PHYSICAL REVIEW B VOLUME 28, NUMBER 4 15 AUGUST 1983

Sagittal elastic waves in infinite and semi-infinite superlattices

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(Received 9 May 1983)

Elastic waves, polarized in the sagittal plane, are investigated in infinite and semi-infinite superlattices made from alternate layers of two isotropic media. By the use of a transfer-matrix method, we obtain explicit equations for the dispersion of the bulk modes as well as of the surface modes of a semi-infinite superlattice. We present a few illustrations of the theory for Al-W superlattices in which the relative thicknesses of the two media or the thickness of the layer at the surface are varied.

I. INTRODUCTION

The study of acoustic wave propagation in layered media[1,2] is an old problem which found its original motivation in studies of the propagation of seismic shocks through the Earth's crust. There is a recent interest in this problem due to the development of a technology for fabricating artificial crystals—superlattices—consisting of alternating layers of two different materials.[3,4] Recent theoretical work on acoustic waves in superlattices has been mainly concerned with the dispersion of the elastic waves propagating in such systems.[5–13] In the particular case when the layer thicknesses are small compared to the wavelength, the superlattice can be described by an effective medium[14–20] whose elastic constants and density are some combinations of the parameters of the two constituents; obviously, the waves are nondispersive in this limit.

There are also recent atomic calculations of the bulk and surface phonons in linear-chain superlattices,[11,21] and even in superlattices made by the association of simple-cubic slabs.[22] These advances are motivated in part by the infrared and Raman measurements in GaAs-AlAs—like superlattices.[21,23–26] We also mention recent new experimental results[26] on the Brillouin scattering of light from thermally excited elastic waves in such structures.

In this paper we investigate the elastic waves of a semi-infinite superlattice that are polarized in the sagittal plane, i.e., in the plane containing the wave vector and the normal to the surface. Recently, Kueny *et al.*[27] reported experimental results for the velocity of Rayleigh waves in a Nb-Cu heterostructure as a function of the layer thickness; later Kueny and Grimsditch[13] presented a numerical calculation of this velocity for an N layer heterostructure deposited on a substrate. In this work, we describe a new method, based on the transfer matrix, for solving this problem in an essentially analytic way. We find the equations from which the bulk bands of the superlattice as well as its free surface modes can be deduced. The outline of the theory and the dispersion relations are given in Sec. II. Section III contains a few illustrations of the theory.

Let us also point out that we recently derived[11,12] explicit results for the condition of existence and the dispersion of transverse surface elastic waves in a superlattice. The possibility of such modes in a semi-infinite superlattice had been shown earlier numerically by Auld *et al.*[10]

II. THEORY OF THE SAGITTAL MODES IN SUPERLATTICES

The superlattice consists of alternating layers of two elastic isotropic media A and A', described by their elastic constants (c_{11},c_{44}) and (c'_{11},c'_{44}) and their densities ρ and ρ', respectively. The geometry of a semi-infinite superlattice is depicted in Fig. 1. The layers as well as the free surface of the superlattice are perpendicular to the x_3 axis. The superlattice period is $D=d+d'$, where $d=2h$ and $d'=2h'$ are the thicknesses of the two media, respectively.

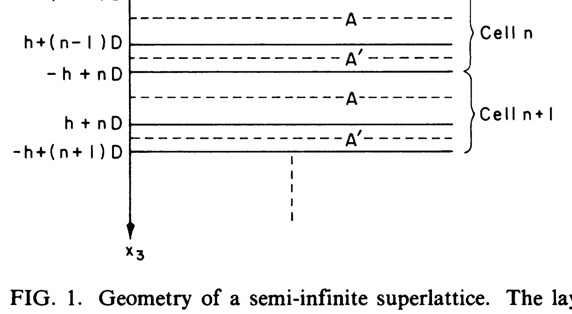

FIG. 1. Geometry of a semi-infinite superlattice. The layer thicknesses in the bulk are $d=2h$, $d'=2h'$, so the superlattice period is $D=d+d'$. The surface layer is made of medium A and has a thickness $h+h_s$. The layers are perpendicular to the x_3 axis.

The surface layer is assumed to be of type A, with a thickness $h+h_s$.

Let us assume that the wave vector $\vec{k}_{\parallel}$ parallel to the surface is along the x_1 axis. Owing to the isotropy of the media there is a decoupling between the waves polarized in the sagittal plane (the x_1x_3 plane) and the transverse modes polarized along x_2. Here we will consider only the former modes since the latter were studied in Refs. 10—12.

A. General formalism

The general form of the displacement field in each medium can be obtained from the equations of motion of elasticity theory, after a Fourier transformation in the coordinates parallel to the surface. The same method has been used previously in surface[28] and interface[29] problems. Then, for example, if x_3 belongs to the medium A' of the layer n we have

$$u_1(x_3)=(A_{nl}e^{-\alpha_l x_3^{(n)}}+B_{nl}e^{\alpha_l x_3^{(n)}}+A_{nt}e^{-\alpha_t x_3^{(n)}}+B_{nt}e^{\alpha_t x_3^{(n)}})e^{i(k_{\parallel}x_1-\omega t)}, \tag{2.1a}$$

$$u_3(x_3)=i\left[\frac{\alpha_l}{k_{\parallel}}A_{nl}e^{-\alpha_l x_3^{(n)}}-\frac{\alpha_l}{k_{\parallel}}B_{nl}e^{\alpha_l x_3^{(n)}}+\frac{k_{\parallel}}{\alpha_t}A_{nt}e^{-\alpha_t x_3^{(n)}}-\frac{k_{\parallel}}{\alpha_t}B_{nt}e^{\alpha_t x_3^{(n)}}\right]e^{i(k_{\parallel}x_1-\omega t)}. \tag{2.1b}$$

We have introduced the variable $x_3^{(n)}=x_3-(n-1)D$ whose range is $-h$ to h; this has the advantage of simplifying the expressions for the coefficients A_{nl}, A_{nt}, B_{nl}, and B_{nt}.

In Eqs. (2.1),

$$\alpha_l=(k_{\parallel}^2-\omega^2/c_l^2)^{1/2},\quad \alpha_t=(k_{\parallel}^2-\omega^2/c_t^2)^{1/2}, \tag{2.2}$$

where $c_l=(c_{11}/\rho)^{1/2}$ and $c_t=(c_{44}/\rho)^{1/2}$ are, respectively, the longitudinal and transverse velocities of sound in medium A; ω is the frequency of the wave.

