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Acoustic waves in finite superlattices

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Acoustic waves of shear horizontal polarization are studied in a finite superlattice (SL) deposited on a substrate with or without a surface cap layer, or sandwiched between two materials. Using a Green's function method, we have obtained closed-form expressions of local and total densities of states as a function of the frequency ω and the wave vector $k_{\parallel}$ parallel to the layers. Due to the substrate-SL-capping layer interaction, different kinds of localized and resonant discrete modes are found and their properties are investigated.

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 superlattice, 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] Such a study can be performed by means of a Green's-function technique, which is also of interest for scattering problems.[13]

In a very recent paper[12] we were able to obtain closed-form expressions of Green's function and DOS for a semi-infinite SL with a free surface (with or without a cap layer) or in contact with a substrate. In this paper we are dealing with the more general situation of a finite SL deposited on a substrate, and covered with a surface cap layer. Let us mention that Raman experiments were performed to study the substrate-SL-capping layer interactions on Si-$Ge_m Si_n$-Si,[14] and some of the observed peaks were interpreted as resonant modes associated with the presence of the cap layer and the substrate. Very recently, high-resolution Raman measurements[15] on finite Si-$Si_{1-x}Ge_x$ SL's have revealed the existence of a fine structure in the folded longitudinal-acoustic phonons as a set of nearly equally spaced satellite lines; these small peaks may be interpreted as the confined phonons of the whole SL considered as a thin film deposited on the substrate. In this paper the dispersion of the waves and the vibrational DOS are derived and discussed as a function of the wave vector $k_{\parallel}$ (parallel to the layers) as well as the number N of periods of the SL and the nature of the substrate and the cap layer. Although our results are in general obtained for shear horizontal vibrations (for which the displacement is in the plane of the layers and perpendicular to $k_{\parallel}$), they can also be used for longitudinal waves propagating along the axis of the SL, provided the transverse velocities are replaced by the longitudinal ones.

The Green's function (from which the DOS is deduced) is calculated by using the interface response theory[16] in composite materials in which the solution is first searched in the restricted space of the interfaces before being extended to the whole material. As a consequence our system becomes, for any given value of $k_{\parallel}$, equivalent to a simple linear chain with a pseudoatom located at each interface of the SL. We avoid the detail of the analysis which is similar, although more cumbersome, to that of Ref. 12 and only report the expression of the total DOS $n(\omega, k_{\parallel})$ in the Appendix.

In the following we give a few illustrations related to a finite GaAs-AlAs SL deposited on a Si substrate with or without a surface GaAs cap layer of different thickness, and for such a finite SL sandwiched between two Si substrates. The thicknesses d_1 and d_2 of the layers in the SL are assumed to be equal, the period of the SL being $D = d_1 + d_2 = 2d_1$.

Figure 1 gives the Love modes, as deduced from the peaks of the DOS (see also Fig. 2), for a finite GaAs-AlAs SL deposited on a Si substrate, assuming that the outermost layers in the SL are both of AlAs type. For the sake of clarity in Fig. 1, the SL only contains $N = 5$ layers of GaAs and $N + 1 = 6$ layers of AlAs. The branches situated below the substrate bulk band correspond to Love waves confined in the finite SL and decaying exponentially into the substrate; they appear as true δ functions in the DOS. The extension of these curves into the substrate band represents resonant modes (also called leaky waves) associated with the deposition of the finite SL on top of the substrate. The recent fine structure observed[15] in the Raman experiments on Si-$Si_{1-x}Ge_x$ SL's seems to be analogous to these waves, in the case of longitudinal vibrations and for $k_{\parallel} D = 0$.

The curves in Fig. 1 can also be classified according to their oscillatory (full lines) or localized character in the SL; the latter are decaying either from the free surface (dashed-dotted lines are also labeled s as surface) or from the SL-substrate interface (dashed lines, also labeled i as interface). The number of branches corresponding to oscillatory waves in the SL increases with the number N of periods [see also Fig. 4(a) for $N = 20$, to be discussed below], leading to the bulk bands of an infinite SL in the limit $N \rightarrow \infty$. On the other hand, the surface and interface localized modes, which are already distinguishable in Fig. 1, even for such a small number of periods as $N=5$, shift only slightly with N when going to the limit of a semi-infinite SL; however, due to the finiteness of the SL, a surface and an interface branch may interact together when falling in the same minigap of the SL, as for $k_{\parallel}D \cong 2.3$ in Fig. 1 (dotted lines).

