

Elastic surface waves in crystals with overlayers: Cubic symmetry

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We study the elastic surface waves of systems formed by semi-infinite cubic crystals with overlayers of cubic symmetry, having (001) free surfaces and interfaces, by using a Green's-function technique, for arbitrary thickness and direction of propagation. For the symmetry directions [100] and [110] in the limit of small thickness of the overlayers, it is possible to obtain the dispersion relation of Rayleigh and Love waves in closed form, to first order in $h\kappa$ (h is the thickness of the overlayer; κ is the parallel wave vector). An application is made to the system formed by a layer of $\text{Ga}_x\text{Al}_{1-x}\text{As}$ on a GaAs substrate, and the influence of the layer composition on the dispersion relation of the elastic surface waves is discussed.

I. INTRODUCTION

The systems formed by solid layers in close mechanical contact with a semi-infinite substrate, i.e., systems with several interfaces, pose interesting theoretical and practical problems. The overlayers are thin; usually their thickness is smaller than the wavelength of the surface wave being studied. Introduction of this layer on top of a former free surface induces dispersion in the wave so that the phase velocity now depends on the frequency.

The interest in surface waves has ranged from seismology¹ to ultrasonic signal processing devices,² with important applications to radar and communications,^{3,4} passing through surface flaw detection.⁵ It is interesting to note that the field of surface-wave devices has grown in sophistication and range, and many of these devices include a thin layer in at least part of the propagation path. These layers can be used for different purposes, such as to provide a desired dispersion characteristic,⁶ as part of transducers for generating surface waves,⁷ or as a guiding region to confine a surface wave laterally.⁸

For these systems it is common to have different independent modes of propagation confined to the surface region, some of which are perturbations of the free-surface Rayleigh waves, but we have also the Love modes which are very different in nature. The dispersion relation of the different modes has been usually obtained by solving the equations of motion jointly with the boundary conditions, for the elastic displacements.⁹ Recently, a method has been instituted and applied to isotropic¹⁰ and hexagonal¹¹ media, allowing us to study the theory of surface waves in systems with overlayers with more generality than has hitherto been possible. In this method the presence of an overlayer of small thickness h compared with the acoustic vibration wavelength λ has been shown to be equivalent to new effective boundary conditions at the surface, in a similar way to other approaches.^{12,13}

We shall consider systems with cubic symmetry due to the fact that this allows for the inclusion of the features of crystalline anisotropy (most of the surface-wave devices use single crystals), and many of the substances of practical interest crystallize in the cubic system. We shall study systems having (001) free surfaces and interfaces in order to avoid too much complication in the calculations, but the same method can be used for any surface orientation or propagation direction. In the limit of small thickness for symmetry directions the dispersion relation of the surface acoustic waves is derived in closed form to first order in $h\kappa$. Experimentally,¹⁴ the frequency variation of the Rayleigh wave appears to be detectable even for a surface coverage of a few hundredths of an adsorbed monolayer. This, together with our analytic expressions, could provide a means of determining the elastic constants of very thin films.

We use a Green's-function method to obtain the frequencies of the system, in spite of its greater complexity as compared with the usual approach,⁹ because this method makes possible the calculation of other properties of such systems, such as, for instance, the mean-square displacements of atoms^{10,15} or the elastic energy of point defects.^{16,17}

For the study of the dispersion relation of anisotropic film/substrate systems this method would constitute merely an alternative to the standard eigenvalue calculations based on a study of the eigenfunctions.^{9,18–20} However, an analysis yielding the Green's function of the system provides a more direct inroad into the calculation of spectral functions—e.g., the projected mode density—of interest for scattering problems.²¹

In Sec. II we present the Green's-function calculation which yields the eigenmodes of the system; for very thin layers, the effective boundary conditions at the surface are derived. In Sec. III we consider the thin overlayers ($h\kappa \ll 1$), giving the dispersion relation of the modes in

closed form for symmetry directions. In Sec. IV an application is done to the system formed by an overlayer of arbitrary thickness of $\text{Ga}_x\text{Al}_{1-x}\text{As}$ on a GaAs substrate for an arbitrary propagation direction, and the possibility of obtaining the elastic constants of the layer is discussed. Finally conclusions are drawn in Sec. V.

