Numerical study of light-beam propagation and superprism effect inside two-dimensional photonic crystals

Natalia Malkova, David A. Scrymgeour, and Venkatraman Gopalan
Materials Research Institute and Department of Materials Science and Engineering, Pennsylvania State University, University Park, Pennsylvania 16802, USA

(Received 20 September 2003; revised manuscript received 26 May 2004; published 29 July 2005)

We numerically study the propagation of Gaussian beams under superprism refraction conditions inside two-dimensional hexagonal photonic crystals. We employ two-dimensional finite difference time domain calculations, and compare them with theoretical predictions based on plane-wave method calculations. The discrepancies are analyzed in terms of the light propagation in a dispersive negative refraction medium.

DOI: 10.1103/PhysRevB.72.045144 PACS number(s): 42.70.Qs, 41.20.Jb, 42.25.–p, 42.30.–d

I. INTRODUCTION

In the last few years, the study of the periodic dielectric structures has received considerable interest because it provides the ability to prevent the propagation of the electromagnetic waves in certain frequency ranges. This isolator property of the photonic crystals can have implications for quantum optics, high-efficiency lasers and optoelectronic devices. Another application of photonic crystals follows from their photon conducting properties, which are determined by the dispersion of the allowed bands. The pioneering paper by Kosaka et al. experimentally demonstrated light-beam steering that is extremely sensitive to incident angle or wavelength. This effect was called the "superprism effect." In particular, negative refraction of the light path inside a photonic crystal was reported, where light stays on the same side of the surface normal of incidence. If Snell’s law is applied without regard to the photonic band anisotropy, this phenomena implies a negative refractive index. In addition, the negative refraction is the attribute of left-hand materials, first theoretically discussed by Veselago, which have simultaneous negative permittivity and permeability \( \varepsilon \) and \( \mu \). The numerical experiments with photonic crystals, namely, photonic structures that show the superprism effect and are characterized by a periodically modulated positive permittivity and permeability equal to one, demonstrated that the propagation of the light through the photonic crystal is similar to the left-hand materials. In practical applications, the novel negative refraction property of the photonic crystals presents an exciting possibility for achieving microphotonic and nanophotonic devices that can collect, focus, disperse, switch, and steer light. In particular, it has been shown that wavelength-division multiplexed filters can be based on photonic crystals exhibiting superprism effect.

Theoretical background for light propagation in strongly modulated photonic crystals has been developed by Notomi, who showed that strong dispersion of the allowed bands near the gap resulted in refraction-like behavior of the beam. Similar physical effects have been theoretically predicted and experimentally observed in grating waveguides. The explanation suggested was based on the dispersion properties of the optical Floquet-Bloch waves in the periodically stratified medium developed in the framework of dynamical theory of x-ray diffraction in crystals. The superprism effect is predicted by momentum conservation in specific directions inside any given photonic crystal. The numerical simulation of the superprism effect using finite difference time domain (FDTD) method often confirm these predictions, but at other times, fails to confirm them. Instead, one sometimes observes no propagation, or nebulous, ill-formed light beams at best, propagating in the directions predicted by the plane wave method. Such failures are often observed in photonic crystals, but the reasons are not currently well understood. This paper is a systematic attempt to understand such discrepancies and, starting from the theory of the light propagation in the strong dispersive medium, characterized by the left-handed behavior, to develop specific conditions under which superprism effect in photonic crystals can be expected to be observed.

The specific system under consideration in this paper is a two-dimensional photonic crystal based on PLZT (lead lanthanum zirconium titanate) material as a matrix medium, dielectric constant \( \varepsilon_p=6.2 \), consisting of cylindrical pores of air, dielectric constant \( \varepsilon_r=1 \), periodically arranged in a hexagonal lattice pattern. This design was developed by our research group, to actively control the superprism effect using the electro-optic effect in PLZT material. By applying an electric field to the photonic crystal, the electro-optic effect changes the dielectric constant of the material, hence modifying the band structure and as a result, the refraction angle inside the photonic crystal. The band structure for the TM mode (electric field is parallel to the cylindrical axis) of the hexagonal photonic crystal with the period of the lattice \( a \) and with the radius of the pores \( R=0.35a \) is shown in Fig. 1. The band structure was calculated by the standard plane-wave technique with 569 plane waves in the basis, giving a relative error of less than 1%. Frequencies close to pseudogap are typically the best operating points for observing the superprism effect. Two relatively close frequencies \( \tilde{\omega} = \omega a / (2 \pi c) = 0.48 \) and 0.49 (shown by the bold and dashed lines in Fig. 1) have been selected for the study. The corresponding iso-frequency surfaces (that is, the plots of equal frequency points in the \( k \)-space) calculated by the plane wave technique, are shown by bold and thin lines in Fig. 2(a).

