Surface elastic waves in superlattices: Sagittal localized and resonant modes

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We investigate the existence and behavior of localized and resonant acoustic modes of sagittal polarization associated with the surface of a semi-infinite superlattice. These modes appear as well-defined peaks of the density of states, either inside the minigaps or inside the bulk bands of the superlattice. The densities of states, which are calculated as functions of the frequency ω and the wave vector $k_{\parallel}$ (parallel to the interfaces), are obtained from an analytic determination of the Green function for a semi-infinite superlattice. We show the existence of δ peaks of weight $-\frac{1}{2}$ at the limits of any bulk band. The conservation of the total number of states leads to the necessary existence of surface localized modes inside the gaps, but also of semilocalized modes which appear as well-defined resonances inside the bulk bands of the superlattice.

A great deal of work has been devoted during the last decade to the study of acoustic vibrations in superlattices (SL's).[1-7] Besides the bulk waves propagating in the whole SL, it has been shown that the presence of inhomogeneities within the perfect SL, such as a free surface, an internal surface (i.e., a substrate/SL interface), or a layer defect, give rise to localized states inside the minigaps separating the bulk bands.[8-11] The knowledge of the density of states (DOS) in these systems also indicates the spatial distribution of the modes, and in particular the possibility of resonant states which may appear as well-defined peaks of the DOS inside the bulk bands.[12-15] Such a study can be performed by means of a Green's function technique which is also of interest for scattering problems.[16]

In some recent works,[12,13] we have studied in detail transverse-acoustic modes in a semi-infinite SL with or without a cap layer, and in a SL in contact with a substrate. For these modes involving only one direction of vibration, the Green's functions have been calculated analytically in the above systems and the density of states obtained as functions of the frequency ω and the wave vector $k_{\parallel}$ (parallel to the interfaces). The localized and resonant modes associated with such inhomogeneities (surface, interface, ...) in the SL appear as well-defined peaks of the density of states either inside the minigaps or inside the bulk bands of the SL. In particular, we have obtained general rules[12] for the existence of transverse localized modes associated with the free surface of a semi-infinite SL, as well as for resonant modes associated with the interface between a SL and a substrate.

Acoustic modes of sagittal polarization have been investigated during the last few years using a transfer matrix method. In particular, surface-localized modes have been obtained and discussed in detail.[8,17] However, to our knowledge, the variation of the total vibrational density of states associated with the above-cited perturbation of the SL, and in particular the existence of surface resonant states, have not yet been studied. In this paper, we study localized and resonant modes together with the variation of the density of states associated with a free surface in a SL. Due to the coupling of two degrees of vibrations, the Green's function calculation, from which the density of states is deduced, becomes rather complicated as compared to the case of transverse vibrations. For this reason, we limit ourselves in this paper to the case of a semi-infinite SL without changing the thickness and the nature of the surface cap layer.

The Green's function is calculated by using the interface response theory in composite materials[18] in which the solution is first searched in the restricted space of interfaces before being extended to the whole material. We avoid the detail of the analysis which is similar to, although more cumbersome than, that for transverse modes.[12,13,15] The detail analytic expressions of the Green's functions are given in Ref. 15. In the following, we shall focus on a few illustrations of these results. In these examples the SL's are made of Al and W with the parameters given in Ref. 8. The thicknesses d_1 and d_2 of the layers in the SL are assumed to be equal, the period of the SL being $D=d_1+d_2=2d_1$.

