Surface and interface elastic waves in superlattices: Transverse localized and resonant modes

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Localized and resonant transverse elastic waves associated with the surface of a semi-infinite superlattice or its interface with a substrate are investigated. These modes appear as well-defined peaks of the vibrational density of states, either inside the minigaps or inside the bulk bands of the superlattice. The densities of states, which are calculated as a function of the frequency ω and the wave vector $\mathbf{k}_{\parallel}$ (parallel to the interfaces), are obtained from an analytic determination of the response function for a semi-infinite superlattice with or without a cap layer, and also for a superlattice in contact with a substrate. Besides, we show that the creation from the infinite superlattice of a free surface or of the substrate-superlattice interface gives rise to δ peaks of weight $(-\frac{1}{4})$ in the density of states, at the edges of the superlattice bulk bands. Then when one considers together the two semi-infinite superlattices obtained by cleavage of an infinite one along a plane parallel to the interfaces, one always has as many localized surface modes as minigaps, for any value of $\mathbf{k}_{\parallel}$. Although these results are obtained for transverse elastic waves with polarization perpendicular to the saggital plane (containing the propagation vector $\mathbf{k}_{\parallel}$ and the normal to the interfaces), they remain valid for the longitudinal waves in the limit of $\mathbf{k}_{\parallel}=\mathbf{0}$. Specific applications of these analytical results are given in this paper for Y-Dy or GaAs-AlAs superlattices. The effect of a Si surface cap layer on the surface of this last superlattice is also investigated.

I. INTRODUCTION

The propagation of acoustic waves in superlattices has been the object of many experimental and theoretical studies over the past decade, summarized in several recent review papers.[1–7] The extended states propagating in the whole superlattice form bulk bands which are separated by small gaps. Localized modes associated with a perturbation of the perfect superlattice may exist inside these gaps. In particular, it was shown that surface acoustic waves may exist,[8] as well as modes localized at the interface between a superlattice and a substrate,[9] or near a planar defect in an otherwise perfect superlattice.[10,11] However, to our knowledge, the variation of the vibrational density of states associated with the above cited perturbations of a superlattice has not yet been studied, apart from a short attempt[8] at showing only in the surface local density of states the peaks associated with surface localized modes. Intense peaks were observed in Raman experiments[12] on Si capped Ge_mSi_n superlattices and interpreted with the help of a simple linear chain model as resonant modes (also called leaky waves). In this paper, we study resonant and localized modes together with the variation of the density of states associated with surfaces and interfaces in superlattices. Closed form expressions are obtained for transverse elastic waves polarized perpendicular to the saggital plane, i.e., the plane containing the propagation vector $\mathbf{k}_{\parallel}$ (parallel to the interfaces) and the normal to the interfaces. However, these results also remain valid in the case of longitudinal waves propagating along the axis of the superlattice, which means in the limit of $\mathbf{k}_{\parallel}=\mathbf{0}$.

These investigations are done with the help of the response functions associated to such heterostructures.[13] The knowledge of these Green's functions enables us to calculate both the local and total density of states. Then, in addition to the dispersion of extended and localized states, one can also obtain the spatial distribution of the modes and, in particular, the possibility of resonant modes which may appear as well-defined peaks of the density of states inside the bulk bands.

The organization of this paper is as follows. Section II presents the model we use for these studies. Section III gives the analytical results obtained for the densities of states in the above-described heterostructures. Section IV shows the numerical results for Y-Dy or GaAs-AlAs semi-infinite superlattices with or without a surface cap layer and for such semi-infinite superlattices in contact with a substrate. The response functions necessary for these studies are given in the Appendix.

II. THE MODEL

The superlattice is formed out of an infinite repetition of two different slabs, labeled by the unit-cell index n. Each of these slabs of width d_i is labeled by the index $i=1$ or 2, within the unit cell n. All the interfaces are taken to be parallel to the (x_1,x_2) plane. A space position along the x_3 axis in medium i belonging to the unit cell n is indicated by (n,i,x_3), where $-d_i/2\le x_3\le d_i/2$. The period of the superlattice is called $D=d_1+d_2$.

We limit ourselves to the simplest case of shear horizontal vibrations where the field displacements $u_2(x_3)$ are along the axis x_2 and the wave vector $\mathbf{k}_{\parallel}$ (parallel to the interfaces) is directed along the x_1 axis. We can then consider with the same general equations the two follow-

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ing cases.

(i) A superlattice built out of cubic crystals with (001) interfaces and $\mathbf{k}_\parallel$ along the [100] crystallographic direction. The corresponding bulk equation of motion for medium i is[2]

$$\left[\rho^{(i)}\omega^2-k_\parallel^2C_{44}^{(i)}+C_{44}^{(i)}\frac{d^2}{dx_3^2}\right]u_2(x_3)=0 , \quad (1)$$

where $\rho^{(i)}$ and $C_{44}^{(i)}$ are, respectively, the mass density and the elastic constant and ω is the frequency of the vibrations.

(ii) A superlattice built out of hexagonal crystals with (0001) interfaces. The isotropy of these interfaces enables us to choose $\mathbf{k}_\parallel$ along any direction within the (x_1,x_2) plane. For simplicity we shall leave $\mathbf{k}_\parallel$ along the x_1 axis. In this case, the bulk equation of motion for medium i becomes[2]

$$\left[\rho^{(i)}\omega^2-k_\parallel^2\left[\frac{C_{11}^{(i)}-C_{12}^{(i)}}{2}\right]+C_{44}^{(i)}\frac{d^2}{dx_3^2}\right]u_2(x_3)=0 , \quad (2)$$

where $C_{11}^{(i)}$, $C_{12}^{(i)}$, and $C_{44}^{(i)}$ are the elastic constants of medium i.

It is well known[2,8] that these transverse waves are not coupled to the other waves polarized in the saggital plane which contains the normal to the interfaces and the vector $\mathbf{k}_\parallel$.

We also took advantage of the infinitesimal translational invariance in directions parallel to the interfaces and Fourier analyzed the equations of motion and all operators according to, for example,

$$g(\omega|\mathbf{x},\mathbf{x}')=\int\frac{d^2k_\parallel}{(2\pi)^2}g(\omega,\mathbf{k}_\parallel|x_3,x_3')e^{i\mathbf{k}_\parallel(\mathbf{x}_\parallel-\mathbf{x}_\parallel')} , \quad (3)$$

where $\mathbf{x}_\parallel\equiv(x_1,x_2)$ is the component parallel to the interfaces of the real-space position $\mathbf{x}$. In the following, we shall drop for simplicity the ω and $k_\parallel$ dependences of the functions g.

Let us define

$$\alpha_i^2=k_\parallel^2-\rho^{(i)}\frac{\omega^2}{C_{44}^{(i)}} \quad (4)$$

for the cubic crystals and

$$\alpha_i^2=k_\parallel^2\left[\frac{C_{11}^{(i)}-C_{12}^{(i)}}{2C_{44}^{(i)}}\right]-\rho^{(i)}\frac{\omega^2}{C_{44}^{(i)}} \quad (5)$$

for the hexagonal ones. Then, as mentioned above, Eqs. (1) and (2) have the same expression,

$$\left[\frac{d^2}{dx_3^2}-\alpha_i^2\right]u_2(x_3)=0 . \quad (6)$$

The corresponding bulk response function for medium i is defined by

$$\left[\frac{d^2}{dx_3^2}-\alpha_i^2\right]G_i(x_3-x_3')=\delta(x_3-x_3') . \quad (7)$$

The response functions associated to the different heterostructures considered here are defined in the same manner taking into account the appropriate boundary conditions.[12,13] We shall give their expressions in the Appendix as they are interesting by themselves for the study of many other physical properties.

