

MICROCAVITÉS ET CRISTAUX PHOTONIQUES *MICROCAVITIES AND PHOTONIC CRYSTALS*

Photonic band structure theory: assessment and perspectives

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Received and accepted 23 November 2001

Note presented by Guy Laval.

Abstract

An attempt is made to provide an assessment on the current state of photonic bandstructure theory, a field of research which is at the heart of rapid progress in photonic crystal research. First, different approaches to calculating photonic bandstructures as well as the optical properties of defect structures in photonic crystals are reviewed. Several highlights and applications of photonic bandstructure theory are presented that help to illustrate the tremendous progress the field has seen. Finally, perspectives of photonic bandstructure theory are briefly discussed and an attempt is made to identify possible future developments. To cite this article: K. Busch, C. R. Physique 3 (2002) 53–66. © 2002 Académie des sciences/Éditions scientifiques et médicales Elsevier SAS

photonic crystals / electromagnetic theory / photonic band structure / photonic band gaps

Résumé

Nous tentons ici de proposer une évaluation de l'état actuel de la théorie de la structure des bandes photoniques, un domaine de recherche qui se situe au cœur des progrès rapides de la recherche sur les cristaux photoniques. Nous rappelons d'abord quelques approches du calcul des bandes photoniques ainsi que des propriétés optiques des structures des défauts dans les cristaux photoniques. On présente ensuite quelques points forts et applications de la théorie de la structure des bandes photoniques, afin d'illustrer les énormes progrès accomplis dans ce domaine. Enfin, nous discutons brièvement les perspectives de la théorie de la structure des bandes photoniques et tentons d'en identifier les futures applications. Pour citer cet article : K. Busch, C. R. Physique 3 (2002) 53–66. © 2002 Académie des sciences/Éditions scientifiques et médicales Elsevier SAS

cristal photonique / théorie électromagnétique / structure des bandes photoniques / bande interdite photonique

1. Introduction

The past two decades have seen a tremendous increase in interest in the field of photonic crystals [1–6]. These microstructured optical materials are characterized through a spatially periodic modulation in their index of refraction. The resulting Bragg-scattering of electromagnetic waves leads to the formation of photonic bandstructures, very much in analogy to the electronic bandstructure of ordinary semiconductors or metals. In fact, under suitable circumstances such as appropriate lattice symmetry and sufficiently

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high variations in the index of refraction, PCs may exhibit complete photonic band gaps (PBGs), i.e., ranges of frequencies over which ordinary (linear) propagation is forbidden, irrespective of the direction of propagation. The multitude of today microstructuring techniques of high-quality optical materials and the resulting flexibility in fabricating PCs substantially contribute to the enormous interest in PCs. The deliberate creation of defect states inside a PBG such as cavity and waveguiding modes enhances the potential of PCs even further. In particular, the potential of judiciously designed PCs in tailoring the electromagnetic dispersion relation and mode structure to almost any need opens entirely new avenues for both basic research as well as technological applications. With PCs it thus becomes possible to manipulate both the radiation dynamics of active materials embedded in them as well as the propagation characteristics of electromagnetic radiation. In fact, the seminal papers of Yablonovitch [7] and John [8] have been concerned with the possibility of inhibiting spontaneous emission [7] and the realization of Anderson-localization of light [8] in these materials. Since then, numerous novel effects regarding the radiation dynamics of active materials in PCs such as fractional localization near a photonic band edge [9] and all-optical transistor action [10] have been proposed. Similarly, the re-examination of classical nonlinear effects such as solitary wave propagation [11] and nonlinear susceptibilities [12] in PCs have revealed a number of interesting results that await experimental confirmation. Furthermore, technological applications of PCs in the immediate future are concerned with the equally exciting realization of PC-based integrated photonics. For instance, suitably engineered cavity modes interacting with waveguiding structures may provide the foundation of several functional elements such as add-drop filters [13] and (de)-multiplexers [14]. Similarly, tunable bandstructures [15] and super-refractive phenomena such as the super-prism effect [16] may provide additional tools in order to develop PCs into a platform technology for optical telecommunication.

Photonic bandstructure theory lies at the heart of many of the interesting developments sketched above; photonic bandstructure calculations determine the structures that exhibit complete PBGs and allow accurate interpretations of measurements. In fact, the prediction of a complete PBG in the diamond structure by Chan, Ho and Soukoulis [17] along with the subsequent confirmation [18] may be regarded as a historical landmark. Recent experimental efforts in the development of the so-called woodpile structures [19,20] as well as inverse opals [21,22] have been strongly motivated by the theoretical works [23,24] that predicted the existence of complete PBGs in these structures. Moreover, the incorporation of nonlinear and optically active materials into PCs along with a detailed understanding of the optical properties of the resulting composite systems may enhance the utility of PCs over and above the conventional linear structures. Here, too, photonic band structure theory provides essential input such as group velocities and local density of states for realistic nonlinear and quantum optical calculations. Finally, the optical properties of defect structures in PCs may be accurately simulated through photonic bandstructure computations and, as a consequence, photonic bandstructure theory represents an important predictive as well as interpretative basis for the PC research.

