Band structure and band-gap control in photonic superlattices

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The photonic band structure as well as the density of photon states of a one-dimensional photonic superlattice comprised of alternate layers of air and GaAs are theoretically investigated within the transfer-matrix formalism. The existence of photonic superlattices of null gap with band-touching phenomena is demonstrated, indicating the importance of one-dimensional photonic superlattices for many important practical applications.

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The propagation of light through a periodic medium has been extensively investigated since the advent of photonic-crystal (PC) materials proposed by Yablonovitch[1] and John,[2] who suggested that such structured materials with a periodic dielectric constant could influence significantly the nature of the photonic modes analogously to the influence of semiconductor crystals on electronic properties.[3–5] In particular, the existence of photonic bands in the energy spectrum as well as photonic band gaps, i.e., forbidden frequency regions for light propagation and optical emission resulting from the Bragg scattering of electromagnetic waves, have permitted quite a number of analogies with physical properties of semiconductor physics. Thus, in the last two decades, investigation of PCs has gained a powerful thrust and resulted in a considerable number of both experimental and theoretical investigations on photonic systems. The microstructuring techniques of high quality optical materials available nowadays yield to a remarkable flexibility in the fabrication of the PCs, resulting in the tailoring of the electromagnetic dispersion relation and mode structure to suit almost any need, opening new perspectives for both basic and technological research purposes.[5] Among many others, superrefractive phenomena such as the superprism effect[6] and tunable band structures[7,8] provide exciting possibilities to realize a variety of optical applications by using PCs.[9,10] In that respect, one-dimensional (1D) photonic band-gap structures[11–14] have been extensively investigated resulting in the proposal of various devices.

In this work we derive, via a transfer-matrix formalism, a transcendental equation for the photonic band structure of a 1D periodic structure made of alternating layers of different materials, such as GaAs and air. In addition to the well known existence of the band gaps, we show that, depending on the width relationship between the layer materials, superlattices with null photonic band gap may exist and the conditions for such occurrences are also established.

Here we focus on a 1D photonic superlattice in the z direction, i.e., a periodic photonic heterostructure composed of alternating layers of different layer materials, such as, e.g., GaAs and air. We choose the origin located at the center of a first slab (with dielectric constant ϵ_1 and magnetic permeability μ_1) of width a with period $d=a+b$, where b is the slab width of the second material (with dielectric constant ϵ_2 and magnetic permeability μ_2). For simplicity, here we restrict the analysis to electromagnetic (EM) plane waves, although the generalization to other EM waves is straightforward. Let us consider the propagation, along the z axis of the superlattice, of an in-plane linearly polarized electromagnetic field of the form $\vec{E}(z,t)=E(z)e^{-i\omega t}\hat{x}$. By using Maxwell's equations for linear and isotropic media, it is not difficult to show that the amplitude $E(z)$ of the electric field satisfies (Ref. 15)

$$\frac{d}{dz}\left[\frac{1}{n(z)Z(z)}\frac{dE}{dz}\right]=-\frac{n(z)}{Z(z)}\frac{\omega^2}{c^2}E, \tag{1}$$

where $n(z)=\sqrt{\epsilon(z)}\sqrt{\mu(z)}$ and $Z(z)=\sqrt{\mu(z)}/\sqrt{\epsilon(z)}$ are the refraction index and impedance, respectively, of each layer material. The solution of Eq. (1) for the electric field within each host material may be quite generally written

$$E(z)=E(z_0)\cos[k(z-z_0)]+\frac{1}{k}\left(\frac{dE}{dz}\right)_{z=z_0}\sin[k(z-z_0)], \tag{2}$$

where $k=\frac{2\pi}{\lambda}=\frac{\omega}{c}|n|$ and z_0 denotes an arbitrary point in each of the layer materials. By introducing the auxiliary function

$$\psi(z)=\begin{pmatrix} E(z) \\ \dfrac{1}{nZ}\dfrac{dE}{dz}\end{pmatrix}, \tag{3}$$

and the transfer matrix $M(z-z_0)$ as

$$\psi(z)=M(z-z_0)\psi(z_0), \tag{4}$$

where

$$M(z-z_0)=\begin{pmatrix} \cos[k(z-z_0)] & \dfrac{nZ}{k}\sin[k(z-z_0)] \\ -\dfrac{k}{nZ}\sin[k(z-z_0)] & \cos[k(z-z_0)]\end{pmatrix}, \tag{5}$$