For given ω and $k_{\parallel}$, the wave vectors along the axis x_3 of the SL which can be deduced from the bulk dispersion relations are called k_3. In the case of sagittal modes in-

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volving two components of the displacement field, there are two pairs of k_3 associated with given $k_\parallel$ and ω, which can be written as[8,17] $\pm(K_1+iL_1)$ and $\pm(K_2+iL_2)$. Now an elastic wave at the frequency ω propagates in the SL if $L_1=0$ or $L_2=0$, while it is attenuated if both L_1 and L_2 are different from zero. Each pair of k_3 (the first, for instance) can take four different forms; it can be

$$\begin{aligned} &\text{(i) pure real } (L_1=0)\ , \\ &\text{(ii) pure imaginary } (K_1=0)\ , \\ &\text{(iii) complex but with } K_1=\pm\frac{\pi}{D}\ , \\ &\text{(iv) complex with } K_1\neq\pm\frac{\pi}{D}\ . \end{aligned} \tag{1}$$

However, in case (iv) the two pairs of k_3 necessarily become

$$K+iL, -(K+iL), K-iL, -(K-iL)\ . \tag{2}$$

Figure 1(a) gives an example of the complex band structure in a W-Al SL showing the combinations of the above-mentioned cases. One can see the presence of direct gaps at the center and the edge of the reduced Brillouin zone, but also the possibility[19] of indirect gaps inside this zone [Fig. 1(b)]. This is a consequence of coupling between the components of the displacement, i.e., the mixing between waves polarized in each constituent as a result of reflection and transmission phenomena at the interfaces. Let us also mention that the imaginary parts of k_3 wave vectors in Fig. 1(a) give the attenuation of the possible localized waves in the gaps.

In Fig. 2 we represented the so-called projected band structure of the bulk and surface modes, namely, ω versus $k_\parallel$. The bulk bands associated with each polarization ($L_1=0$ or $L_2=0$) of the waves are, respectively, represented by horizontally and vertically dashed lines. The ranges of frequencies belonging simultaneously to both types of bands are drawn in black in Fig. 2, while the regions separating the different shaded areas correspond to gaps. Due to the large difference between the elastic parameters of W and Al, these gaps are rather large in contrast to the case of more usual systems like GaAs-AlAs.[17] Inside these gaps, we have represented surface modes corresponding to two complementary semi-infinite SL's obtained by cleaving the infinite W-Al SL in such a way that one obtains one SL with a full W layer at the surface (dashed lines) and its complementary with a full Al layer at the surface (solid lines). In these figures some of the surface modes are very close to the bulk bands and cannot be distinguished from the latter on

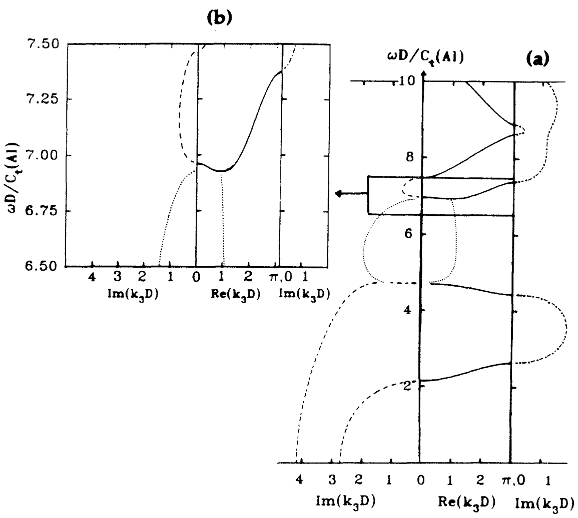

FIG. 1. (a) Complex band structure (ω versus complex k_3) in a W-Al SL with $d_1=d_2=D/2$ and $k_\parallel D=3$. $\omega D/C_t(\mathrm{Al})$ is a dimensionless frequency where $C_t(\mathrm{Al})$ is a transverse velocity of sound in Al given by $(C_{44}/\rho)^{1/2}$. Solid curves are k_3 real (middle panel of the figure). Dashed-dotted curves are k_3 imaginary (left panel). Dashed curves are the imaginary part of k_3 when its real part is equal to π/D (right panel). In addition, when k_3 is a complex quantity [Eq. (2)], the dotted curves give both its real and imaginary parts; in this case the imaginary part is presented in the left panel. (b) Same as in (a) enlarged in the range of frequencies where the indirect gap appears.