The present paper offers an overview of photonic bandstructure theory. Section 1 provides an introduction to photonic bandstructure calculations as well as a discussion of the most prominent methods for their along with some of the most important results. In Section 2, methods for and results of the computation of defect structures in PCs are discussed. Finally, in Section 3 future directions of photonic bandstructure theory are indicated.

2. Methods of bandstructure computation

The simplest but by no means the only way to calculate photonic bandstructures is to adapt the methods of electronic bandstructure calculations to the case of PCs. Various adjustments are necessary in order to take into account the specific differences between electromagnetic waves in PCs and electron waves in semiconductors or metals. These differences may be best appreciated when combining Maxwell's equations

into the wave equation for the electric field $\vec{E}(\vec{r})$ with harmonic time dependence (frequency ω):

$$\nabla \times \nabla \times \vec{E}(\vec{r}) + \frac{\omega^2}{c^2} (\bar{\epsilon} - \epsilon(\vec{r})) \vec{E}(\vec{r}) = \frac{\omega^2}{c^2} \bar{\epsilon} \vec{E}(\vec{r}) \quad (1)$$

Here, c denotes the vacuum speed of light and the average value $\bar{\epsilon}$ of the spatially varying dielectric constant $\epsilon(\vec{r})$ has been introduced. The dielectric constant $\epsilon(\vec{r})$ contains the structural and material information about the PC. In particular, the dielectric constant:

$$\epsilon(\vec{r} + \vec{R}) \equiv \epsilon(\vec{r}) \quad (2)$$

is periodic with respect to the set $\mathcal{R} = \{n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3; (n_1, n_2, n_3) \in \mathcal{Z}^3\}$ of lattice vectors \vec{R} generated by the primitive translations \vec{a}_i , $i = 1, 2, 3$, that describe the structure of the photonic crystal. For instance, the dielectric constant $\epsilon(\vec{r})$ may be expanded in a Fourier series on \mathcal{G} the reciprocal (dual) lattice corresponding to \mathcal{R} .

Equation (1) bears a close resemblance to the stationary Schrödinger equation. The first term on the l.h.s. features a second-order differential operator acting on a wave field and may be interpreted as a ‘kinetic energy’ term. Similarly, the second term on the l.h.s. represents a term with a ‘periodic potential’ and, finally, the r.h.s. may be identified with an ‘energy eigenvalue’ term. The differences to the stationary Schrödinger equation are apparent; the electric field $\vec{E}(\vec{r})$ is vectorial by nature, implying that scalar approximations are insufficient. In addition, even for frequency independent dielectric constants $\epsilon(\vec{r})$, the ‘periodic potential’ term depends on the ‘energy eigenvalue’ itself, a situation not familiar from electronic systems.

2.1. Dispersion relation, Bloch functions and density of states

The goal of photonic bandstructure computation is the solution of the wave equation (1) through the determination of the dispersion relation (eigenfrequencies) and corresponding modestructure (eigenfunctions). This is facilitated by the observation that equation (1) comprises a set of coupled partial differential equations to which the Bloch–Floquet theorem may be applied: due to the discrete translational symmetry of the lattice, the wave vector \vec{k} labeling the solutions may be restricted to lie in the first Brillouin zone (BZ) of the reciprocal lattice. As a consequence, the dispersion relation $\omega_n(\vec{k})$ in the infinitely extended momentum space is folded back onto the first BZ, introducing a discrete band index n . The eigenmodes corresponding to the eigenfrequency $\omega_n(\vec{k})$ exhibit Bloch–Floquet form

$$\vec{E}_{n\vec{k}}(\vec{r}) = e^{i\vec{k}\vec{r}} \vec{u}_{n\vec{k}}(\vec{r}) \quad (3)$$

where $\vec{u}_{n\vec{k}}(\vec{r} + \vec{R}) = \vec{u}_{n\vec{k}}(\vec{r})$ is a lattice periodic function.

The photonic dispersion relation $\omega_n(\vec{k})$ gives rise to a photonic density of states (DOS), which plays a fundamental role in the understanding of the properties of a PC. The photonic DOS $N(\omega)$ is defined by “counting” all allowed states with a given frequency ω , i.e., by the sum of all bands and the integral over the first BZ of a Dirac- δ function:

$$N(\omega) = \sum_n \int_{\text{BZ}} d^3k \delta(\omega - \omega_n(\vec{k})) \quad (4)$$

For applications to quantum optical experiments in photonic crystals it is, however, necessary to investigate not only the (overall) availability of modes with frequency ω but also the local coupling between an excited atom that can emit a photon with frequency ω and the electromagnetic environment provided by

the photonic crystal at the location of the atom. Consequently it is the overlap matrix element of the atomic dipole moment to the photons in this mode that is determining quantum optical properties such as decay rates, etc. This may combined be combined in the local DOS (LDOS), $N(\vec{r}, \omega)$, defined as

$$N(\vec{r}, \omega) = \sum_n \int_{\text{BZ}} d^3k |\vec{E}_{n\vec{k}}(\vec{r})|^2 \delta(\omega - \omega_n(\vec{k})) \quad (5)$$

For an actual calculation, the integrals in equation (4) and equation (5) must be suitably discretized and one may again revert to the methods of electronic band structure calculations.