Let us recall[8] that the implicit expression giving the bulk dispersion relations of such an infinite superlattice is

$$\cos(k_3D)=C_1C_2+\tfrac{1}{2}\left[\frac{F_1}{F_2}+\frac{F_2}{F_1}\right]S_1S_2 , \quad (8)$$

where

$$C_i=\cosh(\alpha_i di) , \quad (9)$$

$$S_i=\sinh(\alpha_i d_i) , \quad (10)$$

$$F_i=\alpha_i C_{44}^{(i)} , \quad (11)$$

and k_3 is the component perpendicular to the slabs of the propagation vector $\mathbf{k}\equiv(\mathbf{k}_\parallel,k_3)$.

III. DENSITY OF STATES

Knowing the response functions given in the Appendix, one obtains for a given value of $\mathbf{k}_\parallel$ the local and total density of states for a semi-infinite superlattice with a surface cap layer. We shall indicate at the end of this section how one can obtain from these quantities similar results for two limiting cases, namely the case of the interface between a superlattice and a homogeneous substrate, and that of a semi-infinite superlattice without a cap layer.

A. The local densities of states

The local densities of states on the plane (n,i,x_3) are given by

$$n(\omega^2,k_\parallel;n,i,x_3)=-\frac{\rho^{(i)}}{\pi}\text{Im}d^+(\omega^2,k_\parallel;n,i,x_3;n,i,x_3) \quad (12)$$

where

$$d^+(\omega^2)=\lim_{\varepsilon\to 0}d(\omega^2+i\varepsilon) \quad (13)$$

and $d(\omega^2)$ is the response function whose elements are given in the Appendix. The density of states can also be given as a function of ω, instead of ω^2, using the well-known relation $n(\omega)=2\omega n(\omega^2)$. From the elements of the response function given in the Appendix, we obtained the following explicit expressions for the local densities of states on the surface of the semi-infinite superlattice with a cap layer ($n=0$, $i=0$) of width d_0,

$$n_s\left[\omega^2,k_\parallel;0,0,\frac{d_0}{2}\right]=-\frac{1}{\pi}\text{Im}\left[\frac{C_1S_2}{F_2}+\frac{C_2S_1}{F_1}+\frac{S_0}{F_0C_0}\left[C_1C_2+\frac{F_1}{F_2}S_1S_2-t\right]\right]\Delta^{-1} , \quad (14)$$

where C_0, S_0, F_0 have the same definitions as C_i, S_i, F_i given by Eqs. (9)–(11) for $i=0$,

$$t=\begin{cases}\eta+(\eta^2-1)^{1/2}\,, & \eta<-1\\ \eta+i(1-\eta^2)^{1/2}\,, & -1<\eta<+1\\ \eta-(\eta^2-1)^{1/2}\,, & \eta>1\end{cases} \tag{15a}$$

with

$$\eta=C_1C_2+\tfrac{1}{2}\left[\frac{F_1}{F_2}+\frac{F_2}{F_1}\right]S_1S_2 \tag{15b}$$

and

$$\Delta=C_1C_2+\frac{F_2}{F_1}S_1S_2-t^{-1}-\frac{F_0S_0}{C_0}\left[\frac{C_1S_2}{F_2}+\frac{C_2S_1}{F_1}\right]. \tag{16}$$

In the same manner the local density of states at the interface between the cap layer and the semi-infinite superlattice was found to be

$$n_i\left[\omega^2,k_\parallel;0,0,-\frac{d_0}{2}\right]=-\frac{1}{\pi}\mathrm{Im}\left[\frac{C_1S_2}{F_2}+\frac{C_2S_1}{F_1}\right]\Delta^{-1}. \tag{17}$$

B. The total density of states

The total density of states for a given value of $k_\parallel$ is obtained by integrating over x_3 and summing on n and i the local density $n(\omega^2,k_\parallel;n,i,x_3)$. A particularly interesting quantity is the variation of the total density of states between the semi-infinite superlattice with the cap layer $n=0$ and the infinite superlattice having the same number of slabs as the semi-infinite superlattice without the cap layer. This variation $\Delta n(\omega^2)$ can be written as the sums of the variations $\Delta_1 n(\omega^2)$ and $\Delta_2 n(\omega^2)$ of the density of states in slabs 1 and 2 and the density of states $n_0(\omega^2)$ inside the cap layer

$$\Delta n(\omega^2)=\Delta_1 n(\omega^2)+\Delta_2 n(\omega^2)+n_0(\omega^2) \tag{18}$$

where

$$\Delta_1 n(\omega^2)=\frac{-\rho^{(1)}}{\pi}\sum_{n=-\infty}^{0}\mathrm{Im}\int_{-d_1/2}^{+d_1/2}[d(n,1,x_3;n,1,x_3)-g(n,1,x_3;n,1,x_3)]dx_3\,, \tag{19}$$

$$\Delta_2 n(\omega^2)=\frac{-\rho^{(2)}}{\pi}\sum_{n=-\infty}^{-1}\mathrm{Im}\int_{-d_2/2}^{+d_2/2}[d(n,2,x_3;n,2,x_3)-g(n,2,x_3;n,2,x_3)]dx_3\,, \tag{20}$$

$$n_0(\omega^2)=\frac{-\rho^{(0)}}{\pi}\mathrm{Im}\int_{-d_0/2}^{+d_0/2}d(0,0,x_3;0,0,x_3)dx_3 \tag{21}$$

and d and g are the response functions of, respectively, the semi-infinite superlattice with the cap layer and of the infinite superlattice. With the help of the explicit expressions of these response functions given in the Appendix we obtained

$$\Delta_1 n(\omega^2)=\frac{-\rho^{(1)}}{\pi}\mathrm{Im}\frac{t}{(t^2-1)^2}\left\{\frac{S_1}{\alpha_1F_1}\left[C_2S_1+\tfrac{1}{2}C_1S_2\left[\frac{F_1}{F_2}+\frac{F_2}{F_1}\right]\right]+\frac{d_1S_2}{2F_2}\left[1-\frac{F_2^2}{F_1^2}\right]\right\}\frac{Y}{\Delta}\,, \tag{22}$$

$$\Delta_2 n(\omega^2)=\frac{-\rho^{(2)}}{\pi}\mathrm{Im}\frac{t^2}{(t^2-1)^2}\left\{\frac{S_2}{\alpha_2F_2}\left[C_1S_2+\tfrac{1}{2}C_2S_1\left[\frac{F_1}{F_2}+\frac{F_2}{F_1}\right]\right]+\frac{d_2S_1}{2F_1}\left[1-\frac{F_1^2}{F_2^2}\right]\right\}\frac{Y}{\Delta}\,, \tag{23}$$

$$n_0(\omega^2)=\frac{-\rho^{(0)}}{2\pi}\mathrm{Im}\left\{\frac{S_0}{\alpha_0C_0}\left[\frac{C_1S_2}{F_2}+\frac{C_2S_1}{F_1}\right]+d_0\left[\left[C_1C_2+\frac{F_1}{F_2}S_1S_2-t\right]\frac{S_0}{F_0C_0}+\frac{C_1S_2}{F_2}+\frac{C_2S_1}{F_1}\right]\right\}\frac{1}{\Delta}\,, \tag{24}$$

where

$$Y=C_2-C_1t-\frac{F_0S_0}{C_0}\left[\frac{S_1}{F_1}t+\frac{S_2}{F_2}\right]. \tag{25}$$

At the limits of the bulk bands of the superlattice given by $t(\omega_0)=\pm 1$, an expansion to first order in $(\omega-\omega_0)$ provides

$$\frac{t}{(t^2-1)^2}=\tfrac{1}{8}\left[\left[\frac{d\eta}{d\omega}\right]_{\omega_0}\right]^{-1}\left[P\left[\frac{1}{\omega-\omega_0}\right]-i\pi\delta(\omega-\omega_0)\right] \tag{26}$$

and then

$$\Delta_1 n(\omega)+\Delta_2 n(\omega)=-\tfrac{1}{4}\delta(\omega-\omega_0)\,. \tag{27}$$

So, the creation of a semi-infinite superlattice from an infinite one gives rise to δ peaks of weight $(-\frac{1}{4})$ in the density of states at the edges of the superlattice bulk bands.