II. GREEN'S FUNCTION FOR A CUBIC OVERLAYER SYSTEM

We shall be concerned with a system formed by a semi-infinite cubic substrate (with elastic constants C_{11} , C_{12} , C_{44} , and density ρ) covered by a cubic overlayer (with elastic constants C'_{11} , C'_{12} , C'_{44} , and density ρ') of thickness h . We take x_3 as the direction perpendicular to both the free surface and the substrate-overlayer interface, and we consider $x_3=0$ and $-h$ as the plane of the interface and that of the free surface, respectively. All the surfaces and interfaces are supposed to be (001).

The eigenmodes of the system are obtained from the poles of the Green's function, which are calculated as usual by solving the equations of motion inside the bulk of each medium together with the boundary conditions at the interface and at the free surface, namely the continui-

ty of the displacements and of the stresses: For an arbitrary thickness and arbitrary direction of propagation, the eigenmodes are obtained from the zeros of a 9×9 determinant. For the symmetry directions [100] and [110] this determinant factorizes into a 6×6 determinant for the sagittal modes and a 3×3 determinant for the transverse (Love) modes. For a very thin layer a simplification is possible by developing the boundary conditions (2.2) in powers of $h\kappa$, and then relating the conditions at $x_3=0$ and at $-h$, as explained elsewhere.¹⁰ In this way for an arbitrary direction of propagation the eigenmodes can be obtained from the zeros of a 3×3 determinant, whereas in the symmetry directions this determinant is factorized into a 2×2 determinant for the sagittal modes and a 1×1 determinant for the transverse modes. This enables us to obtain the dispersion relations of the Rayleigh and Love waves in closed form,³ to first order in $h\kappa$.

The method has been fully explained elsewhere^{10,11} so we shall give here the final expressions for systems of cubic symmetry only. The similarity transformation introduced in²² in order to make the direction of propagation coincide with the x_1 axis of the crystal has been employed. We shall study now the different possible cases, i.e., (i) arbitrary propagation direction, (ii) [100] direction, and (iii) [110] direction.

A. Arbitrary propagation direction

Following the method described in Ref. 10 we obtain the effective boundary conditions for the substrate

$$C_{44} \left[\frac{\partial}{\partial x_3} G_{1j}(x_3, x'_3) + i\kappa G_{3j}(x_3, x'_3) \right]_{x_3=+0} = hC'_{44} \left[\left[\kappa^2 [\lambda'^2 - (\frac{d'}{2}) \sin^2 2\theta] - \frac{\omega^2}{C_t'^2} \right] G_{1j}(x_3, x'_3) - d' \tau \kappa^2 G_{2j}(x_3, x'_3) - \frac{(\lambda'^2 - 2 - d')^2}{\lambda'^2} \kappa^2 G_{1j}(x_3, x'_3) - \frac{i\kappa(\lambda'^2 - 2 - d')}{\lambda'^2} \frac{C_{44}}{C'_{44}} \left[i\kappa(\lambda^2 - 2 - d) G_{1j}(x_3, x'_3) + \lambda^2 \frac{\partial}{\partial x_3} G_{3j}(x_3, x'_3) \right] \right]_{x_3=+0}, \quad (2.1a)$$

$$C_{44} \left[\frac{\partial}{\partial x_3} G_{2j}(x_3, x'_3) \right]_{x_3=+0} = hC'_{44} \left[\left[\kappa^2 \left[1 + \frac{d'}{2} \sin^2 2\theta \right] - \frac{\omega^2}{C_t'^2} \right] G_{2j}(x_3, x'_3) - d' \tau \kappa^2 G_{2j}(x_3, x'_3) \right]_{x_3=+0}, \quad (2.1b)$$

$$C_{44} \left[i\kappa(\lambda^2 - 2 - d) G_{1j}(x_3, x'_3) + \lambda^2 \frac{\partial}{\partial x_3} G_{3j}(x_3, x'_3) \right]_{x_3=+0} = hC'_{44} \left[-\frac{\omega^2}{C_t'^2} G_{3j}(x_3, x'_3) - i\kappa \frac{C_{44}}{C'_{44}} \left[\frac{\partial}{\partial x_3} G_{1j}(x_3, x'_3) + i\kappa G_{3j}(x_3, x'_3) \right] \right]_{x_3=+0}, \quad (2.1c)$$

where

$$\lambda^2 = C_{11}/C_{44}, \quad d = (C_{11} - C_{12} - 2C_{44})/C_{44} = D/C_{44},$$

$$C_t^2 = C_{44}/\rho, \quad \tau = -\sin 4\theta/4,$$

and θ is the angle between the direction of propagation and the x_1 axis.

