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Anomalous index of refraction in photonic bandgap materials

JONATHAN P. DOWLING and CHARLES M. BOWDEN

Weapons Sciences Directorate, AMSMI-RD-WS-ST, Research, Development, and Engineering Center, US Army Missile Command, Redstone Arsenal, Alabama 35898-5248, USA

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Abstract. Near the gap in a photonic bandgap material the effective index of refraction can become less than unity and in fact can approach zero at the band edge itself—leading to ultra-refractive optical effects. We illustrate this effect quantitatively in a simple one-dimensional Kronig–Penney model of a three-dimensional bandgap structure. As a complement to index-enhancing schemes involving lasing without inversion, ultra-refractive optics with photonic band materials has many applications, including laser accelerators and lenses of ultra-short focal lengths.

1. Introduction

Recently Scully and Fleischhauer *et al.* have predicted the existence of an ultra-high index of refraction with zero absorption in a coherently prepared atomic system (called phaseonium) that exhibits lasing without inversion [1, 2]. The present authors have considered local field effects in such systems and have predicted that you can expect a further, frequency-specific, absorptionles index enhancement of many orders of magnitude due to the local field interaction [3]. Scully has pointed out a few of the many applications for such a high-index material, for example, laser accelerators that require a precise control of the optical phase velocity [1, 4], and optical microscopes with increased resolving power. Now that lasing without inversion has been seen experimentally the realization of such high-index materials seems to be near at hand [5].

It seems natural then as a complement to the work of Scully and colleagues, that we could seek additional more easily manufactured materials, other than coherently prepared atomic systems, that can alter the index in such a striking fashion. It is in this vein that we propose photonic bandgap (PBG) materials as a possible candidate. In current prototypes of PBG materials the structure is about 85% air and so losses are less than in a homogeneous dielectric.

It is well understood now, theoretically and experimentally, that a carefully chosen periodic dielectric lattice may exhibit frequency bandgaps for all photon polarizations and directions of propagation [6–13]. In particular, it has been pointed out that the dispersion relation, and hence the optical group and phase velocities, in such a material will have very unusual properties [11, 12]. Although there has been mention of the application of these novel properties to lensing, particularly in the microwave regime where prototypical samples of bandgap materials are currently readily manufactured, no quantitative analysis seems to have been done [14].

In the following, we shall develop the analytical expression for the effective index of refraction in a simple model of a three-dimensional PBG material developed by John and Wang [12]. We find that near certain band edges the phase velocity tends towards infinity, and hence the index of refraction towards zero as you approach the bandgap. Upon noting that the refractive or resolving power of an optical system depends upon the *ratio* of n_1 to n_2, we then may strive to increase the refractive power by either drastically increasing n_1—the Scully approach using phaseonium—or by drastically *decreasing* n_2—the approach we advocate here using PBG materials. In the next Section, we begin by developing the effective index formula in the simple one-dimensional model of a three-dimensional PBG structure of John and Wang [12].

2. A simple model of a photonic band structure

In the model of John and Wang [12] they assume a material such that, regardless, of polarization or propagation direction, the photon always encounters precisely the same periodic index variation. Of course such a material cannot exist—but yet the approximation allows us to treat three-dimensional structure analytically as a one-dimensional problem while maintaining the original three-dimensional flavour. Selecting a particular x axis through the material, we shall assume a periodic step function for the index of the form.

$$n(x)=\begin{cases} n_1, & x\in(b/2, a+b/2)+md, \\ n_2, & x\in(-b/2, b/2)+md, \end{cases} \tag{1}$$

where the steps have index values of n_1 and n_2 with widths a and b, respectively, with $d=a+b$ being the period of the lattice, and $m=0, \pm 1, \pm 2, \ldots$ the translation factor. This periodic array is illustrated in figure 1.