C. Localized states

When the denominator of $\Delta n(\omega^2)$ vanishes for a frequency lying inside the gaps of the infinite superlattice, one obtains localized states within the cap layer which decay exponentially inside the bulk of the superlattice. The explicit expression giving these localized states is

$$C_1S_2\left[\frac{F_0}{F_2}\frac{S_0}{C_0}-\frac{F_2}{F_0}\frac{C_0}{S_0}\right]+S_1S_2\left[\frac{F_1}{F_2}-\frac{F_2}{F_1}\right]+C_2S_1\left[\frac{F_0}{F_1}\frac{S_0}{C_0}-\frac{F_1}{F_0}\frac{C_0}{S_0}\right]=0 \quad (28)$$

together with the condition

$$\left|C_1C_2+\frac{F_2}{F_1}S_1S_2-\frac{F_0S_0}{C_0}\left[\frac{C_1S_2}{F_2}+\frac{C_2S_1}{F_1}\right]\right|>1\ . \quad (29)$$

D. The limit of a semi-infinite superlattice without a cap layer

In the limit when the thickness d_0 of the cap layer goes to zero, $S_0 \to 0$ and the above results (14), (22), (23), (27), (28), and (29) remain valid for a semi-infinite superlattice ending with a complete $i=1$ surface layer. We remark on Eq. (24) that in this limit, $n_0(\omega)$ vanishes.

In the limit where the cap layer $i=0$ is of the same nature as the $i=2$ superlattice layer and $d_0=d_s<d_2$, the same results provide the localized modes for a semi-infinite superlattice ending with an incomplete $i=2$ surface layer. In this case, we can calculate the variation of the density of states between such a semi-infinite superlattice and the same amount of the bulk superlattice, using in Eq. (18) $\Delta_2 n(\omega^2)$ integrated to $d_s/2$ rather than to $d_2/2$ in the last layer, and taking $n_0(\omega^2)=0$.

A particularly interesting result can be obtained when cleaving an infinite superlattice for the variation $\Delta n_c(\omega^2)$ of the total density of states between the two complementary semi-infinite superlattices and the infinite one. It is possible to show by using standard transformation of the trace of the response functions[13] that $\Delta n_c(\omega^2)$ can be obtained from the knowledge of the elements

$d_1(0,2,d_s;0,2,d_s)$ and $d_2(0,2,d_s;0,2;d_s)$

of the surface response function of the two complementary semi-infinite superlattices, namely,

$$\Delta n_c(\omega^2)=\frac{1}{\pi}\frac{d}{d\omega^2}\text{Im}\ln\det[d_1(0,2,d_s;0,2,ds)+d_2(0,2,d_s;0,2,d_s)]\ . \quad (30)$$

Using the expressions given in the Appendix for these elements of the response functions, one finds that $\Delta n_c(\omega^2)$ is zero inside the bulk bands of the superlattice and that at all edges of these bulk bands $\Delta n_c(\omega^2)$ display δ functions of weight $(-\frac{1}{2})$. These two facts, together with the necessary conservation of the number of states, enable us to conclude that when one considers together the two semi-infinite superlattices obtained by the cleavage of an infinite one, one has as many localized surface modes as minigaps for each value of $\mathbf{k}_\parallel$. There is only one very special exception to this general rule for a cleavage done along a plane situated exactly in the middle of a given slab.

E. The limit of an interface between a semi-infinite superlattice and an homogeneous substrate

When the thickness d_0 of the cap layer goes to infinite, $S_0/C_0 \to 1$ in the above expressions which remains valid and enables us to study the interface between a semi-infinite superlattice and an homogeneous semi-infinite substrate. In particular, the results of Eqs. (28) and (29) remain valid in this limit giving the localized interface states, (27) giving δ peaks of weight $(-\frac{1}{4})$ at the edges of the superlattice bulk bands with (22) and (23) giving the variation of the density of states within the space of the superlattice. Within the space of the semi-infinite substrate, rather than $n_0(\omega^2)$ we shall calculate the variation $\Delta_0 n(\omega^2)$ of the density of states between the substrate in contact with the superlattice and the same volume of the infinite substrate, namely

$$\Delta_0 n(\omega^2)=\frac{-\rho^{(0)}}{\pi}\text{Im}\int_0^\infty[d_0(x_3,x_3)-G_0(x_3,x_3)]dx_3\ , \quad (31)$$

where

$$d_0(x_3,x_3')=\frac{-1}{2F_0}e^{-\alpha_0|x_3-x_3'|}+\left[\frac{1}{2F_0}+\frac{1}{\Delta_0}\left[\frac{C_1S_2}{F_2}+\frac{C_2S_1}{F_1}\right]\right]\times e^{-\alpha_0(x_3+x_3')}\ , \quad (32)$$

$$\Delta_0=C_1C_2+\frac{F_2}{F_1}S_1S_2-t^{-1}-F_0\left[\frac{C_1S_2}{F_2}+\frac{C_2S_1}{F_1}\right]\ , \quad (33)$$

and

$$G_0(x_3,x_3')=-\frac{1}{2\alpha_0C_{44}^{(0)}}e^{-\alpha_0|x_3-x_3'|}\ . \quad (34)$$

We obtained like that

$$\Delta_0 n(\omega^2)=\frac{-\rho^{(0)}}{\pi}\times\text{Im}\left\{\frac{1}{2\alpha_0}\left[\frac{1}{2F_0}+\frac{1}{\Delta_0}\left[\frac{C_1S_2}{F_2}+\frac{C_2S_1}{F_1}\right]\right]\right\}\ . \quad (35)$$

Here also it is interesting to calculate the variation of the density of states $\Delta^{(1)}n_I(\omega^2)$ between the semi-infinite superlattice and substrate on one hand and these same elements but coupled. $\Delta^{(1)}n_I(\omega^2)$ can be obtained in the same manner as above [Eq. (30)] but with $d_2(0,2,d_s;0,2,d_s)$ now being the surface element of the response function of a semi-infinite homogeneous substrate. Consider now the semi-infinite superlattice complementary to the one above, in the same cleavage of an infinite superlattice and calculate as above the variation of the density of states $\Delta^{(2)}n_I(\omega^2)$ between this complementary semi-infinite superlattice and the above substrate, on one hand, and these same elements but coupled. Such calculations provide one exact result, namely that the sum of the variation of the density of states of the two complementary systems $\Delta n_{IC}(\omega^2)=[\Delta^{(1)}n_I(\omega^2)+\Delta^{(2)}n_I(\omega^2)]$ is zero for ω belonging at the same time to the substrate and superlattice bulk bands. Bearing in mind the result of Sec. III D regarding the existence of surface states on these two complementary semi-infinite superlattices, we can now expect resonances, associated with the superlattice-substrate interface, which fall within the superlattice gaps and inside the bulk band of the substrate.

