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# Surface and interface optical waves in superlattices: transverse electric localized and resonant modes

M L Bah, A Akjouj†, E H El Boudouti‡, B Djafari-Rouhani and L Dobrzynski

EDI Laboratoire de Dynamique et Structure des Matériaux Moléculaires, Centre National de la Recherche Scientifique (D0 801), Unité de Physique, Université de Lille I, 59655 Villeneuve d'Ascq Cedex, France

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**Abstract.** We investigate the existence and behaviour of localized and resonant optical waves associated with the surface of a semi-infinite superlattice or its interface with a substrate, considering the case of transverse electric modes. In this paper, we present an analytic determination of the response function (Green function) for a semi-infinite superlattice with or without a cap layer, and for a superlattice in contact with a substrate. This calculation enables us to obtain both local and total densities of states as functions of the frequency $\omega$ and the wavevector $\boldsymbol{k}_{\parallel}$ (parallel to the interfaces). Besides the surface and interface localized modes which occur as delta peaks inside the gaps, one can also obtain resonant states as well defined peaks of the density of states inside the bulk bands of the superlattice. In particular, we emphasize the different types of mode induced by a cap layer. In addition, we show that the creation of a semi-infinite superlattice gives rise to delta peaks of weight $-1/4$ in the density of states at every edge of the superlattice bulk bands.

## 1. Introduction

In the past few years, interest has turned to electromagnetic waves in superlattices, which typically are periodic arrays of a sufficiently large number of alternate layers of two different materials. The propagation of electromagnetic waves in superlattices has been the subject of many experimental and theoretical studies over the past decade, summarized in several recent review papers [1–5]. The periodic optical media and specifically stratified periodic structures play an important role in a number of applications [1]. These include Bragg reflection, holography, optical stop bands and multichannel waveguides.

The extended states propagating in the whole superlattice form bulk bands which are separated by gaps. Localized modes associated with a perturbation of the perfect superlattice may exist inside these gaps. In particular, it was shown that surface electromagnetic waves may exist [2–14], as well as localized modes induced by the presence of a cap layer at the surface of the superlattice [12, 15]. The optical modes localized at the surface of a superlattice have been observed [1, 13, 14] in a periodic layer structure which consisted of 12 pairs of alternating layers of GaAs and $Al_{0.2}Ga_{0.8}As$ on a GaAs substrate. However, to our knowledge, the variation in the electromagnetic density of states associated with the above-cited perturbations of a superlattice has not yet been studied, apart from a study [5]

† Author to whom correspondence should be sent.

‡ Present address: Département de Physique, Faculté des Sciences, Université Mohamed I, Oujda, Morocco.

showing only in the local density of states the peaks associated with surface localized modes of a semi-infinite superlattice.

In this paper, we study resonant and localized electromagnetic modes together with the variation in the density of states associated with surfaces and interfaces in superlattice. Closed-form expressions are obtained for s-polarized (transverse electric) waves. We stress in particular that, for the first time to our knowledge, well defined resonant optical waves induced by a cap layer exist and may then be observed by the same experimental methods as localized surface modes.

The theoretical method used here, namely the Green function method, enables us to study these modes in semi-infinite dielectric superlattice with or without a cap layer. Indeed, from knowledge of the response functions [16] in such heterostructures, one can calculate both the local and the total density of states ($\boldsymbol{k}_\parallel$-resolved density of states where $\boldsymbol{k}_\parallel$ is the wave-vector parallel to the interfaces). 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 $\boldsymbol{k}_\parallel$-resolved density of states inside the bulk bands.

The complete response functions can also be used to derive any other physical property of the system at hand. They play a central role in the theories of light scattering (both Brillouin and Raman), as well as in various other physical phenomena [4, 17].

In the simple case of s-polarized modes, the electric field has only one transverse component along the $x_2$ axis, where $x_3$ is the axis of the superlattice and the wavevector $\boldsymbol{k}_\parallel$ (parallel to the interfaces) is directed parallel to $x_1$. The study consist of isotropic dielectric materials of thicknesses comparable with the wavelength of electromagnetic radiation. The retardation is fully taken into account. We are interested in the calculation of the density of states ($\boldsymbol{k}_\parallel$-resolved density of states) and dispersion curves in a semi-infinite superlattice with or without a cap layer at the surface, or in contact with a substrate. After a brief introduction to the theory, we present a discussion of the general behaviour of the $\boldsymbol{k}_\parallel$-resolved density of states as well as a few illustrations of the dispersion curves, in particular in the case of localized and resonant modes induced by the cap layer.

The organization of this paper is as follows. After presenting the model in section 2, section 3 gives the analytical results obtained for the densities of states in the above-mentioned heterostructures. Section 4 shows the numerical results for 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.

## 2. The basic equations for isotropic dielectric superlattices

The superlattice is formed out of an infinite repetition of two different isotropic dielectric slabs, labelled by the unit-cell index $n$. Each of these slabs of width $d_i$ is labelled 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 $-d_i/2 \leqslant x_3 \leqslant d_i/2$. The period of the superlattice is called $D = d_1 + d_2$.

It was shown [16] that all the elements of the response function of layered isotropic dielectrics, and in particular those of a superlattice; $\mathbf{g}(k_\parallel, \omega/x_3, x'_3)$, can be easily deduced from one basic element $g(k_\parallel, \omega/x_3, x'_3)$ where $k_\parallel$ is the modulus of the propagation vector parallel to the interfaces, and $\omega$ the frequency. The bulk basic equation for one homogeneous infinite medium $i$ can be written

$$\left(\frac{F_i}{\alpha_i}\frac{\partial^2}{\partial x_3^2} - \alpha_i^2\right) G_i(k_\parallel, \omega/x_3, x_3') = \delta(x_3 - x_3') \qquad -\infty < x_3, x_3' < +\infty \tag{1}$$

with

$$\alpha_i(k_\parallel, \omega) = \left[k_\parallel^2 - \frac{\omega^2}{c^2}\varepsilon_i\right]^{1/2} \tag{2}$$

where $c$ is the speed of light, $\varepsilon_i$ the dielectric function, $G_i(k_\parallel, \omega/x_3, x_3')$ the bulk response function, and

$$F_i = \alpha_i. \tag{3}$$

The implicit expression giving the bulk dispersion relation for such an infinite superlattice is

$$\cos(k_3 D) = C_1 C_2 + \frac{1}{2}\left(\frac{F_1}{F_2} + \frac{F_2}{F_1}\right) S_1 S_2 \tag{4}$$

where

$$C_i = \cosh(\alpha_i d_i) \tag{5}$$

$$S_i = \sinh(\alpha_i d_i) \tag{6}$$

and $k_3$ is the component perpendicular to the slabs of the propagation vector $\boldsymbol{k} \equiv (\boldsymbol{k}_\parallel, k_3)$ (see for example [18]).

