

Photonic band structure in periodic dielectric structures

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Abstract

Recent experiments have found the existence of "photon bands" in periodic dielectric structures analogous to the electron bands in the solid. One-dimensional crystals are considered here.

1 Introduction

It is well known that the electron forms energy bands in periodic crystals. the deviation from the free-particle dispersion may be thought to be caused by the coherent interference of scattering of electrons from individual atoms. This leads to the formation of gaps and other characteristic aspects in the electron band structure. Analogously, any particle would coherently scatter and form energy bands in a medium that provides a periodic scattering potential with a length scale comparable to the wavelength of the particle. Specifically this should be true for the propagation of classical electromagnetic (EM) waves in periodic dielectric structures.

2 Electromagnetism in Mixed Dielectric Media

All of macroscopic electromagnetism, including the propagation of light in a photonic crystal, is governed by the four macroscopic Maxwell equations. In cgs units, they are,

$$\nabla \cdot B = 0 \tag{1}$$

$$\nabla \times E + \frac{1}{c} \frac{\partial B}{\partial t} = 0 \tag{2}$$

$$\nabla \cdot D = 4\pi\rho \tag{3}$$

$$\nabla \times H - \frac{1}{c} \frac{\partial D}{\partial t} = \frac{4\pi}{c} J \tag{4}$$

where (respectively) E and H are the macroscopic electric and magnetic fields, D and B are the displacement and magnetic induction fields, and ρ and J are the free charges and currents.

We will restrict ourselves to propagation within a mixed dielectric medium, a composite regions of homogeneous dielectric material, with no free charges and currents. With this type of medium in mind, in which light propagates but there are no sources of light, we can set $\rho = J = 0$. We have $D(r) = \epsilon(r)E(r)$. However, for most dielectric materials of interest, the magnetic permeability is very close to unity and we may set $B = H$.

With all of these assumptions in place, the Maxwell equations(1-4) become

$$\nabla \cdot H(r, t) = 0 \tag{5}$$

$$\nabla \times E(r, t) + \frac{1}{c} \frac{\partial H(r, t)}{\partial t} = 0 \tag{6}$$

$$\nabla \cdot \epsilon E(r, t) = 0 \tag{7}$$

$$\nabla \times H(r, t) - \frac{\epsilon(r)}{c} \frac{\partial E(r, t)}{\partial t} = 0. \tag{8}$$

We emply the familier trick of using a complex-valued field for mathematical convenience, remembering to take the real part to obtain the physical fields. This allowa us to write a harmonic mode as a certain field pattern times a complex exponential:

$$H(r, t) = H(r)e^{i\omega t} \tag{9}$$

$$E(r, t) = E(r)e^{i\omega t} \tag{10}$$

To find equations for mode profiles of a given frequency, we insert the above equations into (5-8). The two divergence equations give the simple conditions:

$$\nabla \cdot H(r) = \nabla \cdot D(r) = 0 \tag{11}$$

These equations have a simple physical interpretation. There are no point sources or sinks of displacement and magnetic fields in the medium. Alternatively, the field configurations are built up of electromagnetic waves that are transverse. We can focus on the other two Maxwell equations as long as we are always careful to enforce this transversality requirement.

The two curl equations relate $E(r)$ to $H(r)$:

$$\nabla \times E(r) + \frac{i\omega}{c}H(r) = 0 \quad (12)$$

$$\nabla \times H(r) - \frac{i\omega}{c}\epsilon(r)E(r) = 0 \quad (13)$$

We can decouple these equations in the following way. Divide the equation (13) by $\epsilon(r)$, and then take the curl. Then using equation (12) we can eliminate $E(r)$. The result is an equation entirely in $H(r)$:

$$\nabla \times \left(\frac{1}{\epsilon(r)} \nabla \times H(r) \right) = \left(\frac{\omega}{c} \right)^2 H(r) \quad (14)$$

This is the master equation. In addition to the divergence equation (11), it completely determines $H(r)$. The strategy will be the following: for a given photonic crystal $\epsilon(r)$, solve the master equation to find the modes $H(r)$ for a given frequency, subject to the transversality requirement. Then using equation (13), $E(r)$ can be recovered:

$$E(r) = \left(\frac{-ic}{\omega\epsilon(r)} \right) \nabla \times H(r) \quad (15)$$

By expanding the field pattern into a set of plane waves, it'll convert the differential equation (14) into a system of linear equations that can be solved on a computer. Doing so allows us to determine which are the allowed mode frequencies for a given crystal, and which wave vectors k are associated with those modes.

