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The influence of capping layers on surface phonon polaritons in superlattices

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Abstract. The influence of capping layers on surface phonon polaritons in two-layer superlattices is investigated here theoretically. General analytical expressions are given. A few illustrative applications are presented afterwards, for p-polarized non-retarded polaritons within GaAs–InAs superlattices with or without an InP capping layer. A few dispersion curves for such polaritons are drawn. The variation of the frequencies of these polaritons with the thickness of the capping layer is given.

1. Introduction

Surface phonon polaritons in two-layer superlattices have been studied before theoretically by Yeh *et al* (1977), Giuliani *et al* (1984), Liu *et al* (1985), Lambin *et al* (1985a, b), Haupt and Wendler (1987), Djafari-Rouhani and Dobrzynski (1987), Dereux *et al* (1988), Vetrov and Shabanov (1992), Bah *et al* (1992), and others. Corresponding experimental investigations appeared also, see for example Yeh *et al* (1978), Ng *et al* (1978), Yariv and Yeh (1984), Yeh (1988), Lambin *et al* (1986) and Dumelow *et al* (1993). The surface phonon polaritons can be studied by electron energy loss spectroscopy, infrared reflectivity measurement and attenuated total reflection.

However, to our knowledge the effects of capping layers on surface phonon polaritons in superlattices have not been addressed before. This is the aim of the present paper. The dispersion relation of these excitations can be obtained by different methods. In this work, we have used a Green function approach, based on the interface response theory of Dobrzynski (1987), which also provides the possibility of studying the local and total densities of states in these composite systems (Bah 1995). In section 2 we give the closed form expression of the surface phonon polariton dispersion relation in a superlattice with a cap layer and, as a particular case, the corresponding expression for the interface between a semi-infinite superlattice and a homogeneous substrate. Section 3 contains a few applications of these general results for p-polarized non-retarded polaritons in GaAs/InAs superlattices with or without an InP surface cap layer.

2. The dispersion relation of surface modes

The superlattice is formed from an infinite repetition of two different isotropic dielectric slabs labelled by the index $i = 1$ or 2. Each material i is characterized by its dielectric constant $\varepsilon_i(\omega)$ (where ω is the frequency) and its thickness d_i, the period of the superlattice being $D = d_1 + d_2$. The cap layer will be denoted by the index 0 with the corresponding parameters $\varepsilon_0(\omega)$ and d_0 (see figure 1).

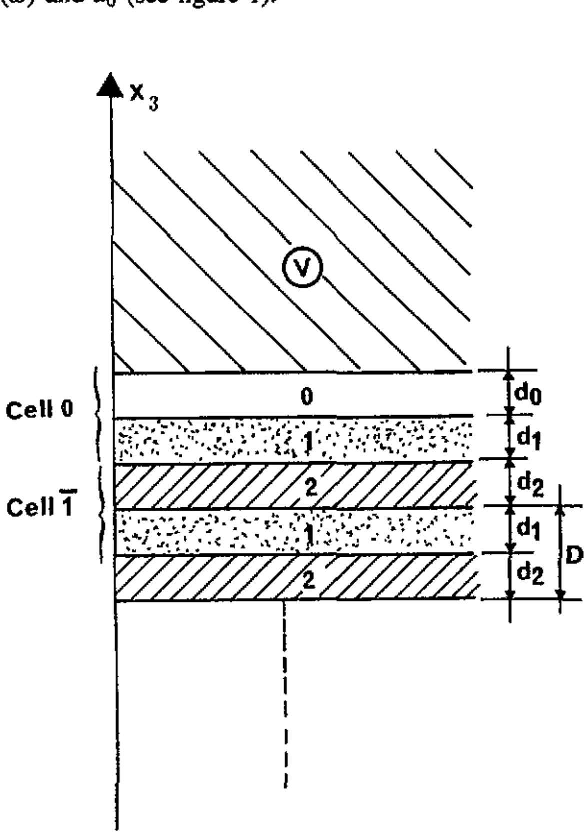

Figure 1. A schematic representation of a semi-infinite two-layer superlattice ($i = 1, 2$) with a cap layer ($n = 0, i = 0$) and in contact with vacuum ($i = \mathrm{v}$). d_0, d_1 and d_2 are respectively the thicknesses of the cap layer and of the two different dielectric slabs out of which the semi-infinite superlattice is built. D is the width of the unit cell.