## 3. Density of states

Knowing the response function given in the appendix, one obtains for a given value of $\boldsymbol{k}_\parallel$ the local and total densities of states for a semi-infinite superlattice with a surface cap layer (figure 1). 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 a semi-infinite superlattice without a cap layer and that of a semi-infinite superlattice in contact with a semi-infinite homogeneous substrate.

### *3.1. The local density of states*

The local density of states on the plane $(n, i, x_3)$ is given by

$$n(\omega^2, k_\parallel; n, i, x_3) = -\frac{\varepsilon_i}{\pi c^2}\,\mathrm{Im}\, d^+(\omega^2, k_\parallel; n, i, x_3; n, i, x_3) \tag{7}$$

where

$$d^+(\omega^2) = \lim_{\Gamma\to 0}[d(\omega^2 + \mathrm{i}\Gamma)] \tag{8}$$

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 $\omega$, using the well known relation $n(\omega) = 2\omega n(\omega^2)$. From the elements of the response function given in the appendix, we obtain the following closed-form expressions for the local densities of states at the interface between vacuum and the cap layer ($n = 0, i = c$) of width $d_c$ (see figure 1):

$$n_s\left(\omega^2, k_\parallel; 0, c, \frac{d_c}{2}\right) = -\frac{1}{\pi}\,\mathrm{Im}\left[\frac{C_1 S_2}{F_2} + \frac{C_2 S_1}{F_1} + \frac{S_c}{F_c C_c}\left(C_1 C_2 + \frac{F_1}{F_2} S_1 S_2 - t\right)\right] \times \frac{1}{(1 + F_v S_c/F_c C_c)\Delta} \tag{9}$$

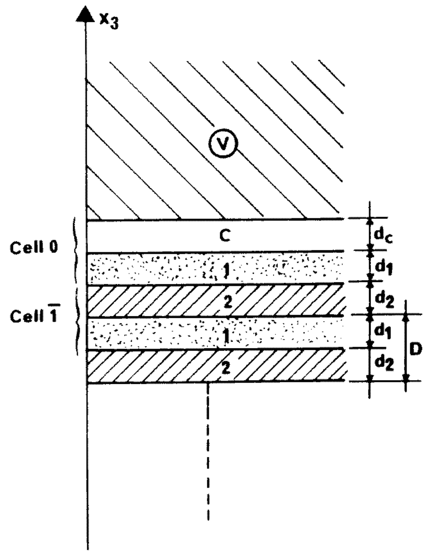


**Figure 1.** Schematic representation of a semi-infinite superlattice ($i = 1, 2$) with a cap layer ($n = 0; i = c$) in contact with vacuum. $d_c, d_1$ and $d_2$ respectively, are, the thicknesses of the cap layer and of the two different slabs out of which the semi-infinite superlattice is built. $D$ is the period of the superlattice.

where

$$t = \begin{cases} \eta + (\eta^2 - 1)^{1/2} & \eta < -1 \\ \eta + \mathrm{i}(1 - \eta^2)^{1/2} & -1 < \eta < 1 \\ \eta - (\eta^2 - 1)^{1/2} & \eta > 1 \end{cases} \tag{10}$$

with

$$\eta = C_1 C_2 + \frac{1}{2}\left(\frac{F_1}{F_2} + \frac{F_2}{F_1}\right) S_1 S_2 \tag{11}$$

$$\Delta = C_1 C_2 + \frac{F_2}{F_1} S_1 S_2 - t^{-1} - R F_v \left(\frac{C_1 S_2}{F_2} + \frac{C_2 S_1}{F_1}\right) \tag{12}$$

$$R = \frac{1 + F_c S_c / F_v C_c}{1 + F_v S_c / F_c C_c} \tag{13}$$

and $S_c, C_c, F_c$ and $F_v$ have the same definitions as $C_i, S_i$ and $F_i$ given by equations (3), (5) and (6).

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

$$n_i\left(\omega^2, k_\parallel; 0, c, \frac{-d_c}{2}\right) = -\frac{1}{\pi} \mathrm{Im}\left(\frac{C_1 S_2}{F_2} + \frac{C_2 S_1}{F_1}\right) \Delta^{-1}. \tag{14}$$

### *3.2. 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 over $n$ and $i$ the local density $n(\omega^2, k_\parallel; n, i, x_3)$.

More particularly we are interested in this total density of states from which the contributions of the infinite superlattice and vacuum alone have been subtracted. This variation $\Delta n(\omega^2)$ can be written as the sums of the variations $\Delta_1 n(\omega^2)$ and $\Delta_2 n(\omega^2)$ in the densities of states in slabs 1 and 2, the density of states $n_c(\omega^2)$ inside the cap layer $i = c$ and the variation $\Delta_v n(\omega^2)$ in the density of states in vacuum:

$$\Delta n(\omega^2) = \Delta_1 n(\omega^2) + \Delta_2 n(\omega^2) + \Delta_v n(\omega^2) + n_c(\omega^2) \tag{15}$$

where

$$\Delta_1 n(\omega^2) = -\frac{\varepsilon_1}{\pi c^2} \sum_{n=-\infty}^{0} \mathrm{Im}\left( \int_{-d_1/2}^{d_1/2} [d(n,1,x_3;n,1,x_3) - g(n,1,x_3;n,1,x_3)]\,\mathrm{d}x_3 \right) \tag{16}$$

$$\Delta_2 n(\omega^2) = -\frac{\varepsilon_2}{\pi c^2} \sum_{n=-\infty}^{-1} \mathrm{Im}\left( \int_{-d_2/2}^{d_2/2} [d(n,2,x_3;n,2,x_3) - g(n,2,x_3;n,2,x_3)]\,\mathrm{d}x_3 \right) \tag{17}$$

$$n_c(\omega^2) = -\frac{\varepsilon_c}{\pi c^2} \mathrm{Im} \int_{-d_c/2}^{d_c/2} d(0,c,x_3;0,c,x_3)\,\mathrm{d}x_3 \tag{18}$$

$$\Delta_v n(\omega^2) = -\frac{\varepsilon_v}{\pi c^2} \mathrm{Im}\left( \int_0^{+\infty} [d(x_3,x_3) - G_v(x_3,x_3)]\,\mathrm{d}x_3 \right). \tag{19}$$

