Large photonic band gaps and transmittance antiresonances in periodically modulated quasi-one-dimensional waveguides

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For quasi-one-dimensional $(Q1D)$ waveguides of width a and with stubs attached periodically, it is shown that the photonic gaps with periodic dielectric contrast can be *many times larger* than those of a Q1D quarterwave structure for sufficiently short *a*. Similar photonic gaps, without dielectric contrast, result from *destructive* interference. When a double stub is inserted in a finite waveguide it can lead simultaneously to transmittance resonances in the gaps and *antiresonances* in the bands that widen, respectively, into new bands and gaps when more stubs are inserted.

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The existence of a photonic band gap (PBG) in materials where the refractive index varies periodically gives rise to many interesting and potentially useful properties, including the localization of light $[1]$, the inhibition of spontaneous emission $[2]$, etc.; see Ref. $[3]$, and references cited therein. These properties become more pronounced when the PBG is made large. Accordingly, the search for crystals with large PBGs has been extensive $[1-4]$. However, to our knowledge this search has had a limited success as it has identified structures with significant PBGs described by a gap-to-midgap frequency ratio of only about 20%.

In this paper, we present results of PBG calculations for quasi one-dimensional $(Q1D)$ waveguides (WGs) of width *a with and without* a periodic dielectric contrast. With inspiration from the microwave stub tuners and recent work on superlattices of *electronic* stub tuners [5], we add double stubs branching off the main WG in a periodic manner. *Without* dielectric contrast a PBG appears when the interference between waves propagating along the main WG and those reflected from the stubs is *destructive*. It can be as much as *one order of magnitude larger* than that of a Q1D quarterwave (qw) structure, with *small, relative* dielectric contrast $\Delta n/n$, where $\Delta n = |n_1 - n_2|$ and $n = (n_1 + n_2)/2$. The $\Delta n=0$ gaps can be further enhanced when the refractive index in the WG varies periodically. In addition, we present results for the transmittance through a finite number of identical units, connected to two infinitely long WGs, and show how one can have simultaneously bound states in the gaps, i.e., transmittance resonances, and *antiresonances*, i.e., resonance dips, in the bands by inserting one stub in a WG with contrast and a *finite* number of units. We present results only for the transverse electric (TE) polarization. We focus on the frequency regime in which only *one* mode propagates in the main WG, so the structures we consider always exhibit *full* PBGs. The results for transverse magnetic (TM) polarization are similar and will be presented elsewhere together with the full *vector* calculation.

The general unit cell of the periodically modulated WGs we consider is depicted in Fig. 1. It consists of two segments with refractive indices n_1 and n_2 , and corresponding lengths L_1 and L_2 . The two stubs have dimensions s_1 and s_2 , the total length is $L = L_1 + L_2$, and $h = a + s_1 + s_2$. We consider two types of WGs: (1) the dielectric material is enclosed by perfectly conducting boundaries (here represented by the solid lines), and (2) the WGs are defined by the dielectric contrast, with the enclosing region outside the solid lines has a refractive index $n_{\text{enc}} < n_1$ and n_2 . For type (1), the normal components of the electromagnetic waves vanish at the walls and the wave numbers in the *y* direction are restricted to discrete values. For type (2) , the waves decay exponentially outside of the WGs. This structure, particularly type (2) , is similar to the *corrugated* WGs, known from optoelectronics, which generally involve a *single* dielectric constant $(\Delta n=0)$ in the guiding material. In addition, the variations in the width of this WG are usually quite *small* and approximate theoretical treatments are typically employed. Here, we consider s_1 and s_2 of the same order as *a* and perform *full* calculations.

For the TE polarization, we have $E(r) = (0,0,E)$ and $H(r)=(H_x,H_y,0)$ and the scalar wave equation for *E* reads

$$
\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial x^2}\right)E + \frac{\omega^2}{c^2}n^2E = 0,
$$
\n(1)

where ω is the frequency, c the speed of light, and *n* the refractive index. For type (1) WGs, the solution for $x < 0$ in Fig. 1 can be written as

FIG. 1. The unit cell of a periodic WG with refractive index and stub structure. Perfectly conducting boundaries are assumed.

