Superprism effect and light refraction and propagation in photonic crystals

Wei Jiang[*a], Chuhua Tian[a], Yongqiang Jiang[a], Yihong Chen[b], Xuejun Lu[c], and Ray T. Chen[a]
[a]Microelectronics Research Center and Department of Electrical and Computer Engineering, University of Texas, Austin, Texas 78758
[b]Omega Optics, 10435 Burnet Road, Suite 108, Austin, Texas 78758
[c]Department of Electrical and Computer Engineering, University of Massachusetts, Lowell, MA 01854

ABSTRACT

Photonic crystal based devices received attention in recent years. Based on the superprism effect in photonic crystals, beam steering devices can be made with properties sensitively dependent on the wavelength and incident angle of light. One stumbling block for designing superprism-based demultiplexers is that current numerical methods have difficulties in simulating a *practical* superprism device with commonly available computational facilities. Examining the superprism effect in a more general perspective, we previously developed a rigorous theory to solve the photonic crystal refraction problem for any surface orientation and any lattice type. This paper will compare our theory with other methods with regard to computational workload to demonstrate the advantages of our theory. Excellent agreement of numerical results with the transfer matrix method is also demonstrated. Heuristic discussions on the beam width variation and energy conservation are presented. A technique for direct computation of the dispersion surface is compared with the methods that combine a photonic band solver with certain interpolation or 1D-searching techniques.

Keywords: photonic crystal, superprism effect, refraction, dispersion surface, energy conservation, beam width

1. INTRODUCTION

Photonics research has prospered in the waning years of last century, owing to the rise of wavelength-division-multiplexing(WDM) technology in fiber-optic communications. In recent years, more and more photonics research has shifted toward the direction of nano-structure design and fabrication, with photonic crystals[1,2] regarded as one of the promising approaches in a broad range of applications. Photonic crystals(PCs) are a new class of artificial optical materials with periodic dielectric structures, which result in unusual optical properties[3-9] that may provide revolutionary solutions for many problems. In particular, Kosaka et al. discovered the superprism effect,[6] which can be utilized for WDM[6] and superlens[9] applications.

This paper will examine the superprism effect from a broader perspective, which considers general properties of photonic crystal refraction and light propagation in photonic crystals. We will compare a rigorous PC refraction theory[8] previously developed by us with other methods.

[*] jiang@ece.utexas.edu; phone 1-512-471-2003; fax 1-512-471-8575.

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In addition, how to efficiently compute the dispersion surface seems not adequately discussed in the literature. Although this problem appears to be trivial with a standard photonic band solver,[9,10] we find that an alternative method may be employed to simplify the problem. Another apparently trivial question, the beam width change upon refraction, will also be analyzed to reveal its connection with the energy conservation.

2. LIGHT REFRACTION AT A SURFACE OF A PHOTONIC CRYSTAL

2.1 Anomalous refraction: superprism effect

Light refraction at the surface of a photonic crystal has been subject to extensive study recently.[6] The refraction angle was found to depend on incident angle and wavelength sensitively, which may be utilized for wavelength-division-multiplexing (WDM) applications. These anomalous refraction phenomena were named the superprism effect.[6] Moreover, under certain conditions, the light beam refracts to the opposite side of the surface normal, a phenomenon expected only if the refractive index of one medium happens to be negative. This "negative refraction" phenomenon has been further studied in the context of building superlenses with photonic crystals.[9]

