}(-d_s)$.

The relations (C3) and (C4) suggest that in this case the boundary conditions (C1) can be rewritten as

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} |u_s^+\rangle = 0 \text{ and } (\,1 \quad 0\,)|v_s^+\rangle = 0. \tag{C5}$$

These are reasonable boundary conditions for the substrate of infinite thickness. From the above discussion we can readily conclude that the terms $(\,\hat{0} \quad \hat{1}\,)T_s P_s$ and $(\,0 \quad 1\,)t_s p_S$ are replaced by the terms $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ and $(\,1 \quad 0\,)$ for the case of $d_s \to \infty$.

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