

Dynamics of systems with two interfaces

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Systems with two interfaces (sandwich ABC , planar defect, film) are considered. A symmetrization scheme is used to obtain the symmetrical (S) and antisymmetrical (A) modes of the planar defect and the thin film for arbitrary thickness. When medium B is very thin ($hk_{\parallel} \ll 1$), we obtain the eigenmodes of the planar defect in analytical form, clarifying some discrepancies previously existing in the study of such a system. The interaction energy of point defects is obtained in closed form. The particular case of two adatoms is considered.

I. INTRODUCTION

Interface waves¹⁻⁶ are of great interest from an experimental and theoretical point of view. Systems with several interfaces introduce interesting theoretical problems⁷ and must be studied with sophisticated experimental techniques.^{6,8,9} The surface wave spectrum can differ significantly from that of a single surface and its study is not trivial.

A sandwich $A-B-C$ (the particular case $A-B-A$ is called the planar defect) can be used to guide elastic surface waves in an analogous way to the case of systems with overlayers.¹⁰ If the thickness of medium B is arbitrary the problem is very complicated and the equations must be solved numerically.¹¹⁻¹³ The purpose of this paper is to present an alternative approach which can reduce the computational work considerably.

The planar defect has been studied both in elasticity theory^{14,15} and lattice dynamics¹⁶ with differing results. For example, an equivalent membrane model¹⁵ does not yield a localized sagittal mode for the planar defect in contrast to the results of references.^{14,16} This appeared as a surprise, as the models used in Refs. 14 and 15 were thought to be the same. We shall show that the case considered in Ref. 14 is different from the equivalent membrane model, and that both can be obtained as particular cases of the more general result obtained here.

The key feature of the planar defect case is that it has mirror symmetry ($A-B-A$). This allows us to

use a symmetrization scheme which yields the symmetric and antisymmetric eigenmodes for the arbitrary thickness, h , of medium B . This is not possible for the unsymmetric case ($A-B-C$), but then the problem can be fairly simplified for $hk_{\parallel} \ll 1$, a condition often met in practice. Both these cases are studied in Sec. II. The eigenmodes are obtained from the poles of the Green's function of the system and this is constructed using an approach recently developed.¹¹⁻¹³ In Sec. III we consider the problem of the thin film in which we use symmetrical and antisymmetrical Green's functions in order to simplify the problem. We discuss there the elastic waves of such a system and also the elastic energy of interaction of defects. This has been discussed previously for surfaces,¹⁷ interfaces¹⁸ and systems with overlayers,¹² and is treated here for the first time for the thin film. The conclusions are discussed in Sec. IV.

II. ELASTIC WAVES
IN A SANDWICH $A-B-C$

The three media A , B , and C are assumed to be isotropic, with the following elastic constants and densities: C_{11}, C_{44}, ρ (for A), C'_{11}, C'_{44}, ρ' (for B), and $C''_{11}, C''_{44}, \rho''$ (for C). For each medium we also have sound velocities $C_t = (C_{44}/\rho)^{1/2}$, $C_l = (C_{11}/\rho)^{1/2}$ (for A), etc. The eigenmodes of the sandwich can be obtained from the poles of the Green's function of the system.

For isotropic media, as is well known, there is a factorization in modes polarized in the sagittal plane ($x_3, k_{||}$) and those polarized perpendicularly to this plane (direction x_2), if we take $k_{||}$ along x_1). As a result, the sagittal $\{A-B-C\}$ localized

eigenmodes are the roots of an (8×8) determinant, instead of a (4×4) determinant as for a plane interface AB (it is this that in general requires numerical solution).

Let us now study first the symmetric case.

A. Planar defect (A-B-A)

In this case it proves convenient to define $x_3=0$ as the mirror symmetry plane bisecting medium B . The two interfaces are at $x_3 = \pm h/2$ and we define the symmetrical (S) and antisymmetrical (A) states in the following form:

$$|S\rangle \equiv \left[\frac{|x_3,1\rangle + |-x_3,1\rangle}{\sqrt{2}}, \frac{|x_3,2\rangle + |-x_3,2\rangle}{\sqrt{2}}, \frac{|x_3,3\rangle - |-x_3,3\rangle}{\sqrt{2}} \right], \quad (2.1a)$$

$$|A\rangle \equiv \left[\frac{|x_3,1\rangle - |-x_3,1\rangle}{\sqrt{2}}, \frac{|x_3,2\rangle - |-x_3,2\rangle}{\sqrt{2}}, \frac{|x_3,3\rangle + |-x_3,3\rangle}{\sqrt{2}} \right], \quad (2.1b)$$

where 1, 2, and 3 stand for the Cartesian direction indices ($1 \equiv x$, etc.) and x_3 for the coordinate normal to the surface of a point of the system. In this way it is easy to show that for $x_3 > 0$,

$$G_{11}^{S,A}(x_3, x'_3) = G_{11}(x_3, x'_3) \pm G_{11}(-x_3, x'_3), \quad (2.2a)$$

$$G_{31}^{S,A}(x_3, x'_3) = G_{31}(x_3, x'_3) \mp G_{31}(-x_3, x'_3), \quad (2.2b)$$

$$G_{22}^{S,A}(x_3, x'_3) = G_{22}(x_3, x'_3) \pm G_{22}(-x_3, x'_3), \quad (2.2c)$$

$$G_{13}^{S,A}(x_3, x'_3) = G_{13}(x_3, x'_3) \pm G_{13}(-x_3, x'_3); \quad (2.2d)$$

$$G_{33}^{S,A}(x_3, x'_3) = G_{33}(x_3, x'_3) \mp G_{33}(-x_3, x'_3), \quad (2.2e)$$

where the upper sign corresponds to the symmetrical Green's function and the lower sign to the antisymmetrical one.

The boundary conditions in Green's-function form are

$$G_{11}^{S,A} \left[\frac{h}{2} + 0, x'_3 \right] = G'_{11}{}^{S,A} \left[\frac{h}{2} - 0, x'_3 \right], \quad (2.3a)$$

$$G_{31}^{S,A} \left[\frac{h}{2} + 0, x'_3 \right] = G'_{31}{}^{S,A} \left[\frac{h}{2} - 0, x'_3 \right], \quad (2.3b)$$

$$C_{44} \left[\frac{d}{dx_3} G_{11}^{S,A}(x_3, x'_3) + ik_{||} G_{31}^{S,A}(x_3, x'_3) \right]_{x_3=h/2+0} = C'_{44} \left[\frac{d}{dx_3} G'_{11}{}^{S,A}(x_3, x'_3) + ik_{||} G'_{31}{}^{S,A}(x_3, x'_3) \right]_{x_3=h/2-0}, \quad (2.3c)$$

$$\left[ik_{||} C_{12} G_{11}^{S,A}(x_3, x'_3) + C_{11} \frac{d}{dx_3} G_{31}^{S,A}(x_3, x'_3) \right]_{x_3=h/2+0} = \left[ik_{||} C'_{12} G'_{11}{}^{S,A}(x_3, x'_3) + C'_{11} \frac{d}{dx_3} G'_{31}{}^{S,A}(x_3, x'_3) \right]_{x_3=h/2-0}, \quad (2.3d)$$

(and similar equations for the elements $G_{13}^{S,A}$, $G_{33}^{S,A}$, $G'_{13}{}^{S,A}$, and $G'_{33}{}^{S,A}$ for the sagittal modes, and

$$G_{22}^{S,A} \left[\frac{h}{2} + 0, x'_3 \right] = G'_{22} \left[\frac{h}{2} - 0, x'_3 \right], \quad (2.4a)$$

$$C_{44} \left[\frac{d}{dx_3} G_{22}^{S,A}(x_3, x'_3) \right]_{x_3=h/2+0} = C'_{44} \left[\frac{d}{dx_3} G'_{22}{}^{S,A}(x_3, x'_3) \right]_{x_3=h/2-0}, \quad (2.4b)$$

for the transverse modes.