2.2. Plane wave methods

A straightforward way of solving for eigenvalues and eigenfunctions of equation (1) is to expand the dielectric constant as well as the periodic part of the Bloch function into a Fourier series on the reciprocal lattice, transforming equation (1) into an eigenvalue problem for an infinite matrix which must be suitably truncated to become accessible to an approximate numerical solution. Owing to its simplicity and flexibility in handling practically any geometry of the unit cell, this so-called plane wave method (PWM) has become the work house for most investigations of photonic bandstructures.

In practice, it turns out that rather than solving equation (1) for the electric field $\vec{E}_{\vec{k}}(\vec{r})$ it is more convenient to solve the equivalent wave equation for the magnetic field $\vec{H}_{\vec{k}}(\vec{r})$:

$$\nabla \times \left(\frac{1}{\epsilon(\vec{r})} \nabla \times \vec{H}_{\vec{k}}(\vec{r}) \right) = \frac{\omega^2}{c^2} \vec{H}_{\vec{k}}(\vec{r}) \quad (6)$$

through a corresponding expansion of the inverse dielectric constant and the periodic part of the Bloch function into plane waves. On the one hand, the divergence-free nature of the magnetic field, $\nabla \cdot \vec{H}_{\vec{k}}(\vec{r}) = 0$, allows us to restrict the number of expansion coefficients to only two transverse polarizations for any given plane wave. For a total number of N plane waves, this leads to a $2N \times 2N$ matrix problem instead of the $3N \times 3N$ matrix problem that results from applying the PWM to equation (1). On the other hand, the continuity of the magnetic field $\vec{H}_{\vec{k}}(\vec{r})$ is expected to reduce the number of plane waves necessary for obtaining converged results.

However, as most PCs consist of piecewise homogeneous sections of material, there still remains the question whether such step-like discontinuities of the dielectric constant are accurately represented within the PWM and, as a consequence, the convergence properties of the PWM have been carefully investigated [24,25]. Besides the above-mentioned advantages of the PWM based on the magnetic field, equation (6), it has become apparent that the magnetic field approach exhibits superior convergence properties as compared to PWM based on the electric or the displacement field. Applying PWM to equation (6) involves the computation of the matrix of Fourier coefficients of the inverse of the dielectric constant which can be done in two ways. One can calculate the inverse dielectric constant in real space and then compute its Fourier coefficients. This is referred to as the direct method. Alternatively, one can calculate the matrix of Fourier coefficients of the dielectric constant and then take its inverse to obtain the required Fourier coefficients. The latter method is known as the Ho–Chan–Soukoulis (HCS) method [17]. Since the operations of taking the Fourier transform and inversion commute on the complete set of plane waves, the results for the direct method and for the HCs method must coincide exactly. However, we are numerically restricted to operate on a finite dimensional subspace of the full reciprocal space. This leads to dramatically different rates of convergence of the two methods as the subspace (number of plane waves) is increased. Detailed investigations [25] have clearly demonstrated the superior convergence properties of the HCS method.

2.3. KKR method

Another approach to solving equation (1) is to adapt the method of Kohn, Korringa and Rostocker (KKR method) familiar from electronic bandstructure theory to the case of PCs. Within the KKR method, the wave function is expanded into a series of vector spherical harmonic functions centered around individual lattice sites. Graf addition theorem for Bessel functions then allows a matching of the electromagnetic field resulting from the radiation that emanates from all but the central scatterer to the electromagnetic field expanded around this central scatterer. This procedure maps equation (1) onto an eigenvalue problem of an infinite matrix system both for two-dimensional [26,27] as well as three-dimensional systems [28,29]. As a consequence of this expansion, the discontinuities of the dielectric constant associated with spherically symmetric scatterers may be represented to arbitrary accuracy and it is for these systems that the KKR method proves to be more efficient than PWM, allowing the results of PWM [28] to be gauged. In essence, for spherically symmetric systems, KKR method and PWM may be regarded as complementary. KKR relies on the eigenfunctions of the individual scatterer and, therefore, allows to represent the discontinuities of the dielectric function very accurately while the lattice structure is incorporated via the multicenter expansion technique. Conversely, PWM is based on an accurate representation of the underlying lattice structure via the expansion into an appropriate set of plane waves and attempts to incorporate the discontinuities in the dielectric constant through the corresponding Fourier coefficients. However, for non-spherical scatterers, the KKR method loses its most attractive feature of accurately incorporating the discontinuities of the dielectric constant. In view of the numerous structures with non-spherical scatterers that exhibit complete PBGs, the KKR has, therefore, been unable to replace PWM as the work horse of photonic bandstructure theory.

2.4. Real-space methods

Adapting methods from electronic bandstructure theory to the case of PCs is, however, not the only successful route to computing photonic bandstructures. In particular, the convergence issues associated with PWM and the limitation to spherical scatterers of the KKR method have prompted a number of authors to develop real-space methods for photonic bandstructure computations that allow the efficient treatment of arbitrary scatterer shapes.