IV. APPLICATIONS AND DISCUSSIONS OF THE RESULTS

In what follows, specific results will be given for Y-Dy (Ref. 14) or GaAs-AlAs superlattices and also for this last superlattice with a Si surface cap layer. Tables I and II give the numerical values of the elastic constants and of the mass densities of these crystals.

We shall first consider (Sec. IV A) semi-infinite superlattices, then (Sec. IV B) semi-infinite superlattices with a surface cap layer and finally (Sec. IV C) semi-infinite superlattices on a semi-infinite homogeneous substrate. All the specific results presented here are given for transverse elastic waves with polarization perpendicular to the saggital plane containing the normal to the interfaces and the propagation vector $\mathbf{k}_\parallel$ parallel to the interfaces.

A. Semi-infinite superlattices

The applications presented here refer to a GaAs-AlAs superlattice with $d_1=d_2$ and period $D=d_1+d_2$. Figure 1 gives the dispersion of bulk bands and surface modes as a function of $k_\parallel D$. We have represented the surface modes of the two complementary semi-infinite superlattices obtained by cleaving the infinite GaAs-AlAs superlattice within one GaAs slab, such that the thickness of the remaining surface GaAs layer is, respectively, $d_s=0.3d_2$ and $d_s=0.7d_2$ in each semi-infinite part. As demonstrated in Sec. III D, one obtains as many surface states as gaps and moreover there is one surface state in each gap associated with either one or the other of the complementary semi-infinite superlattices. One can observe that the surface modes are very dependent on the thickness of the last surface layer of GaAs. We shall come back to this point in the discussion of Fig. 3.

For the moment, let us show in Fig. 2, for $k_\parallel D=6$, the variation of the vibrational density of states between the semi-infinite superlattice terminated by a GaAs layer of width $d_s=0.7d_2$ and the same amount of the bulk superlattice, as defined in Sec. III D. The δ functions appearing in this figure are enlarged by the addition of a small imaginary part to the frequency ω. The δ functions associated with the surface localized states are noted as L_i and the δ functions of weight $(-\frac{1}{4})$ situated, respectively, at the bottom and top of the bulk bands are called B_i and T_i. The form of these enlarged δ functions B_i and T_i of weight $(-\frac{1}{4})$ are not exactly the same because of the contributions coming from the divergences in $(\omega-\omega_{T_i})^{-1/2}$ or $(\omega-\omega_{B_i})^{-1/2}$ existing in the density of states in one di-

TABLE I. Elastic constants and mass densities of Y and Dy.

	C_{11} ($\times 10^{10}$ N/m^2)	C_{12} ($\times 10^{10}$ N/m^2)	C_{44} ($\times 10^{10}$ N/m^2)	ρ (kg/m^3)
Y	7.79	2.85	2.431	4450
Dy	7.31	2.53	2.40	8560

TABLE II. Elastic constants and mass densities of GaAs, AlAs, and Si.

	C_{44} ($\times 10^{10}$ N/m^2)	ρ (kg/m^3)
GaAs	5.94	5316.9
AlAs	5.42	3721.8
Si	7.96	2330

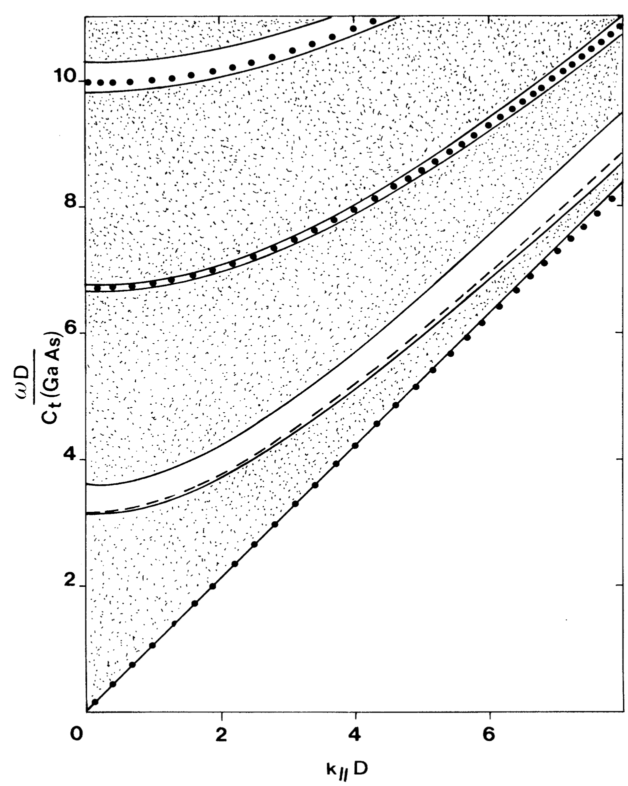

FIG. 1. Bulk and surface transverse elastic waves in a GaAs-AlAs superlattice. The curves give $\omega D/C_t$ (GaAs) as a function of $k_\parallel D$, where ω is the frequency, $k_\parallel$ the propagation vector parallel to the interfaces, C_t(GaAs) the transverse speed of sound in GaAs, and $D=d_1+d_2$ the period of the superlattice. The shaded areas represent the bulk bands. The dotted lines represent the surface phonons for the semi-infinite superlattice terminated by a GaAs layer of thickness $d_s=0.7d_2$. The dashed lines represent the surface phonons for the complementary superlattice terminated by a GaAs layer of thickness $d_s=0.3d_2$.

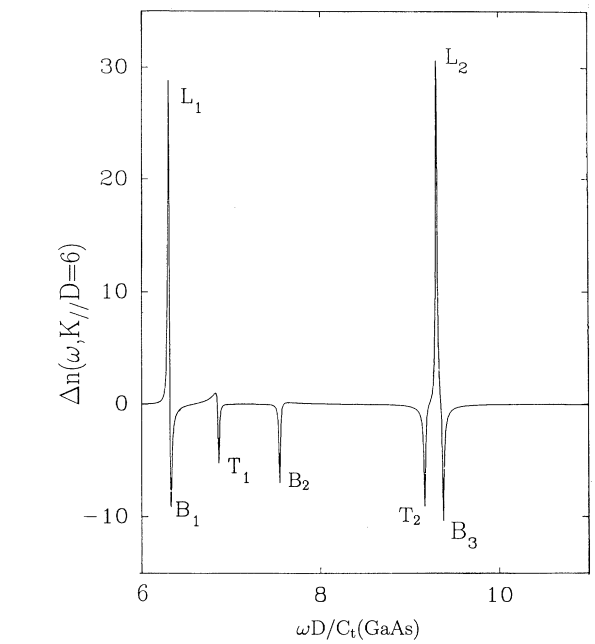

FIG. 2. Variation of the density of states in units of D/C_t (GaAs) between a semi-infinite GaAs-AlAs superlattice terminated by a GaAs layer of width $d_s=0.7d_2$ and the same amount of a bulk superlattice, for $k_\parallel D=6$ and as a function of $\omega D/C_t$(GaAs). B_i and T_i, respectively, refer to δ peaks of weight $(-\frac{1}{4})$ situated at the bottom and the top of the bulk bands and L_i indicates the localized surface modes.

