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Dispersive properties of one-dimensional photonic band gap structures for second harmonic generation

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Abstract. We analyse the dispersive properties of one-dimensional photonic band gap structures, and discuss applications to phase matching conditions in the case of second harmonic generation. Band edge effects such as increased density of modes, large field enhancement, and low group velocity induce highly efficient parametric amplification, provided the proper phase matching conditions can be established. Direct integration of Maxwell's equations in the time domain confirms these conclusions, and shows that parametric amplification in one-dimensional photonic band gap structures provide much larger conversion efficiencies compared with ordinary quasi-phase-matching devices.

Keywords: Optics, nonlinear optics

1. Introduction

During the last few years, one-dimensional periodic dielectric structures, referred to usually as photonic band gap (PBG) crystals [1], have been extensively studied both theoretically and experimentally [2,3]. PBG crystals are usually composed of alternating high and low index materials, in an arrangement that gives rise to a series of forbidden wavelength gaps. That is, light is almost completely reflected by the crystal, while a series of forbidden wavelength pass bands form, in good analogy to the bands and gaps that form as a result of the periodic atomic arrangement in semiconductors. Three-dimensional photonic crystals typically discussed in the literature [1] are topologically much more complicated, and beyond the scope of this work. Since we seek proof-of-principle results, the one-dimensional geometry that we use will suffice to discuss, for example, enhancement of spontaneous emission rates [4]; optical limiting and switching of short pulses [5]; and nonlinear frequency conversion [6], which is the subject of this paper.

Recently [6], the prediction was made that it is theoretically possible to enhance second harmonic (SH) generation (and in general nonlinear frequency conversion) at the band edge of a PBG structure by several orders of magnitude compared with ordinary quasi-phase-matching

techniques. The structure was designed to maximize the density of modes for both the pump and the second harmonic fields. This meant tuning each field near a band edge resonance, which allows for the simultaneous availability of high mode density for both fields. This configuration then leads to a doubly resonant, distributed nonlinear gain condition, where the appropriate phase matching condition can be found and applied provided the dispersive properties of the structure are understood. These conditions are depicted in figure 1, where we plot the transmission characteristics of the structure (solid curve). SH enhancement is predicted to be nearly three orders of magnitude larger than an exactly phase-matched, ideal bulk structure of the same length and of the same nonlinear susceptibility. Clearly, this is an idealized situation, and a simple comparison with an unprocessed bulk material with the same nonlinear coefficient leads to conversion efficiencies better than four or five orders of magnitude. This phenomenon however, depends critically on several factors: (a) an increase in the mode density (i.e. field localization) and a corresponding decrease in group velocity near the band edge. The drop in group velocity can be several orders of magnitude with respect to the bulk group velocity; (b) increased interaction times; (c) strong mode overlap [6]. It was also evident in [6] that phase matching conditions also played a role because maximum

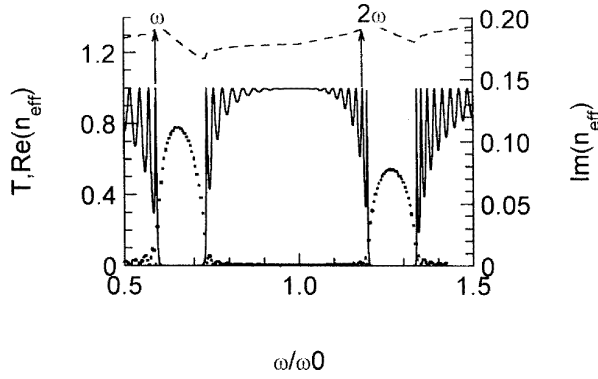


Figure 1. Transmittance (solid curve) and effective index for a 20-period structure, with layer thicknesses $a = \lambda/(4n_1)$, $b = \lambda/(2n_2)$; λ is the free space wavelength. The indices of the layers are: $n_1(\omega) = n_1(2\omega) = 1$; $n_2(\omega) = 1.4285714$ and $n_2(2\omega) = 1.519$. Dashed (dotted) curve: real (imaginary) part of the effective index.

conversion efficiency does not occur where the density of modes is an absolute maximum for both fields. The novelty of the approach outlined in [6] rests on the fact that the only requirement on the structure is a modulation in the linear refractive index along the direction of propagation, and a non-zero $\chi(2)$. It does not require angle tuning of a birefringent crystal, or domain inversion as in quasi-phase matching. The result is a structure where the strength of nonlinear processes can be enhanced by several orders of magnitude compared with a phase-matched or quasi-phase-matched device.