In this work the dispersion relations of the bulk and surface modes are obtained from the poles of the Green functions for the infinite and semi-infinite superlattices. The derivation of these functions follows the method described by Dobrzynski (1988, 1991), except for more elaborate calculations due to the presence of the cap layer at the surface of the superlattice. We do not give here any details about the Green function formalism and limit this section to the presentation of the dispersion relations. This is because the emphasis in this paper is put on the effect of the cap layer on the surface modes rather than on a detailed discussion of the densities of states (Bah 1995).

We first define the two following parameters in each medium $i = 0, 1, 2, \mathrm{v}$ where v stands for vacuum:

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

$$F_i = \alpha_i \qquad \text{for transverse electric (TE) modes} \tag{2}$$

$$F_i = -(\omega^2/c^2)\varepsilon_i(\omega)/\alpha_i \qquad \text{for transverse magnetic (TM) modes.} \tag{3}$$

Here $k_\parallel$ is the modulus of the propagation wave vector parallel to the interfaces and c is the speed of light in vacuum. In each medium i, α_i has the meaning of a wave vector in the direction perpendicular to the layers.

The bulk dispersion relation for the infinite superlattice is (see for example Camley *et al* 1983, Camley and Mills 1984, Dobrzynski 1988)

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

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 in the superlattice $\boldsymbol{k} \equiv (k_\parallel, k_3)$.

When the denominator of the response function vanishes for a frequency lying inside the gaps of the infinite superlattice, one obtains localized states within the cap layer, which decay exponentially into the bulk of the superlattice and into the vacuum. The explicit expression giving these localized states is

$$C_1 S_2(F_2/RF_v - RF_v/F_2) + S_1 S_2(F_2/F_1 - F_1/F_2) + C_2 S_1(F_1/RF_v - RF_v/F_1) = 0 \tag{7}$$

together with the following condition:

$$|C_1 C_2 + (F_2/F_1) S_1 S_2 - RF_v(C_1 S_2/F_2 + C_2 S_1/F_1)| > 1 \tag{8}$$

with

$$R = (1 + F_0 S_0/F_v C_0)/(1 + F_v S_0/F_0 C_0). \tag{9}$$

(8) ensures that these modes decay inside the bulk of the superlattice and inside the vacuum.

These expressions generalize those derived earlier by Dobrzynski (1988) for electromagnetism in dielectric superlattices and by El Boudouti *et al* (1993) for transverse elastic waves in superlattices.

In particular the localized excitations at the interface between a semi-infinite superlattice and an homogeneous semi-infinite substrate can be obtained from (7) and (8) where, in the complementary equation (9), the thickness d_0 of the cap layer goes to infinity, i.e. $S_0/C_0 \to 1$.

In the limit where the cap layer $i = 0$ is of the same nature as the $i = 2$ superlattice layer and $d_0 < d_2$, the same results provide the localized modes for a semi-infinite superlattice ending with an incomplete $i = 2$ surface layer.

Table 1. Transverse and longitudinal frequencies and high-frequency dielectric constants of GaAs, InAs and InP.

	ω_L (cm^{-1})	ω_T (cm^{-1})	ε_∞
GaAs	297	273	10.9
InAs	243	218	12.3
InP	351	307	9.6