Owing to the symmetry of the problem there is a separation between the (*S*) and (*A*) modes. These can be obtained by searching for the general solution of the Green's functions in the form

$$G_{11}^{S,A}(x_3, x'_3) = [G_{11}^{\infty}(x_3, x'_3) \pm G_{11}^{\infty}(-x_3, x'_3)] + A_1 e^{-\alpha_t x_3} + B_1 e^{-\alpha_t x'_3}, \quad (2.5a)$$

$$G_{31}^{S,A}(x_3, x'_3) = [G_{31}^{\infty}(x_3, x'_3) \mp G_{31}^{\infty}(-x_3, x'_3)] + \frac{ik_{\parallel}}{\alpha_t} A_1 e^{-\alpha_t x_3} + \frac{i\alpha_t}{k_{\parallel}} B_1 e^{-\alpha_t x'_3}, \quad (2.5b)$$

$$G_{22}^{S,A}(x_3, x'_3) = [G_{22}^{\infty}(x_3, x'_3) \pm G_{22}^{\infty}(-x_3, x'_3)] + C_1 e^{-\alpha_t x_3}, \quad (2.5c)$$

$$G_{13}^{S,A}(x_3, x'_3) = [G_{13}^{\infty}(x_3, x'_3) \pm G_{13}^{\infty}(-x_3, x'_3)] - \frac{i\alpha_t}{k_{\parallel}} D_1 e^{-\alpha_t x_3} - \frac{ik_{\parallel}}{\alpha_t} E_1 e^{-\alpha_t x'_3}, \quad (2.5d)$$

$$G_{33}^{S,A}(x_3, x'_3) = [G_{33}^{\infty}(x_3, x'_3) \mp G_{33}^{\infty}(-x_3, x'_3)] + D_1 e^{-\alpha_t x_3} + E_1 e^{-\alpha_t x'_3}, \quad (2.5e)$$

and

$$G'_{11}{}^{S,A}(x_3, x'_3) = [G'_{11}{}^{\infty}(x_3, x'_3) \pm G'_{11}{}^{\infty}(-x_3, x'_3)] + A_2 \times \left\{ \frac{\cosh}{\sinh} \right\}(\alpha'_t x_3) + B_2 \times \left\{ \frac{\cosh}{\sinh} \right\}(\alpha'_t x'_3), \quad (2.6a)$$

$$G'_{31}{}^{S,A}(x_3, x'_3) = [G'_{31}{}^{\infty}(x_3, x'_3) \mp G'_{31}{}^{\infty}(-x_3, x'_3)] - \frac{ik_{\parallel}}{\alpha'_t} A_2 \times \left\{ \frac{\sinh}{\cosh} \right\}(\alpha'_t x_3) - \frac{i\alpha'_t}{k_{\parallel}} B_2 \times \left\{ \frac{\sinh}{\cosh} \right\}(\alpha'_t x'_3), \quad (2.6b)$$

$$G'_{22}{}^{S,A}(x_3, x'_3) = [G'_{22}{}^{\infty}(x_3, x'_3) \pm G'_{22}{}^{\infty}(-x_3, x'_3)] + C_2 \times \left\{ \frac{\cosh}{\sinh} \right\}(\alpha'_t x_3), \quad (2.6c)$$

$$G'_{13}{}^{S,A}(x_3, x'_3) = [G'_{13}{}^{\infty}(x_3, x'_3) \pm G'_{13}{}^{\infty}(-x_3, x'_3)] + \frac{i\alpha'_t}{k_{\parallel}} D_2 \times \left\{ \frac{\cosh}{\sinh} \right\}(\alpha'_t x_3) + \frac{ik_{\parallel}}{\alpha'_t} E_2 \times \left\{ \frac{\cosh}{\sinh} \right\}(\alpha'_t x'_3), \quad (2.6d)$$

$$G'_{33}{}^{S,A}(x_3, x'_3) = [G'_{33}{}^{\infty}(x_3, x'_3) \mp G'_{33}{}^{\infty}(-x_3, x'_3)] + D_2 \times \left\{ \frac{\sinh}{\cosh} \right\}(\alpha'_t x_3) + E_2 \times \left\{ \frac{\sinh}{\cosh} \right\}(\alpha'_t x'_3), \quad (2.6e)$$

where $G_{ij}^{\infty}(x_3, x'_3)$ ($i, j = 1, 2, 3$) has been previously calculated,¹⁶⁻¹⁸ and

$$\alpha_t = (k_{\parallel}^2 - \omega^2/C_t^2)^{1/2}, \quad \alpha'_t = (k_{\parallel}^2 - \omega^2/C_t'^2)^{1/2}.$$

Introducing these expressions in Eqs. (2.3) and solving for the coefficients $\{A_1, B_1, D_1, E_1\}$ and $\{A_2, B_2, D_2, E_2\}$, we obtain the secular equations for the (*S*) and (*A*) modes, respectively. This yields the dispersion relations

$$\begin{vmatrix} 1 & 1 & -\cosh \left[\alpha'_t \frac{h}{2} \right] & -\cosh \left[\alpha'_t \frac{h}{2} \right] \\ \frac{k_{\parallel}}{\alpha_t} & \frac{\alpha_t}{k_{\parallel}} & \frac{k_{\parallel}}{\alpha'_t} \sinh \left[\alpha'_t \frac{h}{2} \right] & \frac{\alpha'_t}{k_{\parallel}} \sinh \left[\alpha'_t \frac{h}{2} \right] \\ -C_{44} \frac{\alpha_t^2 + k_{\parallel}^2}{\alpha_t} & -2C_{44} \alpha_t & -C'_{44} \frac{\alpha_t'^2 + k_{\parallel}^2}{\alpha'_t} \sinh \left[\alpha'_t \frac{h}{2} \right] & -2C'_{44} \alpha'_t \sinh \left[\alpha'_t \frac{h}{2} \right] \\ -2C_{44} k_{\parallel} & -C_{44} \frac{\alpha_t^2 + k_{\parallel}^2}{k_{\parallel}} & 2C'_{44} k_{\parallel} \cosh \left[\alpha'_t \frac{h}{2} \right] & C'_{44} \frac{k_{\parallel}^2 + \alpha_t'^2}{k_{\parallel}} \cosh \left[\alpha'_t \frac{h}{2} \right] \end{vmatrix} = 0, \quad (2.7)$$

for the (*S*) modes, and

$$\begin{vmatrix} 1 & 1 & -\sinh\left[\alpha'_i \frac{h}{2}\right] & -\sinh\left[\alpha'_i \frac{h}{2}\right] \\ \frac{k_{||}}{\alpha_t} & \frac{\alpha_t}{k_{||}} & \frac{k_{||}}{\alpha'_i} \cosh\left[\alpha'_i \frac{h}{2}\right] & \frac{\alpha'_i}{k_{||}} \cosh\left[\alpha'_i \frac{h}{2}\right] \\ -C_{44} \frac{\alpha_t^2 + k_{||}^2}{\alpha_t} & -2C_{44}\alpha_t & -C_{44} \frac{\alpha_t'^2 + k_{||}^2}{\alpha'_i} \cosh\left[\alpha'_i \frac{h}{2}\right] & -2C'_{44}\alpha'_i \cosh\left[\alpha'_i \frac{h}{2}\right] \\ -2C_{44}k_{||} & -C_{44} \frac{\alpha_t^2 + k_{||}^2}{k_{||}} & 2C'_{44}k_{||} \sinh\left[\alpha'_i \frac{h}{2}\right] & C'_{44} \frac{k_{||}^2 + \alpha_t'^2}{k_{||}} \cosh\left[\alpha'_i \frac{h}{2}\right] \end{vmatrix} = 0, \quad (2.8)$$

for the (A) modes.