In the dipole approximation, SHG can occur in centro-symmetric materials because of the lack of the inversion symmetry at interfaces that separate two dielectric materials [7]. Under ordinary circumstances, efficient SH generation in a bulk medium requires some kind of phase matching condition to be satisfied, i.e. $2k(\omega) = k(2\omega)$ in a forward direction. In a multilayered structure, or a waveguide with a periodic index modulation, however, part of the propagating field is back-reflected from the structure. Therefore, momentum conversion alone cannot be used to arrive at the phase matching conditions for a periodic structure. For either pulsed or continuous wave operation, counter-propagating wave amplitudes can easily be of the same order of magnitude inside the structure. This situation can occur by tuning the pump at the transmission resonance, as in [6, 8]. The reason for this is that the formation of a quasi-standing wave at the transmission resonance, where the transmission is unity, requires both forward and backward propagating components to be present simultaneously, in nearly equal amounts. This then raises the possibility of forward and backward SH generation [6]. In fact, it can be shown that inside the structure, the simple decomposition of the linear eigenmode in its Fourier components reveals unequal forward and backward amplitudes. This creates a kind of asymmetry in the phase matching conditions for forward and backward propagating modes which has its origins in the existence of boundaries for structures of finite length.

In this paper, we examine how phase matching conditions are established in a layered structure, not necessarily periodic. We show that the dispersion of linear

materials can be combined with the dispersion introduced by the geometry of the structure in order to achieve exact phase matching, that is, equivalence of the effective refractive indices at ω and 2ω . As a consequence, the coherence length, defined as

$$L_c = \frac{\lambda}{4|n(2\omega) - n(\omega)|},$$

becomes infinite for all intents and purposes. Phase matching in a layered structure must be compared and distinguished from the usual quasi-phase matching process, where nonlinear domains are inverted every coherence length to form a structure that is periodic in the nonlinear coefficient only, and where the linear background index is constant [7].

2. Effective index

The method that we discuss to describe the dispersive properties of infinite structures, periodic or not, is based on the evaluation of an effective refractive index for a multilayered structure, based on a formulation of the effective dispersion relation. The method is generally valid for many situations, ranging from long fibre gratings with weak periodicity, to deep gratings with high index contrast. Perhaps more importantly, periodicity is not essential, because often, layered structures may be symmetric or quasi-periodic, as in Cantor or Fibonacci fractal codes. The matrix transfer method [9, 10] allows us to construct the spectral transmission function for any layered structure, starting from the knowledge of the thickness and refractive index of each layer, their geometrical complexion, and the given polarization of this incident light. The ‘transfer matrix method’ [9] is based on the recurrence relations for the coefficients of two linearly independent solutions of the wave equation within a given layer (forward and backward modes). Consider two dielectric layers of refractive indices n_2 and n_1 . It is convenient to choose the thicknesses of each of the layers to be $\lambda/4$, although just about any choice of thickness comparable to the incident wavelength will do. Again for convenience, we consider a structure surrounded by two equal semi-infinite layers of refractive index n . The expression for the transmitted electric field, assuming linear polarization of the electric field, parallel to the interface planes of the layers, can be written as follows:

$$t(k_0, L) = 2 \left/ \left(T_{22}^{(N)}(k_0, L) - \frac{T_{21}^{(N)}(k_0, L)}{ik_0 n} - ik_0 n T_{12}^{(N)}(k_0, L) + T_{11}^{(N)}(k_0, L) \right) \right., \quad (1)$$

where i is the imaginary unit, k_0 is the vacuum wavenumber and $T_{hk}^{(N)}$ are the elements of the transfer matrix $T^{(N)}$ of the structure, obtained by the N th iteration of the following recursive relation:

$$T^{(k)}(\varphi) = T^{(k-1)}(\varphi)T_1(\varphi), \quad k = 1, 2, \dots, N, \quad (2)$$

with

$$T^{(0)}(\varphi) = T_2(\varphi), \quad (3)$$

and

$$T_h(\varphi) = \begin{pmatrix} \cos(\varphi) & \frac{1}{k_0 n_h} \sin(\varphi) \\ -k_0 n_h \sin(\varphi) & \cos(\varphi) \end{pmatrix}, \quad h = 1, 2 \quad (4)$$