The transfer matrix method (TMM) of Pendry and McKinnon [30] represents a finite difference frequency domain (FDFD) approach that is based on a discretization of Maxwell's equation for time harmonic electromagnetic fields. In TMM, the calculation starts with the field distribution of a plane wave on a slice through the PC (a line for a two-dimensional PC and a plane for a three-dimensional PC). This is followed by propagating the field slice by slice via a finite difference discretization of the time harmonic Maxwell's equations through the PC over a certain distance in real space. Then, the dispersion relation is given through the eigenvalues of the resulting transfer matrix that connects the field distribution of the final slice to the field distribution on the initial slice. For instance, for given wave vector components k_x , k_y , and frequency ω , the field is propagated over a lattice constant a in the z -direction and the eigenvalues of the transfer matrix are related to the k_z values of the wave vector via the Bloch theorem, equation (3), [30]. Clearly, TMM is a rather versatile method and may be extended to the calculation of transmission and reflection coefficients for finite slabs of PC material [31].

Alternatively, rather than Maxwell's equation one may consider the wave equation either in the time domain or for fields with harmonic time dependence. The former case has been pioneered by Chan et al. [32] and Sakoda et al. [33]. In both approaches, FDTD solutions to the wave equation within the PCs unit cell are obtained for the Bloch boundary condition provided by the wave vector k under consideration. For instance, Chan et al. [32] obtain the eigenfrequencies through a Fourier analysis of the time evolution of the system that is subjected to a δ -impulse excitation. However, in order to obtain the field distribution (Bloch function) for a specific mode, it becomes necessary to consider the time evolution of the electromagnetic field when the system is driven by a dipole oscillator that radiates with the corresponding eigenfrequency. In

fact, this observation is the basis of Sakoda's approach, where for a given wave vector \vec{k} , the rate of energy transfer from a dipole radiating with an arbitrary frequency to the system is monitored. This energy transfer is appreciable only if the dipole frequency corresponds to an eigenfrequency of the system [33] and, thus, the corresponding Bloch function is obtained simultaneously. The flexibility of these methods is manifest in the fact that upon appropriate modifications of the boundary conditions, they may be applied to systems of finite size [32] or defect structures [34]. Nevertheless, although frequency dependent dielectric constants may be treated using Sakoda's method [33], the scanning of frequencies in conjunction with studying the time evolution of the electromagnetic field distribution requires considerable computational resources.

Therefore, in some instances it will be advantageous to attempt the solution of the wave equation in the frequency domain, since sophisticated methods for solving these type of elliptic partial differential equations are well-known in applied mathematics. In fact, a recent application of the multigrid method to the case of photonic bandstructures [35] has proved to be much more efficient than PWM especially when the mode structure (Bloch functions) are required as well.

2.5. Results of bandstructure calculations

Photonic bandstructure theory lies at the heart of numerous developments in the field of PC research. Without attempting to be complete, we want to discuss some of the most significant developments that have had major impacts on the progress in the field of PC research.

2.5.1. Structures exhibiting complete PBGs

Undoubtedly, the first triumph of photonic bandstructure theory lies in the prediction of a complete three-dimensional PBGs in diamond structure [17] (see also Fig. 1). This remarkable discovery along with its subsequent realization in the microwave regime [18] has settled a period of heated debate about whether structures with complete PBGs at all exist.

Since then, numerous structures exhibiting complete PBGs have been suggested [23,36–41], the most notable being the 'woodpile' structure (a variation of the diamond structure) [23], the inverse opal structure [24], and the square spiral structure [41]. The diamond structure [17] and its cousins [23] constitute a family of PCs which are characterized by a large and complete PBG between the second and third band (fundamental gap) in the photonic bandstructure. In particular, the 'woodpile' structure lends itself to a layer by layer fabrication [19,20]. The fcc lattice structure of the inverse opals, on the other hand, does not exhibit a complete PBG between the second and third band. Instead it has a small PBG between the eighth and ninth band in the photonic bandstructure [24]. For instance, a silicon inverse opal exhibits a PBG with a size of about 4.25% of its center frequency (see Fig. 2).

However, photonic bandstructure theory has revealed the potential for a substantial increase in the size of the PBG through a careful control of the material synthesis parameters [42] such as the degree of infiltration

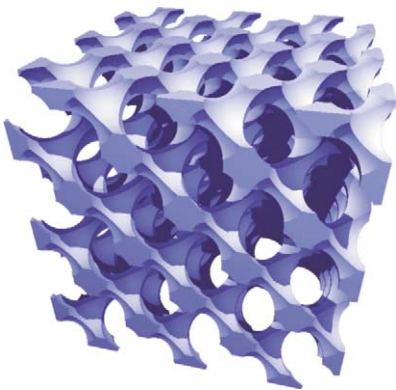
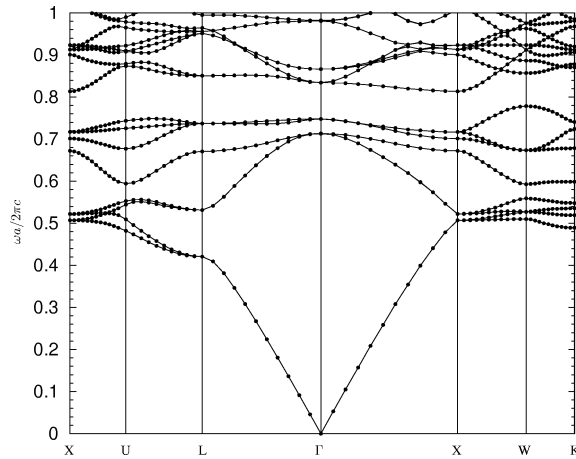