B. [100] direction

We shall consider the boundary conditions for G_{11} and G_{31} [similar equations are obtained for G_{13} and G_{33} (Refs. 10 and 11)] and then for G_{22} . Following the steps given in Ref. 10 we obtain the effective boundary conditions for the substrate

$$C_{44} \left[\frac{\partial}{\partial x_3} G_{11}(x_3, x'_3) + i\kappa G_{31}(x_3, x'_3) \right]_{x_3=+0} = hC'_{44} \left[\left[\lambda'^2 \kappa^2 - \frac{\omega^2}{C_t'^2} \right] G_{11}(x_3, x'_3) - \frac{(\lambda'^2 - 2 - d')^2}{\lambda'^2} \kappa^2 G_{11}(x_3, x'_3) - i\kappa \frac{(\lambda'^2 - 2 - d')}{\lambda'^2} \frac{C_{44}}{C'_{44}} [i\kappa(\lambda^2 - 2 - d)G_{11}(x_3, x'_3) + \lambda^2 \frac{\partial}{\partial x_3} G_{31}(x_3, x'_3)] \right]_{x_3=+0}, \quad (2.2a)$$

$$C_{44} \left[i\kappa(\lambda^2 - 2 - d)G_{11}(x_3, x'_3) + \lambda^2 \frac{\partial}{\partial x_3} G_{31}(x_3, x'_3) \right]_{x_3=+0} = hC'_{44} \left[-\frac{\omega^2}{C_t'^2} G_{31}(x_3, x'_3) - i\kappa \frac{C_{44}}{C'_{44}} \left[\frac{\partial}{\partial x_3} G_{11}(x_3, x'_3) + i\kappa G_{31}(x_3, x'_3) \right] \right]_{x_3=+0}. \quad (2.2b)$$

In the same way we obtain for the transverse modes

$$C_{44} \left[\frac{\partial}{\partial x_3} G_{22}(x_3, x'_3) \right]_{x_3=+0} = h[(C'_{44}\kappa^2 - \rho'/\omega^2)G_{22}(x_3, x'_3)]_{x_3=+0}. \quad (2.2c)$$

The solutions to be used for the Green's function can be written as

$$G_{11}(x_3, x'_3) = G_{11}^{(\infty)}(x_3, x'_3) + A \exp(-\beta_1 x_3) + B \exp(-\beta_2 x_3), \quad (2.3a)$$

$$G_{31}(x_3, x'_3) = G_{31}^{(\infty)}(x_3, x'_3) - \frac{i}{(\lambda^2 - 1 - d)\kappa} \times \left[\frac{\beta_1^2 + \gamma_1^2}{\beta_1} A \exp(-\beta_1 x_3) + \frac{\beta_2^2 + \gamma_1^2}{\beta_2} B \exp(-\beta_2 x_3) \right], \quad (2.3b)$$

with similar solutions for G_{13} and G_{33} , and

$$G_{22}(x_3, x'_3) = G_{22}^{(\infty)}(x_3, x'_3) + C \exp(-\beta_t x_3). \quad (2.3c)$$

In these equations $G^{(\infty)}$ is the bulk Green's function of the substrate.²³ We have

$$\begin{aligned} \beta_t^2 &= \kappa^2 - \frac{\omega^2}{C_t^2}, \\ \beta_1^2 &= \frac{1}{2} [x + (x^2 - 4y^2)^{1/2}], \\ \beta_2^2 &= \frac{1}{2} [x - (x^2 - 4y^2)^{1/2}], \end{aligned} \quad (2.4)$$

where

$$\begin{aligned} x &= -(\gamma_1^2 + \gamma_4^2) - \frac{(C_{12} + C_{44})^2}{C_{11}C_{44}} \kappa^2, \\ y^2 &= \gamma_1^2 \gamma_4^2, \end{aligned} \quad (2.5)$$

with

$$\gamma_1^2 = \frac{(\rho\omega^2 - C_{11}\kappa^2)}{C_{44}}, \quad \gamma_4^2 = \frac{(\rho\omega^2 - C_{44}\kappa^2)}{C_{11}}. \quad (2.6)$$