with $\varphi = k_0 L$. The indices $h = 1, 2$ refer to the layers with refractive index n_1 and n_2 respectively. In these expressions we have assumed equal optical paths for each layer. Note that the k_0 parameter appears only in the off-diagonal elements in the matrix (4), and so it appears only in the off-diagonal elements in the same way in the $T^{(N)}$ matrix, following relation (2). The recursive equation (2) depends on the geometrical sequence of the layers. In expression (1), the transmission depends on the φ variable alone. Moreover, the diagonal and off-diagonal elements of matrix (4) are symmetric and antisymmetric functions respectively. This is also a property of the final matrix $T^{(N)}$. This means that the real part of the transmission (1) is a symmetric function, while its imaginary part is an antisymmetric function of the φ variable. In other words, the magnitude of the transmission is a symmetric function of the frequency, for a fixed optical path L . Moreover the transmission is a periodic function of the frequency because the smallest components of the structures resonate when

$$\varphi = m\pi, \quad (5)$$

where m is an integer. For periodically stratified media, the transmission (equation (1)) takes on a simplified form. In general, however, for any kind of layered sequence [4] the recursive numerical procedure can be performed easily, once the appropriate recursive relation has been established (equations (2) and (3)). This allows us to write the spectral transmission for any kind of layered structure in the following simple form:

$$t \equiv x + iy \equiv \sqrt{T} e^{i\varphi_t} \quad (6)$$

where \sqrt{T} is the transmission amplitude, $\varphi_t = \tan^{-1}(y/x) \pm m\pi$ is the total phase accumulated as the light propagates through the medium, and m is an integer. Starting from the analogy of propagation in a homogeneous medium, we can express the total phase associated with the transmitted field as

$$\varphi_t = k(\omega)D = \frac{\omega}{c} n_{\text{eff}}(\omega)D \quad (7)$$

where $k(\omega)$ is the effective wavevector; and n_{eff} is the effective refractive index that we attribute to the layered structure whose physical length is D . In order to ensure that the phase $\varphi_t(\omega)$ acts as the phase of a travelling wave, we impose that the integer m be uniquely defined so that $\varphi_t(\omega)$ is a monotonically increasing function; this restriction is consistent with the condition that $m = 0$ as $\omega \rightarrow 0$.

The presence of gaps in the transmission spectrum, where the propagation of light is forbidden, suggests that the effective index of the structure should be complex. In particular, the effective index should have a large imaginary component inside the gap, to allow for nearly 100% scattering losses, i.e. destructive interference, reflections and evanescent field modes. Thus, we simply recast the transmission function as follows: first, we assume that $\sqrt{T} = |t| = e^{-\alpha D}$. This implies that an incident field of unit amplitude is ‘attenuated’ by an amount $e^{-\alpha D}$, where $\alpha = (\omega/c)n_i$, and n_i is the imaginary component of the index. According to this picture, we write $\sqrt{T} = e^{\ln \sqrt{T}}$ and the complex transmission becomes $t = e^{i\varphi} = e^{\ln \sqrt{T}} e^{i\varphi_t} = x + iy$. Therefore,

$$i\varphi = i\varphi_t + \ln \sqrt{T} = i \left(\frac{\omega}{c} \hat{n}_{\text{eff}} D \right) \quad (8)$$

where we still have $\varphi_t = \tan^{-1}(y/x) \pm m\pi$ as before, which allows us to rewrite (8) as

$$\hat{n}_{\text{eff}} = (c/\omega D)[\varphi_t - (i/2) \ln(x^2 + y^2)]. \quad (9)$$

Equation (9) suggests that at resonance, where $T = x^2 + y^2 = 1$, the imaginary part of the index is identically zero. Inside the gap, where the transmission is small, ‘losses’ are expected to be high, leading to evanescent waves. We can also define the effective index as the ratio between the speed of light in vacuum and the effective phase velocity of the wave in the medium. We have

$$\hat{k}(\omega) = \frac{\omega}{c} \hat{n}_{\text{eff}}(\omega). \quad (10)$$

This equation represents the effective dispersion relation of the finite structure, regardless of periodicity. Usually, the dispersion relation for periodic structures is obtained by applying periodic boundary conditions to the wave equation for an infinite, periodic structure. According to Bloch’s theorem [4, 10, 11] equations (2) and (3) reduce to

$$\cos(k(\omega)d) = \frac{1}{2} \text{Tr}[M], \quad (11)$$

or

$$\cos(k(\omega)d) = \left[\cos\left(\frac{n_1 \omega a}{c}\right) \cos\left(\frac{n_2 \omega b}{c}\right) - \frac{n_1^2 + n_2^2}{2n_1 n_2} \sin\left(\frac{n_1 \omega a}{c}\right) \sin\left(\frac{n_2 \omega b}{c}\right) \right]. \quad (12)$$