Similarly, for x_3 belonging to the medium A' of the layer n,

$$u_1(x_3)=(A'_{nl}e^{-\alpha'_l x_3'^{(n)}}+B'_{nl}e^{\alpha'_l x_3'^{(n)}}+A'_{nt}e^{-\alpha'_t x_3'^{(n)}}+B'_{nt}e^{\alpha'_t x_3'^{(n)}})e^{i(k_{\parallel}x_1-\omega t)}, \tag{2.3a}$$

$$u_3(x_3)=i\left[\frac{\alpha'_l}{k_{\parallel}}A'_{nl}e^{-\alpha'_l x_3'^{(n)}}-\frac{\alpha'_l}{k_{\parallel}}B'_{nl}e^{\alpha'_l x_3'^{(n)}}+\frac{k_{\parallel}}{\alpha'_t}A'_{nt}e^{-\alpha'_t x_3'^{(n)}}-\frac{k_{\parallel}}{\alpha'_t}B'_{nt}e^{\alpha'_t x_3'^{(n)}}\right]e^{i(k_{\parallel}x_1-\omega t)}, \tag{2.3b}$$

where the variable $x_3'^{(n)}=x_3-(n-1/2)D$ ranges from $-h'$ to h'. The parameters α'_l, α'_t, c'_l, and c'_t are defined as above.

The unknown coefficients A_{nl}, B_{nl}, A_{nt}, B_{nt}, A'_{nl}, B'_{nl}, A'_{nt}, and B'_{nt} are determined from the boundary conditions on the displacements and the stresses at the different interfaces as well as at the free surface. For example, in layer n, at the interface between the media A, and A', we have

$$u_\alpha(x_3)\,|_{x_3^{(n)}=h-0}=u_\alpha(x_3)\,|_{x_3'^{(n)}=-h'+0},\quad \alpha=1,3, \tag{2.4a}$$

$$c_{44}\left[\frac{du_1}{dx_3}+ik_{\parallel}u_3\right]_{x_3^{(n)}=h-0}=c'_{44}\left[\frac{du_1}{dx_3}+ik_{\parallel}u_3\right]_{x_3'^{(n)}=-h'+0}, \tag{2.4b}$$

$$\left[ic_{12}k_{\parallel}u_1+c_{11}\frac{du_3}{dx_3}\right]_{x_3^{(n)}=h-0}=\left[ic'_{12}k_{\parallel}u_1+c'_{11}\frac{du_3}{dx_3}\right]_{x_3'^{(n)}=-h'+0}. \tag{2.4c}$$

Similary, at the interface between the medium A' of layer n and the medium A of layer $n+1$, the boundary conditions are

$$u_\alpha(x_3)\,|_{x_3^{(n+1)}=-h+0}=u_\alpha(x_3)\,|_{x_3'^{(n)}=h'-0},\quad \alpha=1,3, \tag{2.5a}$$

$$c_{44}\left[\frac{du_1}{dx_3}+ik_{\parallel}u_3\right]_{x_3^{(n+1)}=-h+0}=c'_{44}\left[\frac{du_1}{dx_3}+ik_{\parallel}u_3\right]_{x_3'^{(n)}=h'-0}, \tag{2.5b}$$

$$\left[ic_{12}k_{\parallel}u_1+c_{11}\frac{du_3}{dx_3}\right]_{x_3^{(n+1)}=-h+0}=\left[ic'_{12}k_{\parallel}u_1+c'_{11}\frac{du_3}{dx_3}\right]_{x_3'^{(n)}=h'-0}. \tag{2.5c}$$

Finally, at the free surface, the vanishing of the stresses can be expressed as

$$c_{44}\left[\frac{du_1}{dx_3}+ik_{\parallel}u_3\right]_{x_3=-h_s}=0, \tag{2.6a}$$

$$\left[ic_{12}k_{\parallel}u_1+c_{11}\frac{du_3}{dx_3}\right]_{x_3=-h_s}=0. \tag{2.6b}$$

One method for obtaining the eigenfrequencies of a superlattice is to solve these sets of linear equations for each $k_{\parallel}$. Thus for a superlattice of N layers with two free surfaces we have a determinant of rank $8N$. If the N layers are deposited on an infinite substrate the rank of the determinant will be $8N+2$. Instead of using this heavy numerical approach,[13] we shall present a new method which gives explicit equations from which the limits of the bulk bands of the superlattice as well as the free surface modes can be deduced.

In the following, instead of the expressions (2.1) and (2.3), it is more convenient to use another form of the displacement field, expressed in terms of hyperbolic cosines and sines rather than in terms of exponentials. Thus we write Eqs. (2.1) as

$$u_1(x_3)=[P_{nl}\cosh(\alpha_l x_3^{(n)})-Q_{nl}\sinh(\alpha_l x_3^{(n)})+P_{nt}\cosh(\alpha_t x_3^{(n)})-Q_{nt}\sinh(\alpha_t x_3^{(n)})]e^{i(k_\parallel x_1-\omega t)}\,, \tag{2.7a}$$

$$u_3(x_3)=i\left[\frac{\alpha_l}{k_\parallel}Q_{nl}\cosh(\alpha_l x_3^{(n)})-\frac{\alpha_l}{k_\parallel}P_{nl}\sinh(\alpha_l x_3^{(n)})+\frac{k_\parallel}{\alpha_t}Q_{nt}\cosh(\alpha_t x_3^{(n)})\right.$$
$$\left.-\frac{k_\parallel}{\alpha_t}P_{nt}\sinh(\alpha_t x_3^{(n)})\right]e^{i(k_\parallel x_1-\omega t)}\,, \tag{2.7b}$$

where

$$P_{n\mu}=\frac{A_{n\mu}+B_{n\mu}}{2},\quad Q_{n\mu}=\frac{A_{n\mu}-B_{n\mu}}{2}\,,\qquad \mu=l \text{ or } t\,. \tag{2.8}$$

Similar equations will be used instead of the expressions (2.3).

B. Transfer-matrix method

Let us introduce, in each layer n, two column vectors

$$|\psi_n\rangle=\begin{bmatrix}P_{nl}\\P_{nt}\\Q_{nl}\\Q_{nt}\end{bmatrix},\quad |\psi'_n\rangle=\begin{bmatrix}P'_{nl}\\P'_{nt}\\Q'_{nl}\\Q'_{nt}\end{bmatrix}. \tag{2.9}$$

The boundary conditions (2.4) and (2.5) can then be written in the following matrix forms:

$$\underline{H}\,|\psi_n\rangle=\underline{K}'\,|\psi'_n\rangle\,, \tag{2.10a}$$

$$\underline{K}\,|\psi_{n+1}\rangle=\underline{H}'\,|\psi'_n\rangle\,, \tag{2.10b}$$

respectively, where $\underline{H}$, $\underline{K}$, $\underline{H}'$, and $\underline{K}'$ are 4×4 matrices independent of the index n. The expressions for $\underline{H}$ and $\underline{K}$ are given in the Appendix; those for $\underline{H}'$ and $\underline{K}'$ can be deduced from the latter by replacing all the unprimed quantities by the primed ones.

