

Dielectric crystals that act on photons as semiconductors do on electrons – forbidding certain wavelengths to propagate – promise highly efficient lasers and novel photonic materials

# Photonic band gaps

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MANY major discoveries in physics this century originate from the study of waves in periodic structures. Examples include X-ray and electron diffraction by crystals, electronic band structure and holography. Analogies between disciplines have also led to fruitful new avenues of research. An exciting example is the recent discovery of three-dimensionally periodic dielectric structures that exhibit what is called a “photonic band gap” (PBG), by analogy with electronic band gaps in semiconductor crystals. Photons in the frequency range of the PBG are completely excluded so that atoms within such materials are unable to spontaneously absorb and re-emit light in this region; this has obvious beneficial implications for producing highly efficient lasers. Given that electrons and photons obey almost the same differential wave equation, the idea of a PBG is clearly far from crazy. It does, however, demand a radical rethink of how light behaves in periodic structures.

Conventionally, optical gratings are regarded as devices for converting one wave into another by Bragg diffraction, rather than as synthetic dielectric crystals with their own peculiar densities of photonic states, “stop-bands” and “pass-bands”. A periodic structure is characterised by two parameters – a spatial period (pitch or lattice constant) and the amplitude, or modulation depth, of the ripple in potential or refractive index. Most 3-D optical gratings (such as volume holograms) have only a weakly modulated periodicity (typically  $<10^{-4}$  of the average value) so light propagation is only forbidden in rather narrow ranges of wavevector. These so-called “stop-bands” appear around the Bragg scattering points in  $k$ -space and their widths are roughly proportional to the modulation depth (see Yeh *et al.*, Zengerle, and the author in Further reading). It has only been suggested recently, mainly through the pioneering efforts of Sajeev John of the University of Toronto, Canada, and Eli Yablonovitch of Bellcore, US, that a complete PBG should appear if the modulation depth is increased enough in a structure with multiple periodicities (the stop-bands should become so

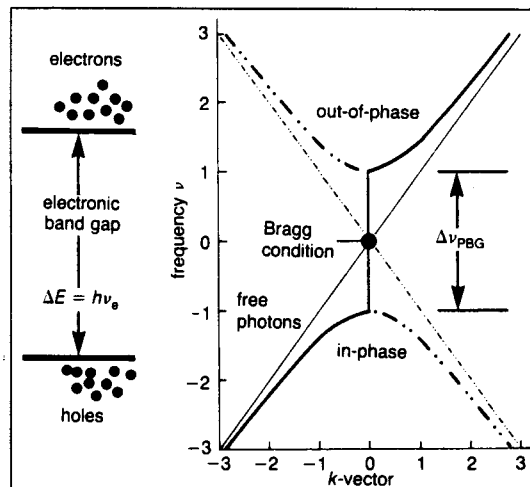
wide that they coalesce and forbid propagation in all directions within a certain range of frequencies). Despite the difficulties of designing and constructing the right kind of structure, and of detecting what happens, Yablonovitch’s team

have observed a PBG at microwave frequencies in a specially drilled dielectric material (microwave refractive index of 3.6) with a face-centred-cubic lattice. This “dielectric crystal” was produced by drilling evenly spaced (8 mm pitch) sets of holes at three carefully chosen angles. To obtain a band gap at optical frequencies requires a very much smaller lattice spacing ( $\sim 400$  nm for  $1.5 \mu\text{m}$  light in GaAs) and is much more challenging to produce. Although techniques involving reactive ion beam etching are being actively developed, no success has yet been reported.

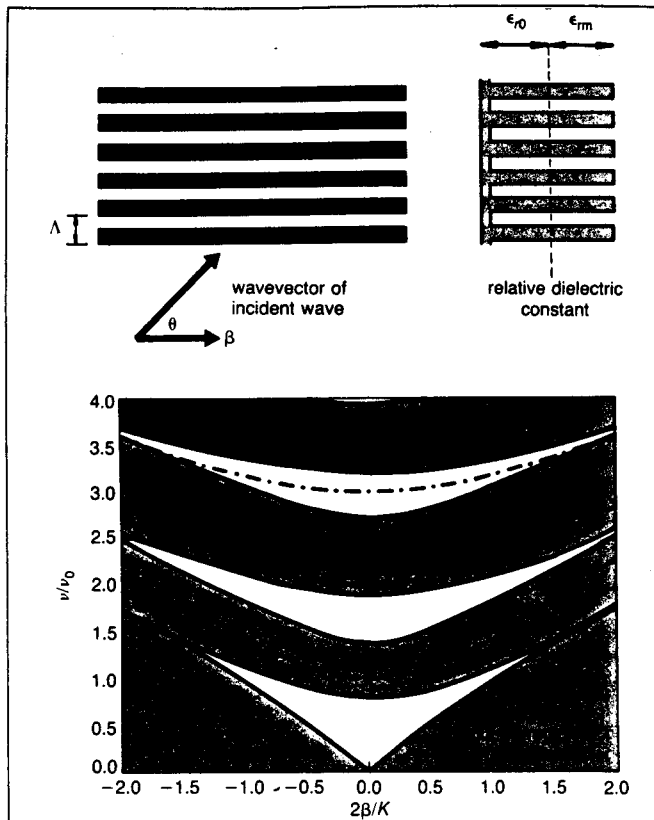
Apart from novelty, PBGs offer fascinating possibilities for new types of electron-photon interactions, and suggest new ways of thinking about the behaviour of light in periodic structures. So, what precisely is a material with a photonic band structure, and how and why does it work?