The general behavior of the resonant states in the DOS is illustrated in Fig. 2 where the widths of the peaks are due to the interaction between the SL states and the substrate. In particular, we have shown the mixing of the surface and interface states, around $k_{\parallel}D=2.3$ in Fig. 1, into a resonant peak r whose weight is almost equal to two states; this peak remains very near to the free surface mode of a semi-infinite SL. The interaction between the surface and interface states disappears by increasing N; this decoupling occurs in the present example for N of the order of 10–15.

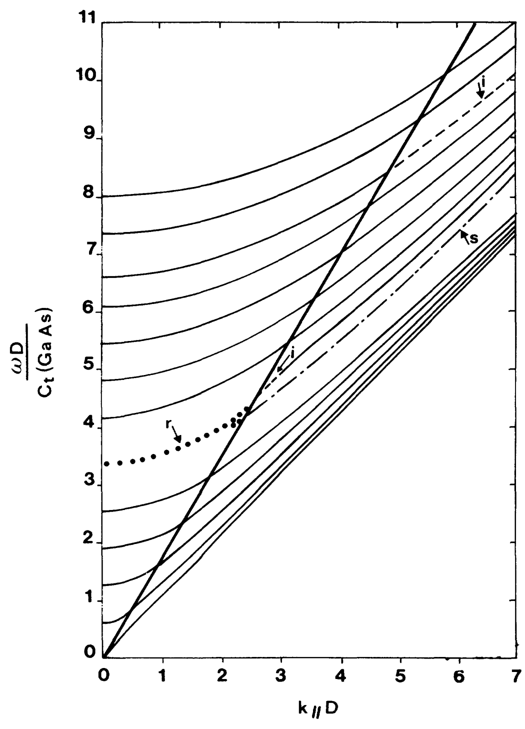

FIG. 1. Dispersion of Love waves associated with the deposition of a finite GaAs-AlAs SL on a Si substrate. The SL contains $N=5$ layers of GaAs and 6 layers of AlAs. The heavy line corresponds to the sound line of the substrate, separating the Love modes confined within the SL from their extension as resonant waves into the substrate bulk band. When the dispersion curves belong to the SL minibands, they are drawn as full lines; when falling inside the SL minigaps, they are represented by dashed-dotted lines (labeled s) or dashed lines (labeled i) corresponding, respectively, to attenuated waves in the SL either from the free surface or from the SL-substrate interface. The label r refers to a resonance obtained from the mixing of a surface and an interface mode. Dimensionless quantities are reported on both axes. c_t(GaAs) is the transverse velocity of sound in GaAs.

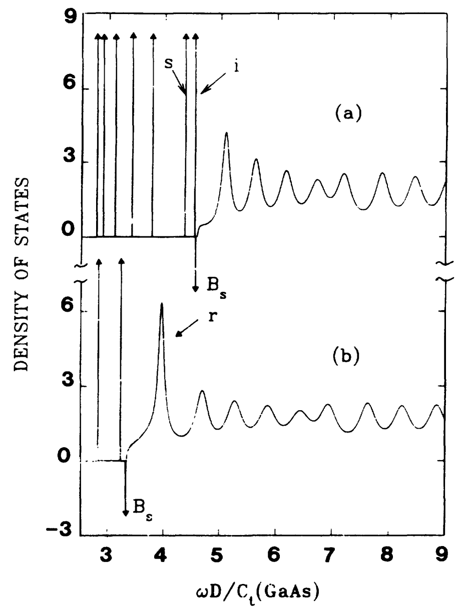

FIG. 2. DOS $n(\omega,k_{\parallel})$, in units of D/C_t(GaAs), depicted for (a) $k_{\parallel}/D=2.6$ and (b) $k_{\parallel}D=1.9$ in Fig. 1. The Love modes localized within the SL give rise to δ peaks represented by arrows. The symbols s, r, and i have the same meanings as in Fig. 1. (The bulk contribution of the substrate to the DOS is subtracted. B_s is a δ function of weight $-\frac{1}{4}$ appearing at the bottom of the substrate bulk band.)