The elimination of the vector $|\psi'_n\rangle$ between the equations (2.10) gives

$$|\psi_{n+1}\rangle=\underline{T}\,|\psi_n\rangle\,, \tag{2.11}$$

where the matrix $\underline{T}$,

$$\underline{T}=\underline{K}^{-1}\underline{H}'\underline{K}'^{-1}\underline{H}\,, \tag{2.12}$$

can be considered a "transfer matrix." The elements T_{ij} of this matrix are given in the Appendix. The transfer matrix has the property of relating the coefficients of the wave function in one cell to those in the preceding cell. For example, by choosing a reference layer n_0, one has

$$|\psi_n\rangle=\underline{T}^{(n-n_0)}\,|\psi_{n_0}\rangle\,. \tag{2.13a}$$

In the semi-infinite superlattice, this reference layer can be chosen to be the surface layer ($n_0=1$); then

$$|\psi_n\rangle=\underline{T}^{(n-1)}\,|\psi_1\rangle\,. \tag{2.13b}$$

One should remember that in the latter case the coefficients P_{1l}, P_{1t}, Q_{1l}, and Q_{1t} defining $|\psi_1\rangle$ satisfy two additional equations which result from the boundary conditions (2.6) at the free surface.

In the following we shall show that the eigenvalues and eigenmodes of the superlattice can be obtained from the diagonalization of the $\underline{T}$ matrix. We consider an infinite and a semi-infinite superlattice in turn.

C. Infinite superlattice

Due to the periodicity perpendicular to the layers, the vector $|\psi_n\rangle$ must satisfy the Bloch theorem

$$|\psi_{n+1}\rangle=e^{ik_3D}\,|\psi_n\rangle\,, \tag{2.14}$$

where k_3 is the wave vector in the x_3 direction. From a comparison of Eqs. (2.11) and (2.14) we find that

$$\underline{T}\,|\psi_n\rangle=e^{ik_3D}\,|\psi_n\rangle\,. \tag{2.15}$$

It follows that the eigenvalues of the infinite superlattice are the roots of the determinant

$$|\underline{T}-e^{ik_3D}\underline{1}|=0\,, \tag{2.16}$$

where $\underline{1}$ is the 4×4 unit matrix. In other words, for given ω and $k_\parallel$, Eq. (2.16) gives the values of k_3. This proves the statement that the eigenvalues of the superlattice are obtained from the diagonalization of the $\underline{T}$ matrix. Let us expand on this result, before giving explicit expressions for these eigenvalues. By defining

$$\lambda=e^{ik_3D} \tag{2.17}$$

and expanding the deteminant of Eq. (2.16) one arrives at the equation

$$(\lambda^2-2s_1\lambda+1)(\lambda^2-2s_2\lambda+1)=0\,, \tag{2.18}$$

where the definitions of the coefficients s_1, s_2 will be given below.

The four solutions λ_1, λ'_1, λ_2, and λ'_2 of Eq. (2.18) satisfy the conditions

$$\lambda'_1=\frac{1}{\lambda_1},\quad \lambda'_2=\frac{1}{\lambda_2}\,, \tag{2.19}$$

which are a general property of the $\underline{T}$ matrix.

We shall prove this property of the eigenvalues of the $\underline{T}$

matrix, and at the same time will obtain explicit expressions for them as well as for the corresponding eigenvectors. Let $|\psi\rangle$ be an eigenvector of $\underline{T}$ associated with an eigenvalue λ; this means that

$$\underline{T}\,|\psi\rangle=\lambda\,|\psi\rangle\ . \tag{2.20}$$

Obviously, $|\psi\rangle$ is an eigenvector of the matrix $\frac{1}{2}(\underline{T}+\underline{T}^{-1})$ with the eigenvalue $\frac{1}{2}(\lambda+\lambda^{-1})$,

$$\tfrac{1}{2}(\underline{T}+\underline{T}^{-1})\,|\psi\rangle=\tfrac{1}{2}(\lambda+\lambda^{-1})\,|\psi\rangle\ . \tag{2.21}$$

The point is that (see the Appendix) $\underline{T}^{-1}$ is related to $\underline{T}$ by

$$\underline{T}^{-1}=\begin{bmatrix} T_{11} & T_{12} & -T_{13} & -T_{14} \\ T_{21} & T_{22} & -T_{23} & -T_{24} \\ -T_{31} & -T_{32} & T_{33} & T_{34} \\ -T_{41} & -T_{42} & T_{43} & T_{44} \end{bmatrix}, \tag{2.22}$$

and thus

$$\tfrac{1}{2}(\underline{T}+\underline{T}^{-1})=\begin{bmatrix} T_{11} & T_{12} & 0 & 0 \\ T_{21} & T_{22} & 0 & 0 \\ 0 & 0 & T_{33} & T_{34} \\ 0 & 0 & T_{43} & T_{44} \end{bmatrix}, \tag{2.23}$$

where (see the Appendix) $T_{33}=T_{11}$, $T_{44}=T_{22}$, $T_{34}=-\alpha_l\alpha_t/k_{\parallel}^2T_{21}$, and $T_{43}=-(k_{\parallel}^2/\alpha_l\alpha_t)T_{12}$. It follows from Eq. (2.23) that the matrix $\frac{1}{2}(\underline{T}+\underline{T}^{-1})$ has two eigenvalues, s_1 and s_2, each of which is doubly degenerate. By introducing the following definitions

$$\begin{aligned} R&=\tfrac{1}{2}(T_{11}+T_{22})\ ,\\ P&=\tfrac{1}{2}(T_{11}-T_{22})\ ,\\ \Pi&=\tfrac{1}{2}[(T_{11}-T_{12})^2+4T_{12}T_{21}]^{1/2}\ , \end{aligned} \tag{2.24}$$

we obtain straightforwardly that

$$s_1=R+\Pi,\quad s_2=R-\Pi\ . \tag{2.25}$$

Finally, by solving the equations $\frac{1}{2}(\lambda+1/\lambda)=s_{1,2}$ one arrives at the $\underline{T}$-matrix eigenvalues

$$\begin{aligned} \lambda_{1,2}&=s_{1,2}+(s_{1,2}^2-1)^{1/2}\ ,\\ \lambda'_{1,2}&=s_{1,2}-(s_{1,2}^2-1)^{1/2}\ , \end{aligned} \tag{2.26}$$

which satisfy the relations (2.19).

With each of these λ is associated a value of the wave vector k_3 in the x_3 direction [Eq. (2.17)]. According to the relations (2.19), these k_3 can be written formally as

$$K_1+iL_1,\ -K_1-iL_1, K_2+iL_2,\ \text{and}\ -K_2-iL_2\ . \tag{2.27}$$

Depending on whether k_3 is real or has an imaginary part, the corresponding wave propagates through the superlattices (bulk bands) or is damped (gaps). Let us consider this point further.