The physical mechanism behind the superprism effect lies in the photonic band structure, because the direction of light...
propagation inside the photonic crystal is determined by the isofrequency surface of the photonic bands. The essential explanation of the effect has been suggested in Refs. 5 and 10. The approach is based on the analysis of the wave vector diagrams, as illustrated in Fig. 2(a). The momentum conservation rule requires that the incident wave vector \( \mathbf{k}_i \) and transmitted (refracted) wave vector \( \mathbf{k}_t \) are continuous for the tangential components parallel to the crystal edge. Given an incident wave vector, which in turn is determined by the frequency and incident angle, the propagation direction is obtained through the momentum conservation rule and the concept of the group velocity \( \mathbf{v}_g = \frac{\mathbf{k}}{\omega} \), where \( \omega \) is an effective operating point for the superprism effect.17 On the other hand, a small group velocity of the light leads to a large sensitivity of the output angle to the frequency of the light, making band-edge frequencies attractive operating points for the superprism effect.17 On the other hand, a small group velocity of the light leads to a large effective dielectric constant of the propagating mode in the crystal, resulting in a large reflection coefficient.18 This might be a reason that limits the ability to observe this effect. Thus, we can assume that the light intensity inside the crystal in the case of \( \tilde{\omega} = 0.49 \) is not sufficient to observe the propagating beam. However, the transmission for frequency \( \tilde{\omega} = 0.49 \) should be higher than for \( \tilde{\omega} = 0.48 \), since it is farther from the pseudoband-gap.19 Moreover, our numerical experiment showed that reflection from the crystal at \( \tilde{\omega} = 0.49 \) is comparable at \( \tilde{\omega} = 0.48 \).

The aim of this paper, therefore, is to understand the interplay between the large sensitivity of the output angle inside the crystal to small frequency changes. In order to understand the noted mismatch between the plane-wave prediction of the effect and the numerical simulation, we have considered the light beam propagation inside the two-dimensional hexagonal photonic crystal for a number of frequencies and incident angles both for the simplest circular isofrequency surface and for the “monster” like surfaces. We analyze the results starting from the theory of propagation of the light beam through a highly dispersive medium. Finally,
we exploit the general idea of the light propagation through the medium characterized by the negative refraction.

The outline of this paper is as follows. In Sec. II we describe the plane-wave method for the calculation of the isofrequency surfaces and the numerical technique used for the FDTD simulation of a Gaussian beam propagation inside the photonic crystal. The numerical results for the two kinds of iso-frequency surfaces with the circular and “monster” like shapes are presented in Sec. III. We compare our theoretical predictions from the plane-wave calculations with the FDTD simulations. A discussion of the observed effects is given in Sec. IV. Section V concludes the paper with a brief summary.

II. NUMERICAL MODEL

We consider the simple hexagonal lattice based photonic crystal described in the Introduction, with the lattice parameter \( a = 0.66 \) \( \mu m \), and the radius of the pore \( R = 0.35a \). The dielectric constant of the background \( \varepsilon_b = 6.2 \) (PLZT material) and the dielectric constant of the cylindrical pores \( \varepsilon_p = 1 \) (air), while the magnetic permeability is a constant, equal to 1 for the entire crystal.

The calculations of the isofrequency surfaces are performed in the framework of the plane wave technique. We divide the nontrivial space of the Brillouin zone into 300 \( \times \) 300 grid cells. Then for a given frequency, we scanned the

FIG. 2. (Color online) Propagation of the TM mode of the Gaussian beam with \( \omega = 0.48 \) and 0.49 incident on the (01) plane of the crystal. (a) The isofrequency surfaces in the air (dashed and dashed-dotted circles for \( \omega = 0.48 \) and 0.49, respectively) and inside the crystal (bold and thin lines for \( \omega = 0.48 \) and 0.49, respectively) illustrate the generation of the negative refracted beam. Group velocities, and incident and transmitted momenta are shown. The distribution of the magnitude of the \( E_z \) component of the TM mode of the Gaussian beam after 10 000 steps incident at an angle of 8° to the surface normal for frequencies of \( \omega = 0.48 \) (b) and 0.49 (c). The surface of the crystal and the normal are shown by dashed lines. The incident, reflected and refracted beams are overlaid.
Brillouin zone over each grid cell. It is worth mentioning that in the case of the discontinuous surface, when derivative to the surface is undefined (specially at the points close to main axes), the calculation of the isofrequency surface cannot be absolutely accurate. The reason for this is that for such frequencies, the isofrequency surface changes dramatically within the 1% error of our plane-wave calculations. However, this error does not affect the presented data since we avoid the most sensitive points, by taking the incident angle of the light within the limits of 4° to 30°.

The numerical experiment is based on the FDTD technique. Our computation domain contained ~400 × 100 unit cells of the photonic crystal and 400 × 5 unit cells of empty space (air). By techniques described in 20, the bottom part of the empty space was a scattered-field zone, from which we can get information about the scattered field. Each unit part of the empty space was a scattered-field zone, from which we can get information about the scattered field. Each unit part of the empty space was a scattered-field zone, from which we can get information about the scattered field. The total number of the time steps was varied between 10 000 and 20 000 with each step \( \Delta t = \Delta x/2c \), where \( c \) is light velocity in vacuum.