As a matter of completeness, we have also studied the spatial distribution of this resonance r in the SL by presenting (Fig. 3) the local DOS integrated over each period of the SL in the cases $N=5$ and 20. The two sets of results present both similarities and differences. In both cases, the intensity of the peak in the DOS decreases by penetrating from the surface into the SL, as a result of the decay of the surface acoustic wave; also, in both cases, the DOS near the interface with the substrate remains very broad, covering the whole minigap of the SL. On the contrary, by increasing N, the DOS near the surface becomes very narrow and almost similar to a δ function; near the interface, the DOS loses small features which exist for a very thin SL as in the case $N=5$. The modification of the DOS inside the substrate, due to the deposition of the SL on its top, is a small quantity oscillating around zero.

It has been shown[8,12] that surface localized modes in semi-infinite SL's are very sensitive to the nature and width of the outermost cap layer. Considering here the case of the finite SL with $N=20$ and with a GaAs cap layer of varying thickness d_c, Fig. 4(a) presents the frequencies of the discrete modes versus d_c, for a given value of $k_{\parallel}$, namely, $k_{\parallel}\ D=3$. The classification of the curves is similar to that in Fig. 1. We shall be interested in the branches L and R (dashed-dotted lines), which are associated with the free surface of the SL and are rather close to the surface modes of a semi-infinite SL. The former branches L correspond to attenuated waves in the substrate; they take place when the lowest discrete mode emerges from the bulk (an effect which is periodically reproduced as a function of d_c). This branch interacts with the SL-substrate interface branch i giving rise to the lifting of degeneracy at the crossing points around $d_c/d_2 \cong 1.45$, 3.1, etc. This interaction is more important for smaller values of N, as emphasized in Fig. 4(b) around $d_c/d_2 \cong 1.45$. The branches R are resonant with the substrate bulk band; the corresponding peaks in the DOS become wider and decrease in intensity when N decreases, as illustrated in Fig. 4(c) in the case of $d_c/d_2 = 1.8$. This behavior can be attributed to the finiteness of the SL and the interaction between the capped SL modes with the substrate; indeed, in the limit of $N \rightarrow \infty$, the resonant mode at $d_c/d_2 = 1.8$ becomes a surface localized mode of a semi-infinite SL and appears as a δ peak in the DOS. We can push further this discussion by considering again the local DOS integrated over each period of the SL; the surface mode R at $d_c/d_2 = 1.8$ extends over 10–15 periods of the SL and therefore its interaction with the substrate is significant as far as N does not exceed this order of magnitude.

Finally, we have illustrated in Fig. 5 the dispersion curves of a finite GaAs-AlAs SL sandwiched between two semi-infinite Si substrates. This geometry, which is the same as the one studied in Ref. 11 by a transfer matrix method, is interesting for resonant transmission of acoustic waves from one substrate to the other. It can be obtained as a particular case of our general result when the thickness of the cap layer d_c goes to infinity (see the Appendix). Figure 5 refers to a SL with $N = 5$, with its outermost layers being of AlAs type. Besides the oscillatory modes inside the minibands of the SL, one can again observe interface modes associated with the SL-substrate interface (dashed lines); these modes, which are two times degenerate in the limit of a thick SL, interact together for a thin SL when falling in the same minigap; this happens in Fig. 4, in both the first and second minigap of the SL. However, the resonance r resulting from the mixing of two interface states is rather wide and not a very well-defined feature.