$d$ and $g$ are the response functions of the coupled (superlattice–cap layer–vacuum) system and of the infinite superlattice, respectively; $G_v$ represents the response function of the infinite homogeneous vacuum. With the help of the explicit expressions for these response functions given in the appendix we obtain

$$\Delta_1 n(\omega^2) = -\frac{\varepsilon_1}{\pi c^2} \mathrm{Im}\left( \frac{t}{(t^2-1)^2} \left\{ \frac{S_1}{\alpha_1 F_1} \left[ C_2 S_1 + \frac{1}{2} C_1 S_2 \left( \frac{F_1}{F_2} + \frac{F_2}{F_1} \right) \right] + \frac{d_1 S_2}{2F_2} \left( 1 - \frac{F_2^2}{F_1^2} \right) \right\} \frac{Y}{\Delta} \right) \tag{20}$$

$$\Delta_2 n(\omega^2) = -\frac{\varepsilon_2}{\pi c^2} \mathrm{Im}\left( \frac{t^2}{(t^2-1)^2} \left\{ \frac{S_2}{\alpha_2 F_2} \left[ C_1 S_2 + \frac{1}{2} C_2 S_1 \left( \frac{F_1}{F_2} + \frac{F_2}{F_1} \right) \right] + \frac{d_2 S_1}{2F_1} \left( 1 - \frac{F_1^2}{F_2^2} \right) \right\} \frac{Y}{\Delta} \right) \tag{21}$$

$$n_c(\omega^2) = -\frac{\varepsilon_c}{2\pi c^2} \mathrm{Im}\left\{ \frac{S_c}{\alpha_c C_c} \frac{1}{1 + F_v S_c / F_c C_c} \left[ \frac{C_1 S_2}{F_2} + \frac{C_2 S_1}{F_1} - \frac{F_v}{F_c^2} \left( C_1 C_2 + \frac{F_1}{F_2} S_1 S_2 - t \right) \right] + d_c \left[ \frac{C_1 S_2}{F_2} + \frac{C_2 S_1}{F_1} + R \frac{F_v}{F_c^2} \left( C_1 C_2 + \frac{F_1}{F_2} S_1 S_2 - t \right) \right] \right\} \frac{1}{\Delta} \tag{22}$$

and

$$\Delta_v n(\omega^2) = -\frac{\varepsilon_v}{\pi c^2} \mathrm{Im}\left[ \frac{1}{2\alpha_v} \left( \frac{1}{2F_v} + \{C_1 S_2/F_2 + C_2 S_1/F_1 + (S_c/F_c C_c)[C_1 C_2 + (F_1/F_2) S_1 S_2 - t]\} [(1 + F_v S_c / F_c C_c)\Delta]^{-1} \right) \right] \tag{23}$$

where

$$Y = C_2 - C_1 t - R F_v \left( \frac{S_1}{F_1} t + \frac{S_2}{F_2} \right). \tag{24}$$

At any edge of the superlattice bulk bands, we have $t(\omega_0) = \pm 1$; an expansion to first order in $\omega - \omega_0$ provides

$$\frac{t}{(t^2-1)^2} = \frac{1}{8}\left[\left(\frac{\mathrm{d}\eta}{\mathrm{d}\omega}\right)_{\omega_0}\right]^{-1}\left[P\left(\frac{1}{\omega-\omega_0}\right) - \mathrm{i}\pi\,\delta(\omega-\omega_0)\right] \tag{25}$$

and then

$$\Delta_1 n(\omega) + \Delta_2 n(\omega) = (-1/4)\delta(\omega - \omega_0). \tag{26}$$

So, the creation of a semi-infinite superlattice from an infinite superlattice gives rise to $\delta$ peaks of weight $-1/4$ in the density of states at the edges of the superlattice bulk bands.

### *3.3. 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 both into the bulk of the superlattice and into vacuum. The explicit expression giving these localized states is

$$C_1 S_2\left(\frac{F_2}{RF_v} - \frac{RF_v}{F_2}\right) + S_1 S_2\left(\frac{F_2}{F_1} - \frac{F_1}{F_2}\right) + C_2 S_1\left(\frac{F_1}{RF_v} - \frac{RF_v}{F_1}\right) = 0 \tag{27}$$

together with the condition

$$\left|C_1 C_2 + \frac{F_2}{F_1} S_1 S_2 - RF_v\left(\frac{C_1 S_2}{F_2} + \frac{C_2 S_1}{F_1}\right)\right| > 1. \tag{28}$$

### *3.4. The case of a semi-infinite superlattice without a cap layer*

This system is obtained when the thickness $d_c$ of the cap layer is going to zero; then $S_c \to 0$ and the above results (9), (20), (21), (23), (27) and (28) remain valid for a semi-infinite superlattice ending with a complete $i = 1$ surface layer in contact with vacuum. Let us note that in this limit $n_c(\omega)$ (equation (22)) vanishes.

In the limit where the cap layer $i = c$ is of the same nature as the $i = 2$ superlattice layer and $d_c = d_s < d_2$, the same results provide the localized modes for a semi-infinite superlattice ending with an incomplete $i = 2$ surface layer (see figure 1). In this case, we can calculate the variation in the density of states between such a semi-infinite superlattice and the same amount of the bulk superlattice, using in equation (17) $\Delta_2 n(\omega^2)$ integrated to $d_s/2$ rather than to $d_2/2$ in the last layer, and taking $n_c(\omega^2) = 0$.

A particularly interesting result is obtained when considering two superlattices obtained by cleaving an infinite superlattice along the space position $x_3 = d_s$ in such a way that one obtains one superlattice with an incomplete surface layer $d_s$ and its complementary superlattice with a surface layer of width $d_2 - d_s$. The variation in the $\boldsymbol{k}_\parallel$-resolved density of states when creating two complementary semi-infinite superlattices from an infinite superlattice is equal to zero [19] for frequencies $\omega$ which belong simultaneously to a superlattice bulk band and are above the light line in vacuum.

### *3.5. The case of an interface between a semi-infinite superlattice and an homogeneous substrate*

This system is obtained by replacing the vacuum by an homogeneous substrate. All the above expressions (9)–(28) and limits (section 3.4) remain valid on replacing the index $v$ by $s$ for the substrate.

## 4. Applications and discussion of the results

In what follows, specific results will be given for superlattices consisting of alternate layers of materials 1 and 2 with or without a cap layer at the surface (denoted by subscript $c$), and also for such superlattices in contact with substrate. The constituents are assumed to be dielectric materials with their dielectric constants denoted $\varepsilon_1$, $\varepsilon_2$ and $\varepsilon_c$. The corresponding layer thicknesses will be denoted $d_1$, $d_2$ and $d_c$, and the period of the superlattice $D = d_1+d_2$. The calculations are performed for $\varepsilon_1 = 3$, $\varepsilon_2 = 10$ and $\varepsilon_c = 2$, and layer thicknesses $d_1 = 2$, $d_2 = 2D/3$ (see figure 7(a)).