The source has been simulated as a sine wave for a given frequency in the time domain and as a Gaussian beam in the space domain. The beam is launched from the air, close to the edge of the empty space in the calculation domain. To get a non-normal incident beam, we rotated the phase-front of the incident wave in the empty space. For a plane-wave behavior of the Gaussian beam with well-defined wave vector, the width of the beam \( \Delta r \) has been taken as equal to 10 times the incident wavelength, that is, \( \Delta r = 20\pi c/\omega \).

The numerical model has been tested by Snell’s law for light propagation from the vacuum into a homogeneous dielectric medium with \( \varepsilon = 6.2 \) and \( \mu = 1 \). The numerical FDTD experiment showed that with an error \( \sim 1\% \), the incident \( \Theta_i \), reflected \( \Theta_r \), and transmitted (refracted) \( \Theta_t \) angles were related by the Snell’s law

\[
\Theta_i = \Theta_r, \tag{1}
\]

\[
\sin(\Theta_i)/\sin(\Theta_r) = n, \tag{2}
\]

where \( n = \sqrt{\varepsilon \mu} \) is the refractive index. In our numerical experiment we could also measure the transmitted and reflected amplitudes of the z-component of electric field and find the ratio of the reflected and transmitted field amplitudes with respect to the incident one. The relative reflected \( r \) and transmitted \( t \) amplitudes of the electric field were in good agreement with Fresnel’s formulas

\[
r = \frac{\cos(\Theta_i) - \sqrt{n^2 - \sin(\Theta_t)^2}}{\cos(\Theta_i) + \sqrt{n^2 - \sin(\Theta_t)^2}}, \tag{3}
\]

\[
t = 1 + r. \tag{4}
\]

Throughout this paper, all the angles are measured from the normal to the crystal edge.

### III. Numerical Results

At first we consider the simplest case, when for a given frequency, the isofrequency surface has a near-circular shape, but is characterized by negative refraction. As a first example, we take the second allowed band (Fig. 1). We analyze the frequency interval \( \tilde{\omega} = 0.40 : 0.46 \). The data obtained by the FDTD simulations in this interval were similar. We select \( \tilde{\omega} = 0.44 \) as a test frequency. The corresponding isofrequency surface is shown in Fig. 3(a). It consists of one central quasi-circle part and six segments around each J point.

We study here only the case when the beam is incident on (01) plane of the crystal, being tilted by an angle \( \Theta_i \), measured from the GX axis, leaving the problem of the light incident on (10) plane, when the incident beam can simultaneously excite the positive and negative refracted beams for future investigation. In this case, as shown by the plane-wave calculations, the central circle is excited by the beam incident under small angles \( \Theta_i < 20° \), and the segments at the zone boundary are excited by the beams incident at larger angles as shown in Fig. 3(a).

The pattern of intensity of the z-component of electric field for the TM mode of the Gaussian beam incident at an angle of 8° after 2000 time steps, and at the angle 26° after 5000 time steps, is presented in Figs. 3(b) and 3(c), respectively. We note from Fig. 3(b) that two beams are excited inside the photonic crystal. The first beam, with a small intensity, has a positive refraction angle. The second beam, with much larger intensity, shows negative refraction. The appearance of the positive refracted beam simply follows Snell’s law, if the photonic crystal is treated as a homogeneous medium with an average index. For a given \( \tilde{\omega} < 0.5 \), the wavelength of the incident light, determined by \( \lambda = a/\tilde{\omega} \), is larger than the scaling of the lattice \( a \). That is why, the incident beam should show a normal refraction from a quasi-homogeneous material with \( \varepsilon = \varepsilon^v \), where the average dielectric constant is defined by \( \varepsilon^v = \varepsilon_0 + f(\varepsilon_1 - \varepsilon_0) \) with the filling factor \( f = \pi R^2/\lambda^2 \). For the structure studied \( \varepsilon^v = 5.04 \). The refraction and reflection angles for this positive refracted beam satisfy Snell’s law (1.2) at \( \varepsilon = \varepsilon^v \). Moreover, the relative reflected field amplitude is in good agreement with Fresnel’s formula (3), predicting the value \( r \sim -0.5 : -0.6 \) for different incident angles, while the transmitted field intensity is \(-5 \) times less than that predicted by Fresnel’s formula (4).

This means that most of the incident light energy goes into exciting the second, negatively refracted beam.