One can see from the expressions for T_{11}, T_{12}, T_{21}, and T_{22} in the Appendix that these four quantities are all real. It follows that R and P [Eq. (2.24)] are both real while Π can be either real or pure imaginary.

(i) For Π real, s_1 and s_2 are also real; if $|s_1|$ *or* $|s_2|$ is smaller than 1, then $|\lambda_1|=|\lambda'_1|=1$ or $|\lambda_2|=|\lambda'_2|=1$; the corresponding k_3 is real ($L_1=0$ or $L_2=0$), and we are in a bulk band; if $|s_1|$ *and* $|s_2|$ are larger than 1, then the corresponding k_3 are pure imaginary ($K_1=K_2=0$); this corresponds to a gap.

(ii) For Π imaginary, s_1 and s_2 are complex conjugate quantities, as are the wave vectors k_3 which have the forms $K+iL$, $-K-iL$, $K-iL$, and $-K+iL$; this also corresponds to a gap.

Finally, we give the eigenmodes $|\psi_1\rangle$, $|\psi_2\rangle$, $|\psi'_1\rangle$, and $|\psi'_2\rangle$ of the $\underline{T}$ matrix associated with λ_1, λ_2, λ'_1, and λ'_2, respectively. We first introduce[30] the two eigenmodes of the upper left-hand 2×2 matrix in $\frac{1}{2}(\underline{T}+\underline{T}^{-1})$,

$$|S_1\rangle=\begin{bmatrix} -T_{12} \\ P-\Pi \\ 0 \\ 0 \end{bmatrix},\quad |S_2\rangle=\begin{bmatrix} -T_{12} \\ P+\Pi \\ 0 \\ 0 \end{bmatrix}. \tag{2.28}$$

These are associated with the eigenvalues s_1 and s_2, respectively. One can easily check that

$$\left.\begin{matrix}|\psi_1\rangle\\|\psi'_1\rangle\end{matrix}\right\}=|S_1\rangle\pm\frac{\frac{1}{2}(\underline{T}-\underline{T}^{-1})\,|S_1\rangle}{\frac{1}{2}(\lambda_1-\lambda'_1)}=\begin{bmatrix} -T_{12} \\ P-\Pi \\ \pm\dfrac{1}{\frac{1}{2}(\lambda_1-\lambda'_1)}[-T_{12}T_{31}+(P-\Pi)T_{32}] \\ \pm\dfrac{1}{\frac{1}{2}(\lambda_1-\lambda'_1)}[-T_{12}T_{41}+(P-\Pi)T_{42}] \end{bmatrix}. \tag{2.29}$$

For this it is sufficient to apply the $\underline{T}$ matrix in the form $\frac{1}{2}(\underline{T}+\underline{T}^{-1})+\frac{1}{2}(\underline{T}-\underline{T}^{-1})$, to $|\psi_1\rangle$. Similarly, we find that

$$\left.\begin{matrix}|\psi_2\rangle\\|\psi'_2\rangle\end{matrix}\right\}=|S_2\rangle\pm\frac{\frac{1}{2}(\underline{T}-\underline{T}^{-1})\,|S_2\rangle}{\frac{1}{2}(\lambda_2-\lambda'_2)}=\begin{bmatrix} -T_{12} \\ P+\Pi \\ \pm\dfrac{1}{\frac{1}{2}(\lambda_2-\lambda'_2)}[-T_{12}T_{31}+(P+\Pi)T_{32}] \\ \pm\dfrac{1}{\frac{1}{2}(\lambda_2-\lambda'_2)}[-T_{12}T_{41}+(P+\Pi)T_{42}] \end{bmatrix}. \tag{2.30}$$

We should point out that the eigenvectors given above are not normalized. Although $|S_1\rangle$ and $|S_2\rangle$ were derived from the upper left-hand 2×2 matrix in $\frac{1}{2}(\underline{T}+\underline{T}^{-1})$ [Eq. (2.23)] the same procedure can be based on the lower right-hand 2×2 matrix in Eq. (2.23).

D. Semi-infinite superlattice

In this subsection we are concerned with the existence and dispersion of surface waves in the gaps separating the bulk bands. The amplitudes of these modes decrease exponentially with increasing distance into the interior layers of the superlattice.

We investigate such a mode as a combination of solutions such as (2.7)–(2.14), but allow the wave vector k_3 to be complex, $k_3=K+iL$, with

$$L>0 \tag{2.31}$$

to insure the decrease of the wave amplitude with increasing distance into the superlattice.

As mentioned previously, for given ω and $k_{\parallel}$ the four wave vectors k_3, corresponding to the four eigenvalues of the $\underline{T}$ matrix, can be written in the form (2.27). Among these wave vectors only two can satisfy the condition (2.31) and, as a result, the two others should be rejected. We then write the solution for the surface mode in layer n as [see Eq. (2.7)]

$$\begin{aligned}
u_1(x_3)&=\sum_{r=1,2} A_r[P_{nl}^{(r)}\cosh(\alpha_l x_3^{(n)})-Q_{nl}^{(r)}\sinh(\alpha_l x_3^{(n)})+P_{nt}^{(r)}\cosh(\alpha_t x_3^{(n)})-Q_{nt}\sinh(\alpha_t x_3^{(n)})]e^{i(k_{\parallel}x_1-\omega t)}\,,\\
u_3(x_3)&=\sum_{r=1,2} A_r i\left[\frac{\alpha_l}{k_{\parallel}}Q_{nl}\cosh(\alpha_l x_3^{(n)})-\frac{\alpha_l}{k_{\parallel}}P_{nl}\sinh(\alpha_l x_3^{(n)})\right.\\
&\qquad\left.+\frac{k_{\parallel}}{\alpha_t}Q_{nt}\cosh(\alpha_t x_3^{(n)})-\frac{k_{\parallel}}{\alpha_t}P_{nt}\sinh(\alpha_t x_3^{(n)})\right]e^{i(k_{\parallel}x_1-\omega t)}\,.
\end{aligned} \tag{2.32}$$

The two vectors $|\psi_n^{(r)}\rangle$ corresponding to this solution,

$$|\psi_n^{(r)}\rangle=\begin{bmatrix}P_{nl}^{(r)}\\ P_{nt}^{(r)}\\ Q_{nl}^{(r)}\\ Q_{nt}^{(r)}\end{bmatrix},\quad r=1,2\,,$$

are the two eigenvectors of the $\underline{T}$ matrix associated with the two retained eigenvalues; they are given by Eqs. (2.29) and (2.30). Moreover the $|\psi_n^{(r)}\rangle$ are related to $|\psi_1^{(r)}\rangle$ by means of Eq. (2.13a).