one may write that

$$\psi\left(\frac{a+b}{2}\right)=T(a,b)\psi(0), \tag{6}$$

$$T(a,b)=M_2\left(\frac{b}{2}\right)M_1\left(\frac{a}{2}\right)=\begin{pmatrix} P & Q \\ R & S\end{pmatrix}, \tag{7}$$

$$P=\cos\frac{bk_2}{2}\cos\frac{ak_1}{2}-\frac{Z_2n_2}{Z_1n_1}\frac{k_1}{k_2}\sin\frac{bk_2}{2}\sin\frac{ak_1}{2}, \tag{8}$$

$$Q = \frac{Z_1 n_1}{k_1} \cos \frac{bk_2}{2} \sin \frac{ak_1}{2} + \frac{Z_2 n_2}{k_2} \sin \frac{bk_2}{2} \cos \frac{ak_1}{2}, \quad (9)$$

$$R = -\frac{k_2}{Z_2 n_2} \sin \frac{bk_2}{2} \cos \frac{ak_1}{2} - \frac{k_1}{Z_1 n_1} \cos \frac{bk_2}{2} \sin \frac{ak_1}{2}, \quad (10)$$

$$S = \cos \frac{bk_2}{2} \cos \frac{ak_1}{2} - \frac{Z_1 n_1}{Z_2 n_2} \frac{k_2}{k_1} \sin \frac{bk_2}{2} \sin \frac{ak_1}{2}, \quad (11)$$

$k_1 = \frac{\omega}{c}|n_1|$, $k_2 = \frac{\omega}{c}|n_2|$, and one may note that $PS - QR = 1$. Moreover,

$$M_1\left(\frac{a}{2}\right) = \begin{pmatrix} \cos\left(k_1 \frac{a}{2}\right) & \frac{Z_1 n_1}{k_1} \sin\left(k_1 \frac{a}{2}\right) \\ -\frac{k_1}{Z_1 n_1} \sin\left(k_1 \frac{a}{2}\right) & \cos\left(k_1 \frac{a}{2}\right) \end{pmatrix}, \quad (12)$$

$$M_2\left(\frac{b}{2}\right) = \begin{pmatrix} \cos\left(k_2 \frac{b}{2}\right) & \frac{Z_2 n_2}{k_2} \sin\left(k_2 \frac{b}{2}\right) \\ -\frac{k_2}{Z_2 n_2} \sin\left(k_2 \frac{b}{2}\right) & \cos\left(k_2 \frac{b}{2}\right) \end{pmatrix}. \quad (13)$$

Similarly,

$$\psi\left(-\frac{a+b}{2}\right) = T(-a,-b)\psi(0), \quad (14)$$

$$T(-a,-b) = M_2\left(-\frac{b}{2}\right) M_1\left(-\frac{a}{2}\right) = \begin{pmatrix} P & -Q \\ -R & S \end{pmatrix}, \quad (15)$$

and, by using the Bloch condition

$$\psi(z+d) = e^{iqd}\psi(z), \quad (16)$$

where q is chosen within the first Brillouin zone (BZ) of the photonic superlattice, i.e., $-\pi/d \leq q \leq \pi/d$, one may then obtain, with $\lambda = e^{iqd}$, the secular equation

$$PS(1-\lambda)^2 - QR(1+\lambda)^2 = 0, \quad (17)$$

which leads to the two following equivalent relations:

$$\sin^2\left(\frac{qd}{2}\right) = -QR, \quad (18)$$

$$\cos^2\left(\frac{qd}{2}\right) = PS. \quad (19)$$

Note that the solutions of either (18) or (19) lead to the $\omega = \omega(q)$ dispersion relationship or photonic band structure of the periodic superlattice, with the corresponding solutions for the in-plane electric field being straightforwardly obtained through Eqs. (3)–(5). Based on the dispersion relation obtained above, one may now proceed to obtain the photonic density of states,[16] by calculating the number of allowed states for a frequency ω that is, by performing the integral over the BZ and all bands, i.e.,