We shall first consider (section 4.1) semi-infinite superlattices, then (section 4.2) semi-infinite superlattices with a surface cap layer and finally (section 4.3) semi-infinite superlattices on a semi-infinite homogeneous substrate.

### *4.1. Semi-infinite superlattices*

Figure 2 gives the dispersion of bulk bands and surface modes as a function of $k_\parallel D$. The slab at the surface of the superlattice is either 1 or 2 with the same thickness as in the bulk. The shaded areas are the bulk bands separated by gaps where surface electromagnetic modes are represented for either material 1 (full lines) or material 2 (broken lines) at the surface. One can observe that these surface modes are very dependent on the type of material which is at the surface. On the assumption that the latter is material 1 and choosing $k_\parallel D = 6$, figure 3 shows the $k_\parallel$-resolved density of states of the semi-infinite superlattice in contact with vacuum from which the contributions of the infinite superlattice and the infinite vacuum have been subtracted as defined in section 3.2. The $\delta$ functions appearing in this figure are enlarged by adding a small imaginary part to the electromagnetic frequency $\omega$. The $\delta$ functions of weight 1 associated with the localized surface electromagnetic modes are labelled $\mathrm{L}_i$. Also, we have shown that $\delta$ peaks of weight $-1/4$ appear in the variation $\Delta n(\omega, k_\parallel)$ in the total density of states at both the bottom and the top of every bulk band of the superlattice (these peaks are labelled $\mathrm{B}_i$ and $\mathrm{T}_i$, respectively). This result was also found by El Boudouti *et al* [20] for the propagation of transverse acoustic waves in superlattices. The form of the enlarged $\delta$ functions for $\mathrm{B}_i$ and $\mathrm{T}_i$ of weight $-1/4$ are not exactly the same because of the contributions coming from the divergence in $(\omega - \omega_{\mathrm{B}_i})^{-1/2}$ or $(\omega-\omega_{\mathrm{T}_i})^{-1/2}$($\omega_{\mathrm{B}_i}$ and $\omega_{\mathrm{T}_i}$ are the frequencies of the bottom and the top of every bulk band of the superlattice) existing near the band edges in the density of states in one dimension. Apart from the above $\delta$ peaks and the particular behavior near the band edges, the variation $\Delta n(\omega, k_\parallel)$ in the density of states does not show any other significant effect inside the bulk bands of the superlattice.

Now we assume that the surface cap layer is of the same nature as those of the bulk but with a different thickness. Figure 4 represents the variation in the frequencies of surface electromagnetic modes, for $k_\parallel D = 6$, as a function of $d_c/D$ where $d_c$ is the width of the surface layer made of material 1 (broken lines) or material 2 (full lines). These frequencies are very sensitive to the width $d_c$; when $d_c$ increases, the frequencies of the existing localized 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 long as their frequencies remain in the vicinity of the band edges. Let us mention that, for any given frequency $\omega$ in figure 4, there is a periodic repetition of the modes as a function of $d_c$.

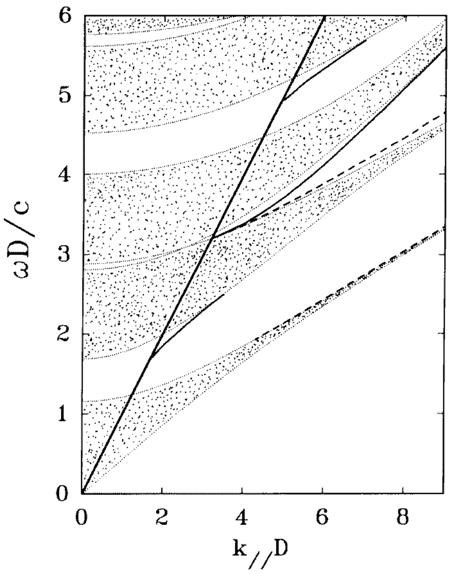


**Figure 2.** Bulk and surface transverse electric waves in a superlattice made of two dielectric materials. The curves give $\omega D/c$ as a function of $k_{\parallel} D$, where $\omega$ is the frequency, $c$ the velocity of light, $k_{\parallel}$ the propagation vector parallel to the interfaces and $D = d_1 + d_2$ the period of the superlattice. The shaded areas represent the bulk bands. The solid lines represent the surface electric waves for the semi-infinite superlattice terminated by the slab of material 1 ($\varepsilon_1 = 3$). The shaded lines represent the surface electric waves for the complementary superlattice terminated by the slab of material 2 ($\varepsilon_2 = 10$). The bold line indicates the light line of vacuum.

### *4.2. Semi-infinite superlattices with a surface cap layer*

The cap layer is in contact with material 1 of the superlattice. Figure 5 gives the dispersion of localized and resonant electromagnetic modes induced by the cap layer of relative width $d_c/D = 3$. They are obtained as well defined peaks in the variation $\Delta n_c(\omega)$ in the total density of states between the coupled (superlattice–cap layer–vacuum) and the uncoupled (infinite superlattice and vacuum alone) systems. An example of $\Delta n(\omega)$ is plotted in figure 6, for $k_{\parallel} D = 6$. These localized and resonant modes are very sensitive to the thickness and to the nature of the cap layer [21]. Most of these can be understood as modified (shifted and broadened) confined modes of a free slab and are therefore different from the surface modes of a superlattice without a cap layer. One can, however, see the existence of interface modes localized at the superlattice–cap layer interface. Among the resonances appearing in figures 5 and 6, the most intense resonance $R_2$ is the lowest, situated just above the cap layer light line. The next resonances are less intense, especially at higher frequencies where the separation between the successive branches increase.

With the help of equations (9) and (14), we also studied local densities of states. We found that they change with the position $x_3$ where they are calculated. In particular, we found that the local density of states at the surface of the cap layer shows the same resonances as the total density of states illustrated in figure 6. On the contrary, in the local density of states at the superlattice–adlayer interface the resonances are shifted with respect to those in figure 6. These behaviours can be understood by the very different boundary conditions existing on these two planes.