We have investigated the existence of sagittal modes exhibiting an exponential decay inside the two media A, that is, with velocities $C < C_t$. Two cases are considered (Figs. 1 and 2), one (Al-W-Al or W-Al-W) for which there exists a Stoneley wave at a single interface AB, and the other (Al-Ni-Al or Ni-Al-Ni) without the Stoneley wave at the single interface AB. In order to make a clear discussion of this system we must consider the existence of a Stoneley wave and the condition, $C'_t < C_t$ or $C_t < C'_t$, separately.

If there exists a Stoneley wave at the single interface AB, then the first (S) and the first (A) modes go to the Stoneley wave when $hk_{||} \rightarrow \infty$ (Fig. 1). When $C'_t < C_t$ we find below C_t an infinity of (S) and (A) modes, due to the fact that in the region $C'_t < C < C_t$, the expressions $\cosh(\alpha'_i h)$, $\sinh(\alpha'_i h)$, etc., are transformed in the periodic functions $\cos(\alpha'_i h)$, $\sin(\alpha'_i h)$, etc. This can be seen in Fig. 2(b). Thus, if there exists a Stoneley wave at the single interface the first (S) and the first (A) modes go to the Stoneley wave, while the remaining ones tend to go to C'_t , when $hk_{||} \rightarrow \infty$.

If $C_t < C'_t$ (W-Al-W and Al-Ni-Al), there is not an infinity of modes below C_t . For W-Al-W we find an (S) mode and an (A) mode which tend to approach the velocity of the Stoneley wave when $hk_{||} \rightarrow \infty$ [Fig. 1(a)]. For Al-Ni-Al we find an (A) mode which merges with C_t around $hk_{||} = 10$ [Fig. 2(a)]. The parameters used as input in the calculation are given in Table I.

Thus, although the number of roots of the secular equation increases for increasing h , in the limit $h \rightarrow \infty$, there is in fact only one surface wave velocity. Indeed, if we take $hk_{||} \rightarrow \infty$ in Eqs. (2.7) and (2.8), both equations give the dispersion relation for a Stoneley wave.²

Equations (2.7) and (2.8) are generally valid for any thickness h and can be used to recover some results known for particular cases, thus providing a

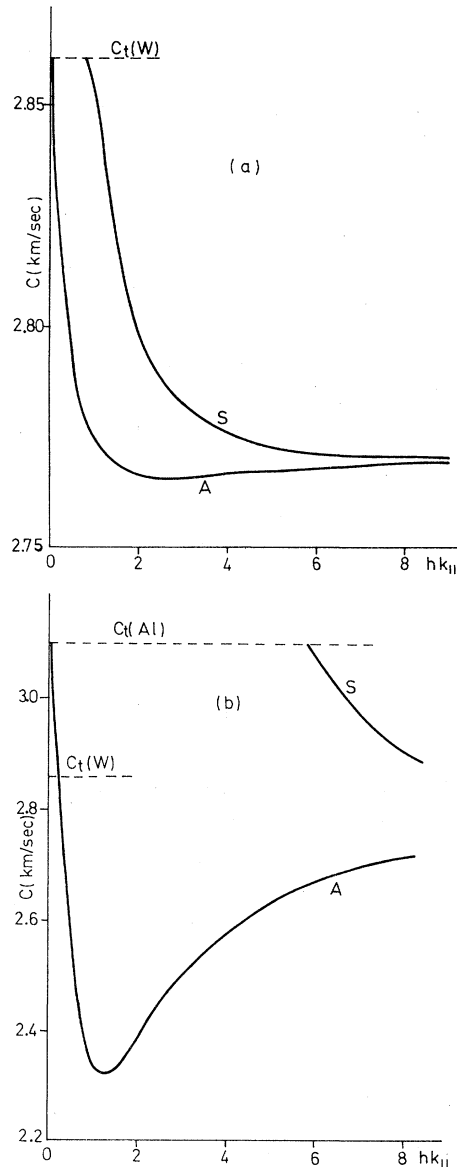


FIG. 1. Symmetrical (S) and antisymmetrical (A) modes at planar defects: (a) W-Al-W and (b) Al-W-Al, as a function of the thickness of the planar defect. The parameters are taken from Ref. 11.

check on our analysis. For example, a thin film is obtained if A is the vacuum, i.e.,

$$\rho = C_{44} = C_{12} = C_{11} = 0.$$

Then, Eqs. (2.7) and (2.8) reduce to

$$(k_{\parallel}^2 + \alpha_i'^2)^2 \tanh \left[\alpha_i' \frac{h}{2} \right] = 4k_{\parallel}^2 \alpha_i' \alpha_i' \tanh \left[\alpha_i' \frac{h}{2} \right], \quad (2.9)$$

and

$$(k_{\parallel}^2 + \alpha_i'^2)^2 \tanh \left[\alpha_i' \frac{h}{2} \right] = 4k_{\parallel}^2 \alpha_i' \alpha_i' \tanh \left[\alpha_i' \frac{h}{2} \right], \quad (2.10)$$

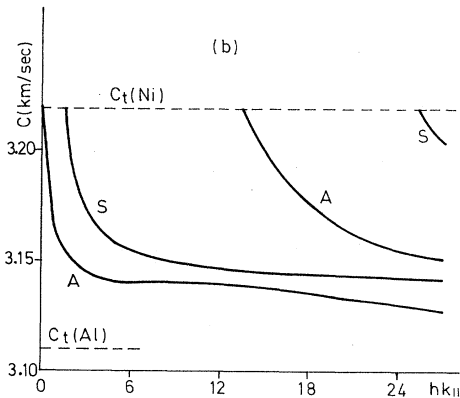
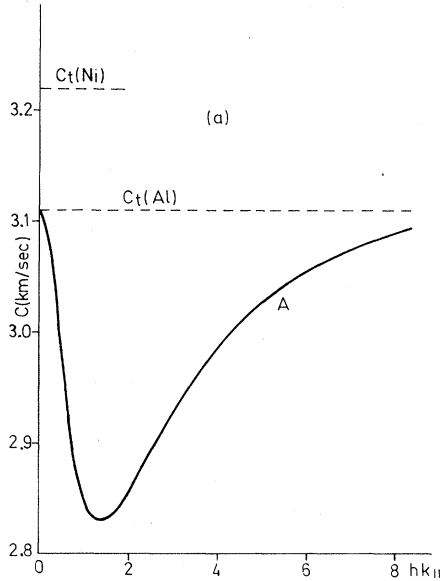


FIG. 2. Same as Fig. 1 for planar defects: (a) Al-Ni-Al and (b) Ni-Al-Ni.

respectively. These are indeed the dispersion relations for the (S) and (A) modes of a thin film.²⁰

Now we can discuss the planar defect. It can be seen that for $hk_{\parallel} \ll 1$, Eq. (2.8) admits as a solution a localized mode given by

$$\omega^2 = C_i^2 k_{\parallel}^2 [1 - A(hk_{\parallel})^2 + O(h^2)], \quad (2.11)$$

with

$$A = \frac{C_{44}}{2C'_{44}} + \left[\frac{\rho'}{2\rho} - 1 \right]. \quad (2.12)$$

The frequency of this mode differs from that of the transverse bulk band only by terms of order k_{\parallel}^3 . The result given in Eq. (2.11) was obtained previously in the particular case $\rho = \rho'$ from elasticity theory¹⁴ and from the elastic limit of Rosenzweig's model.¹⁶ The reason for the discrepancies mentioned above would now be clear. The different results¹⁴⁻¹⁶ are all correct by themselves, but entail different approximations based on h finite, when $hk_{\parallel} \ll 1$. If one takes the limit $h \rightarrow 0$ according to the prescription of Ref. 15, then one obtains the equivalent membrane model as it will be seen in the case of the sandwich ABC . Thus, according to Ref. 15, we have $h\rho = hC_{ij} = 0$, and $h\rho' = \rho_s$, $hC'_{ij} = C_{ij}^s$, when $h \rightarrow 0$. In this way the displacements are continuous at the interface and the conditions on the stresses are modified with respect to the case of h finite. This amounts to a different approximation and has a different solution.¹⁵