As noted previously, the displacement field in the layer at the surface should also satisfy the boundary conditions (2.6) at the free surface situated at $x_3=-h_s$. This leads to two homogeneous linear equations for the two unknowns A_1 and A_2. The surface modes are then solutions of the 2×2 determinant obtained from this system,

$$\begin{vmatrix}D_{11} & D_{12}\\ D_{21} & D_{22}\end{vmatrix}=0\,, \tag{2.33}$$

with

$$\begin{aligned}
D_{1r}&=2\alpha_l[P_{1l}^{(r)}\sinh(\alpha_l h_s)-Q_{1l}^{(r)}\cosh(\alpha_l h_s)]+\left[\alpha_t+\frac{k_{\parallel}^2}{\alpha_t}\right][P_{1t}^{(r)}\sinh(\alpha_t h_s)-Q_{1t}^{(r)}\cosh(\alpha_t h_s)]\,,\\
D_{2r}&=\left[\left[1-2\frac{c_{44}}{c_{11}}\right]-\frac{\alpha_l^2}{k_{\parallel}^2}\right][P_{1l}^{(r)}\cosh(\alpha_l h_s)-Q_{1l}^{(r)}\sinh(\alpha_l h_s)]-2\frac{c_{44}}{c_{11}}[P_{1t}^{(r)}\cosh(\alpha_t h_s)-Q_{1t}^{(r)}\sinh(\alpha_t h_s)],\quad r=1,2\,.
\end{aligned} \tag{2.34}$$

III. BAND STRUCTURE FOR BULK AND SURFACE SAGITTAL MODES

We present here a few illustrations of the band structure for sagittal elastic modes in a superlattice. In these examples the superlattices are made of Al and W with the parameters given in Table I. The choice of these materials is consistent with the assumption of isotropic media for the theoretical calculation. This is far from being the case in other systems studied previously[11–13] for practical reasons (GaAs-AlAs and Nb-Cu). However, in cubic materials with a (001) surface and propagation along [100], the description of the transverse elastic waves is formally identical to that in isotropic materials. This point does not apply to the sagittal modes studied here.

The Al-W superlattice also has the advantage of presenting large gaps between bulk bands (Figs. 2–4), even

TABLE I. Elastic constants and densities of Al and W. The elastic constant c_{12} is taken to be $c_{12}=c_{11}-2c_{44}$ to satisfy the isotropy assumption.

	c_{11} (10^9 N/m^2)	c_{44} (10^9 N/m^2)	ρ (g/cm^2)
W	52.33	16.07	19.317
Al	10.68	2.82	2.733

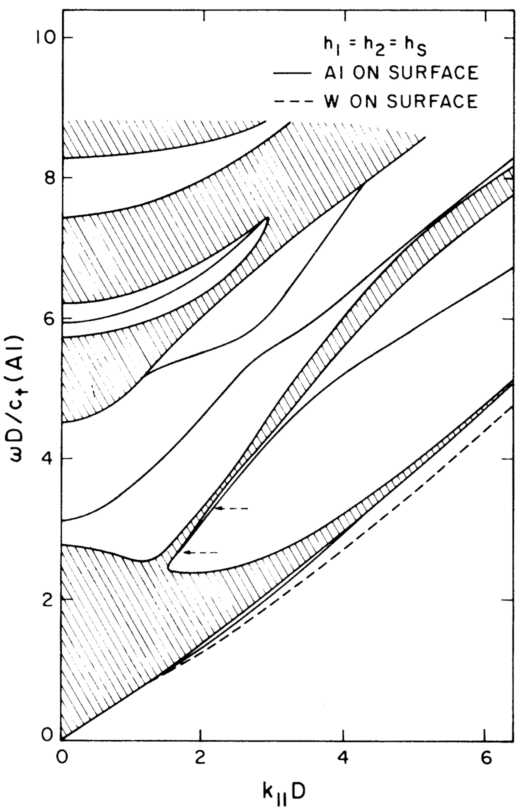

FIG. 2. Bulk bands and surface wave dispersion for an Al-W superlattice with $d_{\mathrm{Al}}=d_{\mathrm{W}}$. The shaded areas are the bulk bands. The surface modes are presented either for an Al layer (solid line) or a W layer (dashed line) at the surface. The surface-layer thickness is assumed to be the same as that of a corresponding bulk layer. We present dimensionless quantities on the two axes. $c_t(\mathrm{Al})$ is the transverse velocity of sound in Al $[c_t(\mathrm{Al}) =(c_{44}/\rho)^{1/2}_{\mathrm{Al}}]$. Some of the surface modes are very near to the bulk bands and cannot be distinguished on the scale of the figure. However, the arrows indicate the location of these surface modes.

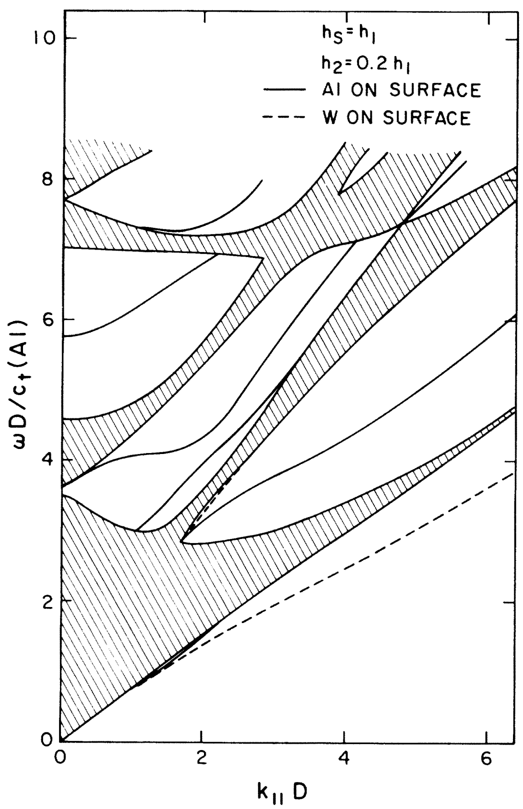

FIG. 3. Same as in Fig. 2 but with $d_{\mathrm{Al}}=5d_{\mathrm{W}}$.

at $k_{\parallel}=0$, in contrast to the other systems mentioned. As a matter of fact, there is a large ratio (about 5) between the parameters of Al and W which is not the case in other systems. Moreover, at an interface between two semi-infinite Al and W crystals there is a Stoneley (interface) wave; in a superlattice this gives rise, in the limit of thick layers, to bulk bands at the frequency of the Stoneley mode.