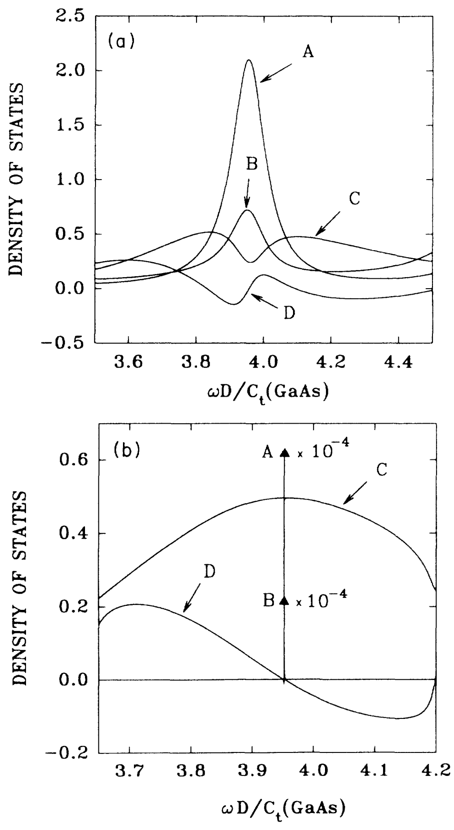

FIG. 3. (a) Spatial distribution of the resonance r depicted in Fig. 2(b): curves A and B, respectively, represent the local DOS integrated over the first and the third period of the SL from the free surface; curve C refers to the same quantity for the period in contact with the substrate, whereas curve D gives the modification of the substrate DOS after the deposition of the SL on its top. (b) Same as in (a) but for a SL containing $N = 20$ layers of GaAs and 21 layers of AlAs. Note that the local DOS at the surface becomes like a δ function.

In conclusion, the closed-form expressions we have obtained for the local and total DOS enable us to derive the dispersion of both localized and resonant states for a finite SL deposited on a substrate, their spatial distribution, and their behavior as a function of the thickness of the SL. This calculation may also be extended to more general geometries, for instance, when the transition from the substrate to the SL takes place through an epilayer, in which new interface states can be expected. Finally, it is worthwhile to mention that our results can be transposed straightforwardly to two other physical problems, namely, the electronic structure of SL's in the Kronig-Penney model[17] and the propagation of polaritons in these heterostructures when each constituent is characterized by a local dielectric constant $\varepsilon(\omega)$.[18] This is because both the equations of motion and the boundary conditions in the above problems involve similar mathematical equations.

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APPENDIX

Each material i ($i = 1,2$) in the SL is characterized by its elastic constant $C_{44}^{(i)}$, mass density $\rho^{(i)}$, and thickness d_i. Similarly, the substrate and the cap layer involve, respectively, the parameters $(C_{44}^{(s)}, \rho^{(s)})$ and $(C_{44}^{(c)}, \rho^{(c)}, d_c)$, and they can be either in contact with the materials 1 or 2 of the SL.

Let us first define the following equations in each material $i = 1, 2, s$, or c:

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

$$C_i = \cosh(\alpha_i d_i), \quad S_i = \sinh(\alpha_i d_i) ,$$

$$F_i = \alpha_i C_{44}^{(i)}, \quad i = 1,2,s,c ,$$

$$t_i = \exp(ik_3 D) ,$$

where k_3 is a wave vector along the axis of the SL and satisfying the following dispersion relation in the infinite SL:[8]

$$\cos k_3 D = C_1 C_2 + \frac{1}{2}\left[\frac{F_2}{F_1}+\frac{F_1}{F_2}\right] S_1 S_2 \ .$$

Then we introduce four specific quantities, namely, Y_1^c and Y_2^c corresponding to the free surface and Y_1^s and Y_2^s associated to the SL/substrate interface,

$$Y_1^c = C_1 C_2 + \frac{F_2}{F_1} S_1 S_2 - t - \frac{F_c S_c}{C_c}\left[\frac{C_1 S_2}{F_2}+\frac{C_2 S_1}{F_1}\right] ,$$

$$Y_2^c = C_2 - C_1 t - F_c \frac{S_c}{C_c}\left[\frac{S_1}{F_1} t + \frac{S_2}{F_2}\right] ,$$