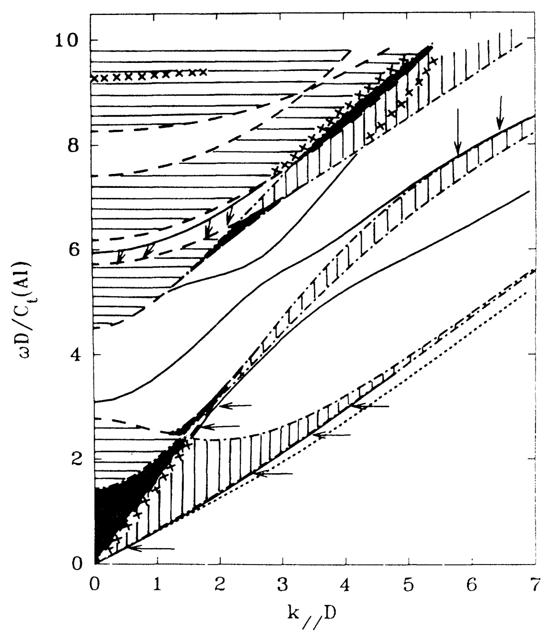

FIG. 2. Bulk and surface sagittal elastic waves in W-Al SL. The curves give $\omega D/C_t(\mathrm{Al})$ as a function of $k_\parallel D$, where ω is the frequency, $k_\parallel$ the propagation vector parallel to the interfaces, $C_t(\mathrm{Al})$ the transverse speed of sound in Al, and $D=d_1+d_2$ the period of the SL. The horizontally and vertically shaded areas correspond to bulk bands associated with each of the two polarizations of the waves. The range of frequencies belonging simultaneously to these two types of bands is represented in black. The surface modes associated with two complementary SL's (ending, respectively, with a full W layer or a full Al layer) are represented by dashed lines (W at the surface) and solid lines (Al at the surface). Some of the surface modes are very close to the bulk bands and cannot be distinguished from the latter at the scale of the figure; they are indicated by arrows. The extensions of the localized modes into the bulk bands as resonances are indicated by crosses.

the scale of the figure; we have indicated their positions by arrows.

Besides the localized modes which appear as δ peaks inside the gaps, the variational density of states (discussed below in Figs. 3 and 4) also contains well-defined features falling inside the bulk bands of the SL. These peaks can be considered as resonant states associated with the surface of the SL's. Their dispersion is plotted in Fig. 2 by crosses; some dispersion curves appear to be continuations of localized branches into the bulk bands of the SL. Let us remark that these resonant modes may be localized with respect to one type of band and propagating with respect to the other. This situation, which can occur when the vibrations involve at least two degrees of freedom, is of course without analogue in the case of transverse waves.[12]

The behavior of localized and resonant modes in the density of states is illustrated in Figs. 3 and 4 where the variation of the total density of states is sketched when two complementary semi-infinite SL's are created by the cleavage of an infinite SL. For the sake of clarity and despite the analytic nature of our calculation, the δ peaks in the density of states are broadened by adding a small imaginary part to the frequency ω (i.e., $\omega \rightarrow \omega + i\varepsilon$).