Depending on their frequencies, the modes induced by the cap layer may propagate

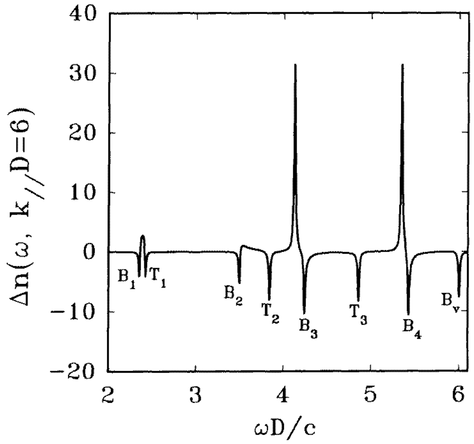


**Figure 3.** Density of states (in units of $D/c$) of the semi-infinite superlattice with a layer of material 1 ($\varepsilon_1 = 3$) at the surface, for $k_\parallel D = 6$. The contributions of the infinite superlattice and vacuum have been subtracted. $B_i$ and $T_i$ refer to $\delta$ peaks of weight $-1/4$ at the edges of the bulk bands, $L_i$ indicates the modes localized at the surface and $B_v$ refers to the $\delta$ peak of weight $-1/4$ situated at the light line of vacuum.

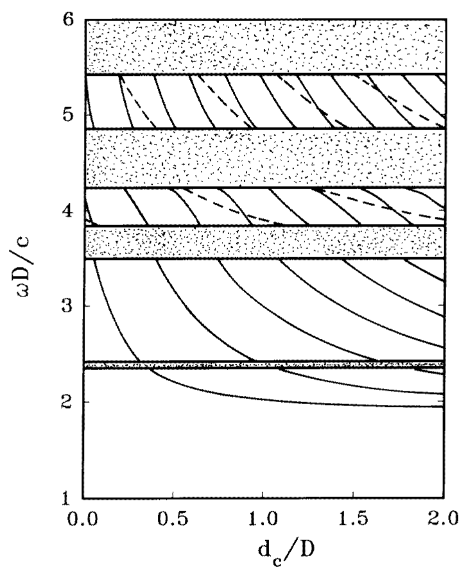


**Figure 4.** Variation in the dimensionless frequencies $\omega D/c$ of the surface modes of a semi-infinite superlattice, for $k_\parallel D = 6$, as a function of $d_c/D$, where $d_c$ is the width of the surface layer made of material 1 (broken lines) or material 2 (full lines). The shaded areas show the first three bulk bands of the superlattice.

along the direction perpendicular to the interfaces in both the superlattice and the cap layer, or they may propagate in one and decay in the other, or finally they may decay on both sides of the superlattice–adlayer interface. The latter, which corresponds to an interface localized mode is labelled by the index $i$ in figures 5 and 6. To illustrate these three types of behaviour, we have plotted in figures 7(b), (c) and (d) the local densities of states

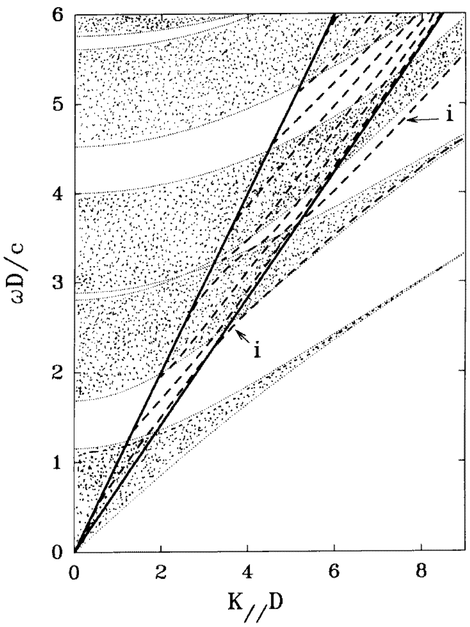


**Figure 5.** Dispersion of localized and resonant modes (broken lines) induced by a cap layer of material $c$ of thickness $d_c = 3D$ and dielectric constant $\varepsilon_c = 2$, deposited on the top of the superlattice formed of materials 1 and 2 and terminated by a layer of material 1. The shaded areas are the superlattice bulk bands. The bold lines indicate the light line in vacuum and in material $c$, respectively. The branches labelled (i) correspond to modes localized at the superlattice–cap layer interface.

as functions of the space position $x_3$ for a given wavevector $k_\| D = 6$ and for different reduced frequencies $\omega D/c = 4.458$, 4.981 and 4.027 corresponding to a resonant mode $R_3$, a localized mode $L_1$ and an interface mode i, respectively, in figure 6. This local density of states reflects the spatial behaviour of the square modulus of the electric field.

In the first case (figure 7b), the reduced frequency ($\omega D/c = 4.458$) falls inside the bulk band of the superlattice. Consequently, the local density of states corresponding to this resonant mode shows an oscillatory behaviour both in the space of the superlattice and in the space of the cap layer and decays in vacuum. However, the local density of states is on average more important inside the cap layer than in the superlattice. One can also observe that, in the space occupied by the superlattice, this state is mostly concentrated in the layer made of material 1. A similar behaviour was found for electronic states in multiquantum wells where some resonant states are mostly concentrated in the barriers rather than in wells [22]. In the second case (figure 7(c)), the reduced frequency ($\omega D/c = 4.981$) falls inside the gap of the superlattice. Now, the corresponding local density of states shows an oscillatory behaviour in the space occupied by the cap layer and a decaying behaviour either in the superlattice or in vacuum. In the third case (figure 7(d)) corresponding to the reduced frequency of a localized state ($\omega D/c = 4.027$) at the superlattice–adlayer interface, the local density of states decays on both sides of this interface.

The frequencies of the localized and resonant electromagnetic modes vary with the thickness $d_c$ of the cap layer. Figure 8 presents this variation, for $k_\| D = 6$. The lowest branch (chain lines) corresponds to interface modes. The next branches (broken lines)

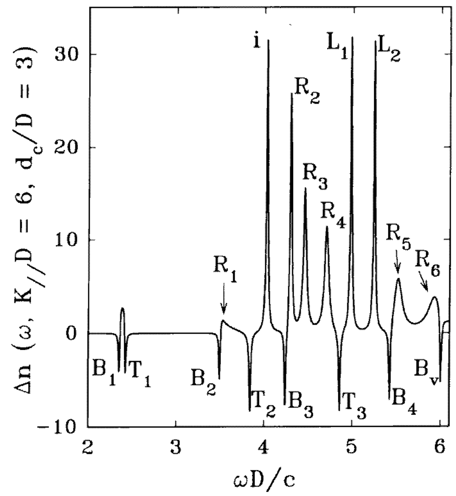


**Figure 6.** Variation in the density of states (in units of $D/c$) corresponding to the case depicted in figure 5, for $k_{\parallel}D = 6$ and $d_c/D = 3$. $B_i$, $T_i$ and $L_i$ have the same meanings as in figure 3; $R_i$ and i refer to the resonant modes and localized mode at the superlattice–adlayer interface, respectively.

become closer to each other when $d_c$ increases, and as a consequence the intensities of the corresponding resonances increase. However, the intensity of the resonant states decreases or may even vanish, in particular when $d_c$ is small or the frequency is high. Moreover, one can observe in figure 8 that the branch corresponding to interface modes remains almost flat (independent of $d_c$) even for small values of $d_c$. Let us mention here too that, for any given frequency in figure 8, there is a periodic repetition of the modes as a function of $d_c$.