and

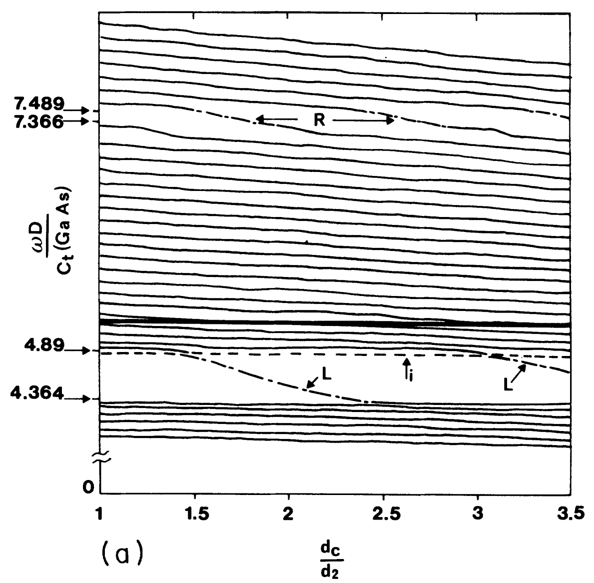
$$Y_1^s = C_1 C_2 + \frac{F_2}{F_1} S_1 S_2 - t - F_s \left[\frac{C_1 S_2}{F_2}+\frac{C_2 S_1}{F_1}\right] ,$$

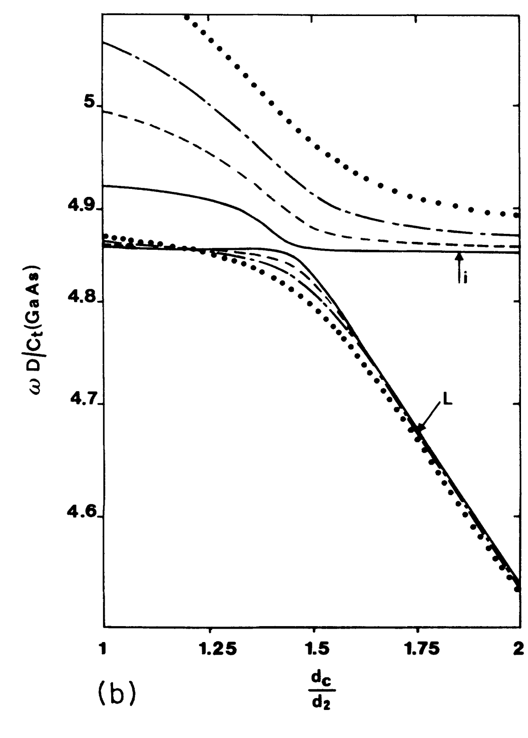
$$Y_2^s = C_2 - C_1 t - F_s \left[\frac{S_1}{F_1} t + \frac{S_2}{F_2}\right] .$$

(a) Expression of the DOS when the substrate and the cap layer are both in contact with the material 1 of the SL. This expression can be written as the sum of four contributions

$$n(\omega^2) = n_1(\omega^2) + n_2(\omega^2) + n_c(\omega^2) + n_s(\omega^2) ,$$

where $n_1(\omega^2)$ and $n_2(\omega^2)$ are the contributions of layers 1 and 2 of the SL, respectively, and $n_c(\omega^2)$ and $n_s(\omega^2)$ come, respectively, from the cap layer and the substrate. Actually, in the latter term, we subtract the contribution of the bulk of the substrate, which is an infinite quantity, and write $n_s(\omega^2) = n_B(\omega^2) + \Delta s n(\omega^2)$. Then we have