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$$
E_1 = \sum_m \left[u_{1m} e^{i\alpha_m x} + \overline{u}_{1m} e^{-i\alpha_m x} \right] \phi_m^w(y),\tag{2}
$$

where $\alpha_m = \sqrt{(n_1\omega/c)^2 - (\pi m/a)^2}$ is the wave number of the *m*th mode and $\phi_m^w(y) = \sqrt{2/a} \sin(m \pi [y - a/2]/a)$. In principle, the sum over *m* should be infinite, but in practice, it is cut off with m_{max} large enough to ensure numerical convergence. Equation (2) also holds for $x \ge L_2$. In the stub regions the solution can be written $[6]$ as

$$
E = \sum_{k} [f_{k} \xi_{k0}(x, y) + \overline{f}_{k} \xi_{0k}(x, y)].
$$
 (3)

The functions ξ_{k0} and ξ_{0k} are Fourier expansions of $X_l(x) \phi_l^s(y)$ and obey appropriate boundary conditions at the interfaces $x=0$ and $x=L_2$. $X_l(x)$ is given in Ref. [6] and $\phi_l^s(y) = \sqrt{\frac{2}{h}} \sin\left(\frac{l\pi [y - d + h/2]}{h}\right)$, where $d = s_1 - s_2$ measures the asymmetry of the stub with respect to the point *y*=0 taken at the center of the $n=n_1$ segments.

Matching the *E* field and its derivative at the boundaries $x=0$ and $x=L_2$ leads to an equation involving a transfer matrix *M* through $\mathbf{u}_1^{\pm} = \mathbf{M} \mathbf{u}_2^{\pm}$, where the *q*th components of matrix *M* through $\mathbf{u}_1 = \mathbf{M}\mathbf{u}_2$, where the *q*th components of the \mathbf{u}_i^{\pm} column vectors are given by $u_i + \overline{u}_i$ for $q \le m_{\text{max}}$ and the \mathbf{u}_i ⁻ column vectors are given by $u_i + u_i$ for $q \le m_{\text{max}}$ and by $u_i - \overline{u}_i$ for $m_{\text{max}} < q \le 2m_{\text{max}}$. The matrix elements M_{ij} , given in Ref. $[6]$ for the electronic case, can be modified in a straightforward manner for the photonic case with minor changes in the wave numbers and the overlap integrals between the stub and WGs, $I_{nm} = \int \phi_n^w(y) \phi_m^s(y) dy$, that enter the expressions for M_{ii} . The matrix for the $n=n_1$ segment $(x>L_2)$ can be obtained in a similar manner and that for the complete unit cell, M_{cell} , is the product of these two matrices. The dispersion for the superlattice is obtained by solving the eigenvalue equation

$$
\mathbf{M}_{\text{cell}} \mathbf{u}^{\pm} = e^{ik_x L} \mathbf{u}^{\pm}.
$$
 (4)

The transmittance through a *finite* superlattice is given by $T = \sum_{mn} |u_{\text{out}}|^2 (\alpha_n / \alpha_m)$, where the $u_{\text{out},n}$ are obtained by solving the transfer matrix equation with the usual conditions solving the transfer mass $u_{in,n} = 1$ and $\bar{u}_{in,n} = 0$.

For type (2) WGs, we use an alternate transfer matrix technique where the scalar wave equation ~1! is *discretized*, the WG mode functions $\phi_m^w(y)$ are expressed as vectors, and *E* is solved on a 2D mesh $|7|$.

In a Q1D superlattice consisting of infinitely wide alternating dielectric slabs, assuming normal incidence, a maximum gap occurs when the phase acquired passing through each slab is $\pi/2$. This quarter-wave condition requires $n_1 L_1 = n_2 L_2$ or equivalently $\pi/2n_2 L_1 = \pi/2n_2 L_2 = \omega_0/c$, where ω_0 is the midgap frequency. Then the PBG $\Delta \omega_{\rm qw}$ is given by

$$
\Delta \omega_{\rm qw} = \omega_0 \frac{4}{\pi} \frac{|n_2 - n_1|}{n_2 + n_1} = \omega_L \frac{2}{\pi} \frac{|n_2 - n_1|}{n_1 n_2},\tag{5}
$$

where $\omega_L = \pi c/L$. We use the parameter ω_L as our results all *scale with unit cell size* and for a more useful comparison with those for fully 2D PBG materials.