A PBG material is formed when a dielectric of high refractive index is riddled with a regular 3-D lattice of cavities. The resulting crystalline structure has islands, or “atoms”, of high refractive index surrounded by interstitial regions where the index is low. In a semiconductor crystal, valence band electrons spend most of their time at the atoms (i.e. low potential energy regions) while conduction band electrons are found mainly in between (high potential energy regions). In the same way, photons in a PBG material have the choice of being concentrated

at the high index “atoms”, or in the low index regions in between. The photon’s position depends on its energy, and if a range of energies exists where neither alternative is possible, a PBG forms. Its appearance and width depend on the refractive index difference between “conduction band” photons and “valence band” photons, i.e. on the modulation depth of the refractive index. Photons with energies lying within the PBG cannot propagate and their wavefunction decays exponentially with position, i.e. they



1 Spontaneous emission is inhibited if the photon released at a radiative electronic transition has an energy  $h\nu_e$  that lies within the PBG. Straight lines are the  $(k, \nu)$  relationship in the absence of periodicity, i.e. for “free photons”. Out-of-phase and in-phase refer to the position of the fringes of the photonic Bloch states relative to the high index regions (see 3); in-phase implies that the peaks of intensity coincide with planes of high refractive index. The group velocity, given by  $2\pi\partial\nu/\partial k$  (thick line), tends to zero at the band gap edges where the slope is zero



2 Band structure of a single grating with high modulation depth  $M = \epsilon_{rm}/\epsilon_{r0}$  (rectangular profile shown to scale top right) for an optical frequency  $\nu$  and wavevector parallel to the interface  $\beta$ . The angle of incidence is  $\theta$ , the Bragg frequency for  $\theta = 90^\circ$  is  $\nu_0$ , and the integral values  $m$  refer to the  $m$ th order Bragg condition, given by  $m\lambda = 2\Lambda \sin\theta$ , where  $\lambda$  is the mean wavelength in the grating. The Fourier series of the grating profile, given by  $M(x) = \sum_n M_n \cos(nKx)$ , has significant harmonics at even values of  $n$  with  $M_0 = 0.56$ ,  $M_2 = -0.18$ ,  $M_4 = 0.10$  and  $M_6 = -0.08$ ; the odd amplitudes are all zero. Eight waves were used in the Bloch expansion. The Bragg conditions follow the dashed curves. As the modulation depth is increased, the range of strong reflection broadens to fill the shaded regions where the density of states is zero – photons are forbidden to exist

are “evanescent”. Precisely the same is true of electrons whose energies lie within the electronic band gap.

In the terminology of band theory, the density of states is zero within the PBG – the photonic states are virtual. Since virtual optical modes cannot propagate, they may be viewed as localised states. For frequencies within the PBG, photons incident from outside the material will be perfectly reflected, just as if it were an ideal metallic object.

Limited photon localisation of this kind is well known in multi-layer dielectric mirrors for a range of incident angles around the Bragg condition. But what would happen if a photon, with an energy lying within the PBG, was created inside a volume of PBG material? This could arise if the material were doped with a fluorescent species. The photons emitted by spontaneous electron–hole recombination at the electronic transitions will be unable to travel away – being reflected back and re-absorbed instead. Spontaneous emission is thus inhibited (figure 1), which has profound implications for the performance of solid-state lasers as first pointed out by Yablonoitch in 1987. By blocking spontaneous emission into undesired optical modes, a PBG lasing structure would be able to improve a laser’s quantum efficiency.

The interest in rare-earth doped glass lasers, in particular frequency up-conversion lasers where the pump frequency is less than the lasing frequency, suggests other applications. The rare-earth ions in these lasers have a multitude

of outer-shell transitions, and the aim of much research is to identify “ladders” of suitable levels up which electrons can “climb”, pumped by cheap infrared diode lasers. Once a suitable level is reached, short wavelength lasing may be achieved. Many possible “ladders” to up-conversion are ruled out because an efficient radiative transition, often in the infrared, exists at some intermediate level. Introducing a PBG to prevent radiative recombination at this level would allow efficient up-conversion lasing, perhaps in the blue or ultraviolet. So far, a great deal of effort in solid-state laser research has been directed towards controlling the environment, and hence the behaviour, of the electronic lasing transitions. Photonic band gap materials provide an extra dimension of control in which the quantum photodynamics are manipulated so as to make the fullest and most efficient use of quantum electrodynamic transitions.