The rate of energy transport for the normal beam is well-known to be determined by the group velocity of the light in a quasi-homogeneous material \( v^g_{p} = c/\sqrt{\varepsilon^p} \), being equal to \( v^g_{p} = 0.44c \). Figure 3(b) shows that the velocity of the positive refracted beam is larger than that of the negatively refracted beam. Therefore, in a number of steps (in this case \( \sim 4000 \) ), the first beam leaves the calculation domain. The second beam propagates inside the calculation domain only, as shown in Fig. 3(c). It is worth noting that the positive refracted beam has been observed in all our numerical experiments. It is of importance that in the case of \( \tilde{\omega} = 0.44 \), the intensity of the positive refracted beam is much less than that of the negative beam, and because of this, the two beams do not show any noticeable interaction (interference). While in
the case of $\bar{\omega}=0.48$ and $0.49$ the intensities of the two beams become comparable, and because of this, the interference fringes have been observed

We turn now to the second refracted beam. First, we note that for the incident angles considered ($\Theta_i < 30^\circ$), we observe the negative refraction of the second beam in accordance with the theoretical model described in Fig. 3(a). Second, it is of importance that in the case of the $\Theta_i < 18^\circ$ the intensity of the negatively refracted beam is almost equal of that of the incident beam, Fig. 3(b). Because of this, the beam is very well defined. However, the negatively refracted beam becomes much more poorly defined for $\Theta_i > 18^\circ$, with the sum of the amplitudes of the negatively refracted beam and the reflected beam measured in the scattered-field zone equal to $\sim 1$. We believe that this is a result of excitation of two different positive and negative refracted beams by the one incident beam. We could also analyze the dynamics of the refracted field change. It turns out that as soon as the second beam has formed, the refracted intensity had increased but only by about 10%.

Third, starting from the dispersion relation $\omega = \omega_0 + k v_g$, we can estimate the wavelength of the light inside the crystal as $\lambda = 2\pi/k$. Using the value $v_g \approx 0.3c$ and $\omega - \omega_0 = 0.05$, obtained from the band spectrum for $\bar{\omega}=0.44$ (Fig. 1), we get $\lambda \approx 6a$. The estimation of the wavelength can also be found from the radius of the isofrequency surface [Fig. 3(a)], which gives the value of the wave vectors. The corresponding wavelength measured from the FDTD simulation agrees with the above estimation. As follows from Fig. 3(b), the magnitude of wavelength is in agreement with the distance between the nearest phase fronts of the second wave. We also note that in accordance with the model, when increasing (decreasing) the frequency up to $\bar{\omega}=0.46$ (down to 0.40), the group velocity decreases (increases). This should result in decreasing (increasing) the wavelength, as confirmed by the FDTD simulations. We observe that for small incident angles of $\Theta_i < 15^\circ$, the phase front of the negative refracted beam was almost perpendicular to the propagation direction, supporting the fact that for the circular isofrequency surface studied, the phase and group velocities are antiparallel as
shown in Fig. 3(a). However, the bigger the incident angle, the greater the deviation of the shape of the isofrequency surface from a circle. As a result, the phase and group velocities become noticeably different from being antiparallel for $\Theta_i > 15^\circ$, resulting in nonperpendicular wavefronts to the propagation direction.

In all our experiments for $\Theta_i > 20^\circ$, besides the phase front of the negative refracted beam, we observed a grating structure parallel to the surface of the crystal [Fig. 3(c)]. This grating structure makes the beam very ill-determined, spreading it out over an angle interval of 90° to 180°. Similar grating structure, or some kind of crablike motion of the light inside a left-hand material has been recently discussed in Ref. 22. It has been shown that such a propagation of the light should be observed in the case of interference of the two beams incident on the crystal that are characterized by different frequencies. Because of this, the two beams are refracted by different angles inside the crystal, interfering with each other. However, we simulated here the propagation of the light with a single frequency. It is possible that we observe the interference of the two beams because of the limited widths of the Gaussian beams. If that were the case, the distance between the interference fringes would be linearly dependent on the width of the beam. Our numerical experiments with different widths of the incident beam show that the distance between the fringes did not change with the width of beam. Moreover, they do not depend on the incident angle either. From these observations, we conclude that the grating structure is determined by the properties of the photonic crystal only. It could be caused by the interference of the negative refracted beam and the positive one, which might appear because of a second-order Bragg’s refraction.

On the other hand, the propagation of the refracted beam through the photonic crystal in this case resembles a system of inhomogeneous plane waves, which appear inside the conducting medium. In such a case, the surface of the constant amplitude is parallel to the interface and does not generally coincide with the plane of constant phase. The wave vector for such a wave contains both the real and imaginary parts, resulting in strong attenuation of the refracted wave inside the conducting medium. We will discuss the attenuation of the refracted waves below.