Let us first consider the band structure at $k_{\parallel}=0$. The sagittal modes are then decoupled into longitudinal and transverse modes, and the band structure is simply a superposition of the band structures for these two types of modes. The description of transverse waves in a superlattice, including surface waves, was given previously[11,12]; at $k_{\parallel}=0$ the same results also apply to waves of longitudinal polarization, if c_{44} is replaced by c_{11}. For example, let us recall[9,12] the well-known dispersion relation for the bulk (transverse or longitudinal) waves at $k_{\parallel}=0$,

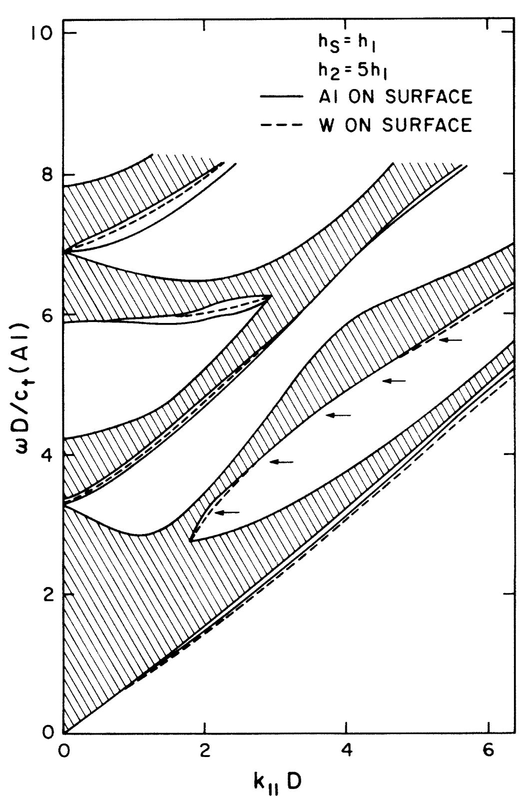

FIG. 4. Same as in Fig. 2 but with $d_{\mathrm{Al}}=0.2d_{\mathrm{W}}$.

$$\cos k_3 D = \cos\left[\frac{\omega d_1}{c}\right]\cos\left[\frac{\omega d_2}{c'}\right] - \frac{1}{2}\left[\frac{\rho c}{\rho' c'} + \frac{\rho' c'}{\rho c}\right]\sin\left[\frac{\omega d_1}{c}\right]\sin\left[\frac{\omega d_2}{c'}\right]. \tag{3.1}$$

In this equation c is the (transverse or longitudinal) velocity of sound in medium A; that is $c=(c_{44}/\rho)^{1/2}$ or $c=(c_{11}/\rho)^{1/2}$, and c' is the corresponding velocity in medium A'. From Eq. (3.1) it is apparent that the existence and the widths of the gaps are very dependent on the ratio $\rho c/\rho' c'$. Finally, we point out that infrared and Raman experiments can be sensitive to zero-wave-vector modes which correspond to the limits of the bulk bands in Figs. 2—4.

Besides the elastic properties of the two materials, a pertinent parameter in the description of the band structure is the relative thickness of the two media. This is illustrated in Figs. 2—4, where the ratio of the thickness of the Al layer to the thickness of the W layer is taken to be 1, 5, and 0.2, respectively. The bulk bands are represented by the shaded areas.

In Figs. 2—4 we have also presented the surface modes when an outermost layer of the superlattice is an Al layer or a W layer, but assuming the same thickness of the surface layer as in the bulk of the superlattice ($h_s = h$ in Fig. 1). In these figures some of the surface modes are very near to the bulk bands and cannot be distinguished from the latter on the scale of the figures.

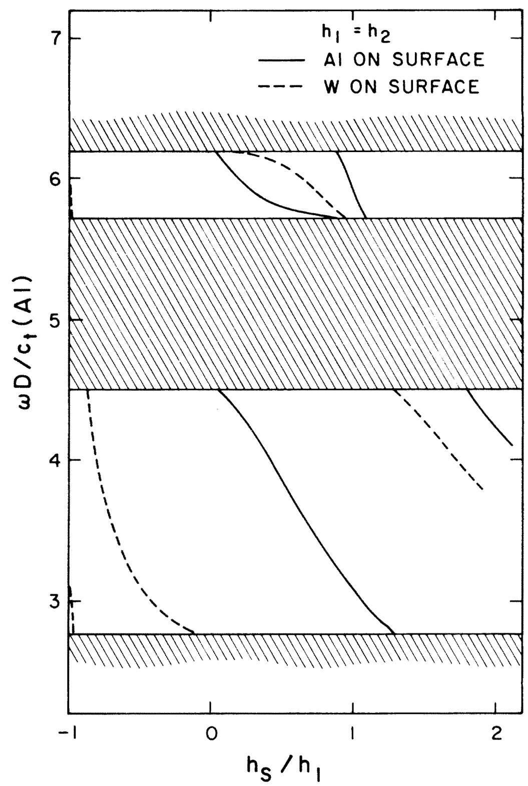

FIG. 6. Frequencies of surface waves, at $k_{\parallel}=0$ in an Al-W superlattice with $d=d'$, as functions of the surface-layer thickness. The figure is restricted to surface waves in the two lowest gaps. We present the surface modes for either an Al layer (solid line) or a W layer (dashed line) at the surface.

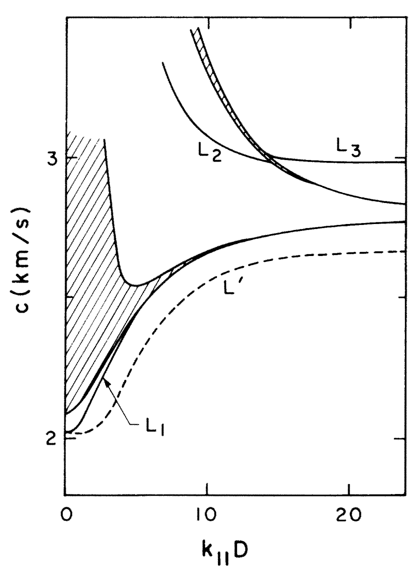

FIG. 5. Phase velocities of the few first surface modes of Fig. 2 for either an Al layer (solid line, L_1,L_2,L_3) or a W layer (dashed line, L') at the surface. The shaded areas are the first bulk bands. In the limit as $k_{\parallel}D \gg 1$: (i) These bulk bands approach the velocity of Stoneley waves at the interface between Al and W; (ii) for a W layer at the surface, the first Rayleigh mode L' goes into the Rayleigh wave on a W substrate; (iii) for an Al layer at the surface a higher surface mode L_3 goes into the Rayleigh wave on an Al substrate.