Figure 1. The inverse diamond structure was one of the first prototype structures predicted to exhibit a large and robust complete PBG [17]. It consists of an overlapping array of air spheres arranged in a diamond lattice. This structure can be mimicked by drilling an array of criss-crossing cylindrical holes into a bulk dielectric [18]. The solid backbone consists of high refractive index material such as silicon leading to a complete PBG as large as 27% of the center frequency. The minimum refractive index (of the backbone) for the emergence of a PBG is roughly 2.0. Practical difficulties in the synthesis of this structure have motivated the simpler but close related designs such as the woodpile structure [23] (courtesy of O. Toader, University of Toronto, Canada).

Figure 2. Photonic bandstructure for a fcc lattice of closed packed air spheres located in a silicon matrix ($\epsilon_{Si} \approx 11.9$ occupying about 26% by volume of the PC). The frequency is plotted in units of $a/2\pi c$, where a is the cubic lattice constant and c denotes the vacuum speed of light. Clearly visible is the complete 4.25% PBG relative to its center frequency between bands 8 and 9.



of the opal template obtained through a self-assembly process [21,22]. Nevertheless, being a higher order PBG, the PBG in inverse opals remains relatively susceptible to disorder [43]. The recently discovered square spiral structure exhibits a large PBG between the fourth and fifth band in the photonic bandstructure and is amenable to micro-fabrication using the so-called glancing angle deposition technique [41].

2.5.2. Comparison with experimental data

The prediction of complete PBGs in the structures discussed above and structures to be discovered, has motivated and will continue to inspire scientists to find novel fabrication techniques in order to realize the corresponding PCs. The resulting samples then have to be characterized spectroscopically allowing a comparison between measured data and the results of photonic bandstructure computations. Conversely, photonic bandstructure theory helps in the interpretation of experimental data. For instance, a plane wave with frequency ω and wave vector \vec{k}_0 impinging on the surface of a PC sample may be incompatible with the symmetry of the Bloch function of corresponding frequency ω and conserved crystal momentum \vec{k}_{\parallel} transverse to the sample surface. Here, the transverse crystal momentum \vec{k}_{\parallel} is defined as that part of the transverse component of the incident wave vector \vec{k}_0 that lies inside the first BZ modulo a reciprocal lattice vector. Therefore, despite the fact that there exists an allowed mode within the PC to which the incoming plane wave could couple, the plane wave may still be reflected and this nil-coupling may complicate the interpretation of measurements. Therefore, in order to understand transmission and reflection spectra from PCs, a detailed symmetry analysis of the corresponding mode structure is of paramount importance [6]. To date, the comparisons between experimental data and photonic bandstructure computations are too numerous to give an exhaustive list of references. However, it is safe to state that photonic bandstructure computation provides an indispensable predictive as well as interpretative tool for the characterization of PCs.

2.5.3. Applications of photonic bandstructures

Simple applications of PCs can be found in the microwave to millimeter wave range. For instance, an antenna mounted on a conventional dielectric substrate emits the majority of its radiation into the substrate itself. If the substrate is engineered into the form of a PC with a PBG at the radiation frequency, the losses can be minimized, leading to highly directional transmitters [44,45]. Other applications include optical filters with tailor made characteristics [46] as well as material exhibiting extremely enhanced effective birefringent behavior [47].

Nevertheless, it is for visible and near-infrared frequencies where PCs are likely to have their most important impact. Here, a novel class of effects, the so-called super-refractive effects [16,49], may have

their most important impact. These effects rely on the fact that the direction of energy flow of an electromagnetic wave packet with center frequency ω and center crystal momentum \vec{k} propagating through a PC is determined by the direction of the group velocity $\vec{v}_g \equiv \nabla_{\vec{k}} \omega(\vec{k})$ (see [48]) and the fact that the dispersion relation $\omega(\vec{k})$ of a PC may far be far from isotropic. In fact, one may derive a number of effects by qualitatively considering the photonic bandstructure and the boundary condition on the interface between a PC and air: similar to the scattering of a plane wave by a PC surface discussed above, when a pulse with center frequency ω and center wave vector \vec{k}_0 propagating in air is incident on this interface, the continuity of the transverse crystal wave vector \vec{k}_{\parallel} determines the mode on the iso-frequency surface $\omega = \omega(\vec{k})$ that will serve as the carrier wave of the energy inside the PC. Depending on the curvature of this generally highly anisotropic iso-frequency surface at the location of the carrier mode one may obtain anomalous refraction properties. Clearly, such anomalous refraction properties lends themselves to the realization of efficient beam steering effects for WDM devices [50] and efficient collimators [51]. Similarly, near special point of the photonic bandstructure, it is possible to utilize the super-refractive behavior of a PC to realize efficient prisms which may perform three orders of magnitude better than conventional prisms and, consequently, this effect has been termed the super-prism effect [16]. As a consequence, super-refractive effects may play an important role in the realization of PC-based devices for optical communication technology such as multiplexers and demultiplexers and the contribution of photonic bandstructure theory will be essential for success [52,53].

