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Bulk and surface phonon polaritons in three-layer superlattices

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Three-layered superlattices are formed from a periodic repetition of three different slabs. Closed-form expressions for the study of bulk and surface polaritons in such materials are given in this paper with a few illustrative applications.

I. INTRODUCTION

The mathematical formalism necessary for the calculation of surface polaritons in dielectric superlattices was shown[1] to be the same as for transverse elastic waves. The surface of a dielectric superlattice is, however, an interface between this superlattice and the semi-infinite vacuum having dielectric constant ε_0. Surface phonon polaritons have been studied theoretically[2-9] and experimentally[10] within two-layer superlattices, but not, to our knowledge within three-layer superlattices.

In Sec. II of this paper we give the closed-form expressions that enable us to study the existence and the frequencies of surface phonon polaritons in three-layer superlattices. This general result is illustrated in Sec. III by a few specific applications.

II. BULK AND SURFACE PHONON POLARITONS IN THREE-LAYER SUPERLATTICES

With the help of the interface response theory of continuous composite systems,[11] applied before to polaritons in two-layer superlattices[7,12] and to surface transverse elastic waves in three-layer superlattices,[13] it is straightforward to obtain the following closed form results enabling one to study the existence and the frequencies of bulk and surface phonon polaritons in three-layer superlattices.

Before giving these results, let us define the following entities: $\mathbf{k} \equiv (\mathbf{k}_{\parallel}, k_3)$ as the propagation vector, where $\mathbf{k}_{\parallel}$ is its component parallel to the interfaces and k_3 its component perpendicular to the interfaces; ω as the frequency of the phonon polaritons; c as the speed of propagation of light; d_i as the width of the slabs $i=1,2,3$ and D as the width of the unit cell

$$D = d_1 + d_2 + d_3 \; ; \qquad (1)$$

ε_i as the dielectric constants

$$\varepsilon_i = 1 \quad \text{for } i=0 \qquad (2)$$

and

$$\varepsilon_i = \varepsilon_\infty \frac{\omega_{\mathrm{L}i}^2 - \omega^2}{\omega_{\mathrm{T}i}^2 - \omega^2} \quad \text{for } i=1,2,3 \; , \qquad (3)$$

where $\omega_{\mathrm{L}i}$ and $\omega_{\mathrm{T}i}$ are, respectively, the longitudinal and the transverse optical phonon frequencies; α_i as the decay

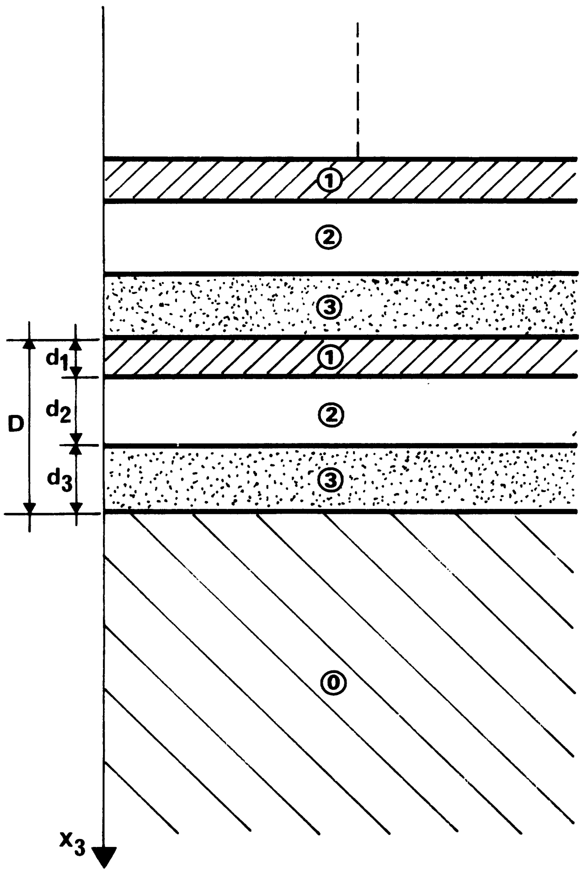

FIG. 1. Schematic representation of a semi-infinite three-layer ($i=1,2,3$) superlattice; d_i ($i=1,2,3$) are the widths of the three different dielectric slabs out of which the semi-infinite superlattice is built; D is the width of the unit cell and $i=0$ stands for the vacuum.