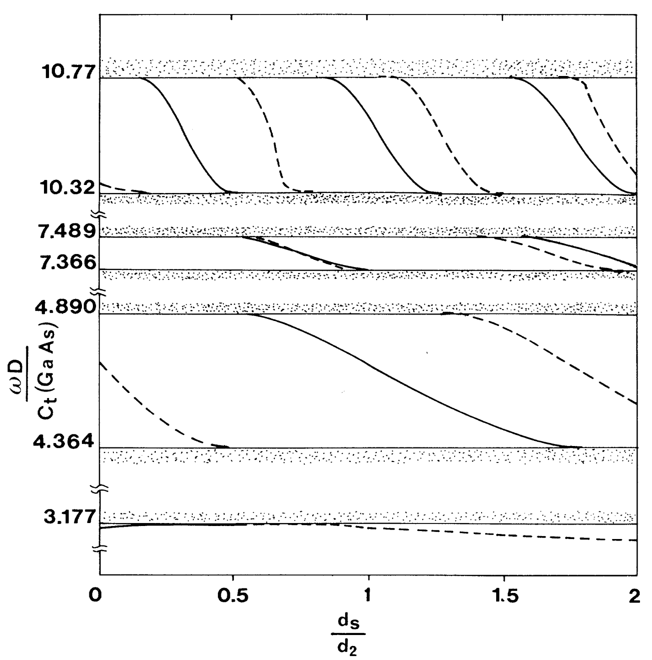

FIG. 3. Variation of the dimensionless frequencies $\omega D/C_t$ (GaAs) of the surface modes of semi-infinite GaAs-AlAs superlattices, for $K_\parallel D=3$, as a function of d_s/d_2, where d_s is the width of the surface layer which may be GaAs (dashed lines) or AlAs (full lines). The shaded areas show the first three bulk bands of the superlattice.

mension. Apart from the above δ peaks and the particular behavior near the band edges, the variation $\Delta n(\omega,k_\parallel)$ of the density of states does not show any other significant effect inside the bulk bands of the superlattice.

Having seen that the frequencies of the surface states is very sensitive to the width d_s of the last surface layer, we present in Fig. 3 the variation of these frequencies, for $K_\parallel D=3$, as a function of d_s/d_2, as well for a surface GaAs layer (dashed lines) as for a surface AlAs layer (full lines). One sees in this figure, for $d_s/d_2\leq 1$, that for all combinations of two complementary superlattices such that $d_{s1}+d_{s2}=d_2$, one always has a surface state in each gap. Let us also note that the same frequency of a surface state reappears with a given periodicity when d_s/d_2 takes values greater than one. When d_s increases, the frequencies of the existing surface modes decrease until the corresponding branches merge into the bulk bands and become resonant states; at the same time new localized branches are extracted from the bulk bands. However, the resonant modes remain well-defined features of the density of states only as far as their frequencies remain in the vicinity of the band edges. Raman investigations of superlattice surface states as a function of the width of the surface layer appeared recently[15] for capped amorphous Ge/SiO superlattices.

B. Semi-infinite superlattices with a surface cap layer

Now we assume that a cap layer of Si, of thickness d_0, is deposited on top of the GaAs-AlAs superlattice terminated by a full GaAs layer. The dispersion of localized and resonant modes induced by a cap layer of relative width $d_0/D=4$ is presented in Fig. 4. Depending on their frequencies, these modes may propagate along the direction perpendicular to the interfaces in both the superlattice and the cap layer, or propagate in one and decay in the other, or decay on both sides of the superlattice-adlayer interface. The interface localized modes corresponding to this last case are labeled by the index i in Fig. 4. Note that when the Si cap layer is deposited on a AlAs layer of the superlattice, different localized and resonant modes appear.[16]

The variation of the density of states $\Delta n(\omega)$ between this superlattice with the Si cap layer and the same amount of the bulk superlattice without the cap layer was calculated as explained in Sec. III B. This $\Delta n(\omega)$ is plotted in Fig. 5, for $k_\parallel D=3$, as a function of $\omega D/C_t$(GaAs). B_i and T_i here also refer to δ peaks of weight $(-\frac{1}{4})$ at the edges of the superlattice bulk bands; L_i and R_i, respectively, indicate the localized and resonant modes induced by the Si cap layer. The most intense resonance R_2 is the lowest one situated just above the Si sound line. The next resonances are less intense, especially at higher frequencies where the separations between the successive branches increase.

With the help of Eqs. (14) and (17), we also studied local densities of states. We found that they change with the position of the plane on which they are calculated. In particular, we found that the local density of states on the surface of the Si adlayer shows the same behavior as the

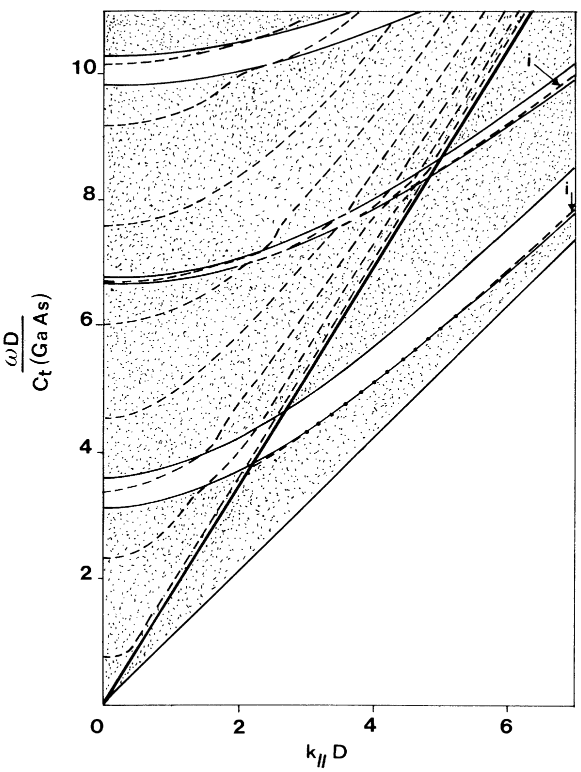

FIG. 4. Dispersion of localized and resonant modes (dashed lines) induced by a Si cap layer of thickness $d_0 = 4D$, deposited on top of the GaAs-AlAs superlattice terminated by a full GaAs layer. The shaded areas are the superlattice bulk bands. The heavy line indicates the bottom of the bulk band of Si. The branches labeled (i) correspond to modes localized at the superlattice-adlayer interface.

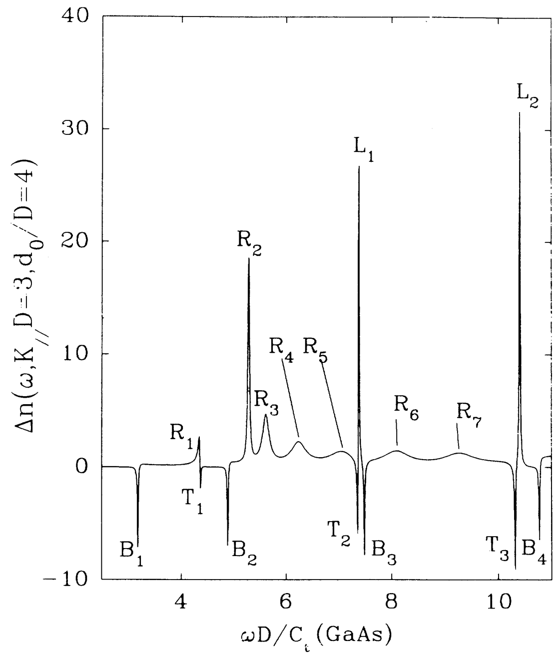

FIG. 5. Density of states [in units of D/C_t(GaAs)] corresponding to the case depicted in Fig. 4, for $k_{\parallel} D = 3$. The contribution of the same amount of the bulk GaAs-AlAs superlattice was subtracted. B_i, T_i, and L_i have the same meaning as in Fig. 2; R_i refers to resonant modes.

total density of states illustrated by Fig. 5. On the contrary, the local density of states at the superlattice-adlayer interface is pretty different. These behaviors can be understood by the very different boundary conditions existing on these two planes.