2.2. Difficulties of prior theories and simulation methods

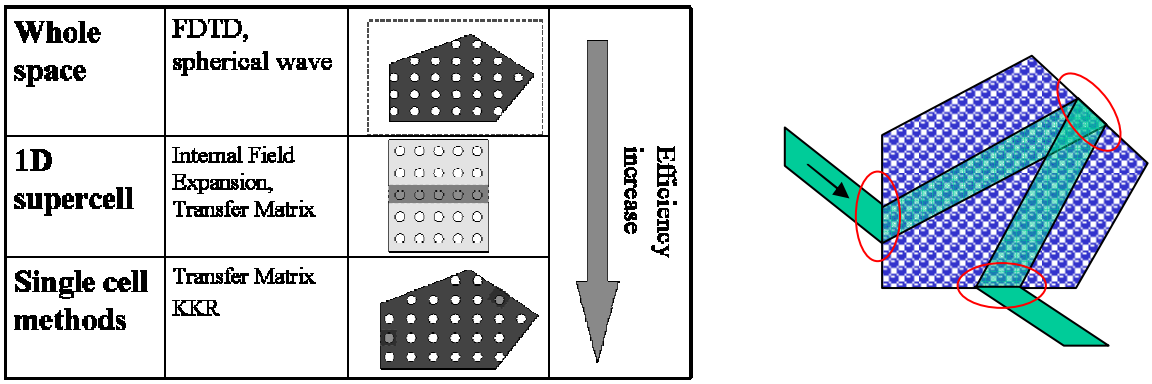
The underpinning physics of the anomalous refraction was attributed to the coupling of the incident light with the propagating modes of the photonic crystal.[6] The light beam direction inside the photonic crystal is given by the group velocity of the eigenmodes of the photonic crystal. The group velocity can be fairly easily determined from the dispersion surface of the photonic crystal. Nevertheless, the coupling amplitude of each excited mode has not been adequately studied, which stymies any realistic design of a WDM demultiplexer.

A variety of theoretical methods are available to calculate the light propagation in photonic crystals, including transfer matrix method,[12-14] the scattering theory of dielectric sphere lattice[15-17] or the multiple scattering method,[18] the internal field expansion method,[19] and the Finite Difference Time Domain simulations.[20] Note some of these methods could have a number of flavors. For example, the transfer matrix method can be based on planar waves or spherical waves.

Based on the effective size of real-space computational domain, all of the methods for photonic crystal transmission can be divided into three categories, as illustrated in Fig. 1(a). The first category can be named the whole-space method,[18,20] which calculates the optical field (electric and/or magnetic field) in the whole space (or in the whole photonic crystal). The second category can be named the 1D supercell methods,[19] which calculates the field in only a supercell of the photonic crystal to solve the transmission problem. This method appears to be applicable to a photonic crystal slab only. The last category is the single-cell method,[14] which calculates the field in a single cell per surface and solves the refraction problem surface by surface. Some methods can be in more than on categories, depending on the detailed implementation. Generally, the last category of methods are most efficient and versatile in practical designs. A detailed comparison of the numerical advantages of these methods is beyond the scope of this paper.

Here, we shall further discuss the most popular approach of the photonic crystal transmission problem. It is our perception that the Finite Difference Time Domain (FDTD) method[9,20] is the most popular numerical approach employed in practice. This is evidently attributed to the wide applicability of FDTD algorithm, the wide availability of the FDTD software with an easy-to-use graphic interface for computer-aided design. However, FDTD simulations can be inefficient in studying photonic crystal refraction. Essentially, *refraction is a phenomenon localized at the interface between two media*. However, in FDTD simulations, one often needs to use a large enough space to enclose the whole photonic crystal, and calculates the field inside the whole computational domain to solve the problem, as illustrated in Fig. 1(b). When the photonic crystal is large enough, such an approach becomes extremely inefficient. On the other hand, when the photonic crystal is small enough such that the surface evanescent waves dominate over the propagating waves inside the *whole* photonic crystal,[21] FDTD simulations can be a good approach to the problem.

However, when such a case occurs, the "photonic crystal" has almost lost its bulk properties and there might be no advantage of considering such a fragment of photonic nano-structure from the perspective of photonic crystals. This reminds us the size effect in other materials.[22] Exploring the limit when the size of a photonic crystal is too small to be a crystal meaningfully is an interesting question.



(a)

(b)

Fig. 1 Comparison of various computational methods for photonic crystal transmission, refraction, and reflection. (a) Three categories of methods, classified by the size of real-space computational domain. (b) Refraction is an effect localized at the surfaces as indicated, whereas the whole space methods must calculate the field in every cell of the photonic crystal to determine the transmission amplitudes along the light path. It is desirable that the photonic crystal refraction problem can be solved on the surface in the same fashion we apply Snell's law to a homogeneous medium.