Finally, when the cap layer is deposited on a superlattice terminated with a full layer of material 2 instead of 1, localized and resonant modes become quite different from those discussed in figures 5–8.

### *4.3. Semi-infinite superlattice in contact with a semi-infinite substrate*

To show the interface localized and resonant modes associated with the deposition of a semi-infinite superlattice on a semi-infinite substrate, we have chosen the same superlattice as before deposited on a substrate with a dielectric constant $\varepsilon_s = 2$. Figure 9 gives the localized and resonant interface modes for two complementary superlattices in which the substrate is in contact with either a full layer of material 2 or a full layer of material 1. In the former case, the two solid lines in the minigaps of the superlattice are localized interface modes which continue (broken lines) as resonances inside the bulk band of the substrate. However, the resonance appearing in the first minigap is rather wide and not a very well defined feature. Now, if the substrate is in contact with material 2, one obtains the dotted branches near the top of the first two bulk bands of the superlattice.

When one creates the two complementary superlattices used in figure 9 from the infinite superlattice and the infinite substrate, the variation $\Delta n_{Ic}(\omega)$ in the density of states is shown to be equal to zero [19] for frequencies $\omega$ belonging at the same time to the bulk bands of the substrate and the superlattice. Bearing in mind the loss of the $-1/2$ state at the limits of any bulk band and the conservation of the total number of states, we are led to the necessary

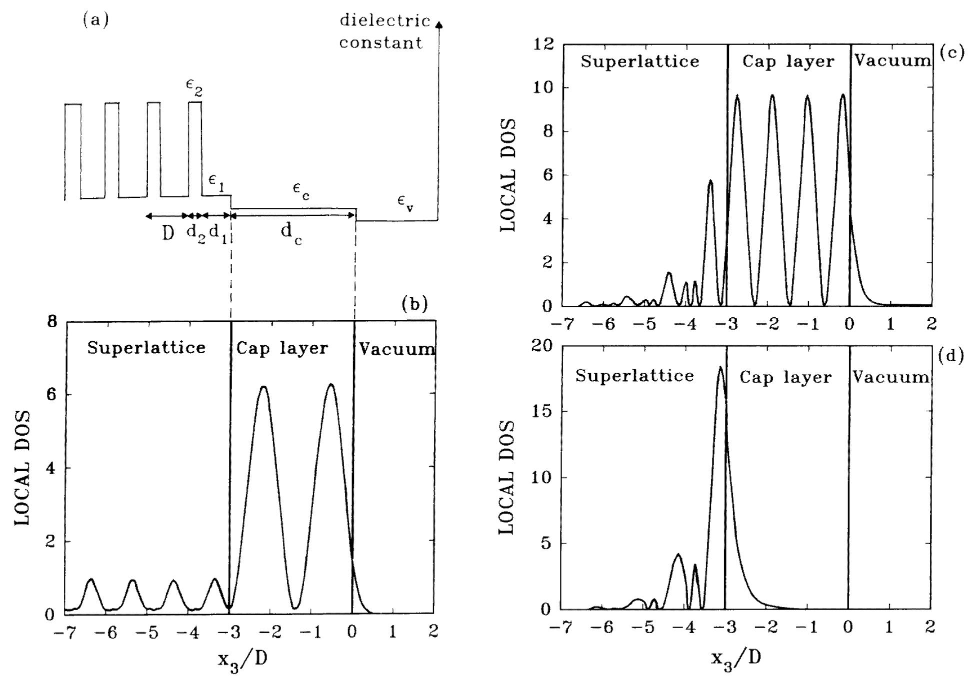


**Figure 7.** (a) A schematic representation of the dielectric constants corresponding to the different constituents of the coupled (superlattice–cap layer–vacuum) system. (b) Spatial representation of the local density of states (DOS) (in units of $D$) at $\omega D/c = 4.458$ and $k_\| D = 6$. (c) The same as in (b) but at $\omega D/c = 4.981$ and $k_\| D = 6$. (d) The same as in (b) but at $\omega D/c = 4.027$ and $k_\| D = 6$.

existence of resonant modes lying at the same time inside the gaps of the superlattice and in the bulk band of the substrate. We have presented in figure 10 an example of this variation in the density of states for $k_\| D = 1$; the loss of states due to the $\delta$ peaks of weight $-1/2$ at every edge of the bulk bands is mostly compensated by the appearance of peaks of the density of states labelled $R_1, R_2, R_3, R_4$ and, $R_5$. Every resonance, of weight almost equal to 1, is distributed differently over each of the two complementary superlattices. One can also check the validity of the statement presented above, namely that $\Delta n_{Ic}(\omega)$ is equal to zero for $\omega$ belonging to the bulk bands of the substrate and the superlattice at the same time.

One can also remark that the position of the interface modes in figures 5 and 9 are almost the same even though in the former case the substrate is replaced by a cap layer of finite thickness $d_c/D = 3$; moreover the localization of the interface modes is similar in both cases.

The frequencies of the interface modes are very sensitive to the nature of the substrate in contact with the superlattice. We have presented in figure 11 the dispersion of interface modes for different values of the parameter $\varepsilon_s$, when $\varepsilon_1 < \varepsilon_s < \varepsilon_2$. In fact, when $\varepsilon_s$ increases, the frequencies of the interface modes shift downwards, in particular the branch which appears above the first bulk band of the superlattice for $\varepsilon_v = 1$ (figure 2) and $\varepsilon_s = 2$ (figure 9) merges into this band for $\varepsilon_s = 3$; when $\varepsilon_s > 3$, an interface branch appears below the first bulk band as illustrated in figure 11 for $\varepsilon_s = 4, 6$ and 8. (Note that, for clarity, we have plotted in this figure the reduced velocity $\omega/ck_\|$ instead of the reduced frequency $\omega D/c$.)