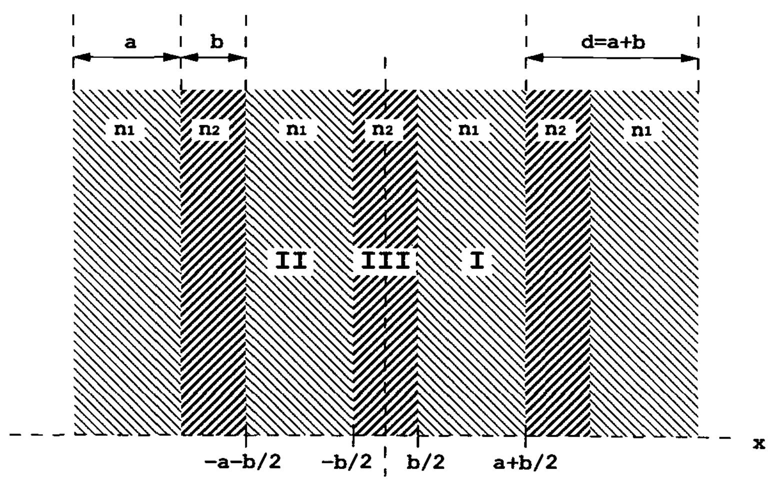

Figure 1. Here, we show a one-dimensional periodic dielectric array used to model a three-dimensional photonic bandgap material. The alternating dielectric regions of indices n_1 and n_2 have width a and b with $d=a+b$ the lattice period. The dispersion relation, $\omega=\omega(k)$, can be obtained by ensuring that the first and second derivative of the modal functions $a_k(x)$ are continuous across the I-III and III-II interfaces, and by invoking Bloch's theorem.

We have given details of the calculation of the Bloch eigenmodes and dispersion relation in this model in a previous work, and we summarize the results here [15]. We seek the solution to the one-dimensional wave equation for the spatial part of the electromagnetic eigenmode $a_k(x)$, namely,

$$a_k''(x)+\frac{n^2(x)\omega_k^2}{c^2}a_k(x)=0, \tag{2}$$

where $n(x)$ is given by equation (1). The eigenvector solution yields the form of the eigenmode function $a_k(x)$, and the eigenvalue solution implies a dispersion relation, $\omega=\omega(k)$, relating the frequency ω to the wave-number k. It is an advantage, in this John and Wang one-dimensional model for a three-dimensional PBG structure, that the solution can be expressed in an analytical and closed-form result. By way of contrast, in an actual PBG material, such as the Yablonovite structure, intensive numerical methods are required to solve the three-dimensional wave equation. To solve equation (2), we first make use of the fact that $n(x)$ is constant in the n_1 and n_2 regions. Hence, equation (2) for the wave equation may be written in a piecewise fashion as

$$a_k''(x)+\frac{n_1^2\omega_k^2}{c^2}a_k(x)=0, \qquad x\in(b/2,a+b/2)+md, \tag{3 a}$$

$$a_k''(x)+\frac{n_2^2\omega_k^2}{c^2}a_k(x)=0, \qquad x\in(-b/2,b/2)+md. \tag{3 b}$$

Let us consider the three regions I, II, and III centred about the origin, as indicated in figure 1. Due to the constancy of index n in these regions, we may immediately write down the most general solutions in regions I and III as

$$a_k^{\mathrm{I}}(x)=A\exp(\mathrm{i}\mu_k x)+B\exp(-\mathrm{i}\mu_k x), \tag{4 a}$$

$$a_k^{\mathrm{III}}(x)=C\exp(\mathrm{i}\nu_k x)+D\exp(-\mathrm{i}\nu_k x), \tag{4 b}$$

where we have defined the unitless parameters $\mu_k\equiv n_1\omega_k/c$, $\nu_k=n_2\omega_k/c$. The unknown constants A, B, and D are to be determined by imposing the appropriate boundary conditions at the dielectric interfaces, as well as the Floquet–Bloch theorem. In fact, Bloch's theorem requires that the solution $a_k^{\mathrm{II}}(x)$ in region II must be identical to that in I with an appropriate translation and a phase factor, namely

$$\begin{aligned} a_k^{\mathrm{II}}(x)&=\exp(-\mathrm{i}kd)\,a_{\mathrm{I}}(x+d)\\ &=\exp(-kd)\{A\exp[\mathrm{i}\mu_k(x+d)]+B\exp[-\mathrm{i}\mu_k(x+d)]\}, \end{aligned} \tag{4 c}$$