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constants

$$\alpha_i=\left[k_{\parallel}^2-\frac{\omega^2\varepsilon_i}{c^2}\right]^{1/2}\ ,\quad i=0,1,2,3\ ; \tag{4}$$

F_i as parameters defined, respectively, for transverse magnetic (TM) modes and transverse electric (TE) modes by

$$F_i=\alpha_i \quad \text{for TE modes}\ , \tag{5a}$$

$$F_i=-\frac{\omega^2}{c^2}\frac{\varepsilon_i}{\alpha_i} \quad \text{for TM modes}\ ,\quad i=0,1,2,3\ ; \tag{5b}$$

and C_i and S_i as condensed notations for

$$C_i=\cosh(\alpha_i d_i) \tag{6a}$$

and

$$S_i=\sinh(\alpha_i d_i)\ ,\quad i=1,2,3\ . \tag{6b}$$

With the above-defined notations the bulk dispersion relation for phonon polaritons in infinite three-layer superlattices is

$$2\cos k_3D=2C_1C_2C_3+\left[\frac{F_1}{F_2}+\frac{F_2}{F_1}\right]S_1S_2C_3+\left[\frac{F_1}{F_3}+\frac{F_3}{F_1}\right]S_1S_3C_2+\left[\frac{F_2}{F_3}+\frac{F_3}{F_2}\right]S_2S_3C_1\ . \tag{7}$$

For the semi-infinite superlattice in contact with the vacuum schematically depicted by Fig. 1, the closed-form expressions enabling one to study within the bulk gaps the existence and the dispersion relations of surface polaritons are

$$\left[F_1-\frac{F_0^2}{F_1}\right]S_1C_2C_3+\left[F_2-\frac{F_0^2}{F_2}\right]S_2C_1C_3+\left[F_3-\frac{F_0^2}{F_3}\right]S_3C_1C_2+\left[\frac{F_1F_3}{F_2}-\frac{F_0^2F_2}{F_1F_3}\right]S_1S_2S_3 -F_0\left[\frac{F_2}{F_1}-\frac{F_1}{F_2}\right]S_1S_2C_3-F_0\left[\frac{F_3}{F_1}-\frac{F_1}{F_3}\right]S_1S_3C_2-F_0\left[\frac{F_3}{F_2}-\frac{F_2}{F_3}\right]S_2S_3C_1=0\ , \tag{8a}$$

together with the condition

$$\left|C_1C_2C_3+\frac{F_1}{F_2}S_1S_2C_3+\frac{F_1}{F_3}S_1S_3C_2+\frac{F_2}{F_3}S_2S_3C_1-\frac{F_0}{F_1}S_1C_2C_3-\frac{F_0}{F_2}S_2C_1C_3-\frac{F_0}{F_3}S_3C_1C_2-\frac{F_0F_2}{F_1F_3}S_1S_2S_3\right|>1\ . \tag{8b}$$

III. A FEW APPLICATIONS TO TM PHONON POLARITONS

This section contains a few dispersion curves of the phonon polaritons bulk bands and localized surface modes for GaAs-InAs-AlAs semi-infinite superlattices. The parameters of these materials are listed in Table I. We shall discuss the general behavior of these phonon polaritons as a function of the thicknesses and the respective positions of the layers. All the curves presented here are given only for *p*-polarized (transverse magnetic modes) retarded polaritons for which F_i takes the values given by Eq. (5b).

The first example of the polariton dispersion of bulk and surface modes as a function of $k_{\parallel}D$ is given in Fig. 2. We have assumed that $d_1=d_2=d_3=D/3$. Here the bulk TM phonon polaritons, solutions of Eq. (7), are presented by the shaded areas and by the solid lines. In the "reststrahlen" regions, defined by the intervals $[\omega_{Ti},\omega_{Li}]$ with $i=1$, 2, and 3, the bulk bands are relatively narrow and well separated. Let us note that in the gaps appearing between the bulk bands in the reststrahlen region, we found surface localized modes. Figure 2 is drawn for AlAs at the surface followed by InAs, GaAs, and so on. In that case, five branches of surface phonon polaritons were found and are presented by the dotted lines.

Figure 3 shows five branches of surface modes for the same superlattice as above but with a GaAs surface layer followed by InAs, AlAs, and so on. Note when comparing Figs. 3 and 2 the variations in the positions of the surface modes.

Figure 4 shows an example in which the layers have the following thicknesses: $d_1/D=\frac{1}{6}$, $d_2/D=\frac{1}{6}$, and $d_3/D=\frac{2}{3}$, for an AlAs surface slab followed by InAs, GaAs, and so on. The qualitative behaviors are similar to the ones presented above (Figs. 2 and 3) but the quantitative results, and in particular the width of the bulk bands, the gaps and the frequencies of the localized modes are very different. Figure 4 shows five branches of surface

TABLE I. Transverse and longitudinal phonon frequencies and high-frequency dielectric constant of GaAs, InAs, and AlAs.