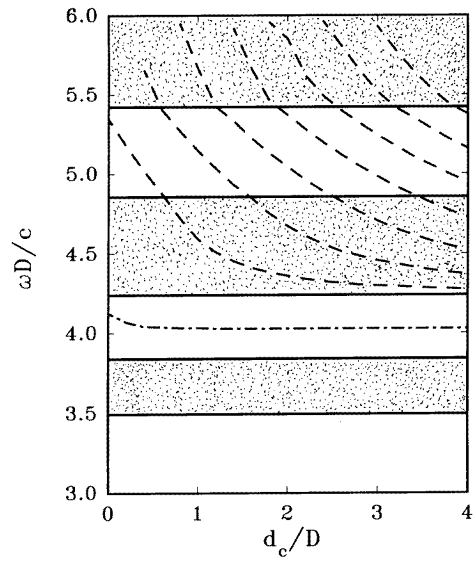


**Figure 8.** Variation in the dimensionless frequencies of localized and resonant modes induced by a cap layer of width $d_c$ deposited on the surface of the semi–infinite superlattice of figure 5, for $k_\parallel D = 6$. The lowest branch (chain lines) correspond to states localized at the superlattice–cap layer interface.

## 5. Conclusion

In this paper we have presented, for the first time to our knowledge, an analytical calculation of the response function for electromagnetic waves in a semi-infinite superlattice, with or without a cap layer. These results have been restricted to isotropic dielectric materials and are applicable to any superlattice system for which the dielectric functions of the component materials can be specified. These complete response functions can be used to study any physical property of the superlattice systems [4, 17]. These include the calculation of light scattering spectra of interface electromagnetic modes, the calculation of the electric and magnetic fields associated with the reflected and transmitted waves, the determination of the dispersion relations for surface (or interface) modes and studies of the attenuation of such modes, and the calculation of the density of states.

Using the interface response theory, we have deduced the closed-form relations of the density of states for electromagnetic waves in a semi-infinite superlattice, with or without a cap layer or in contact with a substrate. These closed-form expressions enabled us to derive the dispersion of both localized and resonant states for these heterostructures and their spatial distribution. Particular attention was devoted to resonances (also called leaky waves) appearing in such heterostructures and to their relations with the localized modes. In particular, we discussed different kinds of localized and resonant mode induced by a cap layer deposited on top of a semi-infinite superlattice. These surface dispersion curves may serve as a tool for the characterization of the material at the surface of the superlattice.

Finally, let us emphasize that the study of other excitations in semi-infinite superlattices, such as transverse elastic waves [20] or electronic states in the Kronig–Penney model [22, 23] involve the same mathematical tool and similar response functions as those derived in this

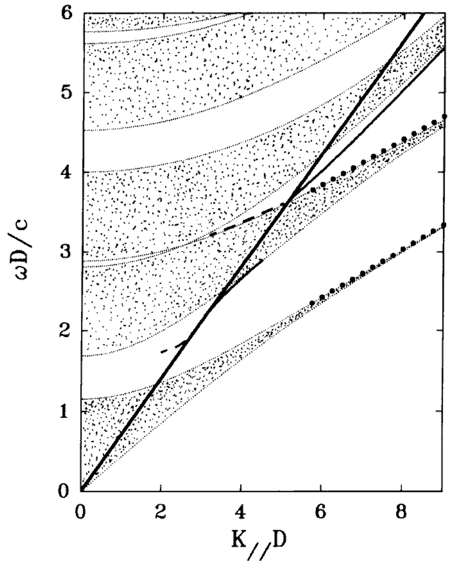


**Figure 9.** Interface localized and resonant modes associated with the two complementary superlattices in which the substrate is either in contact with a full layer of material 1 or 2. The shaded areas are the bulk bands of the superlattice. The bold straight line indicates the bottom of the substrate bulk band. The dielectric constant of the substrate is taken to be $\varepsilon_s = 2$. When the superlattice terminates with a layer 1, the localized (resonant) modes are presented by the full (broken) lines. The dotted lines are interface branches associated with termination of the superlattice by material 2.

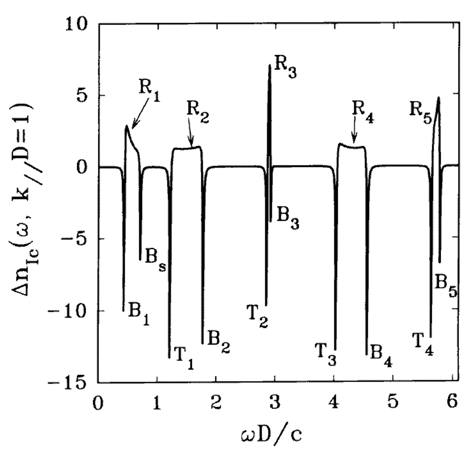


**Figure 10.** Variation in the density of states (in units of $D/c$), at $k_\parallel D = 1$, for the two complementary superlattices of figure 9 created from the infinite superlattice and the infinite substrate. $B_i$ and $T_i$ are $\delta$ peaks of weight $-1/2$ appearing at the edges of the superlattice bulk bands, $B_s$ refers to a $\delta$ peak of weight $-1/2$ situated at the bottom of the substrate bulk band. The loss of states due to the $\delta$ peaks of weight $-1/2$ at every edge of the bulk bands is compensated by the peaks of the density of states labelled $R_i$.

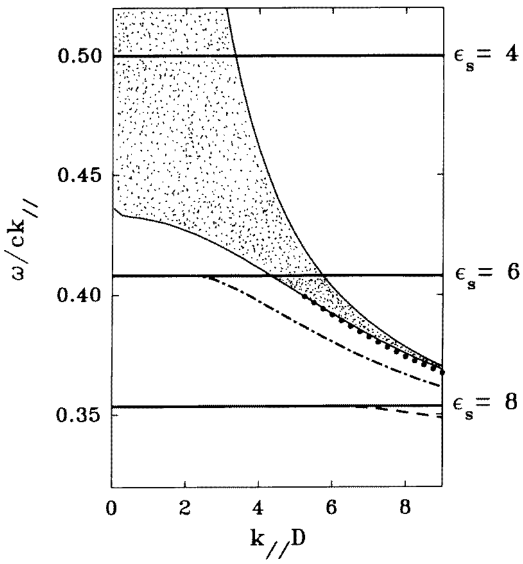


**Figure 11.** Dispersion of the lowest bulk band and interface modes for $\varepsilon_s = 4$ (dotted line), $\varepsilon_s = 6$ (chain line) and $\varepsilon_s = 8$ (broken line). The horizontal bold lines indicate the bottom of the substrate bulk bands characterized by their dielectric constants cited above. In order to obtain good separation between the interface modes, we have represented the reduced velocity $\omega/ck_\parallel$ instead of the reduced frequency $\omega D/c$.

paper. The reason is the mathematical similarity between both the equation of motions and boundary conditions in all the above problems.