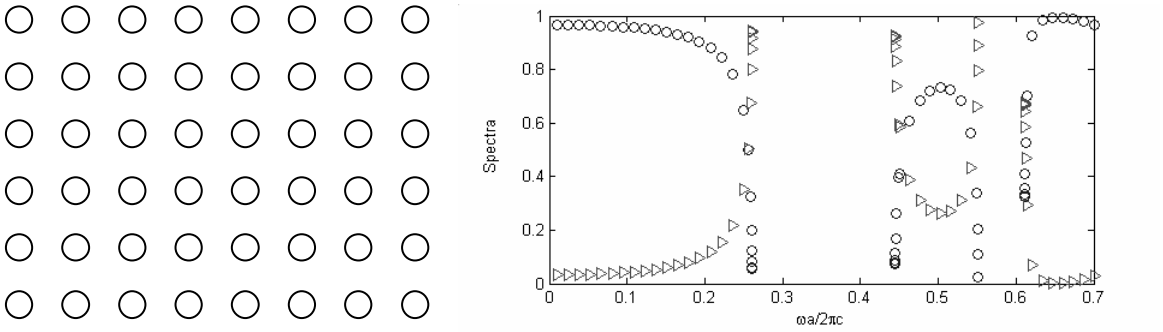
The transfer matrix method is another method widely employed by researchers. For more than two decades, this method has been extensively studied for diffraction gratings, and many flavors of this method have been developed.[23-24] Essentially, it uses a matrix to relate the electromagnetic field on the front and back surfaces of a photonic crystal slab, and this matrix is called the transfer matrix. Typically, the transfer matrix method needs to stratify a 2D or 3D photonic crystal slab into many slices. The transfer matrix of the whole slab equals the product of the transfer matrix of each slice. If each slice consists of a complete layer of photonic "atoms," then one may further slice it into many thin layers, each of which can be regarded homogeneous along the depth direction. Then a plane wave based method can be employed to compute the transfer matrix across each slice.[14] Some spherical-wave approaches can directly compute the transfer matrix of each layer of photonic atoms if the atoms are spherical in shape.[15-17] There are yet other more sophisticated methods. Nonetheless it is our understanding that the plane-wave based "atom"-slicing approach is easiest to understand and implement, and versatile in treating various types of scatterer geometric shapes or spatial dielectric functions. Regardless of the approach, the transfer matrix method generally calculates the eigenvalues $\exp(ik_y d)$, where k_y is the wavevector component normal to the surface and d is certain distance normal to the surface. As we know, some k_y are real, but the others are complex. When k_y appears on the exponent, the eigenvalues $\exp(ik_y d)$ will spread over a larger scale in value due to the nature of the exponential function. Some of the eigenvalues having small magnitudes could be difficult to compute accurately.

In addition, in the scattering matrix approach commonly employed to stabilize the computation, the number of matrix inversion and multiplication grows linearly with the number of layers. It would be preferred that one can find the eigenvalues k_y directly rather than through the exponential form. Also it would be desirable that we can avoid matrix inversions in the computation.

2.3. Theory for single-interface refraction problem

We have developed an analytic theory[8] that not only solves the single-interface refraction problem, but also gives a physical picture of light refraction at the interfaces between photonic crystals and homogeneous media. In addition, it provides an efficient way of calculating the relevant parameters (such as transmission