Substituting the solutions (2.3) into the effective boundary conditions (2.2), we obtain the full Green's function, for this case, the poles of which are the eigenmodes of the system. These modes are then solutions of a 2×2 determinant for the sagittal polarization and of a 1×1 determinant for the transverse polarization. It can be seen that all the expressions obtained here are the same as those for hexagonal crystals¹¹ provided we make the following changes:

$$C_{13} \rightarrow C_{12}, \quad C_{33} \rightarrow C_{11}$$

for the sagittal mode and

$$\frac{C_{11} - C_{12}}{2} \rightarrow C_{44}$$

for the transverse modes.

C. [110] direction

Following the method given in Ref. 10, we obtain the effective boundary conditions for the substrate

$$\begin{aligned}
C_{44} \left[\frac{\partial}{\partial x_3} G_{11}(x_3, x'_3) + i\kappa G_{31}(x_3, x'_3) \right]_{x_3=+0} \\
= hC'_{44} \left\{ \left[\kappa^2 \left[\lambda'^2 - \frac{d'}{2} \right] - \frac{\omega^2}{C_t'^2} \right] G_{11}(x_3, x'_3) - \frac{(\lambda'^2 - 2 - d')^2}{\lambda'^2} \kappa^2 G_{11}(x_3, x'_3) \right. \\
\left. - i\kappa \frac{(\lambda'^2 - 2 - d')}{\lambda'^2} \frac{C_{44}}{C'_{44}} \left[i\kappa(\lambda^2 - 2 - d)G_{11}(x_3, x'_3) + \lambda^2 \frac{\partial}{\partial x_3} G_{31}(x_3, x'_3) \right] \right\}_{x_3=+0}, \quad (2.7a)
\end{aligned}$$

$$\begin{aligned}
C_{44} \left[i\kappa(\lambda^2 - 2 - d)G_{11}(x_3, x'_3) + \lambda^2 \frac{\partial}{\partial x_3} G_{31}(x_3, x'_3) \right]_{x_3=+0} \\
= hC'_{44} \left[-\frac{\omega^2}{C_t'^2} G_{31}(x_3, x'_3) - i\kappa \frac{C_{44}}{C'_{44}} \left[\frac{\partial}{\partial x_3} G_{11}(x_3, x'_3) + i\kappa G_{31}(x_3, x'_3) \right] \right]_{x_3=+0}. \quad (2.7b)
\end{aligned}$$

In the same way we obtain for the transverse modes

$$\begin{aligned}
C_{44} \left[\frac{\partial}{\partial x_3} G_{22}(x_3, x'_3) \right]_{x_3=+0} \\
= hC'_{44} \left\{ \left[\kappa^2 \left[1 + \frac{d'}{2} \right] - \frac{\omega^2}{C_t'^2} \right] G_{22}(x_3, x'_3) \right\}_{x_3=+0}. \quad (2.7c)
\end{aligned}$$

The solutions to be used for the Green's function are written in the same form as (2.3) but now

$$\beta_t^2 = \kappa^2 \left[1 + \frac{d}{2} \right] - \frac{\omega^2}{C_t^2}, \quad (2.8a)$$

$$\begin{aligned}
\gamma_1^2 &= \left[\rho\omega^2 - \left[\frac{C_{11} + C_{12} + 2C_{44}}{2} \right] \kappa^2 \right] / C_{44}, \\
\gamma_4^2 &= (\rho\omega^2 - C_{44}\kappa^2) / C_{11}. \quad (2.8b)
\end{aligned}$$

We can obtain the eigenmodes of the system from the expressions for the hexagonal crystals¹¹ if we make the following changes:

$$C_{13} \rightarrow C_{12}, \quad C_{33} \rightarrow C_{11}, \quad C_{11} \rightarrow \frac{C_{11} + C_{12} + 2C_{44}}{2}$$

for the sagittal modes. For the transverse modes no change is needed.