where $k=k(\omega)$ is the overall wave-number for the lattice. The requirement that the tangential components $\mathbf{E}$ and $\mathbf{B}$ be continuous across the dielectric interfaces becomes a requirement for the continuity of $a_k(x)$ and $a_k'(x)$ at these points [15]. Application of these boundary conditions yields a four-by-four homogeneous matrix equation for the unknown coefficients A, B, C, and D, determining the eigenfunctions $a_k(x)$ and eigenvalues ω_k. However, a solution for such a homogeneous system exists only if the determinant of the coefficient matrix is identically zero. This requires the satisfaction of a dispersion relation of the form [15]

$$k(\omega)=\frac{1}{d}\arccos\left[\cos\left(\frac{n_1\omega a}{c}\right)\cos\left(\frac{n_2\omega b}{c}\right)-\frac{n_1^2+n_2^2}{2n_1n_2}\sin\left(\frac{n_1\omega a}{c}\right)\sin\left(\frac{n_2\omega b}{c}\right)\right]. \quad (5)$$

Note that it is more convenient to give $k=k(\omega)$ rather than the more conventional $\omega=\omega(k)$ due to the nature of the solution. In order to model the Yablonovite structure [6, 7], we choose $n_1=1\cdot0$, $n_2=4\cdot0$, $a/d=0\cdot85$, and $b/d=0\cdot15$ since Yablonovite is mostly air holes of about an 85% filling fraction surrounded by a thin-walled framework of high dielectric constant. Notice that the period length d is arbitrary, and hence so is the scale of the lattice. Our results then hold for wavelengths of arbitrary length, and gaps appear so long as $\lambda\cong d$.

3. Effective index of refraction

In figure 2 we now plot kd versus $\omega d/c$ from equation (5) for the above-mentioned values of the lattice parameters. We see the band and bandgap structure clearly. As in solid state, we note from the slope of the curves that the group velocity $v_g\equiv \mathrm{d}\omega/\mathrm{d}k$ approaches zero at the band edges where a standing wave is formed. More interesting for our purpose here is that the phase velocity $v_\varphi\equiv\omega/k$ tends towards infinity at the three band edges in figure 2 where $kd\rightarrow0$ and $\omega d/c\cong4\cdot0$, $4\cdot8$, and $8\cdot0$, respectively. Since the index of refraction is defined as $n\equiv c/v_\varphi$, this implies that $n\rightarrow0$ at these points. Explicitly, the index is given by

$$\begin{aligned} n\equiv c/v_\varphi&=\frac{kc}{\omega}\\ &=\frac{c}{\omega d}\arccos\left[\cos\left(\frac{n_1\omega a}{c}\right)\cos\left(\frac{n_2\omega b}{c}\right)-\frac{n_1^2+n_2^2}{2n_1n_2}\sin\left(\frac{n_1\omega a}{c}\right)\sin\left(\frac{n_2\omega b}{c}\right)\right]. \quad (6)\end{aligned}$$

In figure 3 we plot n versus $\omega d/c$ for the same lattice parameters, $n_1=1$, $n_2=4$, $a/d=0\cdot85$, and $b/d=0\cdot15$. You can see that the effective index of refraction is

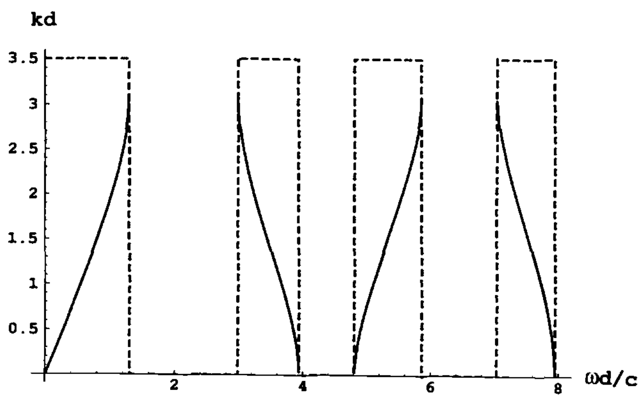

Figure 2. Choosing $n_1=1\cdot0$, $n_2=4\cdot0$, $a/d=0\cdot85$, and $b/d=0\cdot15$ as our lattice parameters—we plot here the dispersion relation, equation (5), in form $k(\omega)d$ versus $\omega d/c$. Notice from the slope of the curve that the group velocity, $v_g\equiv\mathrm{d}\omega/\mathrm{d}k$, tends to zero at the band edges, but that the phase velocity $v_\varphi\equiv\omega/k$ tends to infinity at some of the edges. Hence, standing waves are formed at the band edges—as in solid-state—and the index of refraction $n\equiv c/v_\varphi$ can be zero here.