coefficient) of beam refraction, propagation because this is a single-cell method. Most importantly, this method can solve any surface orientation. We note that surface orientations other than (10), (100) or (111) are not adequately studied in the literature for the transmission and reflection coefficients *R*, *T*. In some prior studies on a rather arbitrary surface orientation,[11,17] only the electromagnetic field pattern simulated through certain whole-space methods are qualitatively examined, but the transmission and reflection coefficients are not quantitatively studied. Recently, Yu and Fan studied the anomalous internal reflection upon surfaces with orientations close to (11) for a PC with rectangular lattice.[25] With FDTD simulations they calculated the reflection efficiency for a beam that contains a continuous set of photonic crystal eigenmodes. The reflection efficiency for a beam was recognized as a collective result of the reflection efficiencies of individual modes. In fact, if the simulation region is large enough, the reflected beam could, we believe, be seen to split into multiple beams. However, the limitation of FDTD simulations did not allow the resolution of the fine constituency of the reflected beams. We first developed a general theory to rigorously calculate the transmission through a PC surface with arbitrary Miller indices, and gave the computation formula for the a quasi-periodic surface.[8] To show the validity of our approach, we show the numerical results (Fig. 2) based on our theory for a single-surface transmission problem studied by Li & Ho.[14] Here a Bloch mode illuminates a surface from the inside of a 2D photonic crystal having a square lattice of dielectric rods with dielectric constant 11.56, as delineated in Fig. 2(a). Excellent agreement is obtained with Li & Ho's original Fig. 8.[14] Those frequency ranges where both the transmission and reflection spectra are absent correspond to the bandgaps of the photonic crystal. As no Bloch mode can exist inside a stop gap, there is no incident mode, so the transmission and reflection spectra are meaningless for these ranges of frequencies.



(a) (b)

Fig. 2 (a) A 2D square lattice of dielectric rods with r=0.18a, ε=11.56. (b) Transmission (circles) and reflection (triangles) spectra for a Bloch mode incident upon the surface from inside the photonic crystal. The abscissa is the dimensionless frequency. Those frequency ranges where both the transmission and reflection spectra are absent correspond to the stop gaps of the photonic crystal.

3. DISCUSSIONS

3.1 Energy conservation

By the type of incident wave assumed, all of the theories or numerical methods for photonic crystal refraction can be divided into two types. The first type assumes the incident wave is a planar wave of infinite width, whereas the second type assumes the incident wave is a beam of finite width. Actually, it can be proved that the result of the first type of theories can be utilized to accurately predict the refraction behavior of a Gaussian beam—if the Gaussian beam is sufficiently wide. Furthermore, it can be proved that the rigorous energy conservation law that can be easily established for a planar incident wave case leads to energy conservation law of a Gaussian beam as well. The proof consists of some fairly length analytical derivations. In this paper, we intend to illustrate the principle through a simpler, or ideal case.

For simplicity, consider a 2D case, although it is straightfoward to extend the following discussion to any 3D case. One shall construct in the *x*-*y* space a large enough contour that encloses the refraction point on the interface. The contour should cut cross the beam at a place sufficiently far from the refraction point so that all the beams separate from each other when they cross the contour. One such contour is illustrated in Fig. 3. For visual clarity, the reflected beams are omitted in the drawing.

Then one can compute the following path integral along contour C

$$0 = \int_C S ds = -\int_{C_{in}} S_{in} ds_{in} + \sum_j \int_{C_{rj}} S_{rj} ds_{rj} + \sum_j \int_{C_{tjj}} S_{tj} ds_{tj} , \qquad (1)$$

where *S* is the magnitude of the Poynting vector, *ds* is the line element along the contour, and the subscripts *in*, *rj*, and *tj* indicate the incident beam, the *j*-th reflected beam (not drawn), and the *j*-th transmitted beam, respectively. Also the whole contour *C* is divided into segements C_{in}, C_{rj}, and C_{tj} that extend across the corresponding beam width. The negative sign in front of the integral for the incident beam is attributed to the convention of using outward surface normal component for surface integral. Here the incident beam has energy flowing into the contour. The integral must varnish because there is no source or absorber inside the contour.