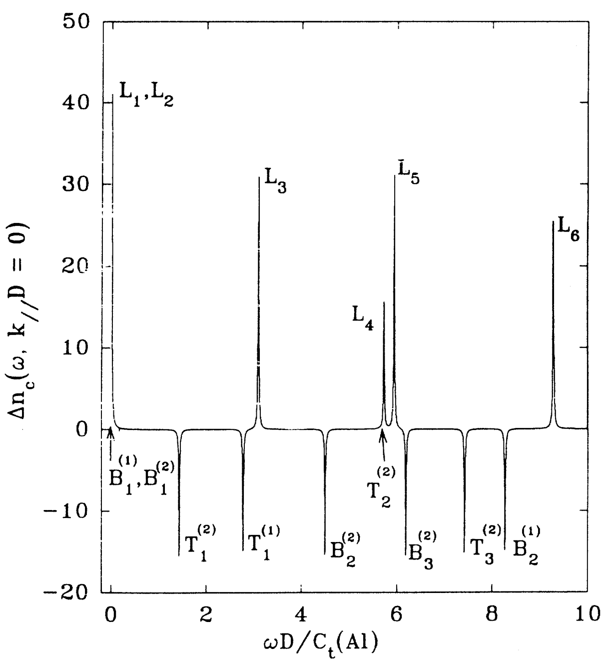

FIG. 3. Variation of the density of states in units of D/C_t(Al) when creating two complementary semi-infinite SL's from the infinite SL. In this figure $k_\parallel D=0$ and as a consequence the sagittal modes are decoupled into transverse and longitudinal modes. One can distinguish the surface transverse modes (labeled L_1, L_2, L_4, and L_6), the surface longitudinal modes (labeled L_2 and L_5), as well as the δ peaks of weight $-\frac{1}{2}$ (($B_i^{(j)}$ and $T_i^{(j)}$)) which appear, respectively, at the bottom and the top of each bulk band i associated with either longitudinal or transverse polarization (labeled, respectively, as $j=1$ and 2). Sometimes the surface modes are located very close to the limits of the bulk bands and therefore mask the band-edge antiresonances.

In Fig. 3 we have chosen $k_\parallel D=0$ and, as a consequence, the sagittal modes separate into decoupled longitudinal and transverse waves. The latter have been investigated in detail in Ref. 12, whereas the former can be studied from the same general expressions when replacing the elastic constants C_{44} by C_{11}. In Fig. 3, the peaks L_1, L_3, L_4, L_6 are associated with transverse surface localized modes whereas L_2 and L_5 give longitudinal surface modes. The mode labeled L_1 is associated with the semi-infinite SL ending with a W surface layer, while the modes labeled L_2, L_3, L_4, L_5, and L_6 belong to the complementary SL having an Al layer at the surface. In Fig. 3, one can also notice δ peaks of weight $-\frac{1}{2}$ (antiresonances) existing at the limits of any bulk band; these peaks are denoted $B_i^{(i)}$ and $T_i^{(j)}$ referring, respectively, to the bottom and top of the band i having the polarization labeled j ($j=1$ for longitudinal and $j=2$ for transverse polarization).

When $k_\parallel D$ departs from zero, both longitudinal and transverse vibrations become coupled, and, some of the localized branches at $k_\parallel D=0$ may now fall inside a bulk band of the SL. Such modes can radiate their energy into the bulk modes and therefore become resonant (or leaky) waves. This, for example, occurs for the mode labeled L_6 in Fig. 3 which appears at $\omega D/C_t(\mathrm{Al}) \cong 9.27$ in Fig. 2. Let us stress that in our approach the signature of such a resonant mode is the existence of a well-defined feature in the density of states. We have checked that the area under this peak approximately corresponds to one state.

Generally speaking, the surface modes can be con-

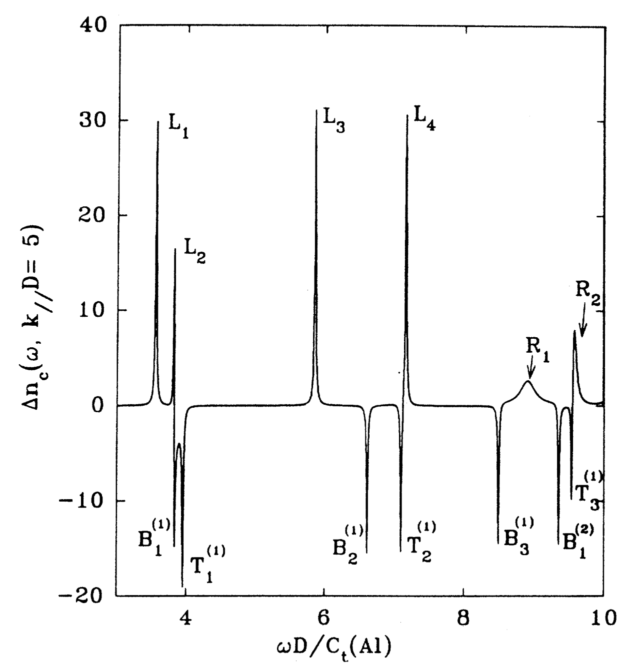

FIG. 4. Same as in Fig. 3 but for $k_\parallel D=5$. In this case the vibrations along the directions x_1 and x_3 are coupled. The surface waves are labeled L_i and the δ peaks of weight $-\frac{1}{2}$ at the limits of the bulk bands are labeled $B_i^{(j)}$ and $T_i^{(j)}$ where j represents the two polarizations called 1 and 2. R_i refers to resonances which appear inside the bulk bands of the SL.