## Bloch expansion

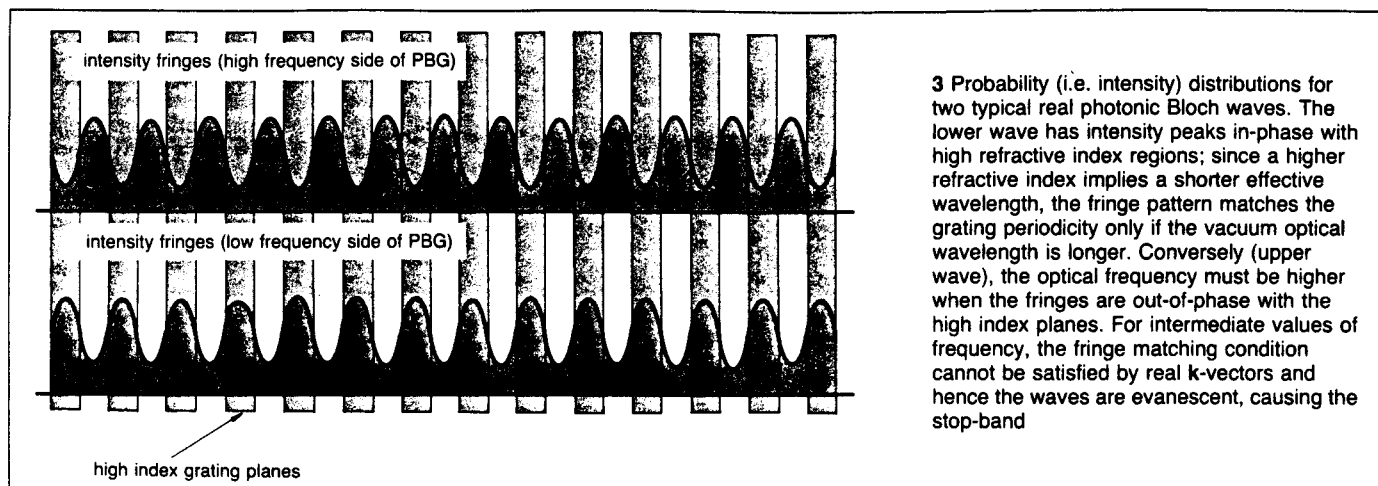
Every study of waves in periodic structures makes use of a single physical principle, enshrined in a theorem proposed by Achille Floquet in 1884, which states that normal modes in periodic structures can be expressed as the superposition of a set of plane waves whose wavevectors are related by momentum conservation:  $\mathbf{k}_n = \mathbf{k}_0 + n\mathbf{K}$ , where  $\mathbf{k}_0$  is an arbitrary initial wavevector,  $\mathbf{k}_n$  the wavevector of the  $n$ th wave,  $\Lambda = 2\pi/|\mathbf{K}|$  is the grating pitch, and  $\mathbf{K}$  is the grating vector. This theorem was later extended to multi-dimensional periodic structures by Bloch in his treatment of electrons in crystals and is referred to as the Bloch expansion.

What is the physical meaning of this theorem? It can be viewed as a direct consequence of the universal ability of waves to image objects. A disturbance such as an electromagnetic wave propagating through a periodic medium must to some degree mimic the periodicity. Since the only way waves can image a static periodic pattern is via two- or multi-beam interference (yielding standing-wave patterns of stationary optical fringes), other waves must therefore appear, travelling in directions such that the resulting pattern of interference fringes matches the periodicity. This is another way of interpreting the equation above; since every wavevector can be turned into any other by adding or subtracting an integral multiple of  $\mathbf{K}$ , and the spacing of the interference fringes between the  $n$ th and the  $m$ th waves is  $2\pi/|\mathbf{k}_n - \mathbf{k}_m|$ , the set of waves with wavevectors given in the equation above will clearly image the grating.

Therefore, the optical modes or Bloch waves of an extended periodic medium consist of stable superpositions of many such waves. A range of results follows from this picture. The simplest is the Bragg condition itself – when the fringe pattern matches the periodicity (or a multiple of it), Bragg diffraction occurs. Perhaps the most profound is that the photonic Bloch waves, possessing stationary optical fringes, can interact much more effectively with the static periodic medium than normal photons can in uniform dielectrics. This permits strong interactions between electrons and photons if the electronic band gap energy matches the photon energy at the top of the PBG – where incidentally the Bloch wave group velocity tends to zero.