One particular surface wave is the Rayleigh wave situated below the bulk bands. When the surface layer is made of Al, this mode is near to the lowest bulk band and disappears at a certain value of $k_{\parallel}$; for a W surface layer, on the contrary, it is well separated from the bulk band. Let us also stress that at very long wavelength ($k_{\parallel}D \ll 1$) the superlattice can be described as an effective medium with hexagonal symmetry.[18] The velocity of the Rayleigh wave is then that of such a medium.[31]

In Fig. 5 we present for a superlattice with $h=h'=h_s$ the phase velocities $\omega/k_{\parallel}$ for the few first surface modes. If a W layer is at the surface, there is a Rayleigh wave L' below all bulk bands whose velocity in the limit $k_{\parallel}D \rightarrow \infty$ approaches the Rayleigh wave velocity of a W substrate. On the other hand, when an Al layer is at the surface, the Rayleigh wave L_1 below the bulk bands disappears at a certain value of $k_{\parallel}D$; however, for increasing $k_{\parallel}D$ the velocity of a higher surface mode L_3 approaches that of the Rayleigh wave on an Al substrate (about 3000 m/s). It is worthwhile to note that as $k_{\parallel}D \rightarrow \infty$ the velocities of the first bulk bands approach the velocity of the (interface) Stoneley wave, about 2800 m/s.

Finally, an important parameter for the existence of the surface modes is the thickness of the surface layer. This statement is illustrated in Fig. 6 where we display, at $k_{\parallel}=0$ and for a Al-W superlattice with $d=d'$, the velocities of the surface modes in the first two gaps (see Fig. 2) as functions of the surface-layer thickness. One can note that the experimental realization of different surface-layer thicknesses, either by molecular-beam epitaxy or by vapor deposition on a macroscopic scale, should be possible.

ACKNOWLEDGMENTS

The work of R.E.C. was supported by the U. S. Air Force Office of Scientific Research Grant No. F49620-78-C-0019. The work of A.A.M. was supported by the National Science Foundation Grant No. DMR 82-14214.

APPENDIX

The matrices $\underline{H}$ and $\underline{K}$ [Eqs. (2.10)] are given by

$$\underline{H}=\begin{bmatrix} U_l & U_t & -S_l & -S_t \\ -\dfrac{\alpha_l}{k_{\parallel}}S_l & -\dfrac{k_{\parallel}}{\alpha_t}S_t & \dfrac{\alpha_l}{k_{\parallel}}U_l & \dfrac{k_{\parallel}}{\alpha_t}U_t \\ 2\alpha_l c_{44}S_l & c_{44}\left[\alpha_t+\dfrac{k_{\parallel}^2}{\alpha_t}\right]S_t & -2c_{44}\alpha_l U_l & -c_{44}\left[\alpha_t+\dfrac{k_{\parallel}^2}{\alpha_t}\right]U_t \\ \left[c_{12}k_{\parallel}-c_{11}\dfrac{\alpha_l^2}{k_{\parallel}}\right]U_l & (c_{12}-c_{11})k_{\parallel}U_t & -\left[c_{12}k_{\parallel}-c_{11}\dfrac{\alpha_l^2}{k_{\parallel}}\right]S_l & -(c_{12}-c_{11})k_{\parallel}S_t \end{bmatrix}, \tag{A1}$$

$$\underline{K}=\begin{bmatrix} U_l & U_t & S_l & S_t \\ \dfrac{\alpha_l}{k_{\parallel}}S_l & \dfrac{k_{\parallel}}{\alpha_t}S_t & \dfrac{\alpha_l}{k_{\parallel}}U_l & \dfrac{k_{\parallel}}{\alpha_t}U_t \\ -2c_{44}\alpha_l S_l & -c_{44}\left[\alpha_t+\dfrac{k_{\parallel}^2}{\alpha_t}\right]S_t & -2c_{44}\alpha_l U_l & -c_{44}\left[\alpha_t+\dfrac{k_{\parallel}^2}{\alpha_t}\right]U_t \\ \left[c_{12}k_{\parallel}-c_{11}\dfrac{\alpha_l^2}{k_{\parallel}}\right]U_l & (c_{12}-c_{11})k_{\parallel}U_t & \left[c_{12}k_{\parallel}-c_{11}\dfrac{\alpha_l^2}{k_{\parallel}}\right]S_l & (c_{12}-c_{11})k_{\parallel}S_t \end{bmatrix}, \tag{A2}$$

where we have used the notations

$$S_{l,t}=\sinh(\alpha_{l,t}h),\quad U_{l,t}=\cosh(\alpha_{l,t}h)\ . \tag{A3}$$

We also introduce the notations

$$V_{l,t}=\sinh(2\alpha_{l,t}h),\quad W_{l,t}=\cosh(2\alpha_{l,t}h)\ , \tag{A4}$$

$$\gamma=\frac{c'_{44}}{c_{44}},\quad \nu=\frac{c_{44}}{c_{11}},\quad \nu'=\frac{c'_{44}}{c'_{11}},\quad \delta=\frac{c_{44}}{\rho}\frac{\rho'}{c'_{44}},\quad \xi=\frac{\rho\omega^2}{c_{44}k_{\parallel}^2}\ , \tag{A5}$$

and

$$z_1=\frac{1}{2\xi}[\gamma\delta\xi+2(1-\gamma)],\quad z_2=\frac{1-\gamma}{\xi},\quad z=\frac{2}{z_1-z_2}\ . \tag{A6}$$

From Eq. (2.12) one can obtain the elements T_{ij} of the $\underline{T}$ matrix. In what follows we present the elements $\tau_{ij}\equiv T_{ij}/z$:

$$\tau_{11}=W_l[W'_l z_1(\tfrac{1}{2}-z_2)-W'_t z_2(\tfrac{1}{2}-z_1)]+\frac{V_l}{2}\left[V'_l\left[z_1^2\frac{\alpha_l}{\alpha'_l}+(\tfrac{1}{2}-z_2)^2\frac{\alpha'_l}{\alpha_l}\right]-V'_t\left[z_2^2\frac{\alpha_l\alpha'_t}{k_{\parallel}^2}+(\tfrac{1}{2}-z_1)^2\frac{k_{\parallel}^2}{\alpha_l\alpha'_t}\right]\right]\ ,$$

$$\tau_{12}=\left[U_lU_tz_1z_2+S_lS_t(\tfrac{1}{2}-z_1)(\tfrac{1}{2}-z_2)\frac{k_{\parallel}^2}{\alpha_l\alpha_t}\right](-W'_l+W'_t)+U_lS_t\left[-V'_l z_1(\tfrac{1}{2}-z_1)\frac{k_{\parallel}^2}{\alpha'_l\alpha_t}+V'_t z_2(\tfrac{1}{2}-z_2)\frac{\alpha'_t}{\alpha_t}\right]$$
$$+S_lU_t\left[-V'_l z_2(\tfrac{1}{2}-z_2)\frac{\alpha'_l}{\alpha_l}+V'_t z_1(\tfrac{1}{2}-z_1)\frac{k_{\parallel}^2}{\alpha_l\alpha'_t}\right]\ ,$$