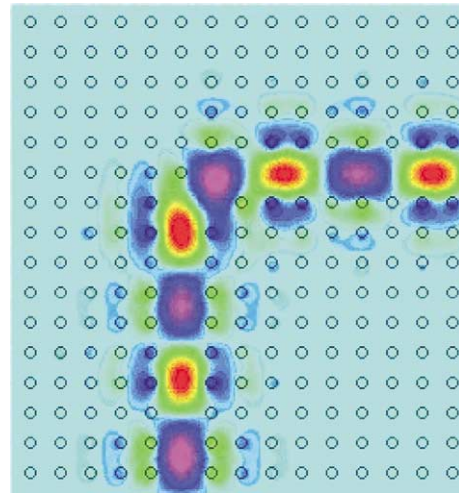
2.5.4. Tunable bandstructures

For many applications it is advantageous to obtain some degree of tunability of the photonic bandstructure through electro-optic effects. This may be useful in routing of signals through an optical communication network and provide flexibility to reconfigure the routing as conditions in the network change. One of the great advantages of PCs is that by volume, most of the material consists of pores. These pores can be infiltrated with other electro-optically active materials which enable reconfiguration of the underlying photonic bandstructure either globally or locally. Tunability may be obtained by controlling one or several forms of optically anisotropy of the constituent materials. For example, the science of liquid crystals has spawned an entire industry related to these electro-optic effects. The large empty volume of PCs is ideally suited for infiltration by a low refractive index liquid crystal with strong optical anisotropy making them efficacious for electro-optic tuning effects. In particular, a change in the orientation of the nematic director field with respect to the isotropic PC backbone by an external electric field can completely open or close the complete three-dimensional PBG [15]. The resulting tunability of spontaneous emission, super-refractive and waveguiding effects (see Sections 2.5.3 and 3, respectively) may considerably enhance the technological value of a composite liquid crystal PC over and above that of either bulk liquid crystal or a conventional PC itself.

3. Defect computation

Optical fibers are replacing electrical wires in shorter distance communications such as local access networks and computer to computer communications. In a completely seamless optical network, communications between nearby computer chips and even within a single computer chip would take place with tiny beams of laser light rather than electricity. Optical communication chips of this type may be faster than their electronic counterparts. The trapping and micro-moulding of the flow of light for the applications suggested above requires materials which allow the fabrication of micro-circuits of light waves that eventually replace today electronic micro-circuits. In electronic micro-circuits, electrical currents are guided by thin metal wires and the electrons are bound within the cross section of the wire by the so-called work function (confining potential) of the metal. As a result, electrical currents follow the path prescribed by the wire without escaping into the background. In contrast, the light in an optical fiber, one of the principal components of today optical communication technology, can easily escape into the background electromagnetic modes of

Figure 3. Sharp bend waveguide channel in a two-dimensional PC. The colors show the propagation of an electromagnetic mode around the bend with no reflection or scattering losses, illustrating the principle of a ‘photonic wire’ (courtesy of J.D. Joannopoulos, Massachusetts Institute of Technology).



empty space if the fiber is bent or distorted on a microscopic scale. Similar considerations apply to the other principal elements of today optical communication technology such as high index waveguiding structures. A major source of interest in PCs manifests itself in their capability to remove this problem by removing all the background electromagnetic modes over the relevant band of frequencies. Light paths and functional elements can be created inside a PBG in the form of engineered waveguide channels, micro-resonators and composite elements consisting of coupled waveguides and/or micro-resonators. An illustrative example of a sharp waveguide bend is depicted in Fig. 3.

The PBG localizes the light and prevents it from escaping the optical micro-circuits. Therefore, the task of photonic bandstructure theory is to provide calculations of the optical properties of finite sized PCs and defect structures embedded in them. This includes the calculation of transmission and reflection coefficients for slabs of PC material as well as eigenfrequencies and mode structures of micro-resonators and waveguiding structures. In addition, time domain simulations of optical signals propagating through functional structures embedded into PCs will be essential in the development of a PC-based optical communication technology.

3.1. Super cell method

Simple defect structures such as micro-cavities may be directly tackled by the methods of photonic bandstructure computation. The reasoning here is that in analogy to the introduction of dopant atoms into a electronic semiconductor, localized defect structures in PCs generate well-localized defect modes (donor or acceptor bound states) with corresponding defect frequencies inside the PBG. In addition, the extended eigenmodes of the underlying PC are turned into comparatively weakly perturbed scattering states (extended states) of the combined PC plus defect system. This state of affairs allows us to model the combined PC plus defect system by a periodic system with a large unit cell (the so-called super cell) centered around the defect to which standard bandstructure computation is applied. If the unit cell is made sufficiently large, the overlap between neighboring unit cells of the decaying wave functions associated with those defect modes whose frequencies are inside the PBG is negligible and very narrow ‘defect bands’ representing the eigenfrequencies of the defect states emerge inside the PBG of the bandstructure of the underlying PC. In fact, the results of calculating defect states using a PWM-based super cell approach where the super cell consisted of up to some 64 unit cells of the underlying PC have been confirmed by experiments [54,55].