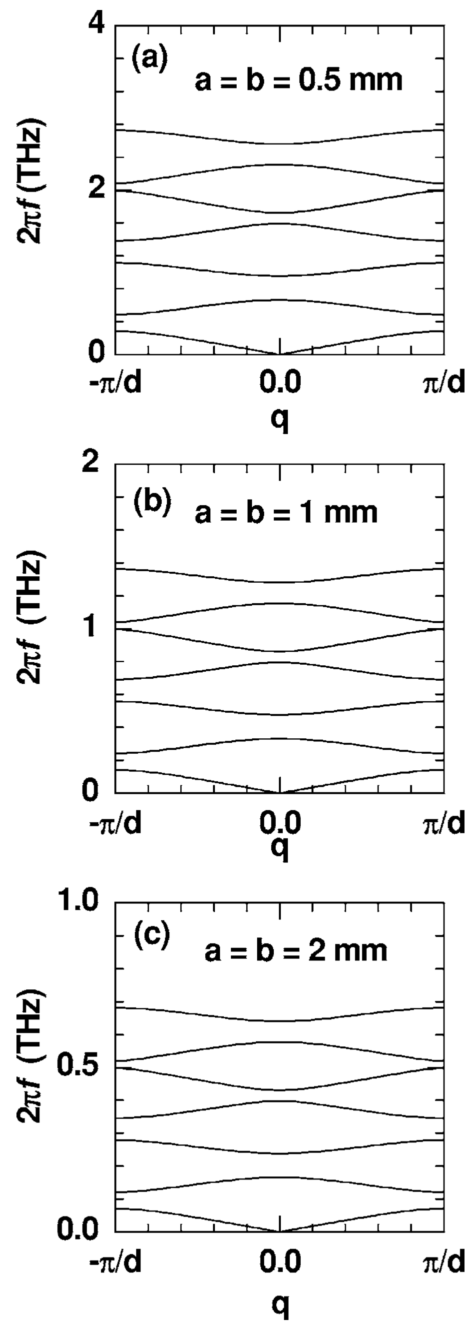

FIG. 1. Photonic band structure ω vs q, with $\omega = 2\pi f$, of a superlattice (period d) with equal alternate layers of air (with thickness a) and GaAs (thickness b and refractive index $n_2 = \sqrt{\epsilon_2} \simeq 3.6$).

$$g(\omega) = \sum_n \int_{BZ} dq\, \delta[\omega - \omega_n(q)], \quad (20)$$

a quantity which is fundamental in the understanding of several properties of a photonic superlattice.

The photonic band structures of a 1D superlattice of period d (with $a = b = d/2$) are depicted in Fig. 1 for various layer widths, illustrating the presence of gaps in the band structure. Figure 2 shows the same results for the photonic band structure, with ω in reduced units, together with the corresponding photon density of states. Band structure results of Figs. 1 and 2 illustrate the presence of the photonic

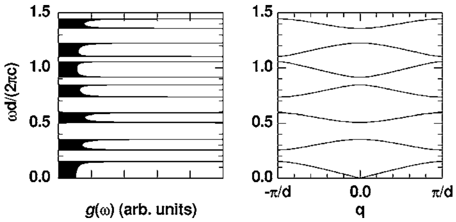

FIG. 2. Photon density of states $g(\omega)$, with $\omega = 2\pi f$, and photonic band structure ω vs q of a superlattice (period d) with equal alternate layers of air (with thickness a) and GaAs (thickness b and refractive index $n_2 = \sqrt{\epsilon_2} \simeq 3.6$), with the angular frequency $\omega = 2\pi f$ in reduced units.

band gaps, and are in agreement with previous work by Longhi and Janner,[12] who used a different theoretical approach.

The modifications introduced in the photonic band structure and photon density of states, when different a and b layer widths are used, are shown in Fig. 3. One clearly sees that, for layers of air (a=5 mm) narrower than the GaAs width (b=15 mm), the corresponding dispersion curves w versus q become flatter, and the band gaps at the BZ edge are quite different than in the case of equal layer widths. One then is able to infer that the group velocity, which is given by the slope of the dispersion curve, may become smaller, indicating a longer interaction time between radiation and matter, an interesting feature for its capability of enhancement of a variety of optical phenomena. To further investigate the effect of the variation of relative air and GaAs widths, we have plotted in Fig. 4 the photonic bands (shaded areas), in the case of the a=5 mm air layer, as functions of the GaAs-layer thickness, obtaining structures, for particular values of the GaAs-layer width, which may be shown to correspond to points with null gaps in the corresponding photonic band structure [see for instance, Fig. 5(d), for a=5 mm and b=1.4 mm]. Note that Eq. (18) [Eq. (19)] indicates that the extrema of the photonic bands at $q=0$ $\left[q = \pm\frac{\pi}{d}\right]$ occur at the