The transverse modes of the planar defect can be obtained in a similar way. The dispersion relations for the (S) and (A) modes are given by

$$C_{44} \alpha_i \cosh \left[\alpha_i' \frac{h}{2} \right] + C'_{44} \alpha_i' \sinh \left[\alpha_i' \frac{h}{2} \right] = 0 \quad (2.13)$$

TABLE I. Input values for the calculation of the velocities given in Figs. 1 and 2.

| | C_{11} (10^{11} N/m ²) | C_{44} (10^{11} N/m ²) | C_t (km/sec) | C_t' (km/sec) |
|----|--|--|-------------------|--------------------|
| W | 5.120 | 1.530 | 5.231 | 2.860 |
| Al | 1.113 | 0.261 | 6.422 | 3.110 |
| Ni | 3.115 | 0.929 | 5.894 | 3.219 |

and

$$C_{44}\alpha_i \sinh \left[\alpha'_i \frac{h}{2} \right] + C'_{44}\alpha'_i \cosh \left[\alpha'_i \frac{h}{2} \right] = 0, \quad (2.14)$$

respectively.

A similar method can be used for $hk_{\parallel} \ll 1$ [Eq. (2.13)], if $C'_i < C_i$ admits the localized mode given by Eq. (2.11) as a solution, with

$$A = \frac{1}{4} \left[\frac{C'_{44}}{C_{44}} - \frac{\rho'}{\rho} \right]^2. \quad (2.15)$$

This result differs from that of Ref. 14 in which no transverse mode was found. However, the existence of this mode in the present analysis admits no doubt.

B. Sandwich ABC

We shall now consider three different elastic media separated by two planes at $x_3=0$ (B/A) and $x_3=-h$ (C/B), for simplicity's sake.

The eigenmodes of the sandwich ABC can be obtained, as usually, from the poles of the Green's function of the system. The method for obtaining this Green's function for $hk_{\parallel} \ll 1$ has been described elsewhere.¹² We shall discuss here only the results obtained from this method.

For the general case of arbitrary h the problem must be solved numerically, but for $hk_{\parallel} \ll 1$ considerable simplifications result by developing the boundary conditions in powers of hk_{\parallel} , reducing the (8×8) determinant, for example, to a (4×4) one. The boundary conditions are given in this case by¹²

$$G_{11}(+0, x'_3) - G'_{11}(-h-0, x'_3) = ik_{\parallel} \left[\frac{C_{44}}{C'_{44}} - 1 \right] G_{31}(+0, x'_3) + h \frac{C_{44}}{C'_{44}} \left[\frac{\partial}{\partial x_3} G_{11}(x_3, x'_3) \right]_{x_3=+0}, \quad (2.16a)$$

$$G_{31}(+0, x'_3) - G'_{31}(-h-0, x'_3) = ik_{\parallel} \frac{C_{11} - 2C_{44} - C'_{11} + 2C'_{44}}{C'_{11}} G_{11}(+0, x'_3) + h \frac{C_{11}}{C'_{11}} \left[\frac{\partial}{\partial x_3} G_{31}(x_3, x'_3) \right]_{x_3=+0}, \quad (2.16b)$$

$$\begin{aligned} & C_{44} \left[\frac{\partial}{\partial x_3} G_{11}(x_3, x'_3) + ik_{\parallel} G_{31}(x_3, x'_3) \right]_{x_3=+0} - C'_{44} \left[\frac{\partial}{\partial x_3} G'_{11}(x_3, x'_3) + ik_{\parallel} G'_{31}(x_3, x'_3) \right]_{x_3=-h-0} \\ & = h \left[\rho' \delta(x_3 - x'_3) + (C'_{11} k_{\parallel}^2 - \rho' \omega^2) G_{11}(x_3, x'_3) - ik_{\parallel} \frac{C_{11}(C'_{11} - 2C'_{44})}{C'_{11}} \frac{\partial}{\partial x_3} G_{31}(x_3, x'_3) \right. \\ & \quad \left. + k_{\parallel}^2 \frac{(C'_{11} - 2C'_{44})(C_{12} - 2C_{44} - C'_{12} + 2C'_{44})}{C'_{11}} G_{11}(x_3, x'_3) \right]_{x_3=+0}, \quad (2.16c) \end{aligned}$$

$$\begin{aligned} & \left[i(C_{11} - 2C_{44})k_{\parallel} G_{11}(x_3, x'_3) + C_{11} \frac{\partial}{\partial x_3} G_{31}(x_3, x'_3) \right]_{x_3=+0} \\ & - \left[i(C'_{11} - 2C'_{44})k_{\parallel} G'_{11}(x_3, x'_3) + C'_{11} \frac{\partial}{\partial x_3} G'_{31}(x_3, x'_3) \right]_{x_3=-h-0} \\ & = h \left[(C_{44} k_{\parallel}^2 - \rho' \omega^2) G_{31}(x_3, x'_3) - ik_{\parallel} C_{44} \frac{\partial}{\partial x_3} G_{11}(x_3, x'_3) \right]_{x_3=+0}, \quad (2.16d) \end{aligned}$$

for sagittal polarization (similar equations hold for G_{13} , G_{33} , G'_{13} , and G'_{33}).

The equations for the transverse polarization are given by

$$G_{22}(+0, x'_3) - G'_{22}(-h-0, x'_3) = h \frac{C_{44}}{C'_{44}} \left[\frac{\partial}{\partial x_3} G_{22}(x_3, x'_3) \right]_{x_3=+0}, \quad (2.17a)$$

$$C_{44} \left[\frac{\partial}{\partial x_3} G_{22}(x_3, x'_3) \right]_{x_3=+0} - C'_{44} \left[\frac{\partial}{\partial x_3} G'_{22}(x_3, x'_3) \right]_{x_3=-h-0} = h \left[\rho' \delta(x_3 - x'_3) + (C'_{44} k_{\parallel}^2 - \rho' \omega^2) G_{22}(x_3, x'_3) \right]_{x_3=+0} \quad (2.17b)$$

Introducing the expressions for \vec{G} and \vec{G}^{11} (Refs. 11 and 12) in Eqs. (2.16) and (2.17) yields the corresponding eigenvalue equation (secular determinants). For sagittal modes,

$$\begin{vmatrix} 1+h \left[\frac{C_{44}-C'_{44}}{C_{44}} \frac{k_{\parallel}^2}{\alpha_t} + \frac{C_{44}}{C'_{44}} \alpha_t \right] & 1 + \frac{h\alpha_t}{C_{44}} (2C_{44} - c'_{44}) & -1 & 1 \\ ik_{\parallel} \left[\frac{1}{\alpha_t} + h \left(\frac{C_{11}-C_{12}+C'_{12}}{C_{11}} \right) \right] & i \left[\frac{\alpha_t}{k_{\parallel}} - hk_{\parallel} \frac{C_{12}-C'_{12}}{C_{11}} + h \frac{\alpha_t^2 C_{11}}{k_{\parallel} C_{11}} \right] & \frac{ik_{\parallel}}{\alpha_t'} & \frac{i\alpha_t'}{k_{\parallel}} \\ - \left[C_{44} \frac{k_{\parallel}^2 + \alpha_t^2}{\alpha_t} \right] & - \left[2C_{44}\alpha_t + h \left[C_{11}k_{\parallel}^2 \right] \right] & -C'_{44} \left[\frac{k_{\parallel}^2 + \alpha_t'^2}{\alpha_t'} \right] & -2C'_{44}\alpha_t' \\ + h \left[C_{11}k_{\parallel}^2 + \frac{C'_{12}}{C_{11}} (C_{12}-C'_{12})k_{\parallel}^2 - K_{\parallel}^2 \frac{C_{11}C'_{12}}{C_{11}} - \rho'\omega^2 \right] & + \frac{C'_{12}}{C_{11}} (C_{12}-C'_{12})k_{\parallel}^2 \frac{C'_{12}C_{11}}{C_{11}} \alpha_t^2 - \rho'\omega^2 \right] & & \\ -ik_{\parallel} \left[2C_{44} + h(C_{44}k_{\parallel}^2 - \rho'\omega^2) \frac{1}{\alpha_t} + hC_{44}\alpha_t \right] & -ik_{\parallel} \left[C_{44} \left[\frac{k_{\parallel}^2 + \alpha_t^2}{k_{\parallel}^2} \right] + h(C_{44}k_{\parallel}^2 - \rho'\omega^2) \frac{\alpha_t}{k_{\parallel}^2} + C_{44}\alpha_t \right] & 2ik_{\parallel}C'_{44} & ik_{\parallel} \frac{C'_{44}(k_{\parallel}^2 + \alpha_t'^2)}{k_{\parallel}^2} \end{vmatrix} = 0 \quad (2.18)$$