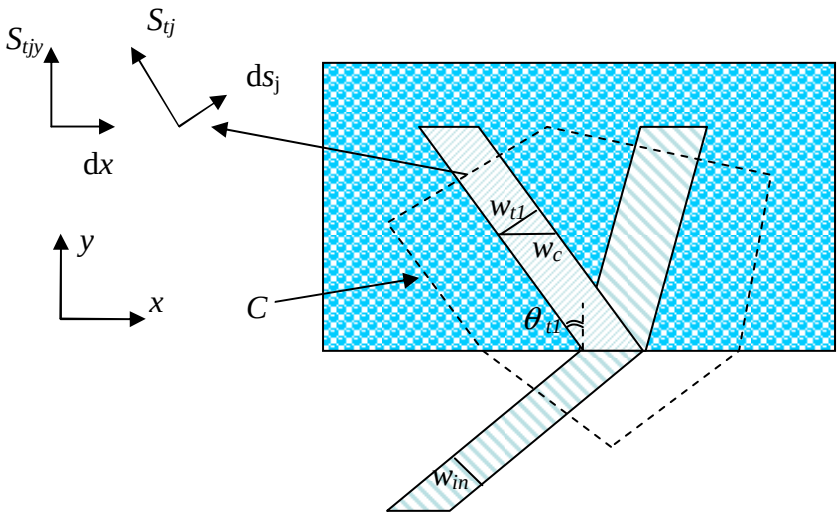


Fig. 3 Schematic drawing for energy conservation in multi-beam refraction.

To gain physical insight, we make a further assumption that each beam is a perfect rectangular beam. Therefore, inside each beam the Poynting vector is a constant(in the sense of cell average); outside the beams, the Poynting vector vanishes. Now Eq. (1) can be simplified to

$$0 = -S_{in} w_{in} + \sum_j S_{rj} w_{rj} + \sum_j S_{tj} w_{tj} , \qquad (2)$$

where the beam widths w_{in}, w_{rj}, and w_{tj} are defined perpendicular to their respective beam propagation directions. Note the beam widths satisfy the following relations

$$\frac{w_{in}}{\cos(\theta_{in})} = \frac{w_{tj}}{\cos(\theta_{tj})} = \frac{w_{rj}}{\cos(\theta_{rj})} = w_c , \qquad (3)$$

where θ_{in}, θ_{rj}, and θ_{tj} are the incident angle, the angle of the *j*-th reflected beam, and that of the *j*-th refracted beam, respectively; w_c is the width of the any beam sectioned by the surface, as indicated in Fig. 3. The relation Eq. (3) appears trivial and intuitively correct for rectangular beams, but a rigorous proof for a Gaussian beam is indeed fairly complicated. In fact, if the incident Gaussian beam width is too narrow, the

refracted field in the photonic crystal may not maintain a decent form of beams. Under such circumstances, the concept of beam may fall down and of course there is no way to apply the Eq. (3). In practical WDM devices, therefore, one shall make every effort in design to preserve a decent form of beams. The *y*-component of the Poynting vector of each beam can be written as

$$(S_{in})_y = S_{in}\cos(\theta_{in}), \qquad (S_{rj})_y = -S_{rj}\cos(\theta_{rj}), \qquad (S_{tj})_y = S_{tj}\cos(\theta_{tj}).$$

Now it is straightforward to show that the conservation of energy gives rise to

$$-(S_{in})_y - \sum_j (S_{rj})_y + \sum_j (S_{tj})_y = 0. \tag{4}$$

A preferred form is probably that

$$\sum_j R_j + \sum_j T_j = \sum_j \frac{-(S_{rj})_y}{(S_{in})_y} + \sum_j \frac{(S_{tj})_y}{(S_{in})_y} = 1. \tag{5}$$

Here we have defined transmission and reflection coefficients R_j and T_j based on the ratios of *y*-components of the corresponding Poynting vectors. To obtain Eq. (5), we have assumed a perfect rectangular beam. A more realistic assumption would be based on Gaussian beams, which is presented elsewhere.[8]

3.2 Calculation of dispersion surface

Dispersion surface, the equi-frequency or iso-frequency surface, in the reciprocal space is a key entity for studying light refraction and propagation in photonic crystals. Mathematically, it is represented by