Next, following the technique described in the Introduction, we calculate the output refracted angle using the plane-wave method, and compare this with the results obtained from the FDTD simulations. The dependence of the output refracted angle as a function of the incident angle is presented in Fig. 4 for the relative frequencies $\tilde{\omega} = 0.40$ (a) and 0.44 (b). The data obtained from the plane wave calculations and from the FDTD simulations are shown by solid lines and by error-bar marked dashed lines, respectively. The results are in reasonable agreement. But we note that, since the beam incident under large angles for this frequency is poorly determined, the error bars in the FDTD estimations for the output angle are larger for $\Theta_i > 18^\circ$. It is worth mentioning that for the case $\tilde{\omega} = 0.40$ the isofrequency surface consists of one central quasi-circular part; because of this, the dependence of the output angle on the incident angle shown in Fig. 4(a) has only one branch. We can conclude that in the case of quasi-circular isofrequency surface, the output angle of the beam is in reasonable quantitative agreement with the values predicted theoretically as a gradient to the isofrequency surface.
Now we consider the Gaussian beam incident on the (01) plane of the crystal with the relative frequencies 0.48 and 0.49. The magnitude of the electric field distribution for $E_z$ component after 10 000 time steps for the TM mode of the Gaussian beam incident at an angle of 8° to the IX axis was presented in Figs. 2(b) and 2(c). First, from the FDTD simulation we note, that in accordance with the iso-frequency diagram presented in Fig. 2(a), the light beam transferring from air to the photonic crystal should undergo negative refraction. In these cases the iso-frequency surfaces have a “monster” like shape, shown by bold and thin lines in Fig. 2(a) for $\omega = 0.48$ and 0.49, respectively. The vectors of momentum and group velocity are not strongly antiparallel to each other, and because of this, the phase front is not perpendicular to the propagation direction anymore. In addition, similar to the case $\omega = 0.44$ at $\Theta_i > 18^\circ$, we observed the grating structure which is always parallel to the interface boundary. Second, by comparing the light path inside the crystal in the case of the pseudocircular iso-frequency surface and in the case of the “monster” like surface, we note that the transmitted (reflected) light intensities decrease (increase) considerably for all the frequencies $\omega = 0.48$–0.50 studied. The case of $\omega = 0.48$ is similar with $\omega = 0.44$ at $\Theta_i > 18^\circ$: we observed the relative amplitudes of both the transmitted field and reflected field measured in the scattered-field zone equal to about one. But there was no noticeable increase in the reflected light intensity when passing from $\omega = 0.48$ to 0.49, while the transmitted intensity dropped three times. In the case $\omega > 0.48$, only separate clouds of the beam, propagating in the right direction, were observed by the FDTD simulations [Fig. 2(c)]. The beam becomes almost undefined and very widely spread out for the frequencies $\omega \geq 0.49$. It is important to note that for $\omega = 0.49$, the beam inside the crystal is not well-defined for all treated incident angles of $2^\circ < \Theta_i < 20^\circ$. From this FDTD simulation, we could not extract the output angle.

From the FDTD simulation we note that in comparison with the previous case $\omega = 0.44$, the velocity of the beam inside the crystal is much less. The reason for small velocities of the beam for these frequencies is understandable from the band structure shown in Fig. 1. For the frequency $\omega = 0.48$ (thin line in Fig. 1) the wave states of the light are very close to the band edge. Because of this, the group velocity, which determines the rate of energy transfer inside the crystal, is extremely low at the points close to the IX direction.

We compare the output refracted angle obtained from the plane wave calculation and from the FDTD simulations, but only for the normalized frequency equal to 0.48. The dependence of the output refracted angle as a function of the incident angle in this case is presented in Fig. 4(c). We note that the results of the FDTD simulations (dashed error-bar line) are in reasonable agreement with the plane wave calculations (solid line). But it is worth mentioning that the beam inside the crystal is not well determined, so the error in the FDTD estimations of the refraction angle is large.

**IV. DISCUSSION**

From the above data we can conclude that the simple theory of the propagation of the wave inside the photonic crystal, developed in Refs. 5 and 10, works reasonably well for all the shapes of the iso-frequency surfaces studied, if the intensity of the refracted beam is strong enough to make it noticeable. In this case, the quantitative agreement between the plane-wave calculations and FDTD simulations has been obtained. But for the “monster” like iso-frequency surfaces, the refracted beams in FDTD simulations are either poorly defined or absent, being very highly divergent. In some special cases when the light frequency is close to the pseudoband-gap, the theory gives insight into the propagation of the beam inside the crystal.

To begin to explain these observations, we can expect that no waves are excited in the photonic crystal at the incident angle $\Theta_i \geq \Theta_{ci} = \arcsin(|n|)$ (where $n$ is effective refractive index). The critical angle $\Theta_{ci}$ corresponds to the total internal reflection for the propagating mode in the photonic crystal. The total internal reflection cannot take place if the light is incident from air ($n_0 = 1$) on to a medium with index $n > 1$. However, in the case of a photonic crystal, the effective refractive index can be less than one, hence allowing for the possibility of total internal reflection. Using the known values of the $\Theta_i$ and $\Theta_{ci}$ for each given frequency, we estimated the effective refractive index from Eq. (2). The dependence of the critical angle on the incident angle for $\omega = 0.44$ (thin line), 0.48 (dashed line), and 0.49 (dashed-dotted line) is presented in Fig. 5. Since all the curves are lying above the dependence $\Theta_{ci} = \Theta_i$ (dotted line), we come to the conclusion that, in the limit of the well-defined effective index, in all cases studied, the incident angles were less than the critical angle.