When no medium *B* exists this equation reduces to the usual Stoneley wave equation for an interface.² However, even for $hk_{\parallel} \ll 1$, it is not possible to obtain from Eq. (2.18) the frequency of the eigenmodes in closed form, in spite of the great simplification achieved. The gain is in a substantial reduction of the computational work.

The equations for the eigenmodes of the planar defect when medium *B* is very thin are readily obtained from Eq. (2.18), thus recovering the eigenmodes obtained previously. It can also be seen from Eq. (2.18) that if one takes the limit $h \rightarrow 0$ as prescribed in Ref. 15, then one obtains the equivalent membrane model.

It is now clear that we can treat the planar defect for arbitrary thickness of medium *B* in a simpler way making use of the symmetry of the system. When medium *B* is very thin we can particularize the general equations to this situation or use the method developed previously¹² to treat such a situation. The more general case of the sandwich *ABC* is more complicated and we cannot simplify the general equations due to the lack of mirror symmetry. Even for a very thin medium *B* we have seen that it is not possible to obtain the eigenmodes in closed form in spite of the great simplification achieved.

III. THIN FILM

As we have just seen the spectrum of systems with two interfaces differs substantially from that of a single interface. We shall now study the simplest system with two interfaces, i.e., the thin film.

The simplification in this case arises from (i) the fact that *A* is the vacuum, so that we need only impose stress-free boundary conditions, and (ii) there is mirror symmetry. Thus, we can use the classification in (*S*) and (*A*) modes, as for the planar defect. The eigenmodes of the thin film (Lamb modes), of course, have long been known.¹⁹⁻²³ The mean-square displacements have also been obtained elsewhere.²⁰ Our main interest here will concern the interaction energy of defects in a thin film. This has been investigated for a single surface¹⁷ or interface¹⁸ and now we propose to study such interaction energy for the thin film as the simplest system with two interfaces. The interaction energy of defects in systems with overlayers has been studied elsewhere¹²; the corrections introduced were small and so was the range of validity of such corrections. The sandwich *ABC* and planar defect also constitute interesting systems for this study but the calculations involved are very heavy and it is difficult to obtain analytical results even for a very thin medium *B*. The thin film, on the other hand, provides an interesting system exhibiting two interfaces, which introduces appreciable changes with respect to a single surface and interface, and for which analytical expressions can be obtained.

We shall consider as our system a material *A* with density and elastic coefficients ρ , C_{11} , C_{12} , and C_{44} , respectively, and bounded by two planes at $x_3 = -h/2$ and $x_3 = h/2$, with mirror symmetry about $x_3 = 0$. Using the above symmetrization scheme the boundary conditions can be expressed as

$$C_{44} \left[\frac{\partial}{\partial x_3} G_{11}^{S,A}(x_3, x'_3) + ik_{\parallel} G_{31}^{S,A}(x_3, x'_3) \right] = 0, \quad (3.1a)$$

$$\left[ik_{\parallel} C_{12} G_{11}^{S,A}(x_3, x'_3) + C_{11} \frac{\partial}{\partial x_3} G_{31}^{S,A}(x_3, x'_3) \right] = 0, \quad (3.1b)$$

$$C_{44} \left[\frac{\partial}{\partial x_3} G_{22}^{S,A}(x_3, x'_3) \right] = 0, \quad (3.1c)$$

$$C_{44} \left[\frac{\partial}{\partial x_3} G_{13}^{S,A}(x_3, x'_3) + ik_{\parallel} G_{33}^{S,A}(x_3, x'_3) \right] = 0, \quad (3.1d)$$

$$\left[ik_{\parallel} C_{12} G_{13}^{S,A}(x_3, x'_3) + C_{11} \frac{\partial}{\partial x_3} G_{33}^{S,A}(x_3, x'_3) \right] = 0, \quad (3.1e)$$

at $x_3 = h/2$. We shall search for the general solution of this Green's function in the following forms:

$$G_{11}^{S,A}(x_3, x'_3) = [G_{11}^{\infty}(x_3, x'_3) \pm G_{11}^{\infty}(-x_3, x'_3)] + A \times \left\{ \frac{\cosh}{\sinh} \right\}(\alpha_l x_3) + B \times \left\{ \frac{\cosh}{\sinh} \right\}(\alpha_l x_3), \quad (3.2a)$$

$$G_{31}^{S,A}(x_3, x'_3) = [G_{31}^{\infty}(x_3, x'_3) \pm G_{31}^{\infty}(-x_3, x'_3)] A \times \left\{ \frac{\sinh}{\cosh} \right\}(\alpha_l x_3) - \frac{i\alpha_l}{k_{\parallel}} B \times \left\{ \frac{\sinh}{\cosh} \right\}(\alpha_l x_3), \quad (3.2b)$$

$$G_{22}^{S,A}(x_3, x'_3) = [G_{22}^{\infty}(x_3, x'_3) \pm G_{22}^{\infty}(-x_3, x'_3)] + C \times \left\{ \frac{\cosh}{\sinh} \right\}(\alpha_l x_3), \quad (3.2c)$$

$$G_{13}^{S,A}(x_3, x'_3) = [G_{13}^{\infty}(x_3, x'_3) \pm G_{13}^{\infty}(-x_3, x'_3)] \frac{i\alpha_l}{k_{\parallel}} D \times \left\{ \frac{\cosh}{\sinh} \right\}(\alpha_l x_3) + \frac{ik_{\parallel}}{\alpha_l} E \times \left\{ \frac{\cosh}{\sinh} \right\}(\alpha_l x_3), \quad (3.2d)$$

$$G_{33}^{S,A}(x_3, x'_3) = [G_{33}^{\infty}(x_3, x'_3) \mp G_{33}^{\infty}(-x_3, x'_3)] + D \times \left\{ \frac{\sinh}{\cosh} \right\}(\alpha_l x_3) + E \times \left\{ \frac{\sinh}{\cosh} \right\}(\alpha_l x_3). \quad (3.2e)$$

Introducing the expressions Eqs. (3.2) in Eqs. (3.1), we obtain the coefficients A, B, C, D, E of the Green's function. Its poles yield the eigenmodes of the system, which have already been given in (2.9) and (2.10). However, we need the Green's function to study the elastic energy of interaction of impurities embedded in the film. The knowledge of this energy can be useful in phenomena such as segregation or diffusion near surfaces. In the case of a film the phenomenon of interest is the competing effect of the two surfaces and its possible consequences on the interaction energy. It is known¹⁸ that the elastic energy of interaction of point defects can be obtained as an integral over the two-dimensional wave vector \vec{k}_{\parallel} of combinations of the elements of the Green's function and its normal derivatives. But, in fact, we only need the knowledge of the static Green's function ($\omega=0$).