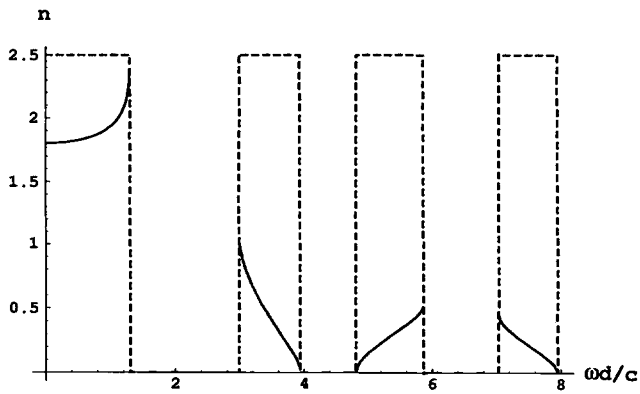

Figure 3. We plot the effective index of refraction $n_{\mathrm{eff}}(\omega) \equiv c/v_\varphi$, given by equation (6). The anomalous index can approach a maximum of only $n \leq \max\{n_1, n_2\}$, but near a band edge we can get $n \rightarrow 0$, leading to unusual refractive properties in a photonic bandgap material.

substantially less than unity at frequencies near the band edges where $\omega d/c \cong 4{\cdot}0$, $4{\cdot}8$, and $8{\cdot}0$.

It was our original hope that we would obtain exceptionally high values of effective n near the photonic band edge, as useful as the high n generated in lasing without inversion systems [1, 5]. However, numerical experimentation and a subsequent analytical analysis have shown that, for this model, the effective index $n_{\mathrm{eff}}(\omega)$ exceeds neither n_1 nor n_2. Our disappointment was short-lived, however, when we realized that a very small index is almost as good as a very large one, since the refractive power is determined by the ratio n_1/n_2. In Scully's proposal he strives for large n_1, but we can obtain the same refractive power (total internal reflection notwithstanding) by taking n_2 to zero near the band edge.

4. Applications

We shall discuss two important applications of the modified index in photonic bandgap materials: laser acceleration of electrons and ultra-refractive optics.

In schemes that invoke the use of lasers as high-energy electron accelerators, the electron velocity must match the phase velocity of the laser in order to extract energy from the field [4]. In the zeroth-order band of our model of a photonic bandgap material, the effective index may range $n_1 \lesssim n_{\mathrm{eff}}(\omega) \lesssim n_2$. Taking $n_1 \approx 1$ for a vacuum, we see then that in this regime the phase velocity $v_\varphi < c$ and a match to the electron velocity is possible. Hence, you can engineer a gradient of phase velocities by controlling the lattice parameters and thus accelerate the electron. In the experiment of Fontana and Pantell [4], the phase velocity is controlled by a background gas in the acceleration tube—limiting the total electron energy gain by electron–atom encounters. However, the Yablonovite structure [7] is mostly empty space with nice built-in acceleration tubes all the way through. We conclude that control of the laser phase velocity without electron-gas collisions seems quite possible in a PBG structure.

A second application, that has immediate practical applications in the microwave regime, is to ultra-refractive optics. Let us consider, in figure 4 (*a*), a