In Fig. 2 we plot the first two branches of the dispersion ω/ω_L vs k_x for three quasi-1D WGs of type (1). To facilitate comparison with the purely 1D case, we have set

FIG. 2. Dispersion relation, ω/ω_L vs k_L/π , for a WG with $(h>a)$ stubs (solid dots) and without $(a=h)$ stubs (crosses). The triangles are for the same WG *without* dielectric contrast. All parameters are given in the text. Notice that adding stubs renders the gaps much larger.

 $L_1=0.5114L=a$, and $L_2=0.4885L$ so that they satisfy the qw condition for $n_1 = 3.4$ and $n_2 = 3.6$. The triangles are for a WG with stubs $(s_1 = s_2 = 0.3068L, h = 1.2273L)$ but *without* dielectric contrast $(n_1=n_2=3.6)$, the solid dots for a WG with the same stubs but *with* contrast $(n_1=3.4,$ n_2 =3.6, Δn =0.2), and the crosses for a stubless WG $(a=h=0.5114L)$ *with* contrast. As can be seen, the first gap *without* contrast is approximately *six* times larger than the qw gap of the stubless WG (equal to $0.022\omega_L$) for this small Δn . As expected, the gap *with* contrast (solid dots) is higher. Higher gaps behave in a similar way; e.g., the second gap is about *four* times larger than the corresponding qw gap (Δn) \neq 0). Note that despite the large increase in the gap, we are still well below the threshold of the second mode in the n_1 segments, which occurs at $\omega = c \pi/n_1 a = 1.15\omega_L$. Similar results follow using type (2) WGs, but the gaps are somewhat smaller.

The gap with $\Delta n \neq 0$, but with no stubs, in Fig. 2 can be increased with a higher Δn and eventually become larger than the $\Delta n=0$ gap. In all cases, however, there is an almost constant increase in the contribution to the gap *coming from the stubs*, $\Delta \omega_s = \Delta \omega - \Delta \omega_{h=a}$, relative to $\Delta \omega_{\rm qw}$ of the infinitely wide WG. This is shown in the inset of Fig. 3 where we plot $\Delta \omega_s / \Delta \omega_{\text{qw}}$ as a function of h/a for various Δn 's, as indicated in the caption, and $a/L = 0.51$. We have fixed $\Delta \omega_{\text{aw}} = 0.0104 \omega_L$, which corresponds to $n_1 = 3.4$, $n_2 = 3.6$. The top three curves, which correspond to type (1) WGs, fall almost on top of each other, despite the different choices for n_1 and n_2 . The lower dotted curve corresponds to a type (2) WG with $n_1 = 3.4$, $n_2 = 3.6$, and $n_{\text{enc}} = 1$. In the latter case, the presence of stubs still increases the gap, but the effect is less dramatic.

The main part of Fig. 3 shows the first gap as a function of a/L for two type (1) WGs, $\Delta n = 3.6 - 3.4 = 0.2$ (solid curve) and $\Delta n = 1.6 - 1 = 0.6$ (long-dashed curve), and for a type (2) WG with $\Delta n = 3.6 - 3.4 = 0.2$ and $n_{\text{enc}} = 1$. In each case, we have fixed $h=a$ (no stubs) and L_1 and L_2 adjusted to the qw condition. In all cases the gap can increase signifi-