For the film problem the Green's function can be obtained by the symmetrization scheme developed above. Taking into account that

$$G_{ij}(x_3, x'_3) = \frac{G_{ij}^S(x_3, x'_3) + G_{ij}^A(x_3, x'_3)}{2} \quad (i, j = 1, 2, 3), \quad (3.3)$$

we obtain, after a lengthy but straightforward calculation, the following expressions:

$$G_{ij}(x_3, x'_3) = G_{ij}^{\infty}(x_3, x'_3) + G_{ij}^F(x_3, x'_3) \quad (i, j = 1, 2, 3), \quad (3.4)$$

where G_{ij}^{∞} is the static Green's function of an infinite crystal,¹⁶ and G_{ij}^F is the term due to the presence of

the two surfaces. We find

$$\begin{aligned}
 G_{11}^F(x_3, x'_3) = & M \{ C^+ \{ \sinh k_{\parallel} h [2k_{\parallel} h (C_{11}^2 - C_{44}^2) - 2(C_{11}^2 + C_{44}^2) - k_{\parallel}^2 h^2 (C_{11} - C_{44})^2] \\
 & + 2k_{\parallel} h \exp(-hk_{\parallel}) (C_{11}^2 - C_{44}^2) \} \\
 & - C^- \{ k_{\parallel} h [2k_{\parallel} h (C_{11}^2 - C_{44}^2) - 2(C_{11}^2 + C_{44}^2) - h^2 k_{\parallel}^2 (C_{11} - C_{44})^2] \\
 & + 2\sinh k_{\parallel} h \exp(-hk_{\parallel}) (C_{11}^2 - C_{44}^2) \} \\
 & + 2k_{\parallel} (x_3 + x'_3) S^+ \{ \sinh k_{\parallel} h [-C_{11}^2 + C_{44}^2 + hk_{\parallel} (C_{11} - C_{44})^2] \\
 & + hk_{\parallel} \exp(-hk_{\parallel}) (C_{11} - C_{44})^2 \} \\
 & - 2k_{\parallel} (x_3 - x'_3) S^- \{ \sinh k_{\parallel} h \exp(-k_{\parallel} h) (C_{11} - C_{44})^2 \\
 & + hk_{\parallel} [-C_{11}^2 + C_{44}^2 + hk_{\parallel} (C_{11} - C_{44})^2] \} \\
 & - 4k_{\parallel} x_3 k_{\parallel} x'_3 (C_{11} - C_{44})^2 (C^+ \sinh k_{\parallel} h + C^- \exp(-k_{\parallel} h)) \}, \tag{3.5a}
 \end{aligned}$$

$$G_{22}^F(x_3, x'_3) = \frac{1}{2C_{44}k_{\parallel} \sinh k_{\parallel} h} [C^+ + C^- \exp(-k_{\parallel} h)], \tag{3.5b}$$

$$\begin{aligned}
 G_{33}^F(x_3, x'_3) = & -M \{ C^+ \{ \sinh k_{\parallel} h [2(C_{11}^2 + C_{44}^2) + 2k_{\parallel} h (C_{11}^2 - C_{44}^2) + (C_{11} - C_{44})^2 h^2 k_{\parallel}^2] \\
 & + 2hk_{\parallel} \exp(-hk_{\parallel}) (C_{11}^2 - C_{44}^2) \} \\
 & + C^- \{ 2\sinh k_{\parallel} h \exp(-hk_{\parallel}) (C_{11}^2 - C_{44}^2) + hk_{\parallel} [2(C_{11}^2 + C_{44}^2) + 2hk_{\parallel} (C_{11}^2 - C_{44}^2) \\
 & + (C_{11} - C_{44})^2 h^2 k_{\parallel}^2] \} \\
 & - 2k_{\parallel} (x_3 + x'_3) S^+ \{ \sinh k_{\parallel} h [C_{11}^2 - C_{44}^2 + hk_{\parallel} (C_{11} - C_{44})^2] \\
 & + hk_{\parallel} \exp(-hk_{\parallel}) (C_{11} - C_{44})^2 \} \\
 & - 2k_{\parallel} (x_3 - x'_3) S^- \{ \sinh k_{\parallel} h \exp(-hk_{\parallel}) (C_{11} - C_{44})^2 \\
 & + hk_{\parallel} [C_{11}^2 - C_{44}^2 + hk_{\parallel} (C_{11} - C_{44})^2] \} \\
 & + 4k_{\parallel} x_3 k_{\parallel} x'_3 (C^+ \sinh k_{\parallel} h - hk_{\parallel} C^-) \}, \tag{3.5c}
 \end{aligned}$$

$$\begin{aligned}
 G_{31}^F(x_3, x'_3) = & iM \{ (S^+ \sinh k_{\parallel} h - S^- \exp(-hk_{\parallel})) [-4C_{11}C_{44}(C_{11} - C_{44}) + h^2 k_{\parallel}^2 (C_{11} - C_{44})^2] \\
 & - 2k_{\parallel} (x_3 + x'_3) C^+ k_{\parallel} h \cosh k_{\parallel} h (C_{11} - C_{44})^2 \\
 & + 2k_{\parallel} (x_3 - x'_3) C^- [\sinh k_{\parallel} h \exp(-hk_{\parallel}) + h^2 k_{\parallel}^2] (C_{11} - C_{44})^2 \\
 & + 2(C_{11}^2 - C_{44}^2) [k_{\parallel} (x_3 - x'_3) \sinh k_{\parallel} h C^+ - C^- k_{\parallel} h k_{\parallel} (x_3 + x'_3)] \\
 & + 4k_{\parallel} x_3 k_{\parallel} x'_3 (C_{11} - C_{44})^2 (S^+ \sinh k_{\parallel} h + S^- \exp(-k_{\parallel} h)) \}. \tag{3.5d}
 \end{aligned}$$

where

$$M = \frac{1}{8C_{44}C_{11}(C_{11} - C_{44})k_{\parallel} [\sinh^2(k_{\parallel} h) - k_{\parallel}^2 h^2]}, \tag{3.6}$$

$$C^{\pm} = \cosh k_{\parallel} (x_3 \pm x'_3), \quad S^{\pm} = \sinh k_{\parallel} (x_3 \pm x'_3). \tag{3.7}$$

$G_{13}^F(x_3, x'_3)$ can be obtained from $G_{31}^F(x_3, x'_3)$ by

exchanging x_3 and x'_3 and taking the complex conjugate.

A. Elastic energy of interaction of one point defect with a film

We shall consider point defects represented by the superposition of three mutually perpendicular

double forces without moment. For such a point defect centered at the point \vec{x}_0 , the distribution of the body force is

$$F_\alpha(\vec{x}) = -A_\alpha \frac{\partial}{x_\alpha} \delta(\vec{x} - \vec{x}_0), \quad \alpha = 1, 2, 3 \quad (3.8)$$

where A_α is a constant with the dimensions of a force times a length. Moreover, we limit ourselves to the case of an isotropic impurity:

$A_1 = A_2 = A_3 \equiv A$. The elastic energy of interaction of such a defect with a film is found to be

$$U_F(x_{03}) = -\frac{A^2}{16\pi C_{44}} \frac{\nu^2}{1-\nu} \frac{1}{x_{03}^3} I(x_{03}) \quad (3.9)$$

(x_{03} is the distance from the center of the film to the defect side), where

$$I(x_{03}) = -\int_0^{\xi_D} \frac{\xi^2 d\xi}{(\sinh^2 \xi h / 2x_{03} - \xi^2 h^2 / 4x_{03}^2)} \times \left[\frac{\xi h}{2x_{03}} - \sinh \frac{\xi h}{2x_{03}} \cosh \xi \right], \quad \xi_D = 2k_D x_{03}. \quad (3.10)$$