$$\tau_{13}=U_l^2\left[-V_l' z_1^2\frac{\alpha_l}{\alpha_l'}+V_t' z_2^2\frac{\alpha_l\alpha_t'}{k_{\parallel}^2}\right]+S_l^2\left[-V_l'(\tfrac{1}{2}-z_2)^2\frac{\alpha_l'}{\alpha_l}+V_t'(\tfrac{1}{2}-z_1)^2\frac{k_{\parallel}^2}{\alpha_l\alpha_t'}\right]$$
$$+V_l[-W_l' z_1(\tfrac{1}{2}-z_2)+W_t' z_2(\tfrac{1}{2}-z_1)]\;,$$

$$\tau_{14}=\left[U_lS_tz_1z_2+S_lU_t(\tfrac{1}{2}-z_1)(\tfrac{1}{2}-z_2)\frac{k_{\parallel}^2}{\alpha_l\alpha_t}\right](W_l'-W_t')+U_lU_t\left[V_l' z_1(\tfrac{1}{2}-z_1)\frac{k_{\parallel}^2}{\alpha_l'\alpha_t}-V_t' z_2(\tfrac{1}{2}-z_2)\frac{\alpha_t'}{\alpha_t}\right]$$
$$+S_lS_t\left[V_l' z_2(\tfrac{1}{2}-z_2)\frac{\alpha_l'}{\alpha_l}-V_t' z_1(\tfrac{1}{2}-z_1)\frac{k_{\parallel}^2}{\alpha_l\alpha_t'}\right]\;,$$

$$\tau_{21}=\left[U_lU_t(\tfrac{1}{2}-z_1)(\tfrac{1}{2}-z_2)+S_lS_tz_1z_2\frac{\alpha_l\alpha_t}{k_{\parallel}^2}\right](W_l'-W_t')+S_lU_t\left[V_l' z_1(\tfrac{1}{2}-z_1)\frac{\alpha_l}{\alpha_l'}-V_t' z_2(\tfrac{1}{2}-z_2)\frac{\alpha_l\alpha_t'}{k_{\parallel}^2}\right]$$
$$+U_lS_t\left[V_l' z_2(\tfrac{1}{2}-z_2)\frac{\alpha_l'\alpha_t}{k_{\parallel}^2}-V_t' z_1(\tfrac{1}{2}-z_1)\frac{\alpha_t}{\alpha_t'}\right]\;,$$

$$\tau_{22}=W_t[-W_l' z_2(\tfrac{1}{2}-z_1)+W_t' z_1(\tfrac{1}{2}-z_2)]$$
$$+\frac{V_t}{2}\left[-V_l'\left[\frac{k_{\parallel}^2}{\alpha_l'\alpha_t}(\tfrac{1}{2}-z_1)^2+z_2^2\frac{\alpha_l'\alpha_t}{k_{\parallel}^2}\right]+V_t'\left[(\tfrac{1}{2}-z_2)^2\frac{\alpha_t'}{\alpha_t}+z_1^2\frac{\alpha_t}{\alpha_t'}\right]\right]\;,$$

$$\tau_{23}=-\frac{\alpha_l\alpha_t}{k_{\parallel}^2}\tau_{14}\;,$$

$$\tau_{24}=U_t^2\left[V_l'(\tfrac{1}{2}-z_1)^2\frac{k_{\parallel}^2}{\alpha_l'\alpha_t}-V_t'(\tfrac{1}{2}-z_2)^2\frac{\alpha_t'}{\alpha_t}\right]+S_t^2\left[V_l' z_2^2\frac{\alpha_l'\alpha_t}{k_{\parallel}^2}-V_t' z_1^2\frac{\alpha_t}{\alpha_t'}\right]+V_t[W_l' z_2(\tfrac{1}{2}-z_1)-W_t' z_1(\tfrac{1}{2}-z_2)]\;,$$

$$\tau_{31}=U_l^2\left[-V_l'(\tfrac{1}{2}-z_2)^2\frac{\alpha_l'}{\alpha_l}+V_t'(\tfrac{1}{2}-z_1)^2\frac{k_{\parallel}^2}{\alpha_l\alpha_t'}\right]$$
$$+S_l^2\left[-V_l' z_1^2\frac{\alpha_l}{\alpha_l'}+V_t' z_2^2\frac{\alpha_l\alpha_t'}{k_{\parallel}^2}\right]+V_l[-W_l' z_1(\tfrac{1}{2}-z_2)+W_t' z_2(\tfrac{1}{2}-z_1)]\;,$$

$$\tau_{32}=U_lU_t\left[V_l' z_2(\tfrac{1}{2}-z_2)\frac{\alpha_l'}{\alpha_l}-V_t' z_1(\tfrac{1}{2}-z_1)\frac{k_{\parallel}^2}{\alpha_l\alpha_t'}\right]+S_lS_t\left[V_l' z_1(\tfrac{1}{2}-z_1)\frac{k_{\parallel}^2}{\alpha_l'\alpha_t}-V_t' z_2(\tfrac{1}{2}-z_2)\frac{\alpha_t'}{\alpha_t}\right]$$
$$+\left[S_lU_tz_1z_2+U_lS_t(\tfrac{1}{2}-z_1)(\tfrac{1}{2}-z_2)\frac{k_{\parallel}^2}{\alpha_l\alpha_t}\right](W_l'-W_t')\;,$$

$$\tau_{33}=\tau_{11}\;,$$

$$\tau_{34}=-\frac{k_{\parallel}^2}{\alpha_l\alpha_t}\tau_{21}\;,$$

$$\tau_{41}=-\frac{\alpha_l\alpha_t}{k_{\parallel}^2}\tau_{32}\;,$$

$$\tau_{42}=U_t^2\left[V_l' z_2^2\frac{\alpha_l'\alpha_t}{k_{\parallel}^2}-V_t' z_1^2\frac{\alpha_t}{\alpha_t'}\right]+S_t^2\left[V_l'(\tfrac{1}{2}-z_1)^2\frac{k_{\parallel}^2}{\alpha_l'\alpha_t}-V_t'(\tfrac{1}{2}-z_2)^2\frac{\alpha_t'}{\alpha_t}\right]$$
$$+V_t[W_l' z_2(\tfrac{1}{2}-z_1)-W_t' z_1(\tfrac{1}{2}-z_2)]\;,$$

$$\tau_{43}=-\frac{\alpha_l\alpha_t}{k_{\parallel}^2}\tau_{12}\;,$$

$$\tau_{44}=\tau_{22}\;.$$

By inverting the matrices $\underline{H}$ and $\underline{K}$ one easily sees that $\underline{H}^{-1}$ ($\underline{K}^{-1}$) can be deduced from $\underline{K}^{-1}$ ($\underline{H}^{-1}$) by changing the parameter h to $-h$. It follows from Eq. (2.12) that one can obtain $\underline{T}^{-1}$ from $\underline{T}$ by changing h and h' to $-h$ and $-h'$, respectively. This leaves all the hyperbolic cosines invariant but changes the signs of the hyperbolic sines. Thus, we obtain the result (2.22).

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