Here, M is the scattering matrix for the elementary unit cell which constitutes the periodic structure [10]; n_1 and n_2 are the refractive indices of layers of thickness a and b respectively, $d = a + b$. Equation (12) is valid only for a periodic structure with an infinite number of layers: that is, if there are no input or output interfaces. Our approach, which was developed principally for finite structures, gives results that are in complete agreement with the results of (12), provided the number of periods is large. The validity of equation (10) is general because it holds for any kind of layered structure, periodic or not.

As an example, let us consider the 20-period, quarter-wave/half-wave structure, already discussed numerically in [6]—see figure 1. Using the matrix transfer method, we construct the transmission function $t = x + iy$, and use the results to calculate the effective index, as given by (9). The results are depicted in figure 1, where we plot the real (dotted curve) and imaginary (short dashes) components of the effective index of refraction. We note that the real part of the index displays anomalous dispersion inside the gap. The imaginary component is small and oscillatory in the pass-bands; it attains its maximum at the centre of each gap, where the transmission is a minimum. By adopting the effective index formulation we have replaced the layered structure with an effective medium of length D . Then, the transmission function for the layered structure depicted in figure 1 can be faithfully reconstructed using (10). This gives us a consistent physical picture of the process, including the accurate predictions of group velocity, density of modes, and spontaneous emission rates [4, 6, 8, 11]. More importantly, the Kramers–Kronig relations for the effective index are

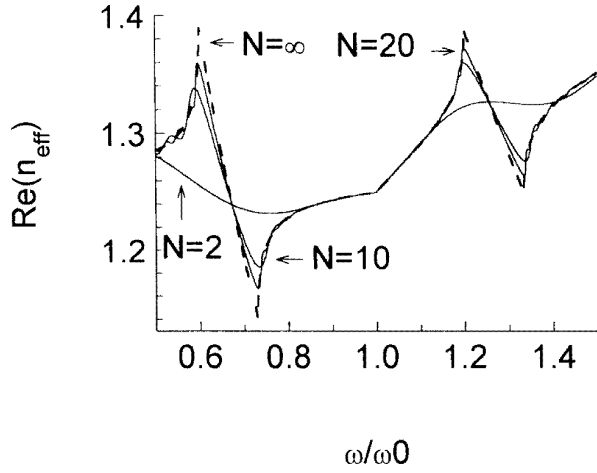


Figure 2. Real part of the effective index for forward propagation with 2, 10, 20, and an infinite number N of periods.

identically satisfied. That is, given the imaginary part of the effective index as $\text{Im}(n_{\text{eff}}) = \frac{1}{2} \ln(x^2 + y^2)$, the real part of the effective index is recovered. We will discuss the details in a future publication [12].

In figure 2, we depict the effective indices upon transmission for 2-, 10- and 20-period structure and compare with the results of the dispersion relation (12). This figure makes it clear that the effective, dispersive properties of the structures are modified by the number of periods. Therefore equation (10) is the appropriate dispersion equation for finite one-dimensional geometry regardless of layer arrangement.

3. Phase matching for nonlinear interactions

Since we are interested in phase matching conditions, let us focus our attention on the real part of the effective index. Again with reference to [6], we have found that for the simple 20-period structure we can generate SH pulses (of similar duration to the pump pulse) whose energy and power levels may be two or three orders of magnitude larger than the energy and power levels produced by an equivalent length of phase-matched bulk medium. The structure is designed so that the pump pulse is tuned near the first-order photonic band gap. The maximum of conversion efficiency has been found numerically by varying the parameters of the structure, assuming ω is fixed at the first transmission maximum near the edge of the gap. The optical path of one type of layer can be modified by simply changing the refractive index in that layer. Maximum conversion efficiency was found when the 2ω field was tuned at the second resonance near the edge of the second-order gap. However, these conditions still correspond to a doubly resonant arrangement, albeit with slightly smaller density of modes compared with the band edge, but with higher conversion efficiency.