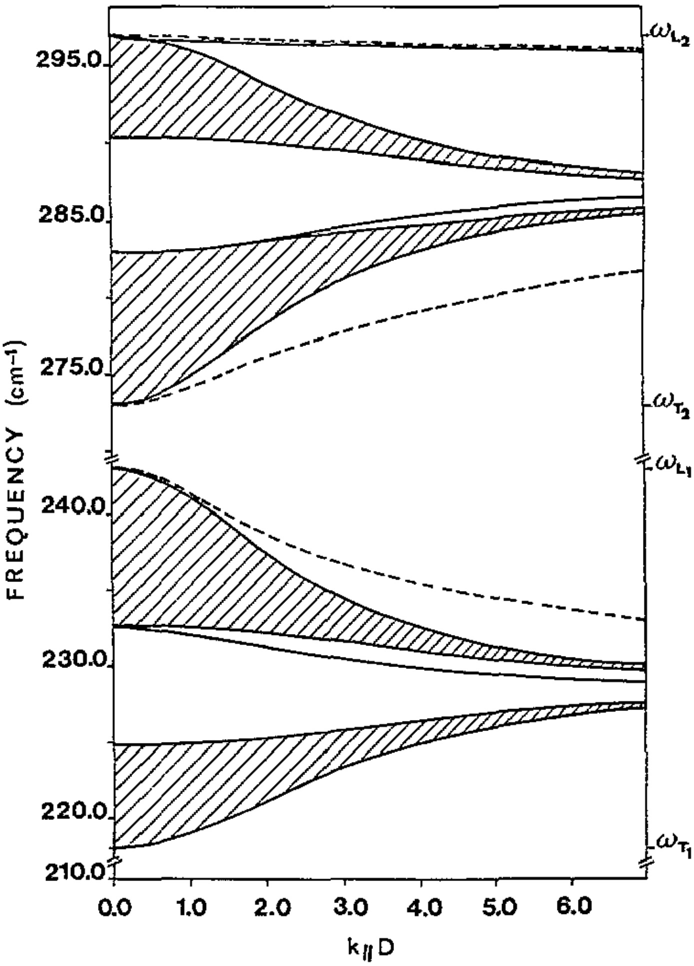

Figure 2. The unretarded bulk and surface phonon polaritons with p polarization for a GaAs–InAs superlattice. The curves give ω (cm^{-1}) as a function of $k_{\parallel}D$, where ω is the frequency, $k_{\parallel}$ the propagation vector parallel to the interface and $D = d_1 + d_2 = 300$ Å the period of the superlattice with $d_1 = 2d_2$. The shaded areas represent the bulk bands. The full lines represent the surface polaritons for the semi-infinite superlattice terminated by a GaAs layer of thickness $d_0 = 0.8d_2$. The dashed lines represent the surface polaritons for the complementary superlattice terminated by a GaAs layer of thickness $d_0 = 0.2d_2$.

3. Application to the surface phonon–polariton modes

In what follows specific results will be given for the GaAs–InAs superlattice and also for this superlattice with an InP surface cap layer. We characterize each material by the usual dielectric constant

$$\varepsilon_i(\omega) = \varepsilon_{\infty i}(\omega_{Li}^2 - \omega^2)/(\omega_{Ti}^2 - \omega^2) \tag{10}$$

where ω_{Li} and ω_{Ti} are the frequencies of the longitudinal and transverse optical phonons and $\varepsilon_{\infty i}$ the high-frequency dielectric constant in material i. The numerical values of ω_{Li}, ω_{Ti} and $\varepsilon_{\infty i}$ are given in table 1.

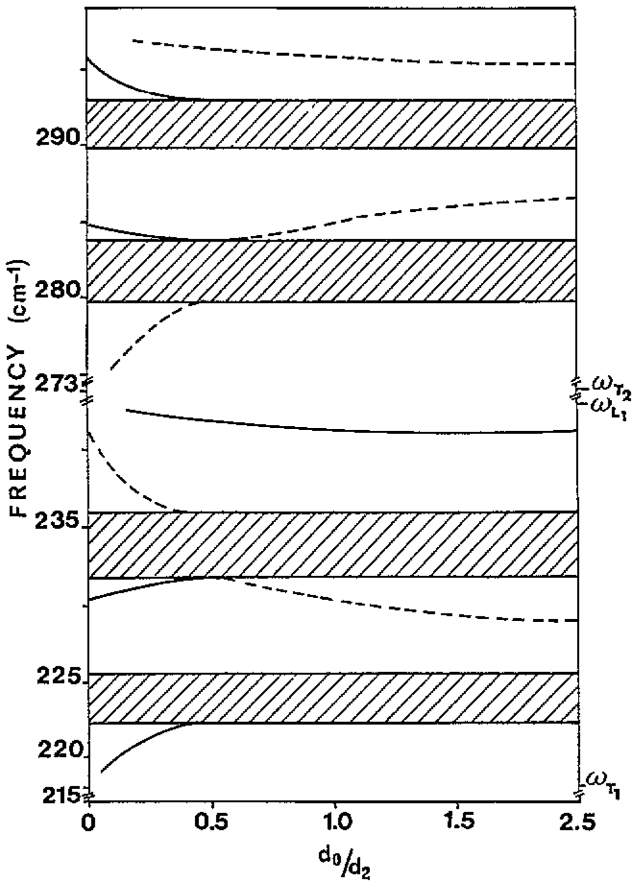

Figure 3. The variation of the frequencies ω of the surface modes of semi-infinite GaAs–InAs superlattices, for $k_\parallel D = 2.5$, as a function of d_0/d_2, where d_0 is the width of the surface layer, which may be GaAs (dashed lines) or InAs (full lines). The shaded areas represent the bulk bands of the superlattice.