III. DISPERSION OF THE ACOUSTIC SURFACE WAVES: THIN OVERLAYER LIMIT

We shall present in this section the analytic form of the dispersion relation for surface waves in symmetry directions and a brief discussion of the dispersion relation for arbitrary direction of propagation.

A. [100] direction

Sagittal modes. The dispersion relation, to first order in $h\kappa$, is given by

$$\omega^2 = C_R^2 \kappa^2 (1 - Ah\kappa) + O(h), \quad (3.1)$$

where C_R is the velocity of the usual Rayleigh wave²⁴ and $A = N/D$, where N and D are the same expressions as those given in Ref. 11 by substituting $C_{13} \rightarrow C_{12}$, $C_{33} \rightarrow C_{11}$.

Love modes. Under the condition $C_t' < C_t$, we have the following dispersion relation:

$$\omega^2 = C_t'^2 \kappa^2 [1 - B(h\kappa)^2] + O(h^2) \quad (3.2)$$

with

$$B = \left(\frac{C'_{44}}{C_{44}} - \frac{\rho'}{\rho} \right)^2.$$

This expression is identical with that for an isotropic crystal.¹⁰

B. [110] direction

Sagittal modes. The dispersion relation, to first order in $h\kappa$, is identical with (3.1) where N and D are now the same expressions as those given in Ref. 11 provided we make the substitution $C_{33} \rightarrow C_{11}$, $C_{11} \rightarrow (C_{11} + C_{12} + 2C_{44})/2$, $C_{13} \rightarrow C_{12}$.

Love modes. Under the condition $C_t' < C_t$, we obtain for the dispersion relation the expression (3.2) where

$$\begin{aligned}
B &= \frac{C_{11} - C_{12}}{2C_{44}} \left[\frac{C'_{11} - C'_{12}}{C_{11} - C_{12}} - \frac{\rho'}{\rho} \right]^2, \\
C_t'^2 &= \frac{C_{11} - C_{12}}{2\rho}, \quad C_t'^2 = \frac{C'_{11} - C'_{12}}{2\rho'}. \quad (3.3)
\end{aligned}$$

This expression is identical with that obtained for hexagonal crystals.¹¹

C. Arbitrary propagation direction

In this case we do not have a factorization into sagittal and transverse modes, but a mode with a mixture of all the polarizations. The dispersion relation can be obtained from the effective boundary conditions by substituting the Green's function in the form ($j=1,2,3$)

$$G_{1j}(x_3, x'_3) = G_{1j}^\infty(x_3, x'_3) + \sum_{l=1}^3 A_{jl} e^{-\beta_l x_3}, \quad (3.4a)$$

$$G_{2j}(x_3, x'_3) = G_{2j}^\infty(x_3, x'_3) + \sum_{l=1}^3 B_{jl} e^{-\beta_l x_3}, \quad (3.4b)$$

$$G_{3j}(x_3, x'_3) = G_{3j}^\infty(x_3, x'_3) + \sum_{l=1}^3 C_{jl} e^{-\beta_l x_3}, \quad (3.4c)$$

where the β_l are the solutions of

$$\beta^6 + \beta^4 \left[\Gamma_0^2 + \Gamma_1^2 + \Gamma_4^2 + \frac{(C_{12} + C_{44})^2}{C_{11} C_{44}} \kappa^2 \right] + \beta^2 \left[(\Gamma_0^2 + \Gamma_1^2) \Gamma_4^2 + \Gamma_0^2 \Gamma_1^2 + \Gamma_0^2 \frac{(C_{12} + C_{44})^2}{C_{11} C_{44}} \kappa^2 - \frac{D^2 \sin^2 4\theta}{16 C_{44}^2} \kappa^4 \right] + \Gamma_0^2 \Gamma_1^2 \Gamma_4^2 - \frac{D^2 \sin^2 4\theta}{16 C_{44}^2} \Gamma_4^2 \kappa^4 = 0 \quad (3.5)$$