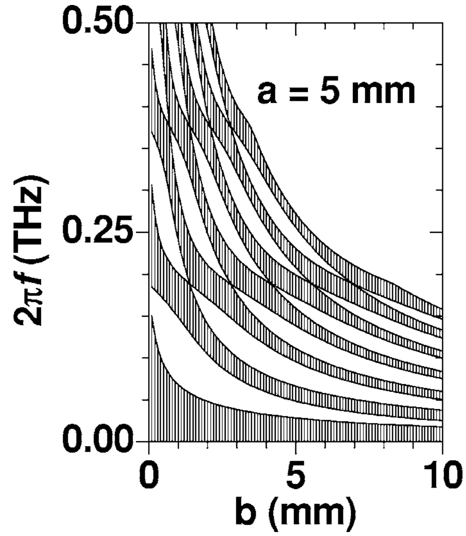

FIG. 4. Photonic bands (shaded areas) of a superlattice (period d) with alternate layers of air (with thickness a) and GaAs (thickness b and refractive index $n_2 = \sqrt{\epsilon_2} \simeq 3.6$).

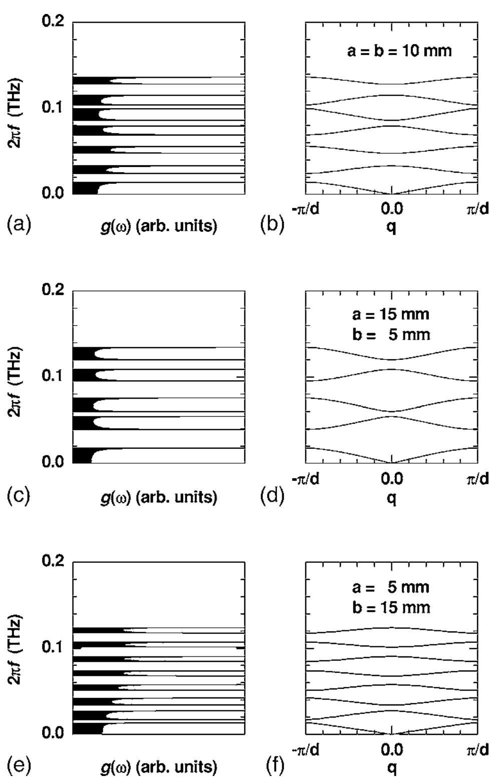

FIG. 3. Density of states $g(\omega)$ [(a), (c), and (e)], with $\omega = 2\pi f$, and photonic band structure ω vs q [(b), (d), and (f)] (period d) with alternate layers of air (with thickness a) and GaAs (thickness b and refractive index $n_2 = \sqrt{\epsilon_2} \simeq 3.6$).

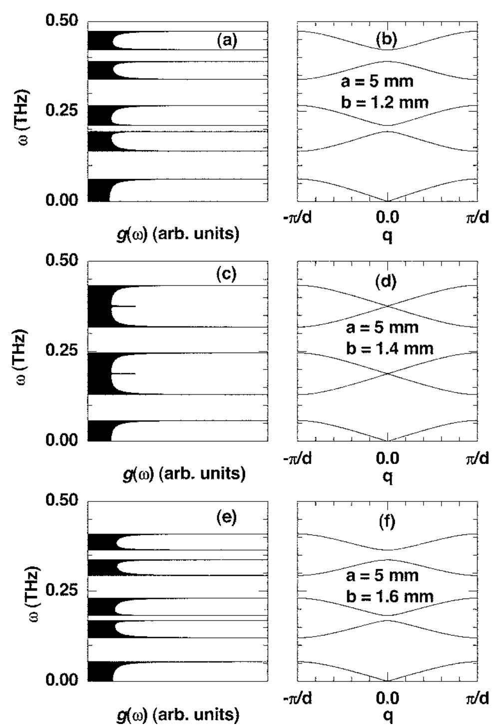

FIG. 5. Density of states $g(\omega)$ [(a), (c), and (e)], with $\omega = 2\pi f$, and photonic band structure ω vs q [(b), (d), and (f)] (period d) with alternate layers of air (with thickness a) and GaAs (thickness b and refractive index $n_2 = \sqrt{\epsilon_2} \simeq 3.6$).