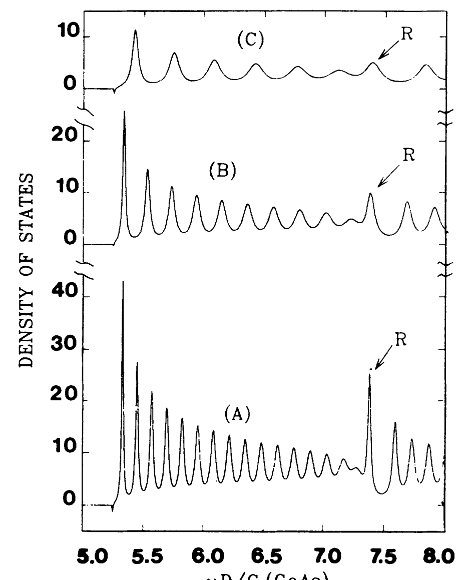


FIG. 4. (a) Variations of the frequencies of the Love modes vs the thickness of the cap layer. The SL contains $N=20$ periods of GaAs-AlAs and is capped with a GaAs layer of varying thickness d_c. The wave vector $k_\parallel$ is chosen such that $k_\parallel D=3$. The symbol i refers to SL-substrate interface modes, whereas L and R refer to free surface modes of the SL, respectively, evanescent in or resonant with the substrate. The heavy line indicates the sound line of the substrate; the arrows give the limits of the SL minigaps. (b) The interaction between the surface and interface states near $d_c/d_2=1.45$, in (a), is emphasized for several values of the number N of periods in the SL: $N=20$ (——), 10 (— — —), 7 (—·—·—·), and 5 (· · · ·). (c) Density of states $n(\omega,k_\parallel)$, for $k_\parallel D=3$ and $d_c/d_2=1.8$, for several values of N: $N=20$ (A), 12 (B), and 7 (C). R corresponds to the resonance depicted in (a). In this figure we have avoided the representation of the δ peaks.

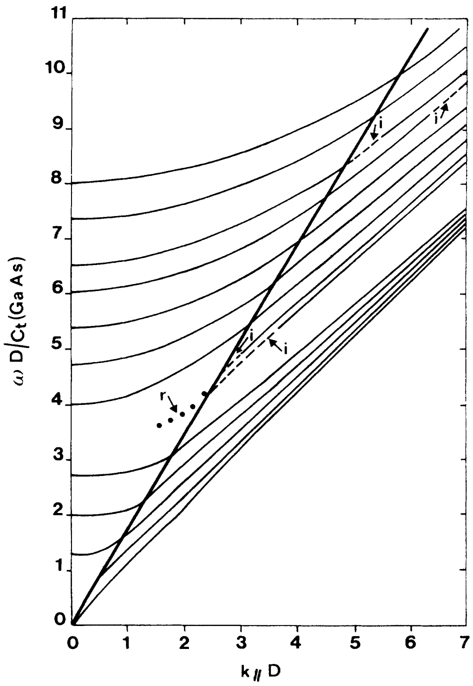


FIG. 5. Dispersion of localized and resonant waves associated with a thin GaAs-AlAs superlattice sandwiched between two Si substrates. The parameters and symbols are the same as in Fig. 1.

$$n_1(\omega^2)=-\frac{\rho^{(1)}}{\pi}\mathrm{Im}\frac{t}{(t^2-1)\Delta_-}\left\{Y\frac{(1-t^{2(N+1)})}{(t^2-1)}\left\{\frac{S_1}{\alpha_1F_1}\left[C_2S_1+\frac{1}{2}C_1S_2\left[\frac{F_1}{F_2}+\frac{F_2}{F_1}\right]\right]+\frac{d_1S_2}{2F_2}\left[1-\frac{F_2^2}{F_1^2}\right]\right\}\right.$$
$$\left.+(N+1)\Delta_+\left\{\frac{d_1}{F_1}\left[C_2S_1+\frac{1}{2}C_1S_2\left[\frac{F_1}{F_2}+\frac{F_2}{F_1}\right]\right]+\frac{S_1S_2}{2\alpha_1F_2}\left[1-\frac{F_2^2}{F_1^2}\right]\right\}\right\}, \tag{A1}$$