(provided that $\text{Re}\beta_j > 0$). With

$$\begin{aligned} \Gamma_0^2 &= \frac{\rho\omega^2}{C_{44}} - \kappa^2 \left[1 + \frac{D}{2C_{44}} \right] \sin^2 2\theta, \\ \Gamma_1^2 &= \frac{\rho\omega^2}{C_{44}} - \kappa^2 \left[\frac{C_{11} - D \sin^2 2\theta / 2}{C_{44}} \right], \\ \Gamma_4^2 &= \frac{\rho\omega^2 - C_{44} \kappa^2}{C_{11}}. \end{aligned} \quad (3.6)$$

Thus the dispersion relation is given by

$$\begin{vmatrix} \Delta_{11} & \Delta_{12} & \Delta_{13} \\ \Delta_{21} & \Delta_{22} & \Delta_{23} \\ \Delta_{31} & \Delta_{32} & \Delta_{33} \end{vmatrix} = 0, \quad (3.7)$$

where ($j=1,2,3$)

$$\Delta_{1j} = \Delta_{1j}^{(0)} - h(\Delta_{1j}^{(a)} + \Delta_{1j}^{(b)}), \quad (3.8a)$$

$$\Delta_{2j} = \Delta_{2j}^{(0)} - h(\Delta_{2j}^{(a)} + \Delta_{2j}^{(b)}), \quad (3.8b)$$

$$\Delta_{3j} = \Delta_{3j}^{(0)} - h(\Delta_{3j}^{(a)} + \Delta_{3j}^{(b)}), \quad (3.8c)$$

with

$$\begin{aligned} \Delta_{ij}^{(0)} &= C_{44} \left[-\beta_j - \frac{(C_{12} + C_{44})}{C_{11}} \frac{\beta_j \kappa^2}{(\beta_j^2 + \Gamma_4^2)} \right], \\ \Delta_{ij}^{(a)} &= \left[C'_{44} \Gamma_1'^2 - \frac{C'_{12}{}^2}{C'_{11}} \kappa^2 \right] - \rho' \omega^2, \\ \Delta_{ij}^{(b)} &= \frac{C'_{12}}{C'_{11}} \kappa^2 \left[\frac{C_{12} C_{44}}{C'_{44}} - \frac{(C_{12} + C_{44}) \beta_j^2}{(\beta_j^2 + \Gamma_4^2)} \right] \\ &\quad + \frac{DD'}{16 C_{44}} \frac{\sin^2 4\theta}{(\beta_j^2 + \Gamma_0^2)} \kappa^4, \end{aligned} \quad (3.9)$$

$$\begin{aligned} \Delta_{2j}^{(0)} &= -\frac{D \sin 4\theta}{4} \frac{\beta_j \kappa^2}{\beta_j^2 + \Gamma_0^2}, \\ \Delta_{2j}^{(a)} &= \frac{C'_{44}}{C_{44}} \frac{D \sin 4\theta \Gamma_0'^2 \kappa^2}{4 \beta_j^2 + \Gamma_0^2}, \\ \Delta_{2j}^{(b)} &= \frac{D' \sin 4\theta}{4} \kappa^2, \end{aligned} \quad (3.10)$$

$$\begin{aligned} \Delta_{3j}^{(0)} &= \left[C_{12} - (C_{12} + C_{44}) \frac{\beta_j^2}{\beta_j^2 + \Gamma_4^2} \right], \\ \Delta_{3j}^{(a)} &= -\rho' \omega^2 \frac{(C_{12} + C_{44})}{C_{11}} \frac{\beta_j}{\beta_j^2 + \Gamma_4^2}, \end{aligned} \quad (3.11)$$

$$\Delta_{3j}^{(b)} = C_{44} \left[1 + \frac{(C_{12} + C_{44})}{C_{11}} \frac{\kappa^2}{\beta_j^2 + \Gamma_4^2} \right] \beta_j.$$

Now it is not possible to obtain a dispersion relation in closed form due to the complexity of the expressions involved, and the secular determinant (3.7) must be solved numerically.