Although the super cell method is not necessarily confined to cavities, it becomes impractical due to the large unit cells that need to be accurately represented when large defect structures with few or no

symmetries are to be investigated. Therefore, practical considerations limit the use of the super cell methods to defect structures of small extend and/or high symmetry such as micro-resonators and straight waveguides.

3.2. Expansion into localized basis sets

The limitations of the super cell method in order to describe the localized modes associated with defect structures embedded into a PC exhibiting a complete PBG suggests the expansion of the corresponding modes into a set of localized basis functions. This can be done by using a universal and complete set of localized functions such Hermite polynomials with a Gaussian envelope [56]. Unfortunately, such universally applicable approaches to defect states in PBGs do not incorporate the information of the underlying perfectly periodic PC which is readily available from the methods of bandstructure computation discussed in Section 2. One way of utilizing this information is to apply a unitary transformation (a ‘quasi’-Fourier transformation) to the extended Bloch functions in order to generate a complete set of localized basis functions, the so-called Wannier functions, that retain information of the underlying PC. This Wannier function approach is well-known from electronic bandstructure theory and may be adapted to the case of PCs. In its simplest form, a tight-binding parametrization of the bandstructure for a certain energy range based on symmetry-adapted localized orbitals is generated and fitted to the results of ab-initio bandstructure computations. Then, the effective Bloch function are transformed into Wannier functions which may then be used as a basis set for expanding the defect wave function. The problem of adapting the tight-binding approach to the description of PCs is the absence of appropriate localized atomic orbitals and the ever-present propagating (extended) low-frequency modes. Until now, satisfactory tight-binding models have only been developed for the TM-polarization of two-dimensional PCs [57]. Very recently, calculations of defect modes such as T-junctions of wave guiding structures have been accomplished for this case [58]. The Wannier function approach offers a number of attractive features such as efficient – possibly semi-analytic – scanning of large parameter spaces for suitable designs of complex defect structures combined with considerable physical insight based on the usage of localized functions that are optimally adapted to the underlying perfectly periodic PC. In particular, the study of wave guiding effects based on ‘photon hopping’ as suggested by Bayindir et al. [59] may be ideally suited to a tight-binding formalism. Nevertheless, it remains unclear how a successful tight-binding description for the TE-polarization in two dimensions and for the full three-dimensional can be developed.

3.3. Finite size KKR methods

Another prominent method of electronic bandstructure theory for defect calculations that may be adapted to electromagnetic problems is the modification of the KKR method (see Section 2.3) to the case of finite sized systems and/or defect structures by appropriately modifying the boundary conditions (see Section 3.4). A number of groups have derived various implementations of closely related finite-size KKR approaches either for the calculations of transmission and reflection characteristics of slabs of PC material [60–62] or for the direct calculation of the corresponding Green’s function [63] (see Section 3.4).

3.4. Green’s function approach

Green’s function approaches represent powerful tools well-known from electronic bandstructure theory that may be adapted to the characterization in the frequency domain of finite sized PCs or defect structures embedded in them. In the case of PCs, the Green’s function is, in fact, a Green’s tensor $\mathbf{G}(\vec{r}, \vec{r}'; \omega)$ and satisfies:

$$\nabla \times \nabla \times \mathbf{G}(\vec{r}, \vec{r}'; \omega) - \frac{\omega^2}{c^2} \epsilon(\vec{r}) \mathbf{G}(\vec{r}, \vec{r}'; \omega) = -4\pi \delta(\vec{r} - \vec{r}') \quad (7)$$

together with the appropriate boundary conditions. For instance, for a finite piece of PC material, the so-called Sommerfeld radiation condition states that the δ -impulse on the r.h.s. of equation (7) gives rise to an

outgoing spherical wave far away from the PC. Physical quantities such as the LDOS $N(\vec{r}, \omega)$ may then be calculated from a knowledge of the Green's function $\mathbf{G}(\vec{r}, \vec{r}'; \omega)$:

$$N(\vec{r}, \omega) = -\frac{2\omega}{\pi c^2} \Im[\text{Tr}(\mathbf{G}(\vec{r}, \vec{r}'; \omega))] \quad (8)$$

where $\Im[\cdot]$ and $\text{Tr}(\cdot)$ denotes the imaginary part and the trace of a matrix, respectively.

In electronic bandstructure theory, a class of efficient methods for obtaining Green's functions is known as the so-called order- N methods. This is to say that these methods scale linearly with the system size N and may be characterized as finite difference or finite element methods either in the frequency or the time domain. To date, there have been several works reporting successful implementations of order- N methods for defect structures in PCs and/or finite sized PCs [32,64]. As discussed in Section 2.4, besides computing photonic bandstructures, TMM may be used to also calculate transmission and reflection properties of finite slabs of PC material. Propagating the electromagnetic field slice by slice represents an order- N FDFD method and allows to treat slabs with defect structures included.

However, due to the fact of having to discretize a large region of space, practical limitations arise from the hardware resources required to treat large defect structures and the numerical stability of the finite difference discretization. In TMM, the former problem may be a less severe but the latter problems merits close attention and additional measures such as multiple scattering treatments familiar from low-energy diffraction theory have to be employed in order to obtain stable numerical results [30].