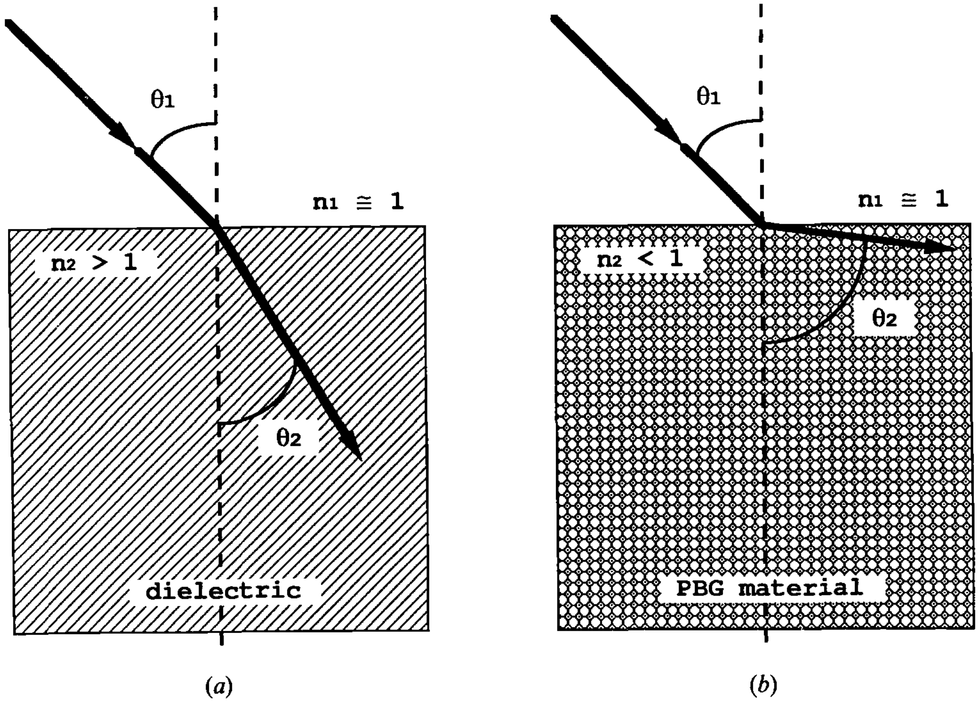

Figure 4. We illustrate schematically Snell's law, equation (7), and compare the refractive ability of a homogeneous dielectric (*a*) to that of a PBG material at a frequency near the band edge (*b*) where $n_{\text{eff}} < 1$.

monochromatic light ray incident from air, $n_1 \cong 1$, upon a homogeneous dielectric slab of index $n_2^{\text{dielectric}} > 1$. This is to be compared to figure 4 (*b*) where the dielectric is replaced with photonic bandgap material whose index is less than unity in the neighbourhood of the ray frequency, in other words, $n_2^{\text{PBG}} < 1$ and the frequency is tuned near the band edge. In both cases, Snell's law applies:

$$\sin\theta_2 = \frac{n_1}{n_2}\sin\theta_1. \tag{7}$$

We illustrate generic refractive rays in figure 4 (*a*) and 4 (*b*) for $n_1 = 1$ and $n_2 > 1$ and $n_2 < 1$, respectively. For $n_1 > n_2$, total internal reflection can occur for incident angles exceeding θ_1^{crit} given by

$$\theta_1^{\text{crit}} = \arcsin\left[\frac{n_2}{n_1}\right], \tag{8}$$

but inside this angular cone—strong refractive power may be obtained. As you approach the bandgap, $n_2 \to 0$ and hence $\theta_1^{\text{crit}} \to 0$, implying that all incident waves are reflected—as you would expect in the gap.

You can also operate in the regime where $n_2(\omega) \gtrsim 1$ for the PBG material and construct ordinary refractive elements. The advantage here is that a heavy dielectric with fixed index may be replaced with a much less massive dielectric lattice (85% air) that can have its index engineered to specifications. Since prototype

PBG materials are readily available in the microwave regime, the applications in this frequency range for refractive elements should be obvious.

5. Summary

We have discussed the novel properties of the effective index of refraction of PBG material when operating near a band edge, using a quantitative and simple one-dimensional model of a three-dimensional PPG structure. Two applications were raised: laser acceleration of electrons and novel refractive optical elements whose indices of refraction vanish near the photonic band edge. No doubt a plethora of other applications can be suggested, such as optical delays, filters, and soliton propagation. In conclusion, we caution that our quantitative study of the John and Wang model is very elementary and neglects the anisotropy of actual three-dimensional photonic crystals. In real structures, the effective index is a tensor quantity so that $\mathbf{k}$ vectors of identical magnitude but different unit directions $\hat{\mathbf{k}}$ will see different refractive indices. Nevertheless, the approach of the phase velocity to infinity at the band edge will still occur, albeit at different rates for different $\hat{\mathbf{k}}$. The purpose of this paper then is to motivate further research into the refractive properties of true three-dimensional dielectric lattices, with an eye towards potential applications.

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