sidered as the poles of the Green's function or equivalently the zeros of its denominator which we shall call $D(\omega)$ (for detailed closed-form expressions, see Ref. 15). Inside the gaps, the function $D(\omega)$ is real and changes sign every time the frequency goes through a localized surface mode. In contrast, inside the bulk bands, the function $D(\omega)$ becomes complex even though the frequency ω is taken to be real variable. The resonant states may be attributed to the maxima of the function $|D(\omega)|^{-2}$ because in the vicinity of one of its maximum ω_R this function can be written in a Lorentzian form

$$|D(\omega)|^{-2} \cong \frac{A}{(\omega-\omega_R)^2+\omega_I^2}$$

centered at $\omega=\omega_R$. In our calculation, we have checked that, for $k_\parallel D \cong 0$ and $\omega D/C_t(\mathrm{Al}) \cong 9.27$, the function $|D(\omega)|^{-2}$ shows a strong maximum which decreases in magnitude as $k_\parallel D$ departs from zero. This branch is associated with the semi-infinite SL having an Al layer at the surface. Let us stress that this frequency ω_R approximately coincides with a zero of the real part of $D(\omega)$. Another approach to obtain the leaky waves would consist of searching the zeros of the complex function $D(\omega)$ when ω is taken to be a complex variable $\omega=\omega_R-i\omega_I$. However, in our case we did not obtain simultaneously the vanishing of the real and imaginary part of $D(\omega)$ for a reasonable range of values of ω_R and ω_I.

Figure 4 gives another illustration of the variational density of states, for $k_\parallel D=5$. Now the polarization of the waves is no longer purely longitudinal nor purely transverse. In this case, one can still notice the existence of antiresonances of weight $-\frac{1}{2}$ at every edge of the bulk bands. The localized surface modes are again denoted L_i, whereas R_1 and R_2 are two resonant modes which appear as extensions of localized modes (see Fig. 2) located in the second and third minigaps into the bulk bands. We have again checked that the function $|D(\omega)|^{-2}$ contains maxima at the frequencies of these resonant states when considering the SL terminated by an Al layer (but not the complementary SL ending with a W layer).

An interesting result is the observation that the variation of the density of states (due to the creation of the two complementary SL's) is exactly equal to zero when the frequency ω belongs simultaneously to the bulk bands of both polarizations (black domains in Fig. 2). This result put together with the existence of antiresonances at the band limits and the conservation of the total number of states implies the necessary existence of surface states which may appear either as localized modes in the gaps or as resonant states belonging to only one type of band (there is no analogue of such resonances in the case of pure longitudinal or pure transverse waves). Let us emphasize that the localized states are a combination of two decaying waves while the eigenvectors of the resonant modes contain one propagating and one decaying component.

In conclusion, the main results of this work (apart from the analytic derivation of the Green's function in the case of sagittal waves[15]) are the existence of antiresonances of weight $-\frac{1}{2}$ at the edges of any bulk band due to the creation of two semi-infinite SL's from an infinite one, and, as a consequence, the necessary existence of localized and resonant surface modes associated with either one or the other complementary SL. The resonant (or leaky) waves which may appear as extensions of localized modes into the bulk bands are presented here for the first time to our knowledge in SL's. Finally, let us mention that the knowledge of the Green's function yields possible a full determination of all eigenvectors[18] in semi-infinite SL's. These quantities are, for instance, involved in the study of Raman scattering by acoustic phonons.[20]

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