3.5. FDTD

The main body of works dealing with the computation of the properties of defects structures in PCs has been carried out using direct FDTD [65] discretizations of Maxwell's equations. This techniques are well-known in the electrical engineering community and while they usually require substantial computational resources, FDTD calculations have been tested and perfected over some 30 years and offer the unique advantage of allowing the time domain simulations of pulses propagating through and interacting with complex defect structures. Therefore, FDTD methods have been instrumental in the development of numerous proposed designs for functional elements for optical communication devices such as waveguide bends [66] (see also Fig. 3), junctions [67], add-drop filters [13] as well as high- Q cavities [68].

3.6. Results: defects

Much of today interest in PCs is the result of calculations of defect structures embedded in PCs. In particular, the MIT group has proposed numerous designs for functional elements [13,66,67] that serve as powerful illustrations of the PCs potential to be developed into a platform technology for optical communication technology. Additional functional elements may include ultra-small beam splitters and Mach–Zehnder interferometers. More recent developments on the basic science side include the discovery of PBGs in photonic quasi-crystals [69,70] that open up for fairly modest index contrasts and studies of the effects of disorder on photonic band structures [43,71–74]. On the technological side, optimized designs for obtaining guided modes in quasi two-dimensional structures [75,76] have been proposed and FDTD calculations have led to the successful design and subsequent realization of an add-drop filter for a dense wavelength division multiplexed optical communication system [14] as illustrated in Fig. 4.

Here, light from an optical fiber carrying many different frequencies f_1, f_2, \dots is inserted into a quasi two-dimensional PC structure by means of a waveguide channel. The frequencies f_1, f_2, \dots lie within the two-dimensional PBG and cannot escape from the waveguide channel except in places where the periodicity of the background pores is disrupted by means of defects. For instance, a hole that is larger than all the other background holes can act as resonator which picks a particular frequency from the waveguide channel, while allowing other frequencies to propagate freely along the waveguide.

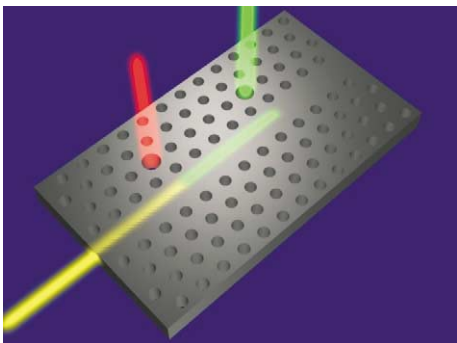


Figure 4. Add-drop filter for a PC-based dense wavelength division multiplexed optical communication system [14]. Multiple streams of data at different frequencies f_1 , f_2 , etc. (yellow) enter the optical micro-chip from an external optical fiber and are carried through the wave guide channel created by the missing row of pores. Data streams at frequency f_1 (red) and f_2 (green) tunnel into the localized defect modes and are routed to different destinations. The frequency of the drop filter is defined by the resonance frequency of the micro-resonator that is determined by the deviation of the defect pore diameter from the pore diameter of the background PC. The experimental realization of the above design has confirmed the corresponding FDTD simulations that led to this design [14] (courtesy of S. Noda, Kyoto University, Japan).

4. Outlook, future developments

In summary, the theoretical description of PCs in the form of photonic bandstructure theory has been the driving force for numerous development in the field of PCs and has matured to the point where it provides a reliable interpretative tool to both material synthesis and spectroscopic analysis of these novel optical materials. The current state of PC research suggest that this field is at a stage comparable to the early years of semiconductor technology shortly before the invention of the solid state electronic transistor by W. Shockley, J. Bardeen and W.H. Brittain.

Besides the obvious necessity for investigations of novel structures that may exhibit PBGs as well as for detailed studies of the effect of fabrication tolerances on the performance of PC-based devices, this state of affairs also points towards a couple of future directions PC research may take: PCs with complete PBGs represent a fundamentally new paradigm for low threshold nonlinear optical phenomena as the absence of modes inside a PBG as well as the extremely low group velocity in the vicinity of a PBG profoundly affect light-matter interaction. For instance, in the context of a three-dimensional PBG where the inhibition of spontaneous emission from atoms and molecules is essentially complete, all textbook results that are derived by retaining spontaneous emission as the leading order process have to be re-examined in the context of the PBG. Novel effects such as low-threshold nonlinear optical response without absorption [12] as well as collective switching and all-optical transistor action [10] have been predicted in these systems. These predictions challenge photonic bandstructure theory to derive realistic models that allow us to calculate effective nonlinear and quantum optical parameters. These efforts will serve as a reliable guide to experimental efforts and help in interpreting data. On the more technological side, the design of efficient coupling elements between PC-based optical chips and the outside world of fiber optics merits considerable attention [77,78]. Similarly, it may be very rewarding to combine defect structures with the concept of tunable optical anisotropies in order to realize semi-passive components for optical communication technologies.

Clearly, these challenges will continue to excite researchers and stimulate further interesting developments in the field of photonic bandstructure theory.

Acknowledgements. K.B. would like to acknowledge the financial support by the Deutsche Forschungsgemeinschaft under Grant Bu 1107/2-1 (Emmy-Noether program).

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