$$n_2(\omega^2)=-\frac{\rho^{(2)}}{\pi}\mathrm{Im}\frac{t}{(t^2-1)\Delta_-}\left\{Y\frac{(1-t^{2N})t}{(t^2-1)}\left\{\frac{S_2}{\alpha_2F_2}\left[C_1S_2+\frac{1}{2}C_2S_1\left[\frac{F_1}{F_2}+\frac{F_2}{F_1}\right]\right]+\frac{d_2S_1}{2F_1}\left[1-\frac{F_1^2}{F_2^2}\right]\right\}\right.$$
$$\left.+N\Delta_+\left\{\frac{d_2}{F_2}\left[C_1S_2+\frac{1}{2}C_2S_1\left[\frac{F_1}{F_2}+\frac{F_2}{F_1}\right]\right]+\frac{S_1S_2}{2\alpha_2F_1}\left[1-\frac{F_1^2}{F_2^2}\right]\right\}\right\}, \tag{A2}$$

$$n_c(\omega^2)=-\frac{\rho^{(c)}}{2\pi}\mathrm{Im}\frac{1}{\Delta_-}\left\{\left[\frac{t^2-1}{t}+Y_1^s\right]\left\{\frac{S_c}{\alpha_cC_c}\left[\frac{C_1S_2}{F_2}+\frac{C_2S_1}{F_1}\right]+d_c\left[\left[C_1C_2+\frac{F_1}{F_2}(S_1S_2-t\right]\frac{S_c}{F_cC_c}\right.\right.\right.$$
$$\left.\left.+\frac{C_1S_2}{F_2}+\frac{C_2S_1}{F_1}\right]\right\}$$
$$\left.-t^{2N}Y_2^s\left\{\frac{S_c}{\alpha_cC_c}\left[\frac{S_1}{F_1}t+\frac{S_2}{F_2}\right]+d_c\left[\frac{S_1}{F_1}t+\frac{S_2}{F_2}+\frac{S_c}{F_cC_c}(C_1t-C_2)\right]\right\}\right\}, \tag{A3}$$

$$\Delta_sn(\omega^2)=-\frac{\rho^{(s)}}{\pi}\mathrm{Im}\frac{1}{2\alpha_s}\left\{\frac{1}{2F_s}+\frac{1}{\Delta_-}\left[\left[\frac{C_1S_2}{F_2}+\frac{C_2S_1}{F_1}\right]\left[\frac{t^2-1}{t}+Y_1^c\right]-t^{2N}\left[\frac{S_1}{F_1}t+\frac{S_2}{F_2}\right]Y_2^c\right]\right\}, \tag{A4}$$

where

$$Y=\frac{(t^2-1)}{t}(Y_2^s+Y_2^c)+2Y_1^sY_2^c$$

and

$$\Delta_\pm=\left[\frac{t^2-1}{t}+Y_1^s\right]\left[\frac{t^2-1}{t}+Y_1^c\right]\pm t^{2N}Y_2^sY_2^c\ .$$

(b) Expression of the DOS when the substrate is in contact with the material 1 of the SL, and the cap layer in contact with the material 2. This expression is given exactly as in the first case, namely,

$$n'(\omega^2)=n_1'(\omega^2)+n_2'(\omega^2)+n_c'(\omega^2)+n_s'(\omega^2)$$

with $n_s'(\omega^2)=n_B'(\omega^2)+\Delta_s' n(\omega^2)$.

Then we have

$$n_1'(\omega^2)=-\frac{\rho^{(1)}}{\pi}\mathrm{Im}\frac{t}{(t^2-1)\Delta'_-}\left\{Y'\left[\frac{1-t^{2(N+1)}}{(t^2-1)}\right]\left\{\frac{S_1}{\alpha_1 F_1}\left[C_2S_1+\frac{1}{2}C_1S_2\left[\frac{F_1}{F_2}+\frac{F_2}{F_1}\right]\right]+\frac{d_1S_2}{2F_2}\left[1-\frac{F_2^2}{F_1^2}\right]\right\}\right.$$
$$\left.+(N+1)\Delta'_+\left\{\frac{d_1}{F_1}\left[C_2S_1+\frac{1}{2}C_1S_2\left[\frac{F_1}{F_2}+\frac{F_2}{F_1}\right]\right]+\frac{S_1S_2}{2\alpha_1F_2}\left[1-\frac{F_2^2}{F_1^2}\right]\right\}\right\}, \tag{A5}$$