## 1-D gratings

How do photonic states in a simple one-dimensional refractive index grating behave as its modulation depth is increased? Stop-bands open up around the Bragg conditions in  $k$ -space (the shaded regions in figure 2). Further, the fringe visibility (the peak-to-peak amplitude divided by



**3** Probability (i.e. intensity) distributions for two typical real photonic Bloch waves. The lower wave has intensity peaks in-phase with high refractive index regions; since a higher refractive index implies a shorter effective wavelength, the fringe pattern matches the grating periodicity only if the vacuum optical wavelength is longer. Conversely (upper wave), the optical frequency must be higher when the fringes are out-of-phase with the high index planes. For intermediate values of frequency, the fringe matching condition cannot be satisfied by real  $k$ -vectors and hence the waves are evanescent, causing the stop-band

twice the mean amplitude) inside the stop-band is 1 (thus preventing power flow across the grating planes) and the fringe pattern is neither exactly in-phase nor out-of-phase with the grating. On the stop-band branches, however, the fringe patterns of the travelling photonic modes are exactly in-phase or out-of-phase, with visibilities less than 1 (figure 3). As explained above, these intensity patterns determine the photon probability distributions, so that in-phase travelling modes experience a higher refractive index on average than out-of-phase ones. A higher refractive index implies a shorter effective wavelength; hence, to satisfy the condition that the fringe pattern should match the periodicity, the vacuum optical wavelength must be longer when the fringes are in-phase with the high index grating planes. Conversely, the optical frequency must be higher when the fringes are out-of-phase with the high index planes – as confirmed in figure 1. For intermediate values of frequency, the fringe matching condition cannot be satisfied by real  $k$ -vectors and hence the waves are evanescent, causing the stop-band.

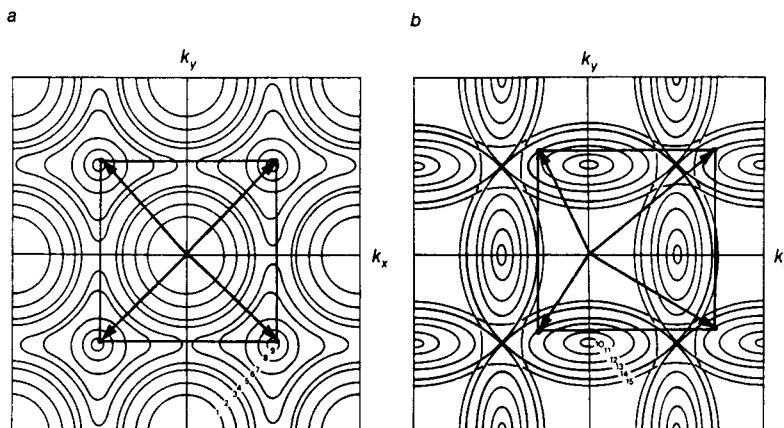
As the modulation depth  $M$  of the relative dielectric constant ( $M = \epsilon_m/\epsilon_0$  where  $\epsilon_m$  is the ripple magnitude and  $\epsilon_0$  the average value) increases (figure 2) the Bragg condition, normally considered inviolate, becomes uncertain, i.e. the range of total reflection broadens as the stop-bands grow in width. Consider a grating with a small number,  $N$ , of periods. For  $M \ll 1$ , the frequency bandwidth is given roughly by  $\nu_0/N$  where  $\nu_0$  is the optical frequency at the Bragg condition. As  $M$  increases, the reflectivity rises without any change in bandwidth, until the reflection per period is so large that practically 100% of the

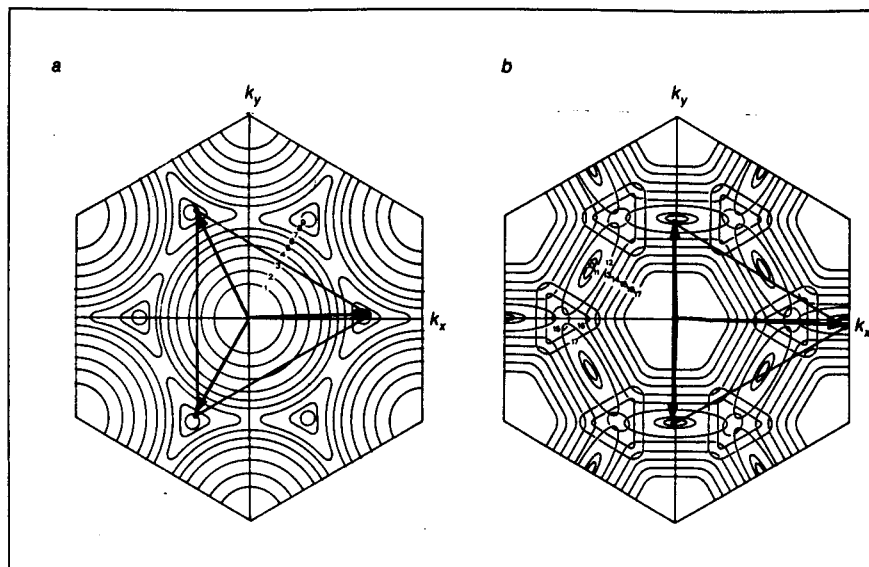
incident beam is reflected before all the grating periods have been used. In the limit of very strong modulation, 100% of the light will be reflected at only one grating period, which then behaves like a mirror with a commensurately huge bandwidth. Even before this limit is reached, the bandwidth can be a substantial fraction of the optical frequency. A trade-off exists between the angular and frequency bandwidths of high reflectivity. Perfect reflection will be obtained for a single-frequency wave over a finite angular bandwidth and for a perfectly collimated beam over a finite range of frequencies. The common multi-layer dielectric mirror behaves just like this. Within a certain angular and wavelength range there are no photonic states inside the multi-layer stack itself; the mirror reflects perfectly (assuming it is thick enough to preclude photon tunnelling through to the substrate).