These expressions can be used, instead of the 9×9 determinant derived from the exact boundary conditions, for the case $h\kappa \ll 1$, because they give fairly accurate results as compared with the exact dispersion relations, with less numerical computation. With these analytical dispersion relations for symmetry directions and the experimental methods capable of detecting frequency variations of the Rayleigh wave even for thin overlayers,¹⁴ one could have a way of determining the elastic constants of these overlayers. We have checked the analytical equations [(3.1)–(3.3)] against the dispersion relations obtained from the exact boundary conditions for several systems, and different values of $h\kappa$ up to $h\kappa=0.01$, and the discrepancies between the simplified expressions for the phase velocities and those obtained from the complete system of equations amounted at most to 0.02 m/s, for the crystals considered. Thus we can conclude that these simplified expressions are reliable as compared to heavier calculations.

IV. $\text{Ga}_x\text{Al}_{1-x}\text{As}$ LAYER ON GaAs SUBSTRATE

In order to obtain the dispersion relations of the different modes appearing by increasing the thickness of the overlayer, we must solve numerically the determinants quoted in Sec. II. As before, for symmetry directions there is a factorization into the sagittal and transverse polarized modes, whereas for arbitrary direction of propagation the uncoupling of the modes does not exist. For symmetry directions it can be shown that the secular determinants are identical with those valid for the hexagonal crystals,¹¹ by making the changes stated in Sec. II. A comprehensive study of the elastic waves in anisotropic film/substrate systems is given in Ref. 9. A brief study of the Al-W system with our method was given elsewhere.²⁵

The Brillouin spectroscopy has been shown to be an excellent technique in which one may obtain the dispersion relation of elastic surface waves for semi-infinite²⁶ and layer/substrate systems.²⁷ Recently, this technique has been applied to the study of surface acoustic waves in superlattices.²⁸ These systems are interesting due to their possible application to microwave electronics and the fabrication of emitting laser diodes. As these structures are produced in the form of thin films, it would be interesting to know the elastic properties of the layer. The present analysis could provide some useful clues if used jointly with experimental evidence, unfortunately not yet available.

We shall consider a $\text{Ga}_x\text{Al}_{1-x}\text{As}$ layer on a GaAs substrate due to the fact that the GaAs-AlAs superlattices and related alloys are among the best studied of these systems, and experimental Brillouin scattering investigations on these materials are in progress.²⁹

The GaAs exhibits pseudo surface waves (PSW's)³⁰ for directions $30^\circ \cong \theta < 45^\circ$. For these directions these modes are the dominant ones. It can be seen that they are very sharp resonances.^{30,31}

Let us assume as a starting point that the elastic constants of the layer are the same as those of the GaAs ($C_{11}=118 \times 10^{10}$ N/m², $C_{12}=53.5 \times 10^{10}$ N/m², $C_{44}=59.4 \times 10^{10}$ N/m², and $\rho=5317$ kg/m³), whereas

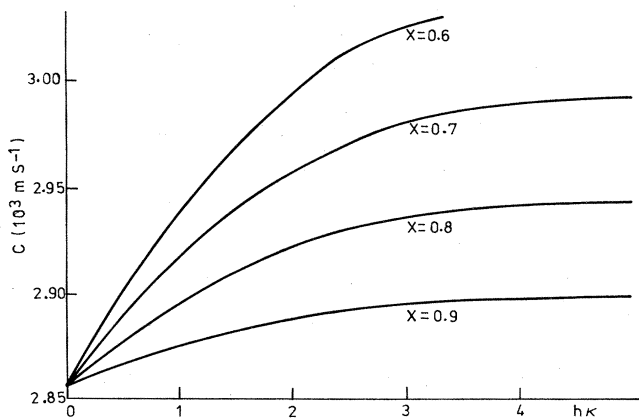


FIG. 1. Dispersion curves for the Rayleigh waves of GaAs/ $\text{Ga}_x\text{Al}_{1-x}\text{As}$ system in the [110] direction for several values of x .