The frequencies of the localized and resonant modes vary with the thickness d_0 of the cap layer. Figure 6 presents these variations, for $k_{\parallel} D = 1$. The first branches become closer one to each other when d_0 increases, and as a consequence the intensities of the corresponding resonances increase. Let us also notice that the curves in this figure are almost horizontal when a localized branch is going to become resonant by merging into a bulk band. The variation with d_0 is faster when the resonant branch penetrates deep into the band, but then the intensity of the resonant state decreases, or may even vanish in particular when d_0 is small or the frequency is high. Finally, let us mention here too that for any given frequency ω in Fig. 6, there is a periodic repetition of the modes as a function of d_0.

When the thickness d_0 of the cap layer goes to infinite, we find the situation of a semi-infinite superlattice in contact with a homogeneous substrate. We address this case in the next section.

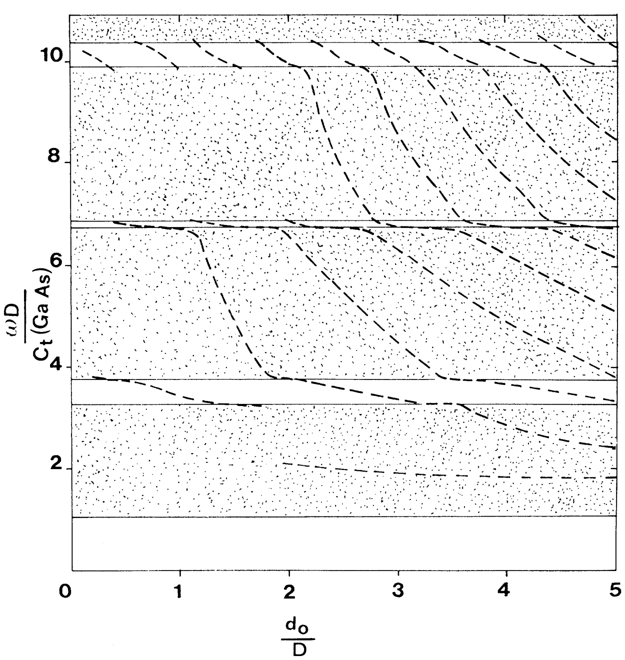

FIG. 6. Dimensionless frequencies $\omega D / C_t$ (GaAs) of the localized and resonant modes induced by a Si cap layer of width d_0 on the semi-infinite GaAs-AlAs superlattice of Fig. 4, for $k_{\parallel} D = 1$.

C. Semi-infinite superlattices on a semi-infinite substrate

The possibility of shear horizontal waves localized at the interface between a superlattice and a substrate was demonstrated before[9] using a transfer-matrix method. Here we show the possibility of resonant modes, associated with this interface, which appear as well-defined features of the density of states. The results will be illustrated, as in Ref. 9, for a Y-Dy superlattice such that $d_1=d_2$ and $D=2d_2$, in contact with a substrate having its transverse speed of sound equal to two times the Dy transverse speed of sound.

In Ref. 9 the existence of localized modes was discussed as a function of the parameter $\gamma=C_{44}^{(s)}/C_{44}^{(\mathrm{Dy})}$ (where the index s refers to the substrate), considering either that a Dy or a Y layer of the superlattice is in contact with the substrate. The interface localized modes originated in general from one of the two following extreme cases: $\gamma=0$ or $\gamma\to\infty$; in the former case the localized modes are those associated with the free surface of the superlattice, whereas in the latter the amplitudes of the vibrations go to zero at the interface and remain vanishingly small in the substrate. To show the interface resonant modes in this section, we present, respectively, in Figs. 7 and 9 two examples in which the elastic constant $C_{44}^{(s)}$ of the substrate takes two very different values, such that $\gamma=C_{44}^{(s)}/C_{44}^{(\mathrm{Dy})}=0.5$ or 4.

(i) Case $\gamma=0.5$. Figure 7 gives the localized and resonant interface modes for both the complementary superlattices in which the substrate is either in contact with a full Y or a full Dy layer. In the former case, the two full lines in the minigaps of the superlattice are localized interface modes which continue (dashed lines) as well defined resonances inside the bulk band of the substrate and within the superlattice minigaps. As the elastic constant $C_{44}^{(s)}$ of the substrate has here a weak value ($\gamma=0.5$), these resonances are close to the surface states of the semi-infinite superlattice ($\gamma=0$). Their intensities, of course, decrease when γ increases.

Now, if the substrate is in contact with a Dy layer, one obtains the dashed-dotted branch near the bottom of the bulk bands, which is partly localized ($k_{\parallel}D\gtrsim 5$) and partly resonant with the superlattice states ($k_{\parallel}D\lesssim 5$). However the dashed lines mentioned in the preceding paragraph are also associated with small resonances in this case.

When one creates the two complementary superlattices used in Fig. 7 from the infinite superlattice and the infinite substrate, the variation of the density of states $\Delta n_{IC}(\omega)$ can again show the new distribution of the states. We have presented such an example in Fig. 8(a), for $k_{\parallel}D=1$: the loss of states due to the δ peaks of weight $-\frac{1}{2}$ at every edge of the bulk bands is mostly compensated by the peaks associated with the resonant states (R_1,R_2,R_3). This compensation can even be observed more easily in Fig. 8(b) showing the variation of the number of states, defined as $\Delta N_{IC}(\omega)=\int_0^{\omega}\Delta n_{IC}(\omega')d\omega'$. One can also check the validity of the statement presented in Sec. III E, namely, that $\Delta n_{IC}(\omega^2)$ is zero for ω belonging at the same time to the substrate and superlattice bulk bands.

(ii) Case $\gamma=4$. In Fig. 9 we have considered the case of a superlattice terminated by a Dy layer. The two localized interface states (full lines) continue by resonances (dashed lines) lying just below the substrate bulk band. They correspond to modes localized on the side of the substrate and progressive on the side of the superlattice. Note also the existence of two other resonances in the minigaps of the superlattice; they are localized on the side of the superlattice and progressive on the side of the substrate. A study of the density of states shows that the resonance appearing in the lowest superlattice minigap is as wide in frequency as the gap and is less sharp than the resonance lying in the second minigap. The frequencies of these last two resonances are rather closed to those of the localized modes appearing on the surface of this superlattice in the limit $\gamma\to\infty$ (Ref. 9) (this imposes on the displacements to vanish on this surface). When γ decreases, the intensities of these resonances decrease and their widths increase over the whole minigaps.