zeroes of either $R(\omega)$ or $Q(\omega)$ $[P(\omega)$ or $S(\omega)]$, and those frequencies for which both $R(\omega)$ and $Q(\omega)$ $[P(\omega)$ and $S(\omega)]$ vanish simultaneously correspond to null gaps. Therefore, the touching of the bands occurs when $R(\omega)=Q(\omega)=0$ at the BZ center, and when $P(\omega)=S(\omega)=0$ at the BZ edge, implying the following zero photonic band-gap conditions, $\frac{a\omega n_1}{c}=N_1\pi$ and $\frac{b\omega n_2}{c}=N_2\pi$, where N_1 and N_2 are integers, and may be viewed as labels for the corresponding points of null gap displayed in Fig. 4 [in Fig. 5(d), for example, $\frac{b}{a}=\frac{n_1}{n_2}=0.28$, and $N_1=N_2=1$ (2) is associated with the first (second) null gap point at $q=0$]. Alternatively, one may write the conditions as $a=N_1\lambda_1/2$ and $b=N_2\lambda_2/2$, which displays the underlying null-gap physics as one of interference effects, and has clear similarities with the corresponding[17] problem of null gaps in the electronic spectra of semiconductor superlattices. At the BZ center N_1 and N_2 are both even or both odd, while at the BZ edge N_1 and N_2 are of opposite parities. One then obtains the occurrence of null gaps if

$$\frac{b}{a}=\frac{n_1}{n_2}\frac{N_2}{N_1}, \tag{21}$$

and at frequencies given by

$$\omega=\frac{N_1\pi c}{n_1 a}=\frac{N_2\pi c}{n_2 b}. \tag{22}$$

Here we note that in a recent work, Liscidini and Andreani[18] analyzed the enhancement of second-harmonic generation in doubly resonant microcavities with periodic dielectric mirrors, and devoted their attention to the photonic gaps themselves, whereas the null-gap points have been altogether ignored, except in a comment on the vanishing of the second-order gap when the so-called $\lambda/4$ condition is fulfilled. The present conditions [Eqs. (21) and (22)] for the vanishing of photonic gaps provide therefore a generalization of the related $\lambda/4$ condition for closed gaps.[19] We then turn to the case of superlattices whose relative widths are in the neighborhood of those that produce null gaps. Figure 5 illustrates the density of photon states as well as the photonic band structures for 1D superlattices with $a=5$ mm air layer and varying GaAs-layer widths. It is clear from Fig. 5(d) that the dispersion curve may be dramatically modified, exhibiting a band touching at the center of the Brillouin zone, with a finite derivative, $\frac{d\omega}{dq}=\pm\frac{d}{2\sqrt{\gamma}}$, with $\gamma=\frac{1}{4}\left[\left(1+\frac{Z_2}{Z_1}\right)\left(1+\frac{Z_1}{Z_2}\right)\alpha^2+\left(1-\frac{Z_2}{Z_1}\right)\left(1-\frac{Z_1}{Z_2}\right)\beta^2\right]$, and $\alpha=\frac{1}{2}\left(\frac{an_1}{c}+\frac{bn_2}{c}\right)$ and $\beta=\frac{1}{2}\left(\frac{an_1}{c}-\frac{bn_2}{c}\right)$, and characterized by a finite peak at the density of photon states, as it is apparent from Fig. 5(c). Of course, such analytical expressions may prove useful in possible applications of the predicted degeneracies in 1D photonic crystals.

Summing up, within the transfer-matrix technique, we have analytically studied the photonic band structures as well as the density of states of a 1D photonic crystal consisting of a superlattice with two alternating layers of air and GaAs of widths a and b, respectively. We have demonstrated the existence of photonic band gaps, as expected. Also, by adequately choosing the width values of the materials constituting the photonic superlattice, we have found photonic band structures with null gaps. Moreover, we find that for particular values of the ratio between these widths, not only a flattening of the bands occurs, but also a dramatic change is presented, with a band-touching effect at the center of the Brillouin zone, which induces a finite peak value at the density of photon states. The flattening of the bands indicates that the group velocity may be greatly reduced so that the interaction time between radiation and matter is longer, yielding to a myriad of optical phenomena. Furthermore, the null gap regions may also be quite useful for future development of filtering optical devices.

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[19] The photonic gap vanishes for a frequency twice as large as the one for which the $\lambda/4$ condition is fulfilled. In a simple periodic system such as the quarter-wave stack (Ref. 1), made up of a number of quarter-wave layers, the optical path of the radiation propagating perpendicularly to the stack is equal to $\lambda/4$ for each alternated layer. In that case $a=\lambda_1/4$, $b=\lambda_2/4$, and $\frac{b}{a}=\frac{n_1}{n_2}$, with $\omega=\frac{\pi c}{2an_1}=\frac{\pi c}{2bn_2}$. Therefore, the gap at the BZ center vanishes for a frequency twice the frequency of the $\lambda/4$ condition [cf. Eq. (22)].