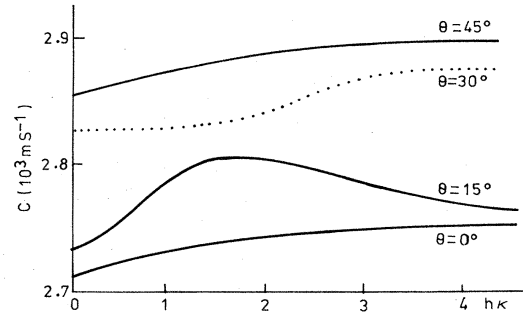


FIG. 2. Dispersion curves for the surface waves of the same system for $x=0.9$ and several directions of propagation. The curves for $\theta=0^\circ$ and 45° correspond to true Rayleigh waves sagittally polarized; for $\theta=15^\circ$ it corresponds to a true surface wave and for $\theta=30^\circ$ it corresponds to a pseudo surface wave.

the density is a function of x (we take the following atomic masses: $M_{\text{Ga}}=70$, $M_{\text{As}}=75$, $M_{\text{Al}}=27$).

The behavior of this system corresponds to those presented in Ref. 9. Thus, for a given direction of propagation, the first Rayleigh mode starts from $C_R(\theta)$ [or $C_{\text{PSW}}(\theta)$] at $h\kappa=0$, going to $C'_R(\theta)$ [or $C'_{\text{PSW}}(\theta)$] for $h\kappa \rightarrow \infty$. It will be a true surface mode or pseudo surface mode depending on its position below or above the bulk minimum velocity $C_b(\theta)$.⁹ In Fig. 1 we give an illustration of this for the [110] direction and different values of x . In Fig. 2 we present the dispersion relation of the surface modes of this system for different directions of propagation and $x=0.9$ (in this case $\rho'=5160$ kg/m³). In Fig. 3(a) we present these same dispersion relations considering that $C'_{ij}=0.95C_{ij}$, $x=0.9$, whereas in Fig. 3(b) we take $1.05C_{ij}$, $x=0.9$ ($ij=11,12,44$). Thus it can be seen that a

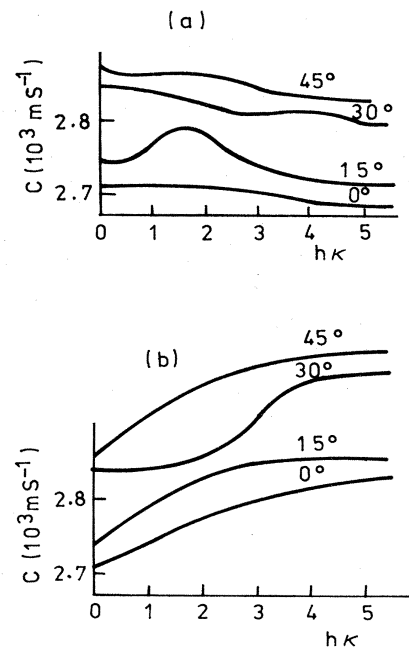


FIG. 3. (a) Dispersion curves for the surface waves of the $\text{Ga}_x\text{Al}_{1-x}\text{As}$ system for several directions of propagation with $x=0.9$ and $C'_{ij}=0.95C_{ij}$. (b) Same as before but with $C'_{ij}=1.05C_{ij}$.

5% variation of the elastic constants of the layer changes drastically the dispersion relation of the surface modes, and this could be tested experimentally. This could be detected with the experimental methods now available.^{14,26-29}

If accurate measurements for the dispersion relations in the thin layer limit were available, it would be possible to use the simplified forms [(3.1)–(3.3)] in order to obtain the elastic constants of the layer. But even in the absence of these measurements we should be able to ascertain whether $C'_{ij} < C_{ij}$ or $C'_{ij} > C_{ij}$ by comparison of experimental dispersion relations for different values of $h\kappa$ with those of Fig. 3.

V. CONCLUSIONS

In the thin-layer limit ($h\kappa \ll 1$) it is possible to obtain in closed form, to first order in $h\kappa$, the dispersion relation

of acoustic surface waves propagating along symmetry directions in a cubic crystal with a cubic overlayer. These expressions could provide a means to obtain the elastic constants of thin overlayers. We have made an application to the GaAs/Ga_xAl_{1-x}As systems and showed that small changes in the elastic constants of the layer induce important changes in the dispersion relation of the surface modes, thus making possible the determination of the elastic constants of the layer.

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