## 2-D and 3-D PBGs

The conclusion from above is that if one seeks complete reflection over a large spread of solid angles and over as wide a range of frequencies as possible, the modulation depth must be large. What about structures with three-dimensional photonic band gaps that are complete over  $4\pi$  steradians? A singly periodic structure clearly cannot forbid propagation along its grating planes. If, however, other sets of grating planes are added and an appropriate three-dimensional crystal structure built up, with a large enough  $M$ , a genuine PBG might appear. Examples (calculated from a simple two-dimensional scalar model) are given in figures 4 and 5. (See Ho *et al.*, Leung and Liu, Zhang and

**4** Approximate 2-D wavevector diagram of a square lattice (see 6), including four waves in the Floquet expansion for the fields, plotted around the origin of wavevector space with optical frequency as a parameter. Modulation depth is  $M = 0.5$ , and the band gap width is  $\sim 0.05$  of the Bragg frequency. As the frequency rises the labels increase from 1 to 15; (a) initially (1–9) the circles grow, coalesce and four increasingly small circles (the loci of real  $k$ -vectors) appear at  $45^\circ$  to the axes, disappearing at the PBG edge when  $\nu/\nu_0 = 0.78$ . As the frequency falls further (b), a point is reached where four small ellipses appear on the axes, growing in size; this is the upper PBG edge and occurs at  $\nu/\nu_0 = 0.83$ . If  $M < 0.4$ , the band gap ceases to be complete. These patterns replicate over all  $k$ -space. The four red wavevectors in (a) and (b) are those of the photonic Bloch waves whose spatial intensity patterns are shown in 6





5 Same as 4 but for a hexagonal sinusoidal lattice with  $M = 0.3$ , including three harmonics in the Bloch expansion. As the frequency rises the labels increase from 1 to 17; (a) initially (1-9) the circles grow, coalesce and six increasingly small "triangles" of real  $k$ -vectors appear spaced  $60^\circ$  apart eventually disappearing at the PBG edge where  $\nu/\nu_0 = 0.87$ ;  $k$ -space is then empty of real states; (b) as the frequency rises further, six small ellipses appear shifted  $30^\circ$  relative to the positions of the triangles; this is the upper PBG edge and occurs at  $\nu/\nu_0 = 0.94$ . Thus the PBG width is  $\sim 0.07$  of the Bragg frequency. A hexagonal geometry produces a PBG more easily than a cubic. The three red wavevectors in (a) and (b) are those of photonic Bloch waves whose spatial intensity patterns are shown in 7

Satpathy, and Yablonovitch and Gmitter in Further reading for rigorous treatments of the 3-D case.) The additional periodicities cause new stop-bands to show up in  $k$ -space, their position depending on the structure. As the modulation depth increases, these extra stop-bands begin to grow in size, crushing the travelling modes (with real  $k$ -vectors) out of existence until the whole of real  $k$ -space is empty within the PBG frequency range.

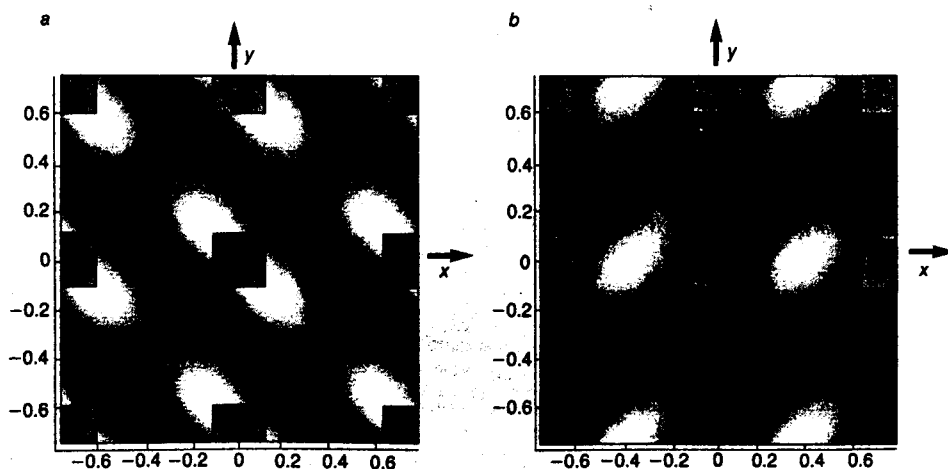
At certain points of high symmetry (for example the W symmetry point in face-centred-cubic lattices), the PBG can (if the "atomic" shape is also highly symmetrical) be suppressed regardless of the modulation strength. This raised a very important issue which could only be clarified with the help of band theorists. Yablonovitch's team originally reported that their structure, consisting of spherical air cavities in a material of refractive index 3.6, showed an experimental band gap at microwave frequencies. The theorists demonstrated that this was not possible, due to the collapse of the PBG at points of high symmetry. It was at first suggested that imperfections in fabrication had disturbed the delicate geometrical symmetry at the W-point, although Yablonovitch later states that his measurement technique had insufficiently high resolution. Working with the theorists, he realised that the attainment of a PBG depends crucially on the microscopic shape of the unit cells. Using a modified drilling technique in which the hole size was increased so that adjacent holes broke into each other,