	ω_T (cm^{-1})	ω_L (cm^{-1})	ε_∞
GaAs	269.2	293	10.9
InAs	218	243	12.3
AlAs	364	403	8.5

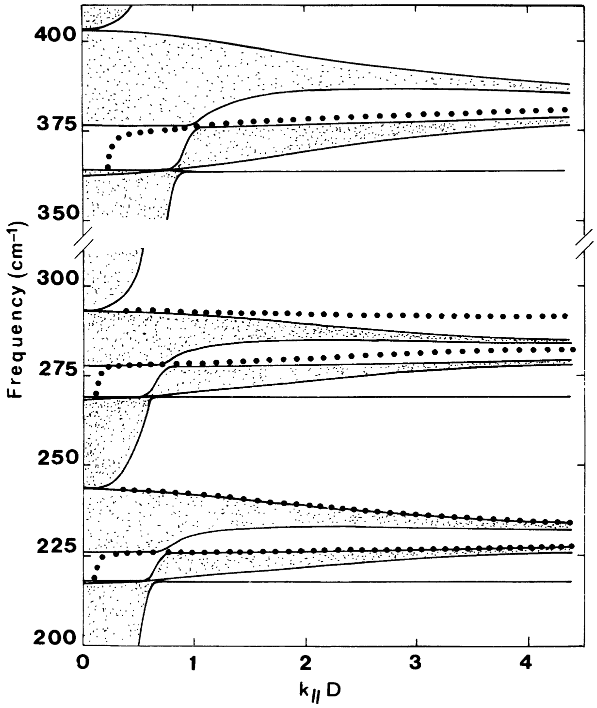

FIG. 2. Bulk and surface phonon polaritons in a three-layer superlattice formed out of AlAs, InAs, and GaAs layers with $d_1=d_2=d_3=D/3$; D is the period of the superlattice. This figure presents the frequencies (cm^{-1}) as a function of $k_{\parallel}D$; $k_{\parallel}$ is the propagation vector parallel to the interfaces. The hatched area presents the bulk bands. The dotted lines appearing in the reststrahlen region $[\omega_{Ti},\omega_{Li}]$, $i=1$, 2, and 3, represent the surface phonon polaritons for a surface AlAs layer followed by InAs and GaAs and so on. The parameters used in these calculations are given in Table I.

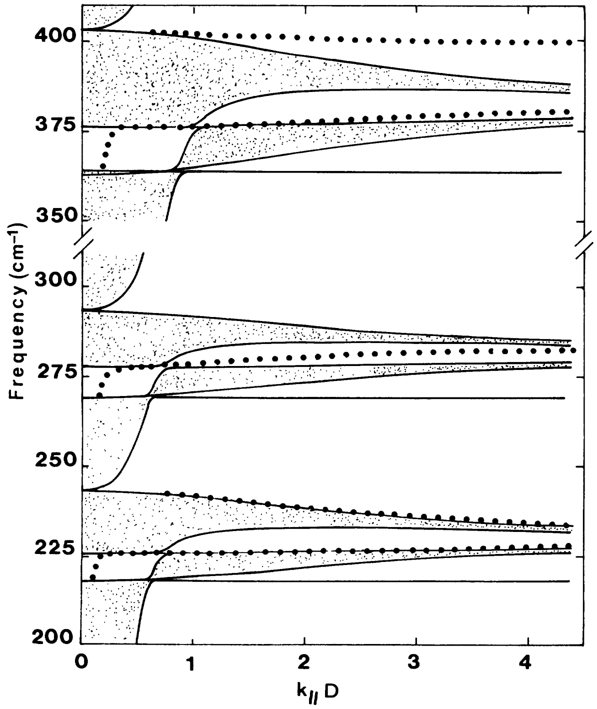

FIG. 3. Same as in Fig. 2 for a surface GaAs layer, followed by InAs and AlAs and so on.