We shall first consider (subsection 3.1) semi-infinite superlattices in contact with a vacuum, then (subsection 3.2) semi-infinite superlattices with a surface cap layer in contact with a vacuum. All the illustrative curves presented here are given for p-polarized non-retarded polaritons for which F_i takes the value given by (3) and the speed of light $c \to \infty$.

3.1. A semi-infinite superlattice in contact with a vacuum

The applications presented here are for a GaAs–InAs superlattice with $d_1 = 2d_2$ and the period $D = d_1 + d_2 = 300$ Å. Figure 2 gives the dispersion of bulk bands and surface modes as a function of $k_\parallel D$, where $k_\parallel$ is the propagation vector parallel to the interface. We have presented the surface modes of two complementary semi-infinite superlattices obtained by cleaving an infinite GaAs–InAs superlattice within one GaAs slab, such that the thickness of the remaining surface GaAs layer is respectively $d_0 = 0.2d_2$ (dashed lines) and $d_0 = 0.8d_2$ (full lines) in each semi-infinite part. One can observe that the frequencies of the surface modes are very dependent on the thickness of the last surface layer of GaAs.

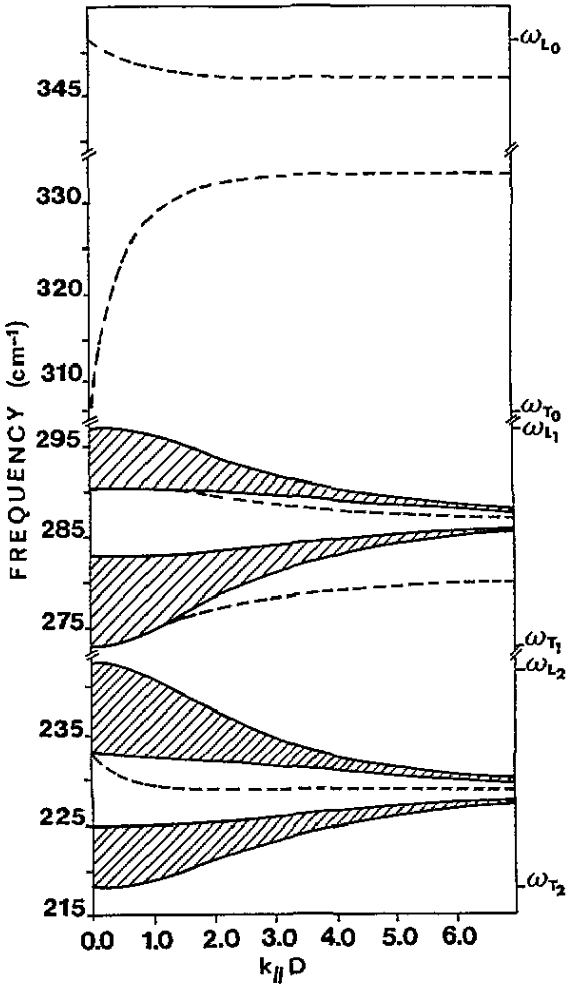

Figure 4. The dispersion of localized phonon polaritons of p polarization for an InP cap layer of thickness $d_0 = D$, deposited on top of the GaAs–InAs superlattice terminated by a full GaAs layer with $d_1 = 0.5d_2$. The shaded areas represent the bulk bands of the superlattice.

Having seen that the frequencies of the surface states are very sensitive to the width d_0 of the last surface layer, we present in figure 3 the variation of these frequencies, for $k_{\parallel}D = 2.5$, as a function of d_0/d_2, both for a surface GaAs layer (dashed lines) and for a surface InAs layer (full lines). All the surface branches that cannot reach the value $d_0 = 0$ actually stop at the frequencies $\omega = \omega_{Li}$ or ω_{Ti} ($i = 1, 2$). Let us note that when d_0 increases, the frequencies of the existing surface modes may either increase or decrease, before going to an asymptotic limit for $d_0/d_2 > 3$. In both cases, for $d_0/d_2 = 0.5$, we observe only one branch of the surface mode, all the other branches become resonant waves (or leaky waves) by merging into the bulk bands of the superlattice.