We take $k_D = 2\pi / (3/4\pi)^{1/3} a_0$ as defined elsewhere.²¹ When $x_{03} \rightarrow 0$, we obtain

$$I(x_{03}) / (2k_D x_{03})^3 = (4 - \frac{3}{2}) / (k_D h) - [2/k_D h + 4/(k_D h)^2 - 4/(k_D h)^3] \times \exp(-k_D h) + \dots$$

This result is in qualitative agreement with the trends found for the vacancy relaxation energies in metal crystal slabs.²² Equation (3.9) must be compared with that obtained for a free surface¹⁷:

$$U_S(x_{03}) = -\frac{A^2}{16\pi C_{44}} \frac{\nu^2}{1-\nu} \frac{1}{x_{03}^3} I_2(\xi_D), \quad (3.11a)$$

with

$$I_2(\xi_D) = \int_0^{\xi_D} \xi^2 e^{-\xi} d\xi. \quad (3.11b)$$

If we set $x_{03} = h/2$ in Eq. (3.9), and then take the limit $h \rightarrow \infty$, we obtain

$$U_s = -\frac{A^2}{6\pi C_{44}} \frac{\nu^2}{1-\nu} k_D^3, \quad (3.12)$$

which gives the interaction energy of a point defect at the free surface.¹⁷

In order to demonstrate the differences between the film and the free surface we can consider tungsten, which is nearly isotropic. In this case,

$$k_D = \frac{3.89}{a_0} = 1.23 \times 10^8,$$

in units of cm^{-1} .

In Fig. 3 we have represented $-I/(2k_D x_{03})^3$ for two values of $k_D h$, i.e., of the thickness h . It can be seen that this function increases very swiftly with the thickness. In order to clarify the analogies and differences with the case of the free surface, we have studied the former function versus $k_D h$ for several values of x_{03} . In Fig. 4 we represent $-I/(2k_D x_{03})^3$ vs $k_D h$ for $x_{03} = 0.5h$. Now the defect is on the surface of the film. Thus we see that when $k_D h \gg 1$, we recover the results of the semi-infinite medium, indicated by a dotted

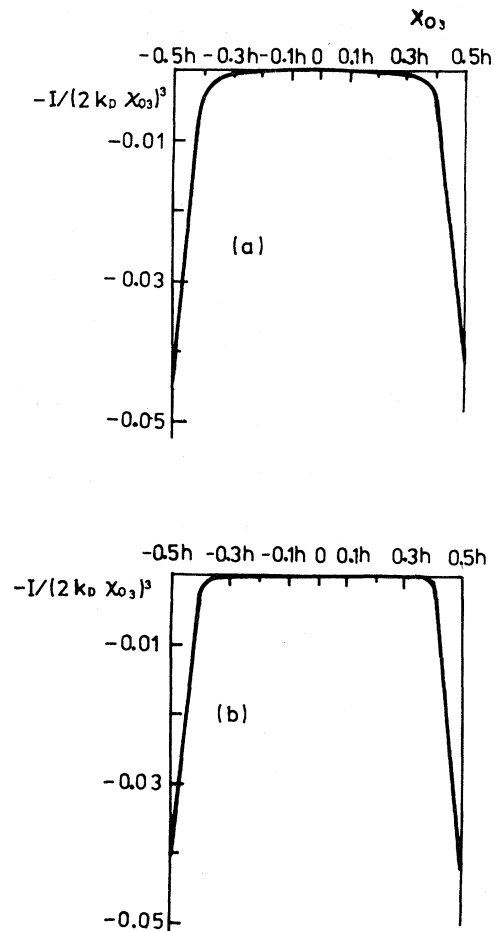


FIG. 3. Behavior of the interaction energy of a point defect with a film: $-I/(2k_D x_{03})^3$ vs x_{03} for (a) $k_D h = 20$, and (b) $k_D h = 50$.

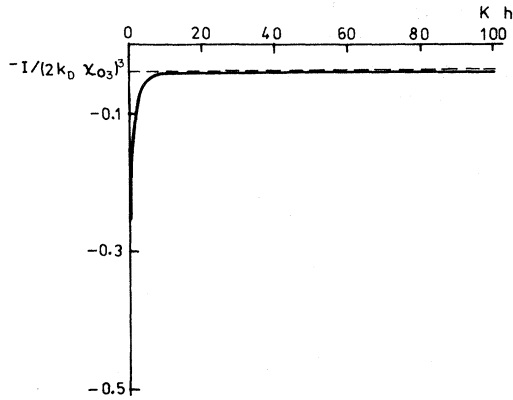


FIG. 4. $-I/(2k_D x_{03})^3$ vs $k_D h$ for $x_{03}=0.5h$. When $k_D h \gg 1$, we recover the value for a free surface (dotted line). For details see text.

straight line on Fig. 4, explained above. In Fig. 5 we give the same representation for $x_{03}=0.1h$, that is, for a defect inside the film. The function increases very steeply with the thickness and for $k_D h \gg 1$, it goes to zero as $1/x_{03}^3$, i.e., the same behavior obtained in the case of the free surface. Figure 6 represents $I_2(\xi_D)/\xi_D^3$ vs ξ_D for the free surface. In Fig. 7 we give the sums of $I_2(\xi_D)/\xi_D^3$ for two surfaces at distances x_{03} and $h - x_{03}$, respectively, for two values of $k_D h$. It can be seen that the existence of the second surface produces a negligible effect when the thickness is great. The effect of the second surface begins to be noticeable for $\xi_D \leq 15$. This gives the value of h for which the effects of the finite thickness of the film begin to be important.

Thus, the behavior of the elastic energy of interaction of a point defect is very different from the case of the free surface only when the thick-

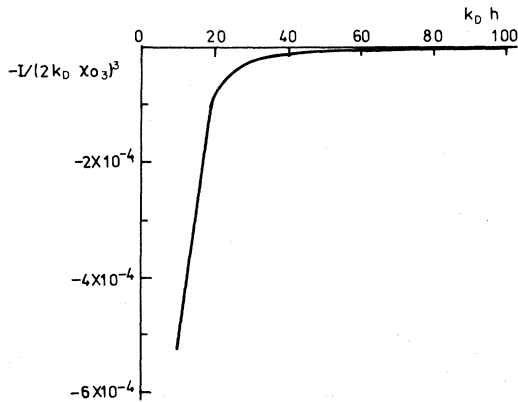


FIG. 5. Same as Fig. 4 for $x_{03}=0.1h$. When $k_D h \gg 1$, $-I/(2k_D x_{03})^3$ goes to zero as $1/x_{03}^3$ in the same way as a free surface.

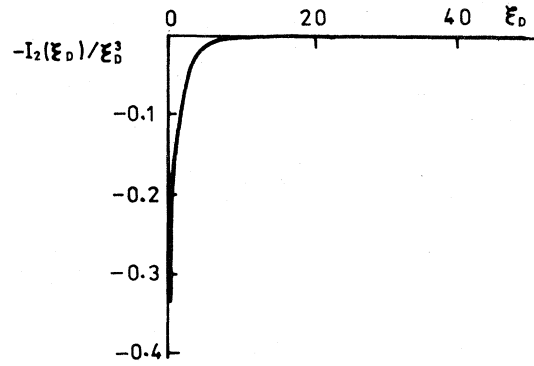


FIG. 6. Free surface: $-I_2(\xi_D)/\xi_D^3$ vs ξ_D .

ness of the film is small in such a way that the point defect is strongly affected by the two surfaces. As the thickness increases and $k_D h \gg 1$, the behavior tends to resemble the case of the free surface due to the fact that the defect is affected more strongly by only one of the surfaces.