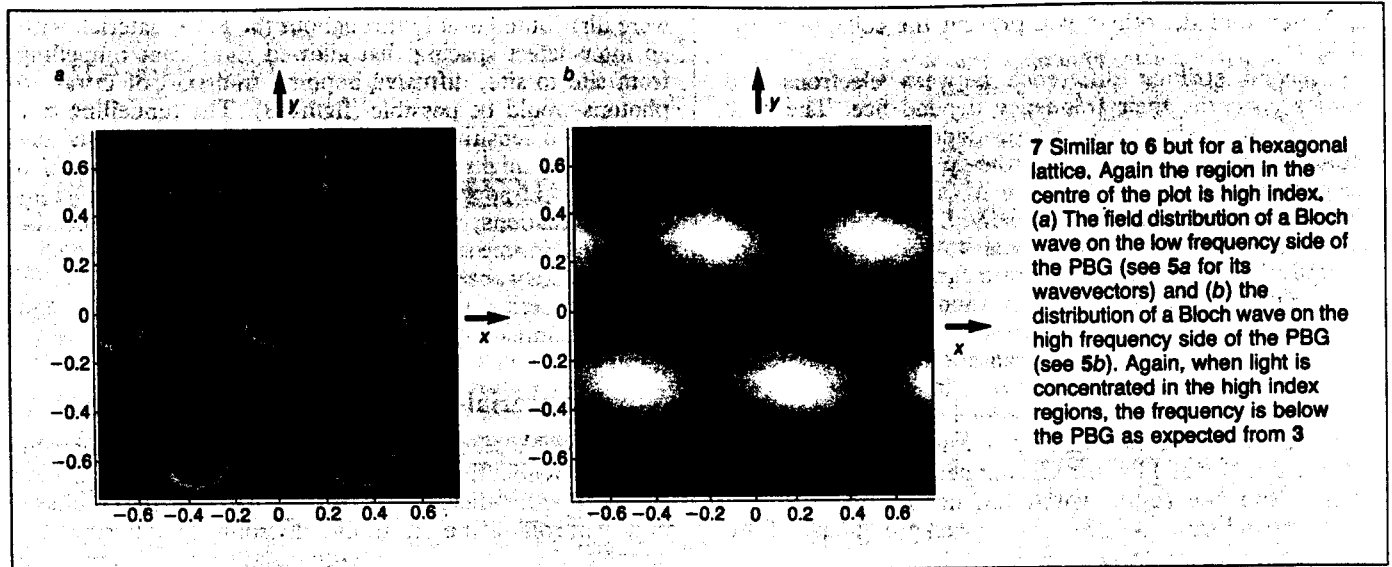
unit cells of non-spherical symmetry were produced and a genuine band gap observed, a result which now agrees with theory.

### Super-resolution

Microscopic field intensity patterns for four selected 2-D photonic states are given in figures 6 and 7. Although these pictures illustrate how photons get redistributed into regions of low and high refractive index, leading to band gap formation, the simplicity of the model (it includes very few waves in Bloch's expansion) means that important harmonics of the basic spatial periodicity are missing. These higher harmonics play an important role in the PBG's sensitivity to unit cell shape, resolving an interesting question: since the wavelength is of the same order as the unit cell dimension, how is it that fine details in the cell geometry should matter since they are below the Rayleigh resolution limit, which states that the smallest feature that light can resolve is half the wavelength? The answer lies in the Bloch expansion. The higher order wavevectors in this are many times larger than the average  $k$ -vector in the medium. Since their effective wavelength, given by  $2\pi/|k_n|$ , is therefore much shorter than on average in the material, and since the amplitudes of the higher order plane waves in the Bloch expansion become large at high modulation depths, a unique kind of super-resolution occurs. A

6 Field intensity distributions in the square case close to the PBG edge, (a) on the low frequency side of the PBG (see 4a for wavevectors) and (b) on the high frequency side of the PBG (4b). The region at the origin (in the centre of the plot) is high index. When the light is concentrated in these high index regions, the frequency is below the PBG as expected from 3





corollary of this is that the exact profile of the periodicity can then become central to whether a PBG appears; as shown by Yablonovitch, asymmetries in the microscopic shape of the "atoms" in the PBG material can upset the symmetry balance and prevent PBG suppression.