Now if the substrate is in contact with a Y layer, the

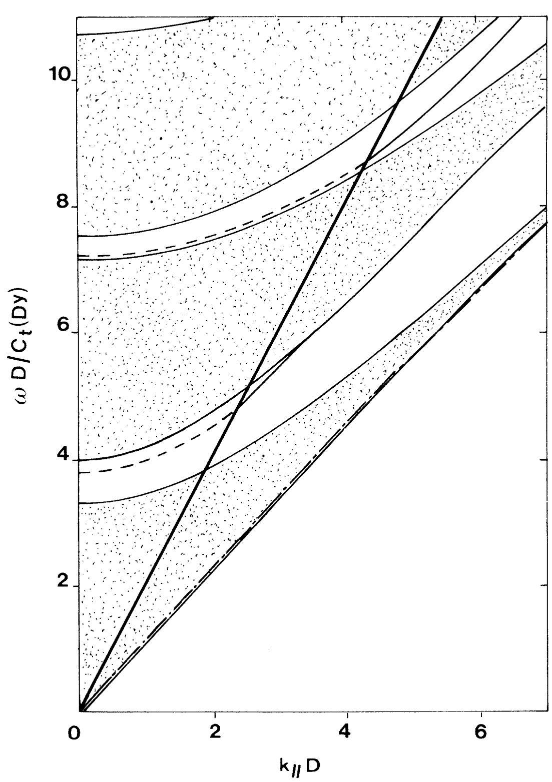

FIG. 7. Interface localized and resonant modes associated with the two complementary Y-Dy superlattices in which the substrate is either in contact with a Y or a Dy layer. The shaded areas are the bulk bands of the superlattice. The heavy straight line indicates the bottom of the substrate bulk band. The parameters of the substrate are defined as $C_t^{(s)}=2C_t^{(\mathrm{Dy})}$ and $\gamma=C_{44}^{(s)}/C_{44}^{(\mathrm{Dy})}=0.5$. When the superlattice terminates with a Y layer, the localized (respectively, resonant) modes are presented by the full (respectively, dashed) lines. The dashed-dotted line is an interface branch associated with a Dy termination of the superlattice.

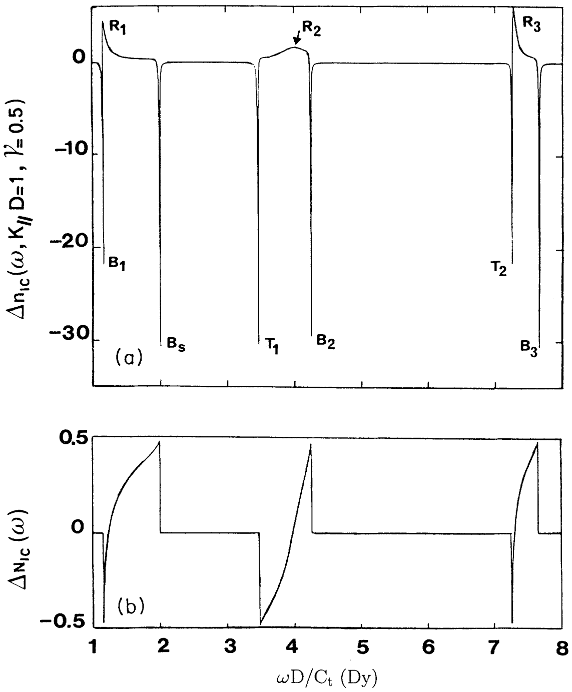

FIG. 8. Variation of the density of states (a) and of the number of states (b), at $K_\parallel D=1$, for the two complementary superlattices of Fig. 7 created from the infinite superlattice and the infinite substrate. B_i and T_i have the same meaning as in Fig. 2, whereas B_s refers to the δ peak of weight $(-\frac{1}{2})$ situated at the bottom of the substrate bulk band.

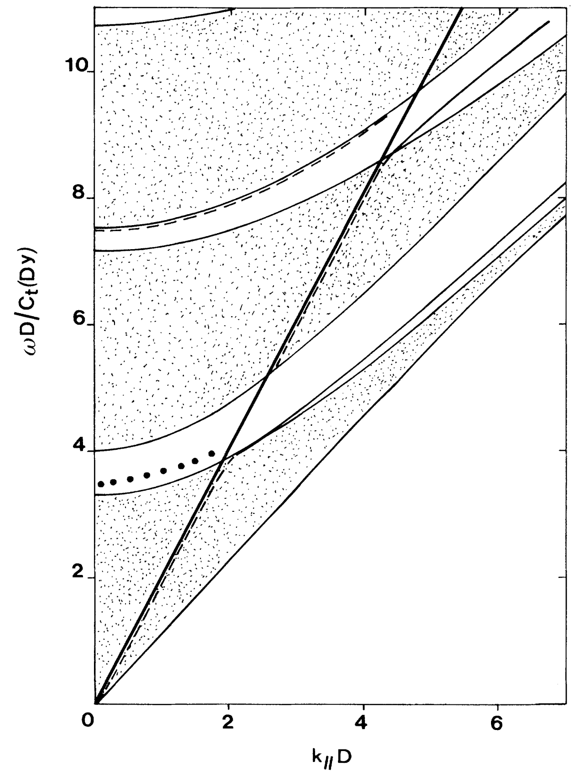

FIG. 9. Interface localized and resonant modes, as in Fig. 7, but for a substrate such that $C_{44}^{(s)}=4C_{44}^{(\mathrm{Dy})}$ and $C_t^{(s)}=2C_t^{(\mathrm{Dy})}$ in contact with a Dy slab of the superlattice.

dashed curves in Fig. 9 still correspond to interface resonant states, which are however less intense than in the case of a superlattice with Dy termination. (The localized modes are, however, different from those presented in Fig. 9.)

In the above discussions, the resonances were defined as peaks in the density of states of the whole system. It is worth mentioning that these features do not necessarily appear in the local density of states at the superlattice-substrate interface. This especially happens when the stiffness of the substrate (parameter γ) is high; indeed, in this case, the frequencies of the resonant modes are practically the same as in the case $\gamma\rightarrow\infty$, but the Green's function (and therefore the local density of states) at the superlattice-substrate interface vanish exactly at the latter frequencies.

V. CONCLUSION

This paper has presented an analytical study of the density of transverse elastic waves for semi-infinite superlattices, for superlattices with a cap layer, and for semi-infinite superlattices in contact with a substrate. Particular attention was devoted to resonances (also called leaky waves) appearing in such heterostructures and to their relations with the localized modes. It was demonstrated in particular that when one considers together the two semi-infinite superlattices obtained by cleavage of an infinite one along a plane parallel to the interfaces, as many localized surface states as minigaps exist for all values of $\mathbf{k}_\parallel$. An extension of these studies to waves polarized in the saggital plane will probably reveal even more interesting resonances.

As a final remark, let us emphasize that the calculations presented here for the transverse elastic waves can be transposed straightforwardly to the electronic structure of superlattices in the effective-mass approximation,[17] or to the propagation of polaritons[18] in these heterostructures when each constituent is characterized by a local dielectric constant $\varepsilon(\omega)$. This is because both the equations of motion and the boundary conditions in the above problems involve similar mathematical equations. Therefore, the general behavior and conclusions obtained in this paper will prove to be useful for the two other physical problems.

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APPENDIX: SUPERLATTICE RESPONSE FUNCTIONS

Following the interface response theory,[13,18] we obtained the following.