From this data we conclude that light can be transmitted into the photonic crystal at all the frequencies studied. Next we note that since the photonic crystal is characterized by a complex band structure, we could expect that the propagation of light should satisfy the theory of beam propagation in the highly dispersive medium.24 We simulate here the incident light as a Gaussian beam in the real space with the width $\Delta r$. Such a beam can be described as a wave packet defined by

$$\Psi(r,t) = \int \phi(\mathbf{k})e^{i(k \cdot r - \omega t)} d\mathbf{k},$$  (5)

where $\Psi(r,t)$ is the Cartesian components of the electric or magnetic field, and $\phi(\mathbf{k})$ is the amplitude function, which for the Gaussian beam is determined by

$$\phi(\mathbf{k}) = A \exp \left( \frac{(k - k_0)^2}{\Delta k^2} \right).$$  (6)

Here $A$ is a normalized constant, $k_0$ is the momentum of the wave packet, $\Delta k$ is the “width” of the wave packet in the momentum space, being related with $\Delta r$ by the uncertainty relation $\Delta r \Delta k \sim 1$. The upper allowable limit of $\Delta k$ is obviously the light momentum $k$. Thus, the following condition must be satisfied:
various plane waves representing the wave packet. Real, but with the different phase velocities $v_g = \omega / k$ associated with the absorption of the energy because the height decreases. The spread of the wave packet is not well-defined in momentum space. Thus the width of the wave packet increases in time while the coefficient is not.

$$\Delta k \sim \frac{1}{\Delta x}.$$  

Since $k = 2 \pi / \lambda$, by taking the width of the wave packet for the incident beam $\Delta x = 10 \lambda$, we guarantee that our incident Gaussian beam satisfies the uncertainty principle, being a well-defined wave packet in momentum space.

It can be easily shown that if the wave packet propagates through the nondispersive medium with a linear dispersion law $\omega(k) = \omega(k_0) + v_g (k - k_0)$ (which is strictly true only for the wave travelling in a vacuum), the form of the wave packet is independent of time, the packet moving as a whole with the group velocity $v_g$. When higher terms in the expansion of $\omega$ as a function of $k$ are taken into account, the packet will spread out, and its form will no longer be time independent. In the case of a dispersive medium defined by the dispersion relation

$$\omega = \omega(k_0) + v_g (k - k_0) + \beta (k - k_0)^2,$$

where $\beta = 1 / 2 \tilde{\omega} \omega / \partial k^2$. The propagation of the Gaussian beam with the initial width $\Delta k \sim 1 / \Delta x$, in the momentum space will be described by

$$|\Psi(x,t)|^2 = \frac{\pi A^2}{(\Delta x_0^2 + \beta^2 t^2)^2} e^{-i\Delta x_0^2 (x - v_g t)^2 / 2(\Delta x_0^2 + \beta^2 t^2)}.$$

As follows from this expression, the intensity of the wave as a function of coordinate $x$ at given time $t$ is a Gaussian curve with width

$$\Delta x = \sqrt{\Delta x_0^2 + \frac{\beta^2 t^2}{\Delta x_0^2}}.$$  

Thus the width of the wave packet increases in time while the height decreases. The spread of the wave packet is not associated with the absorption of the energy because $k$ is real, but with the different phase velocities $v_g = \omega / k$ of the various plane waves representing the wave packet.

From the plane-wave calculations of the photonic crystal studied we have found both the parameters $v_g$ and $\beta$. Using these data the time dependence of the width and normalized amplitude of beam has been calculated. We present in Fig. 6 the evolution in time of the Gaussian beam with the initial width $\Delta x_0 = 10 \lambda$ transferring through the photonic crystal at the frequencies $\tilde{\omega} = 0.44$ (solid lines for the case of $\Theta > 18$ and dotted lines for $\Theta > 20$), 0.48 (dashed-dotted lines) and 0.49 (dashed lines). From the FDTD simulation we could also estimate the evolution in time of the amplitude of transmitted wave intensity for the different frequencies studied. These data are also shown in Fig. 6(b) by the corresponding markers. We note that the theoretical estimations are in reasonable agreement with the FDTD simulations for $\tilde{\omega} = 0.44$ when the isofrequency surface is close to a circle. In all other cases, the FDTD and theoretical data are in qualitative agreement only, showing a big quantitative discrepancy. From our numerical data we could not estimate the width of the beam for the case of a “monster” like isofrequency surface. However, a qualitative comparison of the theoretical and experimental data for the beam width evolution [Fig. 6(a) and Figs. 2 and 3] shows that the Gaussian beam spreads out inside the crystal much faster than is predicted by the theory. From this data, we conclude that for the quasi-circular isofrequency surface, the photonic crystal can be treated as a quasihomogeneous dispersive medium. For the “monster” type of isofrequency surface, such an approach fails. The intensity of beam attenuates inside the photonic crystal much faster than it is predicted by the theory, resembling the attenuation of the light inside the metal, when the wave penetrates only to a depth of the order of an optical wavelength inside the crystal.