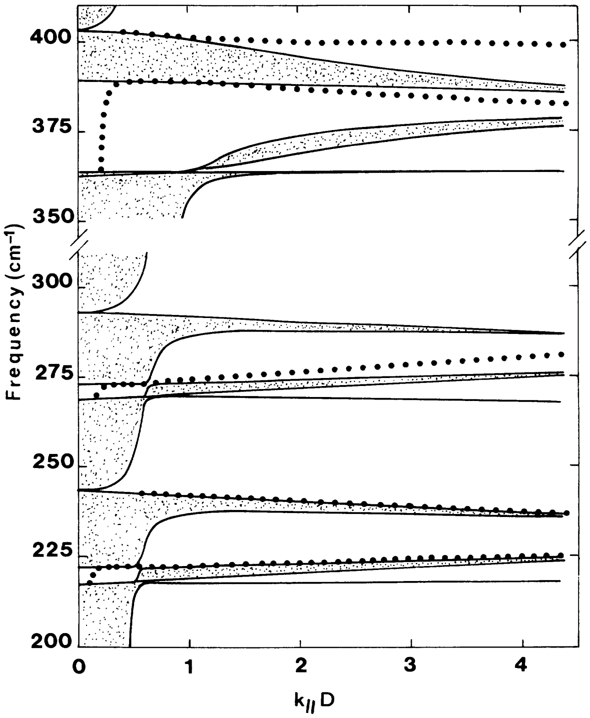

FIG. 4. Same as in Fig. 2 but with $d_1/D=\frac{1}{6}$, $d_2/D_2=\frac{1}{6}$, and $d_3/D=\frac{2}{3}$.

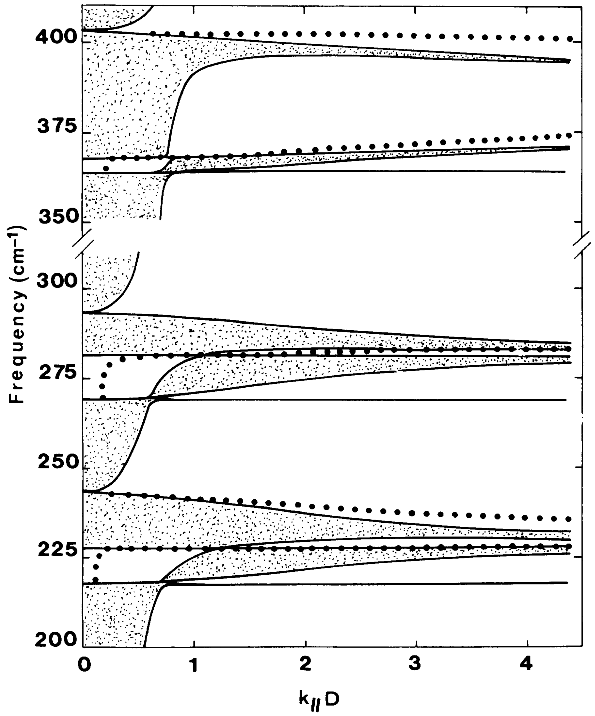

FIG. 5. Same as in Figs. 2 and 4 but for the case $d_1/D=d_2/D=\frac{4}{9}$ and $d_3/D=\frac{1}{9}$.

phonon polaritons presented by the dotted lines. In the reststrahlen regions $[\omega_{Ti}, \omega_{Li}]$, with $i=1$, 2, and 3, the bulk bands are more narrow and more separated than in Figs. 2 and 3.

In Fig. 5, similar observations can be made for the opposite situation $d_1/D=\frac{4}{9}$, $d_2/D=\frac{4}{9}$, and $d_3/D=\frac{1}{9}$ for the surface phonon polaritons. Let us note that the bulk bands in the reststrahlen regions [218–243 cm^{-1}] and [269.2–293 cm^{-1}] are narrower but not well separated. In the reststrahlen region [364–403 cm^{-1}] the bulk bands are narrower and very well separated.

IV. DISCUSSION

In this paper we obtained for the first time to our knowledge bulk and surface phonon polaritons for three-layer superlattices. The existence and the frequencies of these surface modes and the width of the bulk bands were found to be very sensitive to the thickness and the respective positions of the layers.

One can notice that in each specific case considered there is a surface mode whose frequency bends downwards as the light line is approached for each of the three materials. In addition, for two of the materials there is a second surface mode that lies near the top of the respective reststrahlen region and falls inside the bulk band before reaching the light line. Such behavior was already observed before[6] for two-layer superlattices. It is not easy to predict why one material lacks this second surface mode. We can only stress again as in Ref. 6 that the existence and frequencies of these surface modes are very sensitive to the thickness and the respective positions of the layers. Here the introduction of a third superlattice layer and its position in the sequence is a supplementary factor influencing the existence of this supplementary surface mode and the frequencies of all surface modes.

As discussed fully before for two-layer superlattices[6] these surface modes can be studied by electron-energy-loss spectroscopy, infrared reflectivity measurements, and attenuated total reflection.

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