### Electrons versus photons

So far we have blithely been assuming that electrons and photons can be treated as interchangeable. They clearly are not. Electrons have charge and rest mass while photons have neither. Electrons obey Fermi-Dirac statistics whereas photons obey Bose-Einstein statistics, i.e. an unlimited number of photons can be packed into one optical Bloch state, whereas the Pauli exclusion principle permits only two electrons per electronic Bloch state. The governing time-independent differential equations in each case are:

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V(\mathbf{r})\psi = E_c \psi \quad (1)$$

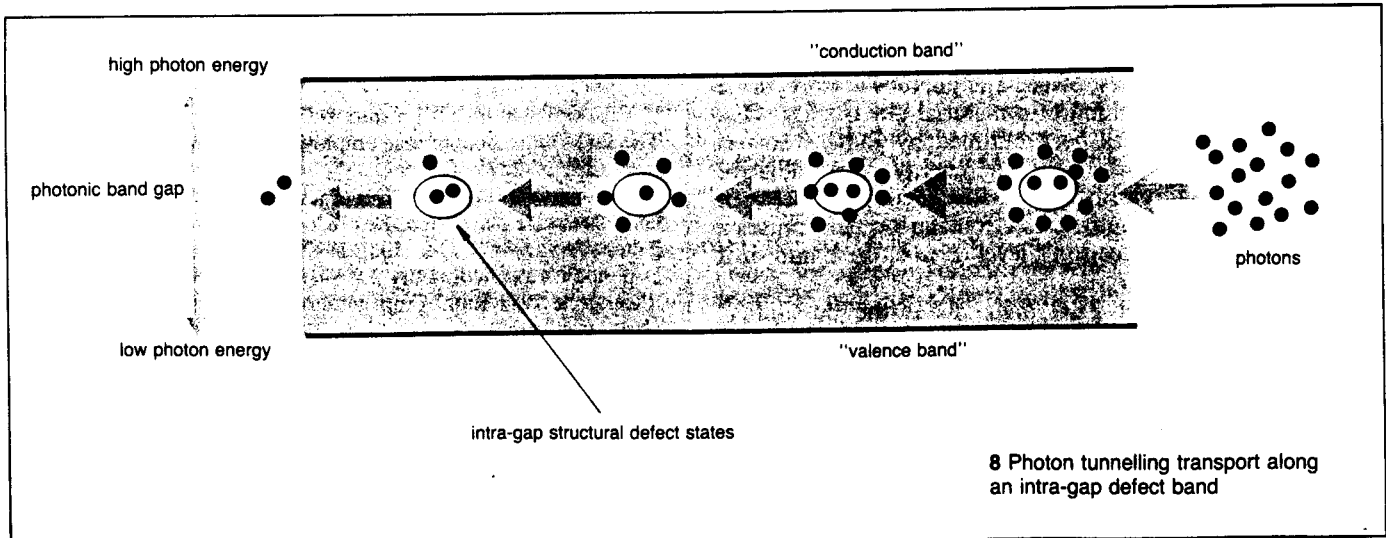
for electrons and

$$-\nabla^2 \mathbf{E} - \nabla(\mathbf{E} \cdot \nabla \ln\{1 + M(\mathbf{r})\}) - k^2 M(\mathbf{r})\mathbf{E} = k^2 \mathbf{E} \quad (2)$$

for photons, where  $k^2 = (\omega/c)^2 \epsilon_r$  scales as the frequency squared and  $\epsilon_r$  is the mean relative dielectric constant.

$V(\mathbf{r})$  and  $M(\mathbf{r})$  describe, respectively, the periodic spatial variation of the electrostatic potential (for electrons) and  $\epsilon_r/\epsilon_0$  (for photons).  $\psi$  is the electron wavefunction,  $\mathbf{E}$  is the electric field,  $E_c$  is the total electron energy and  $m$  the electron rest mass.

Now Schrödinger's equation is scalar, whereas Maxwell's is vector in nature and contains an extra term when the electric field points parallel to the direction of spatial variation of  $M(\mathbf{r})$  (the middle term on the left hand side of (2)). When the electric fields of all the waves represented by the Bloch expansion are parallel to each other and to the reflecting grating planes, strong interference fringes can always form and significant stop-bands appear. If, however, the electric fields point out of a reflecting "atomic" plane, two things can happen that can weaken or prevent the appearance of a PBG, particularly for the large refractive index modulation depths. Firstly, at Brewster's angle (when the electric field of the reflected wave is perpendicular to the electric field of the transmitted wave) the reflected amplitude is zero and the PBG disappears; secondly, only weak (if any) stop-bands can form when the major pair of partial waves in the Bloch expansion are orthogonally polarised. Both problems can be side-stepped by ensuring that a sufficient number of strong non-coplanar reflecting planes exists in the crystal structure so that the partial band gaps created by each set coalesce to cover all  $4\pi$  steradians. If one stop-band shrinks to zero in a particular direction,



the presence of the others will prevent the collapse of the PBG.