3.2. *A semi-infinite superlattice with a surface cap layer*

Now, we assume that a cap layer of InP, of thickness d_0, is deposited on top of the GaAs–InAs superlattice terminated by a full GaAs layer. The dispersions of surface and interface

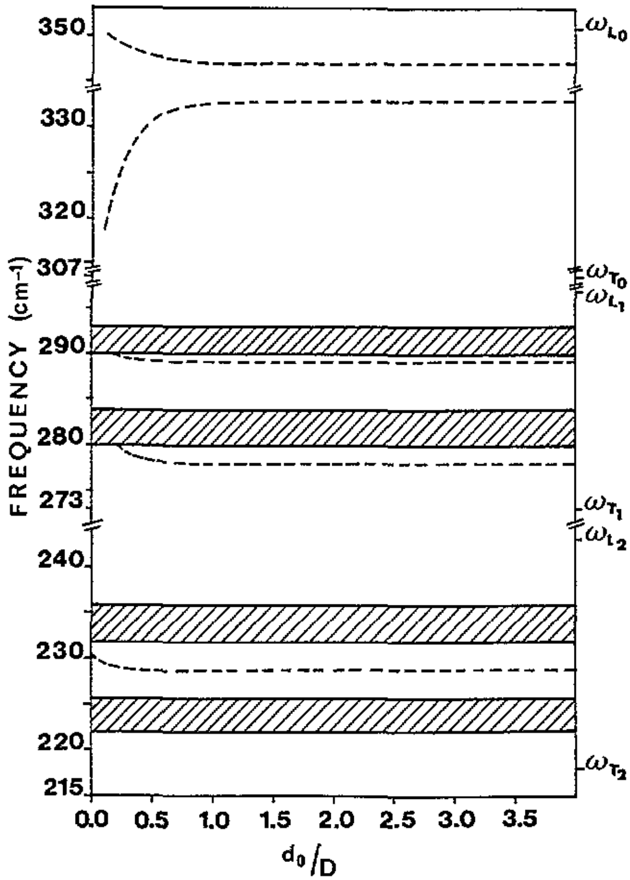

Figure 5. The variation of the frequencies ω of the interface and surface localized modes of an InP cap layer of thickness d_0, deposited on top of the GaAs–InAs superlattice terminated by a full GaAs layer with $d_1 = 0.5d_2$, for $k_{\|}D = 2.5$, as a function of d_0/D.

localized modes are presented in figure 4 for $d_1/d_2 = \frac{1}{2}$ and $d_0/D = 1$. An important variation of the frequencies of the localized modes is obtained with the presence of cap layers. Here the second and third surface modes counted from the bottom of figure 4 are respectively below the third and fourth bulk bands; they become resonant modes by merging into the bulk band at $k_{\|}D \simeq 1$. Without a cap layer, Lambin *et al* (1985a) found these modes above the same bands. Note that different localized modes appear when the InP cap layer is deposited on top of an InAs layer of the superlattice rather than a GaAs layer. These details, as well as the study of the resonances, will be given in the PhD thesis of Bah (1995).

The frequencies of the localized modes show significant variations with the thickness d_0 of the cap layer, as shown in figure 5 for $k_{\|}D = 2.5$. These variations are faster when d_0 is smaller or of the order of D. For $d_0/D < 0.25$, the second and the third localized branches become resonant by merging into the bulk bands. Finally, let us mention that for $d_0/D > 1$, the frequencies of the localized branches reach their asymptotic limits, which correspond, except for the highest branch, to the frequencies of the interface modes between a semi-infinite GaAs–InAs superlattice and a semi-infinite homogeneous InP substrate. In this case, the highest branch corresponds to a localized mode at the interface between the InP cap layer and the vacuum above. These asymptotic limits can be found from (8) and (9) by taking the limit of $d_0 \to \infty$.

4. Conclusion

In this paper we have studied the effect of capping layers on surface phonon polaritons in superlattices. A closed form expression enabling to calculate the corresponding surface phonon polaritons was given here for the first time to our knowledge. A few applications to GaAs–InAs superlattices with or without an InP surface cap layer show that the presence of capping layers has an important effect on the frequencies of the surface polaritons.

As discussed fully before in the case of a superlattice without a cap layer (Dereux *et al* 1988a, b), these surface modes can be studied by electron energy loss spectroscopy, infrared reflectivity measurement and attenuated total reflection.

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