FIG. 3. The first gap $\Delta \omega$ in units of $\Delta \omega_{\rm gw}$, the gap of a Q1D qw structure, as a function of a/L in a stubless ($a=h$) WG. For the solid curve $n_1 = 3.4$ and $n_2 = 3.6$, for the long-dashed curve $n_1 = 1$ and n_2 =1.6 and the WGs are type (1). The short-dashed curve is for a type (2) WG with $n_1 = 3.4$ and $n_2 = 3.6$. Inset: the contribution of the stubs to $\Delta \omega$, in units of $\Delta \omega_{\rm qw}$, as a function of h/a . For the type (1) WGs, the refractive indices for the solid, long-dashed, and dashed-dotted curves are, respectively, $n_1 = 3.4$ and $n_2 = 3.6$, $n_1 = 3.0$ and $n_2 = 3.6$, and $n_1 = n_2 = 3.6$. In each case, we have used $a = L_1 = 0.5114L$, $L_2 = 0.4886L$ and fixed $\omega_{\rm qw}$ at the $n_1 = 3.4$, $n₂=3.6$ value. Note that $\Delta n=0$ for the dashed-dotted curve. The short-dashed curve is for a type (2) WG with $n_1 = 3.4$ and n_2 =3.6.

cantly, by a factor of *three* to *four* for the type (1) WGs and about 1.7 for the type (2) WG at the lowest value of a/L shown. The midgap frequencies show the same dependence on *a*/*L* as the gaps; i.e., they increase with decreasing *a*/*L*. This dependence is inherent in the dispersion relation of a stubless type (1) WG, $(n\omega/c)^2 = \alpha_m^2 + (\pi m/a)^2$, and shows how all frequencies are shifted to higher values when *a* decreases. The same result follows approximately for type (2) WGs. Combining these results with those of the inset, we see that the gap can be more than *one order of magnitude* larger than $\Delta \omega_{\rm qw}$ in type (1) WGs. For type (2) WGs, the full gap at $a/L = 0.51$ with stubs included is $\Delta \omega = 4.55 \Delta \omega_{\rm gw}$, which is still quite large. Importantly, for comparable lattice constants, refractive indices, and frequency ranges, $\Delta \omega_{\text{gw}}$ typically is already about 25% larger than the largest PBG reported so far for 2D systems [8]. The gaps we obtain are also large in comparison to the *midgap* frequency. In the $n_1 = 3.4$, $n_2 = 3.6$ example with stubs, despite the fact that Δn =0.2 is very small, the gap to midgap ratio is 24%.

In analogy with electronic stub tuners explored recently [5,6,9], the origin of the gap when $n_1 = n_2$ in type (1) or (2) WGs is the *destructive* interference between waves propagating along the main WG and those reflected from the stubs. To make this point transparent, we show in Fig. 4 a threedimensional plot of the transmittance T vs frequency ω and width *h* for a type (1) WG with $n_1 = 3.4$, $n_2 = 3.6$, and a, L_1 , and L_2 as in Fig. 1. For fixed ω , *T* varies *periodically with h* and the gaps occur for a change in width, δh , for fixed frequency (indicated by the dashed line), by

$$
\delta h = 2 \pi / \sqrt{(n_2 \omega/c)^2 - (\pi / L_2)^2} = 2 \pi / k_s. \tag{6}
$$

FIG. 4. Transmittance *T* vs ω/ω_L and width *h* for a ten unit cell type (1) superlattice. The unit cells are the same as those of Fig. $3(a)$. The period δh for destructive interference giving rise to the gaps, for fixed ω (dashed line) is given by Eq. (5).

This is just the condition for the *destructive* interference mentioned above, $k_s \delta s_1 = k_s \delta s_2 = \pi/2$ ($\delta h = \delta s_1 + \delta s_2$) since the wavelength in the stub is $\lambda_s = 2\pi/k_s$.

In Fig. 5(a) we plot the transmittance *T* vs ω for $a = L$, $h = 1.227L$, for a type (1) WG. The solid line is for a *finite* superlattice consisting of *three* units with stubs sandwiched between *very long* WGs with $n = n_2$ and width $h=0.7159L$. In the frequency region corresponding to the lowest band of an *infinitely* long superlattice, *T* shows *three* sharp peaks, corresponding to the number of the units, that describe *resonant transmittance* through states *quasibound* in the n_2 segments [10]. These states form a continuous band when the *finite* superlattice is made longer. If the superlattice is instead connected to WGs with $n=n_1$ and width

FIG. 5. (a) The transmittance *T* vs ω/ω_L for a *finite* type (1) superlattice of *three* unit cells (solid curve) connected to *wide* WGs of width $h=1.7159L$ and $n=n_2=3.6$. The dashed curve is for seven units connected to *narrow* waveguides of width $a=0.5114L$ and $n = n_1 = 3.4$. (b) As for the solid curve in (a) but *without* dielectric contrast, $n_1 = n_2 = 3.6$.