We now suggest one of the possible explanations of this finding, based on the idea of the left-hand behavior of the photonic crystal undergoing the negative refraction. It is of importance that for the frequency and incident angle regions studied, the photonic crystal is characterized by negative refraction. Moreover, the propagation of the light might be attributed to the left-handed behavior, determined by the con-
In the general case of the light propagation through the homogeneous medium with both $\epsilon$ and $\mu$ not equal to 1, the relative reflected and transmitted field amplitudes are determined now by the formulas:

$$ r = \frac{|\mu \cos(\Theta_i) - \sqrt{n^2 - \sin(\Theta_i)^2}|}{|\mu \cos(\Theta_i) + \sqrt{n^2 - \sin(\Theta_i)^2}|}, \quad (12) $$

$$ t = 1 + r. \quad (13) $$

In the case of $\epsilon=\mu=-1$, reflection is equal to zero identically, confirming that all of the energy is perfectly transmitted into the left-hand medium from the vacuum. If $\epsilon$ and $\mu$ are equal to each other but do not equal to $-1$, assuming the validity of the Snell’s law, we get

$$ r = \frac{\cos(\Theta_i) - \cos(\Theta_f)}{\cos(\Theta_i) + \cos(\Theta_f)}. \quad (14) $$

Since the superprism effect, regardless of whether the incident beam is positive refracted or negative refracted, implies that $|\Theta_i| < |\Theta_f|$ and, hence, $\cos(\Theta_i) > \cos(\Theta_f)$, reflection $r \geq 0$ and $t \equiv 1$. In the case when the impedance $\sqrt{\mu/\epsilon} \ll 1$ reflection $r$ becomes negative and tends to $-1$, while the transmission $t$ goes to 0.

We invoke the idea that the propagation of the waves in media with a corrugation smaller than the wavelength can be modeled in terms of effective medium. Then, we assume that the photonic crystal can be characterized by frequency dependent effective dielectric permittivity and magnetic permeability, which should satisfy the single condition $\epsilon\mu = n^2 > 0$. Next, following the idea of the left-hand behavior of the photonic crystal undergoing the negative refraction, we assume that in the case of $\tilde{\omega} = 0.44$ at $\Theta_i > 18^\circ$, when the isofrequency surface is close to circle, the photonic crystal can be described as a homogeneous left-hand material with negative effective permittivity and permeability $\epsilon=\mu<0$. In such a case, we can explain a perfect transmission of the crystal in spite of nonzero reflection, which can be caused by the reflection of the first positive refracted beam only. In order to explain the fast attenuation of the light in the cases of $\tilde{\omega} = 0.44$ at $\Theta_i > 18^\circ$ and $\tilde{\omega} = 0.48, 0.49$, we have to attribute to the photonic crystal, both negative effective $\epsilon$ and $\mu$ but not equal to each other, so that the impedance of the crystal $Z < 1$.

We present in Fig. 7 the transmission (a) and reflection (b) of the photonic crystal for $\tilde{\omega} = 0.44$ (solid and dotted line), 0.48 (dashed dotted line), and 0.49 (dashed line). Assuming that the refractive index is determined by Eq. (2), we calculated the relative transmitted field amplitude from Eqs. (12) and (13). When calculating the transmission, we could neglect the first positive refracted beam, which experiences the photonic crystal as a quasihomogeneous medium. The transmitted intensity of this beam is much less than that of the negative refracted beam. However, to calculate the reflected fields we have to take into account the reflection of both the negative and positive refracted beams, because as was discussed in Sec. III the reflection field of the first positive refracted beam was strong, following Eq. (3) with $\epsilon=\epsilon^{*}$. Then, in the scattering field region, we have to see the inter-

---

**FIG. 6.** (Color online) The evolution in time of the width (a) and normalized amplitude (b) of the Gaussian beam with the initial width $\Delta x_0 = 10\lambda$ transferring through the photonic crystal at the frequencies $\tilde{\omega} = 0.44$ (solid lines for the case of $\Theta_i < 18^\circ$ and dotted lines for $\Theta_i > 20^\circ$), 0.48 (dashed-dotted lines) and 0.49 (dashed lines). The data obtained from the FDTD simulations are shown by star, cross, square, and diamond markers for $\tilde{\omega} = 0.44$ at $\Theta_i < 18^\circ$, 0.44 at $\Theta_i > 20^\circ$, 0.48 and 0.49, respectively.

Briefly, the underlying idea behind the left-hand materials is that both the dielectric function and magnetic permeability happen to be negative. In such a case, because of the causality requirement, the sign of the refractive index $n = -\sqrt{\epsilon\mu}$ must be chosen to be negative. But the impedance of the medium