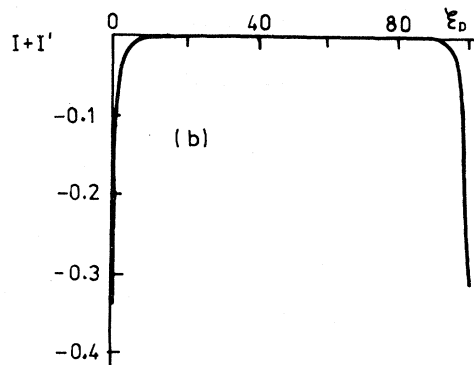
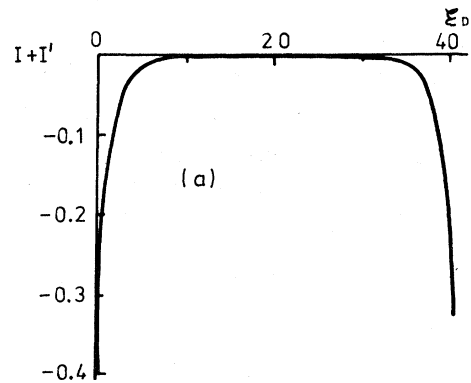


FIG. 7. $I + I' = -I_2(\xi_D)/\xi_D^3 - I_2(\xi'_D)/\xi'^3_D$, $[\xi'_D = 2k_D(h - x_{03})]$ vs ξ_D for two surfaces placed at distances x_{03} and $h - x_{03}$, respectively, for (a) $k_D h = 20$, and (b) $k_D h = 50$.

B. Mutual interaction energy between two impurities and a film

The mutual interaction energy of two point defects is defined as the energy of the system minus the sum of the energies of each impurity alone. Following the method of Ref. 17 we obtain

$$U_F(\vec{x}_0, \vec{x}'_0) = -\frac{AA'}{\pi C_{44}} \frac{\nu^2}{1-\nu} \int_0^{k_D} \frac{k_{||}^2 dk_{||}}{[\sinh^2(k_{||}h) - h^2 k_{||}^2]} J_0(k_{||}R_{||}) \times [\sinh k_{||}h \cosh k_{||}(x_{03} + x'_{03}) - k_{||}h \cosh k_{||}(x_{03} - x'_{03})], \quad (3.13)$$

where $R_{||} = |\vec{x}_{0||} - \vec{x}'_{0||}|$.

If we consider a very thick film ($h \rightarrow \infty$) and the two impurities very close to one surface, Eq. (3.13) reduces to

$$U_F = -\frac{AA'}{\pi C_{44}} \frac{\nu^2}{1-\nu} \int_0^{k_D} k_{||}^2 dk_{||} J_0(k_{||}R_{||}) e^{-k_{||}(X_{03} + X'_{03})}, \quad (3.14)$$

where

$$X_{03} = \frac{h}{2} - x_{03}, \quad X'_{03} = \frac{h}{2} - x'_{03}. \quad (3.15)$$

If we take the limit $k_D \rightarrow \infty$, we obtain

$$U_F = -\frac{2AA'}{\pi C_{44}} \frac{\nu^2}{1-\nu} \frac{1}{(R_{||}^2 + \bar{R}_3^2)^{1/2}} P_2 \left[\frac{\bar{R}_3}{(R_{||}^2 + \bar{R}_3^2)^{1/2}} \right], \quad (3.16)$$

where $\bar{R}_3 = X_{03} + X'_{03}$ and P_2 is the Legendre polynomial of second order. Equation (3.16) is the energy of interaction of two defects in the case of a free surface.¹⁷

Let us return to Eq. (3.13) for a film. The general discussion of this equation is very difficult and we shall consider only the case of two adatoms, that is $x_{03} = x'_{03} = h/2$. Thus, Eq. (3.13) simplifies to

$$U_F = -\frac{AA'}{\pi C_{44}} \frac{\nu^2}{1-\nu} \frac{1}{R_{||}^3} \int_0^{k_D R_{||}} \xi^2 d\xi J_0(\xi) \frac{\sinh \alpha \xi \cosh \alpha \xi - \alpha \xi}{\sinh^2 \alpha \xi - \alpha^2 \xi^2}, \quad (3.17)$$

with $\alpha = h/R_{||}$.

Consider the dimensionless integral

$$I_1 = \int_0^{k_D R_{||}} \xi^2 d\xi J_0(\xi) \frac{\sinh \alpha \xi \cosh \alpha \xi - \alpha \xi}{\sinh^2 \alpha \xi - \alpha^2 \xi^2}. \quad (3.18)$$

This can be decomposed in the following way:

$$I_1 = I_0 + I', \quad (3.19)$$

where

$$I_0 = \int_0^{k_D R_{||}} \xi^2 d\xi J_0(\xi), \quad (3.20a)$$

$$I' = \int_0^{k_D R_{||}} \xi^2 d\xi J_0(\xi) \left[\frac{\sinh \alpha \xi \cosh \alpha \xi - \alpha \xi}{\sinh^2 \alpha \xi - \alpha^2 \xi^2} - 1 \right]. \quad (3.20b)$$

I_0 is related to a single surface exhibiting oscillatory behavior with the upper limit $k_D R_{||}$, such that

$$I_0 = \lim_{\beta \rightarrow 0} \int_0^\infty \xi^2 d\xi J_0(\xi) e^{-\beta \xi} = -1,$$

and it will not be considered here.

We shall study the term I' which has regular behavior. If we take $h > R_{||}$, I' does not depend appreciably on the upper limit $k_D R_{||}$. Thus, we can take $k_D \rightarrow \infty$. The dependence of I' on $\alpha = h/R_{||}$ is given in Fig. 8. In contrast, if we take $h < R_{||}$, the integral I' depends on α and $k_D R_{||}$. The dependence on $k_D R_{||}$ gradually disappears when $R_{||}$ grows.

IV. SUMMARY AND CONCLUSIONS

We have studied the dynamics of systems with two interfaces by using a Green's-function method. For symmetric systems (planar defect or free film) and arbitrary thicknesses of a medium, B , it is possible, by using a symmetrization procedure, to obtain the (S) and (A) modes of such systems.²³ We thus find that the planar defect exhibits interface

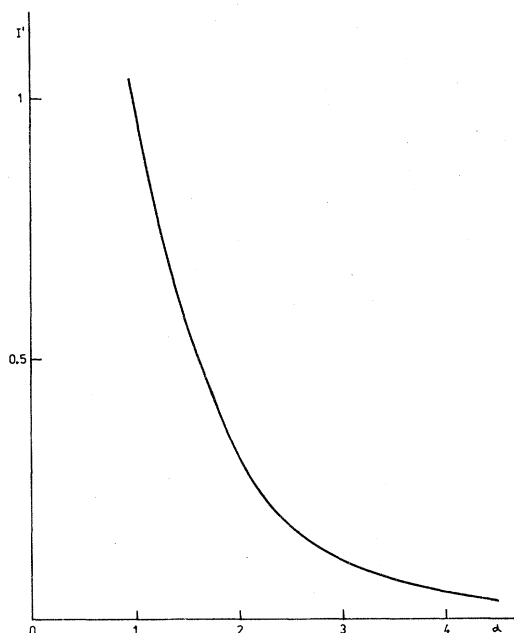


FIG. 8. Interaction energy of two adatoms on one surface of the film. I' vs $\alpha = h/R_{\parallel}$.

waves even for materials in which Stoneley waves are forbidden (Ni-Al-Ni, Al-Ni-Al). When medium B is very thin it is possible to obtain analytical expressions for the eigenmodes of the planar defect and to clarify the discrepancies between the results so far obtained in different treatments of this problem. For the unsymmetric sandwich ABC , when medium B is very thin, the general equations can be simplified by developments in powers of hk_{\parallel} , but it is not possible to obtain the eigenmodes in closed form. Using the symmetrization procedure we have been able to study the interaction energy of point defects with a film obtaining the results in closed form.

Using the symmetrization procedure we have been able to study the interaction energy of point defects with a film obtaining the results in closed form.

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