1. For the infinite superlattice

(a) The elements $g(m,m')$, where $m\equiv(n,i,\pm d_i/2)$ of the response function g between the different interface planes, as functions of C_i, S_i, F_i, t, and η [Eqs. (9)–(11) and (15)], are

$$g\left[n,1,-\frac{d_1}{2};n',1,-\frac{d_1}{2}\right]=\left[\frac{C_1S_2}{F_2}+\frac{C_2S_1}{F_1}\right]\times\frac{t^{|n-n'|+1}}{t^2-1}, \tag{A1}$$

$$g\left[n,1,-\frac{d_1}{2};n',1,+\frac{d_1}{2}\right]=\frac{S_2}{F_2}\frac{t^{|n-n'|+1}}{t^2-1}+\frac{S_1}{F_1}\frac{t^{|n-n'-1|+1}}{t^2-1}, \tag{A2}$$

$$g\left[n,1+\frac{d_1}{2};n',1,-\frac{d_1}{2}\right]=\frac{S_2}{F_2}\frac{t^{|n-n'|+1}}{t^2-1}+\frac{S_1}{F_1}\frac{t^{|n-n'+1|+1}}{t^2-1}, \tag{A3}$$

$$g\left[n,1,+\frac{d_1}{2};n',1,+\frac{d_1}{2}\right]=\left[\frac{C_1S_2}{F_2}+\frac{C_2S_1}{F_1}\right]\times\frac{t^{|n-n'|+1}}{t^2-1}. \tag{A4}$$

(b) The element of this response function between any two points of the infinite superlattice was found to be

$$g(n,i,x_3;n',i',x_3')=\delta_{nn'}\delta_{ii'}U_i(x_3,x_3')+\frac{1}{S_iS_{i'}}\left\{\sinh\left[\alpha_i\left[\frac{d_i}{2}-x_3\right]\right];\sinh\left[\alpha_i\left[\frac{d_i}{2}+x_3\right]\right]\right\}g(M_m,M_{m'})\times\begin{bmatrix}\sinh\left[\alpha_{i'}\left[\frac{d_{i'}}{2}-x_3'\right]\right]\\ \sinh\left[\alpha_{i'}\left[\frac{d_{i'}}{2}+x_3'\right]\right]\end{bmatrix}, \tag{A5}$$

where

$$U_i(x_3,x_3')=-\frac{1}{2F_i}\exp[-\alpha_i|x_3-x_3'|]+\frac{1}{2F_iS_i}\left\{\sinh\left[\alpha_i\left[\frac{d_i}{2}-x_3'\right]\right]\exp\left[-\alpha_i\left[\frac{di}{2}+x_3\right]\right]+\sinh\left[\alpha_i\left[\frac{d_i}{2}+x_3'\right]\right]\exp\left[-\alpha_i\left[\frac{di}{2}-x_3\right]\right]\right\}. \tag{A6}$$

In Eq. (A5) the last three terms are the product of a (1×2) matrix by the $g(M_m,M_{m'})$ (2×2) matrix and by a (2×1) matrix. $g(M_m,M_{m'})$ is the (2×2) matrix formed out of the elements given by Eqs (A1)–(A4), for $m=(n,1,\pm d_1/2)$ and $m'=(n',1,\pm d_1/2)$.

2. For the semi-infinite superlattice with a surface cap layer

The semi-infinite superlattice with a surface cap layer under consideration here is terminated by the unit cell $n=0$ formed of a surface layer $i=0$ of width d_0 deposited on the $i=1$ layer of the semi-infinite superlattice. The underneath unit cell $n=-1$ is formed out of the $i=2$ and then the $i=1$ layers of the superlattice and so on.

(a) In this paper, we need the following elements of the response function d between different interface planes:

$$d\left[0,0-\frac{d_0}{2};0,0,\frac{d_0}{2}\right]=d\left[0,0,\frac{d_0}{2};0,0,-\frac{d_0}{2}\right]=\frac{1}{C_0\Delta}\left[\frac{C_1S_2}{F_2}+\frac{C_2S_1}{F_1}\right], \tag{A7}$$

$$d\left[0,0,\frac{d_0}{2};0,0,\frac{d_0}{2}\right]=\frac{1}{\Delta}\left[\frac{C_1S_2}{F_2}+\frac{C_2S_1}{F_1}+\frac{S_0}{F_0C_0}\left[C_1C_2+\frac{F_1}{F_2}S_1S_2-t\right]\right], \tag{A8a}$$

$$d\left[0,0,-\frac{d_0}{2};0,0,-\frac{d_0}{2}\right]=\frac{1}{\Delta}\left[\frac{C_1S_2}{F_2}+\frac{C_2S_1}{F_1}\right], \tag{A8b}$$

and for n and $n'\le 0$ and $i\neq0$,

$$d\left[n,1,-\frac{d_1}{2};n',1,-\frac{d_1}{2}\right]=\frac{t}{t^2-1}\left\{\left[\frac{C_1S_2}{F_2}+\frac{C_2S_1}{F_1}\right]t^{|n-n'|}-t^{-n-n'}\left[\frac{S_1t}{F_1}+\frac{S_2}{F_2}\right]\frac{Y}{\Delta}\right\}, \tag{A9}$$

$$d\left[n,1,-\frac{d_1}{2};n',1,\frac{d_1}{2}\right]=\frac{t}{t^2-1}\left\{\frac{S_2t^{|n-n'|}}{F_2}+\frac{S_1t^{|n-n'-1|}}{F_1}-t^{-n-n'}\left[\frac{C_1S_2}{F_2}+\frac{C_2S_1}{F_1}\right]\frac{Y}{\Delta}\right\}, \tag{A10}$$

$$d\left[n,1,\frac{d_1}{2};n',1,-\frac{d_1}{2}\right]=\frac{t}{t^2-1}\left\{\frac{S_2t^{|n-n'|}}{F_2}+\frac{S_1t^{|n-n'+1|}}{F_1}-t^{-n-n'}\left[\frac{C_1S_2}{F_2}+\frac{C_2S_1}{F_1}\right]\frac{Y}{\Delta}\right\}, \tag{A11}$$

$$d\left[n,1,\frac{d_1}{2};n',1,\frac{d_1}{2}\right]=\frac{t}{t^2-1}\left\{\left[\frac{C_1S_2}{F_2}+\frac{C_2S_1}{F_1}\right]t^{|n-n'|}-t^{-n-n'-1}\left[\frac{S_1}{F_1}+\frac{S_2}{F_2}t\right]\frac{Y}{\Delta}\right\}, \tag{A12}$$

where Δ and Y are given by Eqs. (16) and (25).

(b) The elements of this response function between any two points of this heterostructure can also be obtained in closed form. In the present study we need only the trace of this response function, so we give here only these expressions for two points belonging both either to the superlattice or to the surface cap layer.

(i) When the two points are inside the superlattice $d(n,i,x_3;n',i',x_3')$ is given by Eq. (A5) in which one has to replace $g(M_m,M_{m'})$ by $d(M_m,M_{m'})$ given by Eqs. (A9)–(A12).

(ii) When the two points are inside the surface cap layer

$$d(0,0,x_3;0,0,x_3')=U_0(x_3,x_3')+\frac{1}{S_0^2}\left\{\sinh\left[\alpha_0\left[\frac{d_0}{2}-x_3\right]\right];\sinh\left[\alpha_0\left[\frac{d_0}{2}+x_3\right]\right]\right\}d(M_0,M_0)\begin{bmatrix}\sinh\left[\alpha_0\left[\frac{d_0}{2}-x_3'\right]\right]\\ \sinh\left[\alpha_0\left[\frac{d_0}{2}-x_3'\right]\right]\end{bmatrix}, \tag{A13}$$

where

$$U_0(x_3,x_3')=-\frac{1}{2F_0}\exp[-\alpha_0|x_3-x_3'|]+\frac{1}{2F_0S_0}\left\{\sinh\left[\alpha_0\left[\frac{d_0}{2}-x_3'\right]\right]\exp\left[-\alpha_0\left[\frac{d_0}{2}+x_3\right]\right]+\sinh\left[\alpha_0\left[\frac{d_0}{2}+x_3'\right]\right]\exp\left[-\alpha_0\left[\frac{d_0}{2}-x_3\right]\right]\right\}, \tag{A14}$$

and $d(M_0,M_0)$ is the (2×2) matrix formed out of the elements given by Eqs. (A7)–(A8), for $M_0=(0,0,\pm d_0/2)$.

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