$$ Z = \sqrt{\frac{\mu}{\epsilon}} \quad (11) $$

keeps the positive sign. When $\epsilon=\mu=-1$, the medium is a perfect match to free space and the interfaces show no reflection.
simulated right after the photonic crystal edge when the second negative refracted beam had just been formed. The experimental data for reflected field has been measured in the scattered-field zone. The numerical data for transmitted and reflected fields are shown by star markers for \( \tilde{\omega} = 0.44 \), by square markers for \( \tilde{\omega} = 0.48 \) and by diamond markers for \( \tilde{\omega} = 0.49 \). First, we note from the numerical data that the magnitude of the reflected fields for \( \tilde{\omega} = 0.48 \) and 0.49 do not change much while the transmitted fields are two times less for \( \tilde{\omega} = 0.49 \) as compared to \( \tilde{\omega} = 0.48 \). Second, both the theoretical and experimental data are in qualitative agreement for \( \tilde{\omega} = 0.44 \) and 0.49, while for \( \tilde{\omega} = 0.48 \) we could not reach an agreement for the reflected and refracted fields simultaneously, using just the same parameter \( \mu / \varepsilon \). We note the discrepancy \( \sim 40\% - 10\% \) between experimental and theoretical data for the reflected field. This discrepancy is not surprising for a very rough theoretical model to be used. It is also worth mentioning that we have not used any fitting technique to find the best relation for \( \mu / \varepsilon \). From these data we conclude that this simplified theory can be used for qualitative explanation of the FDTD numerical experiment. We believe that further progress of the present phenomenological theory, resulting in a quantitative agreement between the theory and experiment, can be achieved by taking into account, the phase shift between the two excited beams as well as the strong anisotropy of the dispersion properties of the photonic crystal.

V. CONCLUSION

We have presented in this paper the numerical analysis of the propagation of the light inside a two-dimensional photonic crystal with a simple hexagonal lattice. In the current theories, the propagation of the light is treated as an excitation of the wave packet which transfer the energy with the group velocity \( \mathbf{V}_g = \mathbf{V}_0 \omega(k) \), where \( \omega(k) \) is the dispersion relation for the photonic crystal studied. We have compared the prediction for the propagation angle of the light inside the crystal obtained from the plane-wave calculations with the FDTD simulation. Our analysis shows that the FDTD numerical experiment follows the simple model only for some special cases when the isofrequency surface has a simple circular shape. We report discrepancies between the plane-wave calculation and FDTD simulation for the case when the isofrequency surface had “monster” like shapes and showed poorly formed beams inside the crystal. We analyze this discrepancy in the frame of the theory of Gaussian beam propagation inside highly dispersive material that is characterized by the negative refraction. We consider the left-handed behavior of a refracted light inside a photonic crystal constructed from materials with a relative permeability equal to 1 and a constant positive permittivity. We follow the idea that, in such a case, the propagation of the light through the photonic crystal may be described by the negative effective refractive index \( n = -\sqrt{\varepsilon} \mu \). Then we assume that the photonic crystal can be characterized by frequency dependent effective dielectric permittivity and magnetic permeability, which should satisfy the single condition \( \varepsilon \mu = n^2 > 0 \). This basic assumption of the model can be motivated by the periodic

![Figure 7](https://example.com/figure7.png)

FIG. 7. (Color online) (a) The transmission of the negative refracted beam inside photonic crystal calculated from Eqs. (12) and (13) for \( \tilde{\omega} = 0.44 \) (solid line for \( \mu = \varepsilon \) and dotted line for \( \mu = \varepsilon \) at \( \Theta_i < 20^\circ \) and \( \mu = 0.3 \varepsilon \) at \( \Theta_i > 20^\circ \)), 0.48 (dotted-dashed line, \( \mu = 0.5 \varepsilon \)), and 0.49 (dashed line, \( \mu = 0.2 \varepsilon \)). The relative magnitude of the z-component of the electric field extracted from the FDTD are shown by star, square, and diamond markers for \( \tilde{\omega} = 0.44, 0.48, \) and 0.49, respectively. (b) The corresponding reflection of the photonic crystal calculated as a sum of magnitude \( \tilde{r} \) [Eq. (14)] and \( r \) [Eq. (3)]. The experimental data for the reflected field shown has been measured in the scattered-field zone.
properties of the photonic crystal, resulting, at first, in strongly modulated band structure, which, in turn, causes a large contrast of the effective dielectric and magnetic constants with the original constants of the constituent components. As a consequence, for the quasi-circular isofrequency surface we have to assume that $|\mu| < |\varepsilon|$ or impedance equal to one. In such a case, the energy is perfectly transmitted through the photonic crystal, giving a well-defined beam path inside the crystal. For the “monster” like isofrequency surface, the transmission properties of the photonic crystal can be explained by assuming $\varepsilon = \mu$ or impedance equal to one. The bigger mismatch of the impedances of vacuum and photonic crystal, the less effective the transmission of the beam through the photonic crystal. We show that this results in metal-like behavior of the photonic crystal, when the light penetrated into the crystal on the depth of the wavelength only.

To conclude, the idea of designing electromagnetic “metamaterials,” synthetic structures that exhibit effective properties different from their constituents is of great interest now. It has been recently reported that magnetic emitters can be created in nonmagnetic photonic crystals. We believe that our study will attract attention towards the negatively refraeted photonic crystals as a promising candidate for “metamaterials.”

ACKNOWLEDGMENTS

This work was supported by National Science Foundation Grant Nos. DMR-00800190, DMR-0507146, DMR-9984691, and DMR-0349632. We thank the Materials Simulation Center (Penn State) for the provision of the computer facilities. We are grateful to Professor Krauss for the kindly presented preprint of Ref. 17 prior to publication.

8 Electronic address: nmalkova@mail.arc.nasa.gov
9 Electronic address: dscrymg@sandi.gov