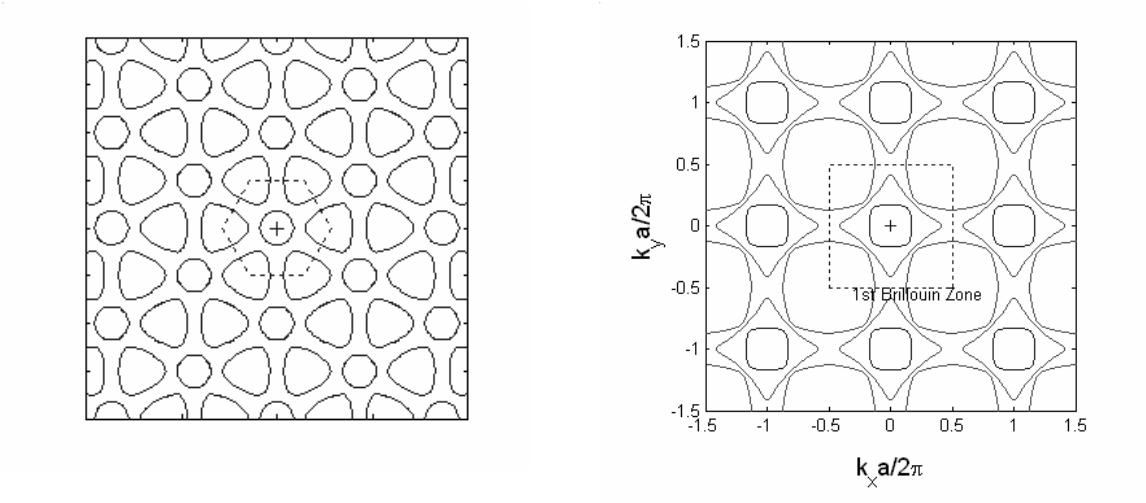
$$\omega(k_x, k_y, k_z) = \omega_c$$

for a given frequency ω_c. One may use the photonic crystal band solver to draw such a surface in the reciprocal space. Starting with an arbitrary initial wavevector $\mathbf{k}_0$, one can calculate the frequency $\omega_0 = \omega(\mathbf{k}_0)$ with the band solver. Then one can search the reciprocal space, starting from $\mathbf{k}_0$, to find a point $\mathbf{k}_{c0}$ that is on the dispersion surface, i.e. $\omega_c = \omega(\mathbf{k}_{c0})$.[9] From this point, one may search the reciprocal space again to find other points on the dispersion surface. Evidently, this approach needs an extra searching algorithm in addition to the eigenvalue solver. Another approach is to calculate the photon bands in the first Brillouin Zone on a sufficiently fine 3D grid; then one may interpolate to draw the contour surface in the reciprocal space.[10] Again, an extra interpolation process is needed in addition to the extensive computation on a grid. In both approaches, we need to calculate the frequencies at a large number of reciprocal-space points that are not on the dispersion surface. Evidently, redundant work exists in these two approaches.

Computing the eigenvalues k_y for a given ω_c on a 2D grid of (k_x,k_z) appears to be a better choice for computing the dispersion surface. Note this is exactly the way we solve the eigenvalues for the refraction problem. For each (k_x,k_z) on a 2D grid, one can calculate the corresponding k_y on the dispersion surface. In this way, not a single compuated eigenvalue is off the dispersion surface. Therefore, this approach appears more efficient compared to those methods based on the photonic band solvers. Illustrated in Fig. 4 is the dispersion surface computed through this technique. Note that for the 2D cases shown in Fig. 4, one actually computes eigenvalues k_y on a 1D grid of k_x for a given frequency ω_c.

4. CONCLUSION

In conclusion, various types of theoretical and numerical methods are compared for studying the refraction problem. The efficiency of a theory we priorly developed is presented. The energy conservation is related to the beam width change upon refraction, and the computation of dispersion surface is discussed.



(a) (b)

Fig. 4 Dispersion surfaces for 2D photonic crystals for a (a) triangular lattice (b) square lattice(multiple frequencies).

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