## Appendix

Knowing the Green function for an infinite homogeneous medium given by

$$G_i(x_3, x_3') = \frac{-1}{2F_i} \exp(-\alpha_i |x_3 - x_3'|)$$

we obtained the following results with the help of the interface response theory [15].

### A1. 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 $\eta$ (equations (2), (3), (5), (6), (10) and (11)), are

$$g\left(n, 1, \frac{-d_1}{2}; n', 1, \frac{-d_1}{2}\right) = \left(\frac{C_1 S_2}{F_2} + \frac{C_2 S_1}{F_1}\right) \frac{t^{|n-n'|+1}}{t^2 - 1} \tag{A1}$$

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

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

$$g\left(n, 1, \frac{+d_1}{2}; n', 1, \frac{+d_1}{2}\right) = \left(\frac{C_1 S_2}{F_2} + \frac{C_2 S_1}{F_1}\right) \frac{t^{|n-n'|+1}}{t^2 - 1}. \tag{A4}$$

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

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

where

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

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

### A2. 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 $i = c$ of width $d_c$ 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 (see figure 1).

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

$$d\left(0, c, -\frac{d_c}{2}; 0, c, \frac{d_c}{2}\right) = d\left(0, c, \frac{d_c}{2}; 0, c, -\frac{d_c}{2}\right) = \frac{C_1 S_2/F_2 + C_2 S_1/F_1}{(1 + F_v S_c/F_c C_c) C_c \Delta} \tag{A7}$$

$$d\left(0, c, \frac{d_c}{2}; 0, c, -\frac{d_c}{2}\right) = \frac{C_1 S_2/F_2 + C_2 S_1/F_1 + (S_c/F_c C_c)[C_1 C_2 + (F_1/F_2) S_1 S_2 - t]}{(1 + F_v S_c/F_c C_c)\Delta} \tag{A8}$$

$$d\left(0, c, -\frac{d_c}{2}; 0, c, -\frac{d_c}{2}\right) = \frac{1}{\Delta}\left(\frac{C_1 S_2}{F_2} + \frac{C_2 S_1}{F_1}\right) \tag{A9}$$

and, for $n$ and $n' \leqslant 0$ and $i \neq c$,

$$d\left(n, 1, -\frac{d_1}{2}; n', 1, \frac{-d_1}{2}\right) = \frac{t}{t^2 - 1}\left\{ \left(\frac{C_1 S_2}{F_2} + \frac{C_2 S_1}{F_1}\right) t^{|n-n'|} - t^{-n-n'} \left(\frac{S_1 t}{F_1} + \frac{S_2}{F_2}\right) \frac{Y}{\Delta} \right\} \tag{A10}$$

$$d\left(n, 1, -\frac{d_1}{2}; n', 1, \frac{+d_1}{2}\right) = \frac{t}{t^2 - 1}\left\{ \frac{S_2 t^{|n-n'|}}{F_2} + \frac{S_1 t^{|n-n'-1|}}{F_1} - t^{-n-n'} \left(\frac{C_1 S_2}{F_2} + \frac{C_2 S_1}{F_1}\right) \frac{Y}{\Delta} \right\} \tag{A11}$$

$$d\left(n, 1, \frac{d_1}{2}; n', 1, -\frac{d_1}{2}\right) = \frac{t}{t^2 - 1}\left\{ \frac{S_2 t^{|n-n'|}}{F_2} + \frac{S_1 t^{|n-n'+1|}}{F_1} - t^{-n-n'} \left(\frac{C_1 S_2}{F_2} + \frac{C_2 S_1}{F_1}\right) \frac{Y}{\Delta} \right\} \tag{A12}$$

$$d\left(n,1,\frac{d_1}{2};n',1,\frac{d_1}{2}\right)=\frac{t}{t^2-1}\left\{\left(\frac{C_1S_2}{F_2}+\frac{C_2S_1}{F_1}\right)t^{|n-n'|}-t^{-n-n'}\left(\frac{S_1}{F_1}+\frac{S_2}{F_2}t\right)\frac{Y}{\Delta}\right\} \tag{A13}$$

where $\Delta$ and $Y$ are given by equations (12) and (24).

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

(i) When the two points are inside the superlattice, $d(n,i,x_3;n',i',x_3')$ is given by equation (A5) in which one has to replace $\mathbf{g}(M_m,M_{m'})$ by $\mathbf{d}(M_m,M_{m'})$ given by equations (A10)–(A13).

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

$$d(0,c,x_3;0,c,x_3')=U_c(x_3,x_3')+\frac{1}{S_c^2}\left[\sinh\left[\alpha_c\left(\frac{d_c}{2}-x_3\right)\right];\sinh\left[\alpha_c\left(\frac{d_c}{2}+x_3\right)\right]\right]$$
$$\times\mathbf{d}(M_c,M_c)\begin{bmatrix}\sinh\left[\alpha_c\left(\frac{d_c}{2}-x_3'\right)\right]\\ \sinh\left[\alpha_c\left(\frac{d_c}{2}+x_3'\right)\right]\end{bmatrix} \tag{A14}$$

where

$$U_c(x_3,x_3')=-\frac{1}{2F_c}\exp\left[-\alpha_c|x_3-x_3'|\right]+\frac{1}{2F_cS_c}\left\{\sinh\left[\alpha_c\left(\frac{d_c}{2}+x_3'\right)\right]\right.$$
$$\times\exp\left[-\alpha_c\left(\frac{d_c}{2}+x_3\right)\right]+\sinh\left[\alpha_c\left(\frac{d_c}{2}+x_3'\right)\right]$$
$$\left.\times\exp\left[-\alpha_c\left(\frac{d_c}{2}-x_3\right)\right]\right\} \tag{A15}$$

and $\mathbf{d}(M_c,M_c)$ is the $(2\times2)$ matrix formed by the elements given by equations (A7)–(A9), for $M_c=(0,c,\pm d_c/2)$.

(iii) When the two points are inside vacuum,

$$d(x_3,x_3')=\frac{-1}{2F_v}+\left(\frac{1}{2F_v}+[C_1S_2/F_2+C_2S_1/F_1+(S_c/F_cC_c)(C_1C_2+(F_1/F_2)S_1S_2-t)]\right.$$
$$\left.\times\{(1+F_vS_c/F_cC_c)\Delta\}^{-1}\right)\exp[-\alpha_v(x_3+x_3')] \tag{A16}$$

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