Using the effective index approach we can therefore understand the circumstance under which maximum conversion efficiency occurs. We find that the effective refractive indices have precisely the same value at the pump and second harmonic frequencies, as shown in figure 1. *That is, the conditions for efficient SH generation reported in [6] are also those that satisfy exact phase matching between*

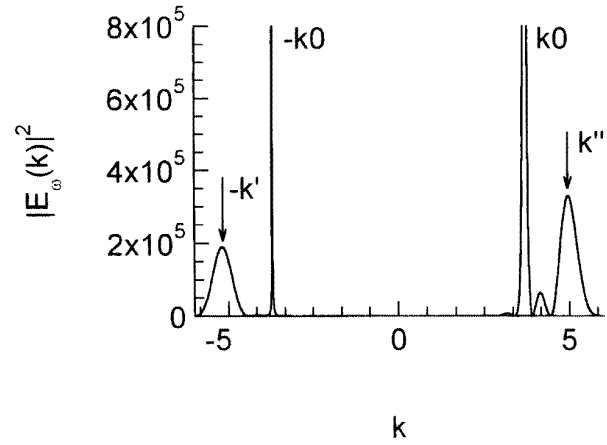


Figure 3. Fourier components for pump wavepackets at a time when the peak of the pulse reaches the structure. Pump tuned at low frequency band edge, $\omega/\omega_0 = 0.591$, obtained using the beam propagation method. $\pm k_0$ are free space components; $-k'$ and k'' are the carrier wavevectors inside the structure, are transient, and correspond to the effective wavevectors.

the fields, i.e. $n_{\text{eff}}(\omega) = n_{\text{eff}}(2\omega) \approx 1.334$ in this case. It is evident that modifying material dispersion, number of periods and layer thickness also modifies the effective index since all these quantities modify the transmission spectrum. In this manner, structures can be designed to satisfy different criteria, third harmonic generation, sum-frequency and/or frequency down-conversion, for example.

The results presented above were obtained by using simple arguments that follow from the application of the matrix transfer method. These results suggest that this phase mismatch may be the reason why, in this case, the forward propagating field is preferentially enhanced, as the results of [6] suggest. To confirm these results, starting from Maxwell's equations, we have examined pulse propagation in a finite PBG structure, as described in [6]. In the calculation, we use a Gaussian input pulse that is approximately one picosecond in duration, and it is tuned to the first resonance near the first-order band edge, at $\omega/\omega_0 = 0.591$ (see figure 1). The pulse length is hundreds of times longer than the length of the structure [6], and the pulse bandwidth can be considered to be much smaller than band-edge transmission resonances. In figure 3, we plot the Fourier transform $|E_\omega(k)|^2$ of the incident pump field as a function of the wavevector k when the peak of the pulse has reached the structure. In the dynamics, four components can be identified. Two correspond to free space propagation, at $\pm k_0$, i.e. portions of the pulse have been transmitted and reflected from the structure. The other two components are transient, and they are clearly visible as long as energy lies inside the structure. An analysis of the other two components reveals that the locations of the centre of gravity of each wavepacket, denoted by $-k'$ and k'' and which represent two packets that travel in opposite directions in the structure, are consistent with the values obtained using the simple effective index calculation depicted in figure 3. In fact then we have $k'' = n_{\text{eff}} k_0$.

We note that the wavepackets of figure 3 are quite broad, and in fact their widths correspond to a range of effective refractive indices. Unlike the free space components at $\pm k_0$, the widths of the wavepackets at $-k'$ and k'' are independent