$$n_2'(\omega^2)=-\frac{\rho^{(2)}}{\pi}\mathrm{Im}\frac{t}{(t^2-1)\Delta'_-}\left\{Y''t\left[\frac{1-t^{2(N+1)}}{(t^2-1)}\right]\left\{\frac{S_2}{\alpha_2 F_2}\left[C_1S_2+\frac{1}{2}C_2S_1\left[\frac{F_1}{F_2}+\frac{F_2}{F_1}\right]\right]+\frac{d_2S_1}{2F_1}\left[1-\frac{F_1^2}{F_2^2}\right]\right\}\right.$$
$$\left.+(N+1)\Delta'_+\left\{\frac{d_2}{F_2}\left[C_1S_2+\frac{1}{2}C_2S_1\left[\frac{F_1}{F_2}+\frac{F_2}{F_1}\right]\right]+\frac{S_1S_2}{2\alpha_2F_1}\left[1-\frac{F_1^2}{F_2^2}\right]\right\}\right\}, \tag{A6}$$

$$n_c'(\omega^2)==\frac{\rho^{(c)}}{2\pi}\mathrm{Im}\left\{\left[\frac{t^2-1}{t}+Y_1^s\right]\left\{\frac{S_c}{\alpha_c C_c}\left[\frac{C_1S_2}{F_2}+\frac{C_2S_1}{F_1}\right]+d_c\left[\left[C_1C_2+\frac{F_2}{F_1}S_1S_2-t\right]\frac{S_c}{F_cC_c}\right.\right.\right.$$
$$\left.\left.+\frac{C_1S_2}{F_2}+\frac{C_2S_1}{F_1}\right]\right\}$$
$$\left.-t^{2N+1}Y_2^s\left\{\frac{S_c}{\alpha_cC_c}\left[\frac{S_2}{F_2}t+\frac{S_1}{F_1}\right]+d_c\left[\frac{S_2}{F_2}t+\frac{S_1}{F_1}+\frac{S_c}{F_cC_c}(C_2t-C_1)\right]\right\}\right\}, \tag{A7}$$

$$\Delta_s'n(\omega^2)=-\frac{\rho^{(s)}}{\pi}\mathrm{Im}\frac{1}{2\alpha_s}\left\{\frac{1}{2F_s}+\frac{1}{\Delta'_-}\left[\left[\frac{C_1S_2}{F_2}+\frac{C_2S_1}{F_1}\right]\left[\frac{t^2-1}{t}+Y_1^{c'}\right]-t^{2N+1}Y_2^{c'}\left[\frac{S_1}{F_1}t+\frac{S_2}{F_2}\right]\right]\right\}, \tag{A8}$$

where

$$Y'=\left[\frac{t^2-1}{t}+Y_1^{c'}\right]Y_2^s+\left[\frac{t^2-1}{t}+Y_1^s\right]tY_2^{c'},$$

$$Y''=\left[\frac{t^2-1}{t}+Y_1^{c'}\right]Y_2^s+\left[\frac{t^2-1}{t}+Y_1^s\right]\frac{Y_2^{c'}}{t},$$

and

$$\Delta'_\pm=\left[\frac{t^2-1}{t}+Y_1^s\right]\left[\frac{t^2-1}{t}+Y_1^{c'}\right]\pm t^{2N+1}Y_2^sY_2^{c'}.$$

The elements $Y_1^{c'}$ and $Y_2^{c'}$ are obtained from Y_1^c and Y_2^c by exchanging the indices 1 and 2.

In both cases, the localized waves are given by the poles of the Green's function, namely,

$$\Delta_-=0 \text{ or } \Delta'_-=0 .$$

(c) Particular cases. From these general expressions (A1)–(A4) and (A5)–(A8), one can deduce easily two limiting cases corresponding to a finite SL without a cap layer (i.e., $d_c=0$ and then $S_c=0$) or deposited between two substrates (i.e., $d_c\to\infty$ and then $S_c/C_c\to 1$).

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