A second striking difference between electrons and photons concerns their frequency dependence. The total energy  $E_e$  of an electron is independent of the potential  $V$  it finds itself in. As  $E_e$  falls (i.e. the de Broglie wavelength rises), the kinetic energy  $T = E_e - V$  can become negative, at which point the electron is localised. In contrast, as the photon energy falls (i.e. the optical wavelength increases), the equivalent terms in the electromagnetic wave equation scale together, meaning that localisation can never occur in a homogeneous dielectric. In a perfect metal, on the other hand,  $k^2$  is negative, yielding localisation at all frequencies (so long as  $\epsilon_0$  remains negative). It is interesting to speculate on the behaviour of photons in the converse of a dielectric crystal – a metallic crystal. Such a structure could be formed in a metal by introducing periodically spaced air cavities, and the result would be the opening up of a photonic band window (PBW) in the background gap of the metal at appropriate regions of the spectrum – the opposite of the photonic band gap that appears in the background window for a dielectric. In this PBW, certain photonic states, their periodic field intensities peaking in the interstices between the metallic sites, would manage to sneak through without attenuation.

A third major difference, not evident from the equations, involves Coulomb forces between electrons and the lattice potential. In the solid state, composite particles such as excitons, polaritons, magnons and plasmons arise through these interactions. They are not expected to have any photonic analogue in PBG structures.

## Novel effects

There are, however, a number of novel interactions unique to PBG structures which have no direct analogue in electronic band theory. Sajeev John has shown that intra-gap photon-atom bound states appear if the PBG material is doped with a fluorescent species whose electronic transition energy lies within the PBG. He goes on to propose mid-gap impurity bands where photons can hop from site to site and thus enjoy limited mobility at an otherwise forbidden energy level. These bands have some properties in common with electron-impurity-bands in semiconductors.

As the edge of the PBG is approached from below or above, the group velocity and momentum of the photonic Bloch waves both tend to zero, i.e. the photon becomes increasingly localised (see figure 1). Strong resonant interactions between the stationary lattice and the localised photons can then occur – in a sense, this is why the stop-band opens up in the first place. The photons acquire, close to a band edge, something of a material-like quality. One consequence of this has been outlined by John, who has shown that if the electronic gap energy of a radiative transition is close to a PBG edge, strong coupling between bound electron and photonic electromagnetic field causes a novel splitting of the electronic level, akin to the Lamb shift in quantum field theory.

A related aspect of PBG materials is the possibility, suggested by Yablonovitch and Gmitter (in collaboration with Meade and co-workers at MIT), of intra-gap photonic, rather than electronic, donor/acceptor states. These may be created by introducing structural defects inside which the local intra-gap  $k$ -vector is real – creating a localised real photonic state. They differ from the photon-atom bound states of John in that they are bosonic states, permitting an unlimited number of photons to be trapped. If such traps

were distributed evenly throughout the PBG material, with an inter-defect spacing that allowed significant tunnelling from site to site, diffusive hopping transport of intra-gap photons would be possible (figure 8). The tunnelling rate will depend sensitively on the spacing, which suggests that these media might exhibit large stress-optical effects. Also for a photon trapped in an intra-gap defect state, zero-point field fluctuations, which give rise to noise and cannot be eliminated in free space or in isotropic homogeneous media, are completely absent. The drawback is that this cannot be verified experimentally except by breaking the crystal and thereby eliminating the effect!

## Novel materials, radical properties

PBG materials seem set to revolutionise optoelectronics by making possible the design and creation of a range of new materials with radical properties. By switching the emphasis from controlling the electronic environment (altering, for example, the fluorescence life-time and phonon energies) to engineering a new photonic environment (altering the energy-momentum relationship for photons via a PBG), a world of possibilities, just beginning to be explored, opens up. Work on PBG materials may eventually result in semiconductor diode lasers with improved quantum efficiencies, new schemes for frequency up-conversion lasers in rare-earth doped glasses and crystals, materials with photonically resonant or anti-resonant optical nonlinearities, and novel photon-electron particles. So far, however, PBGs have been observed only at microwave frequencies in FCC structures drilled into commercial high index dielectric. The race is on to demonstrate an optical PBG, perhaps using the Bellcore scheme based on reactive ion beam etching of GaAs. The moment when PBG structures are used – in anger – to control the behaviour of optoelectronic lasing and nonlinear materials is rapidly approaching. And, perhaps even more exciting, the field is still certain to turn up further discoveries.

## Further reading

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