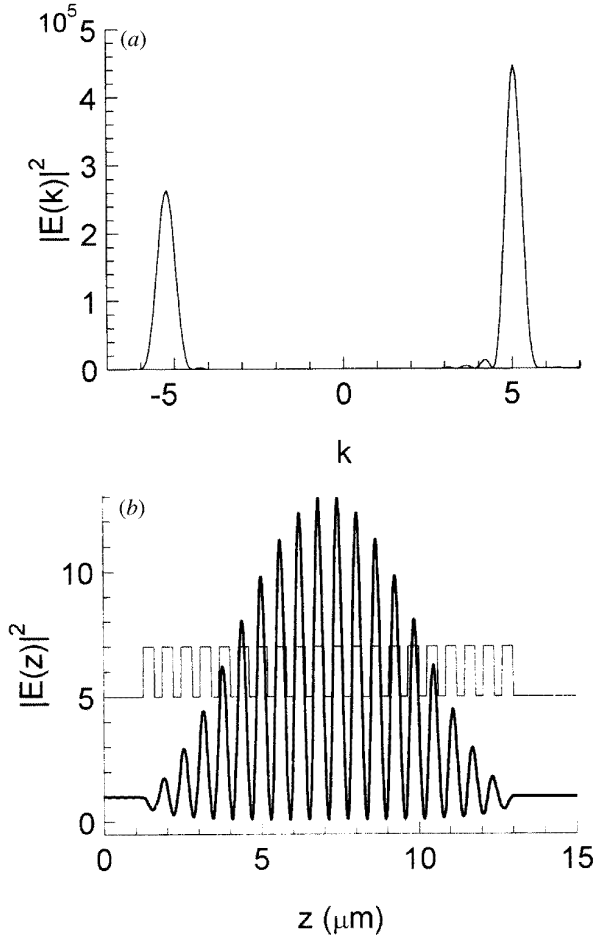


Figure 4. (a) Eigenmode profile at the fundamental frequency, (b) its Fourier transform calculated via the matrix transfer method.

of incident pulse width, an effect that persists in the quasi-monochromatic and plane wave regime. Therefore, we interpret this effect as a simple consequence of the sudden confinement of the incident wave to a space of width D , which excites a range of wavevectors such that $\Delta k \cong 1/D$. This result has been confirmed by calculating the eigenmode of the field, and decomposing in its Fourier components. We find exactly the spectrum that we show in figure 3, except for the free space components. The eigenmode, which represents the spatial distribution of the electric field inside the structure, is obtained using the transfer matrix method at any given frequency, and represents a monochromatic field. Figure 4(a) represents the eigenmode at the band edge for the fundamental field, and figure 4(b) is its Fourier spectrum.

The heights of the two wavepackets are different, a fact which shows that there is an asymmetry between forward and backward propagating fields inside the structure. This behaviour is somewhat unexpected if one thinks of an ordinary standing wave inside a cavity, but it must reflect the properties of the simple linear Fourier decomposition of the fields, and may help to explain why forward components are preferentially enhanced. To conclude this section, we note that the equations of motion have been integrated using a FFT-BPM [6], and a FDTD integration scheme that makes no approximations, both giving results similar to those described above.

Mindful of the limitations imposed by the simple model that we use, our results show that the effective index approach explains well the phase matching conditions present in nonlinear frequency conversion in periodic structures. Our calculations suggest that this is true for second and third harmonic generation, which we have also simulated, and we believe that it may be true in general for any kind of one-dimensional geometry, including quasi-periodic and random structures.

For phase matching in periodic structures, a simple connection can be made between our effective index approach and Bloch's phase β [4, 13, 14] for infinite structures. While we leave the details for exposition in a future work [12], it can be shown that beginning with the phase matching condition that we find, that is $n(\omega) = n(2\omega)$, and taking advantage of the analytical expression of the transmission of a finite structure written as a function of the Bloch phase [4], then the condition $\beta_2(2\omega) = 2\beta_1(\omega)$ is satisfied for SH generation, as one might expect for infinite structures. This is obviously a particular case (for periodic structures) of the more general phase matching conditions as expressed by the effective index approach. That the phase condition is satisfied by the Bloch phase should not be surprising. However, where the phase matching occurs is just as important, and cannot be left as an unresolved issue, since it is the combination of high mode density and phase matching that leads to the enhancement process.

4. Conclusions

To summarize, the effective index approach provides a unique, simple, and fast method to achieve and optimize phase matching conditions in dispersive media via the matrix transfer method. Normal material dispersion can be overcome by proper choice of layer thicknesses. In addition to phase matching, photonic band gap structures offer several other advantages, such as increased density of modes, large field enhancements, low group velocity, and field overlap. The combination of band edge effects and phase matching through anomalous dispersion provides efficiencies orders of magnitude larger than quasi or exact-phase-matching alone. These results are valid for layered structures with large index contrast, long grating structures or waveguides having small index modulation depth, and structures that are not periodic. Although we have specifically addressed the lowest frequency band gaps, similar arguments apply to higher-order band gaps. The advantage of using higher frequency gaps is that the periodicity of the index modulation can be on a longer length scale, which would ease fabrication tolerances for grating structures. As a note of caution, we have also indirectly shown how boundary conditions can lead to phase matching conditions and other effects that cannot be generalized from dispersion relations obtained with calculations that assume structures of infinite length. We predict that one will have to pay particular attention in three-dimensional systems, where dispersive effects may be more severe. Finally, the analogy that is usually drawn between photonic and electronic band structure brings us full circle to predict the same phenomena described above for electrons in finite, solid state nanostructures.

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