FIG. 6. Transmittance *T* vs ω/ω_L for an eight unit type (1) superlattice (dashed curve) with $n_1=2.0$, $n_2=3.6$, $L_1=0.643L=a$, $L_2=0.357L$, connected to WGs of width *a* with $n=n_1=2.0$. The solid curve is for the same superlattice with the n_2 segment of the fourth unit in the form of a double stub with $n=n_2$. This "defect" leads simultaneously to resonances in the first gap and antiresonances the first and second bands.

 $a=0.5114L$, these resonance peaks disappear, as shown by the dashed line, because this band is now below the propagation threshold of the attached WGs and the transmittance only begins with the second band in the dispersion. We have used seven units for the dashed curve to show how the higher gaps begin to show up when the superlattice is made longer. The second of them stands out at $\omega/\omega_l \approx 0.77$. An important observation is that these quasibound states occur even when the dielectric contrast is absent. This is illustrated in Fig. $5(b)$ for $n_1 = n_2 = 3.6$ and is in line with the existence of the $\Delta n=0$ gap; cf. Fig. 1. Notice, however, that the threshold for transmittance is now lower, at ω/ω_L =0.57 since the gap is smaller.

We now consider defects introduced in a finite type (1) WG superlattice. In line with the previous studies in 1D and 2D, defects involving the interchange of refractive indices introduce states in the gaps, i.e., transmittance peaks, with the *peak* position largely determined by *dimensions* of the defect. A qualitatively different defect is a double stub inserted in a WG with contrast. In Fig. 6 we show the transmittance for an eight-unit superlattice in which the n_2 portion of the fourth unit has the form of a double stub. Apart from the usual resonance peaks in the gaps, transmittance *antiresonances* are now apparent in the first and second bands. This simultaneous appearance of peaks and dips, *by the same defect*, is understood as follows. When one mode is allowed in the main WG and a resonance or antiresonance occurs, the solution in the stub is a *standing wave* obeying $\sin(k_5 h) = 0$ or $k_5 h = q \pi$, *q* being an odd integer. Odd *q*'s correspond to a wave with even symmetry with respect to the *y* axis. In the n_1 regions, $q=1$, the peak corresponds to $q=5$ and the two antiresonances satisfy this condition for $q=3$ and $q=7$, respectively *in the stub*. The *T* minima can be interpreted as occurring due to resonant *reflection* from a bound state, a phenomenon noted in the electronic case $[5,6]$. There is no coupling to odd symmetry $(q \text{ even})$ waves due to orthogonality, unless the stub is made asymmetric $[5]$. When more stubs are inserted in the middle of the WG, the resonances and antiresonances widen into bands in the gaps and gaps in the bands, respectively. These same results follow for the type (2) case.

In conclusion, we have shown that periodically modulated quasi-1D WGs exhibit *complete* PBGs. By reducing their width and adding structure such as stubs, the size of the PBGs can be enlarged *by several times* in comparison to the purely 1D case, the effect being more dramatic when the WG is enclosed by perfectly conducting boundaries. Moreover, we have shown that PBGs exist *without dielectric contrast* when the interference between waves propagating along the main WG and those reflected from the stubs are *destructive*. Finally, the transmittance results for a *finite* superlattice, with and without dielectric contrast, show that bound states exist and they occur before the propagation threshold for the main WG; they form the lowest band when the superlattice has a sufficiently large number of units. If a stub is inserted in the middle of a WG, both resonances in the gaps and *antiresonances* in the bands occur that widen into *new* bands in the gaps and gaps in the bands when more stubs are stubs are inserted.

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