3 Physical Origin of Photonic Band Gaps

We know every crystal has two lattices associated with it: the crystal lattice and the reciprocal lattice. Two lattices are related by the definitions: $A = 2\pi \frac{b \times c}{a \cdot b \times c}$; $B = 2\pi \frac{c \times a}{a \cdot b \times c}$; $C = 2\pi \frac{a \times b}{a \cdot b \times c}$ where, a, b, c are primitive vectors of the crystal lattice, and A, B, C are primitive vectors of the reciprocal lattice.

Any vector G of the form

$$G = hA + kB + lC \quad (16)$$

is called a reciprocal lattice vector, (h, k, l =integers), and any vector T

$$T = ua + vb + wc \quad (17)$$

is called crystal translation, (u, v, w =integers).

In order to know what happens to electromagnetic wave inside the crystal, let's consider a dielectric configuration with discrete translational symmetry.

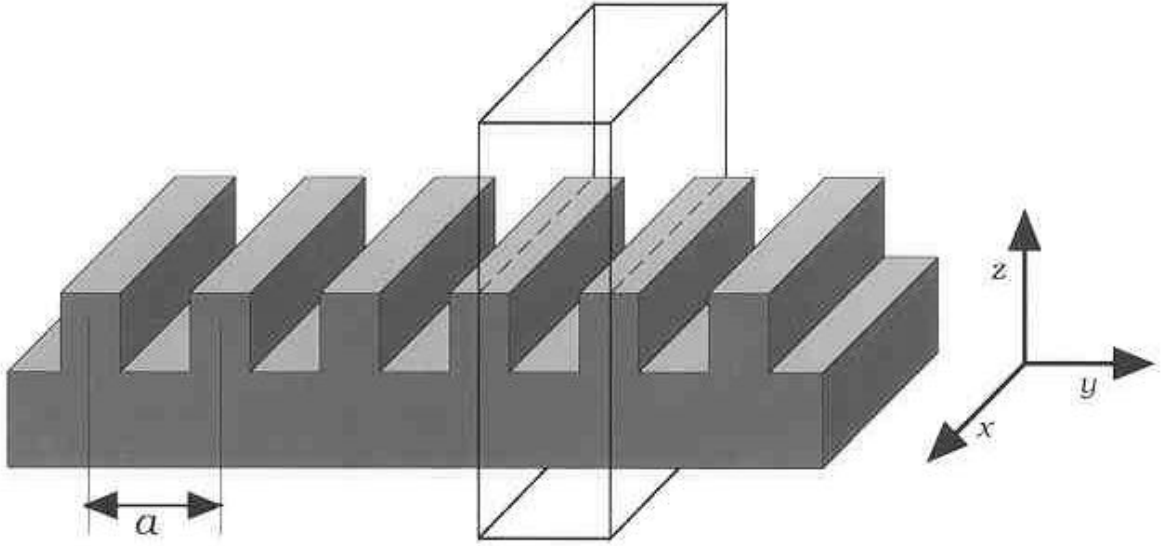
Figure 1: A dielectric configuration with discrete translational symmetry.

For magnetic field, propagating in the x-y plane, this system has continuous translational symmetry in the x-direction. And discrete translational symmetry in the y-direction. The basic step length is the lattice constant a , which is also the primitive lattice vector.

A system with continuous translational symmetry is unchanged by a translation through a displacement d . For each d , we can define a translation operator T_d . A system with continuous symmetry in the x-direction is invariant under all of the T_d 's for that direction. A mode with the functional form $e^{ik_x x}$ is an eigenfunction of any translation operator in the x-direction:

$$T_d e^{ik_x x} = e^{ik_x(x+d)} = (e^{ik_x d}) e^{ik_x x} \quad (18)$$

The corresponding eigenvalue is $e^{ik_x d}$. The dielectric unit that we consider to be repeated over and over, highlighted in the figure with a box, is know as the unit cell. In this example, the unit cell is an xz-slab of dielectric material with width a in the y-direction.



The translational operators for lattice vectors $R = la$ (l =integer) in the y -direction is T_R , whose eigenfunction is plane wave:

$$T_R e^{ik_y y} = e^{ik_y(y+la)} = (e^{ik_y la}) e^{ik_y y} \quad (19)$$

We can begin to classify the modes by specifying k_x and k_y . However, not all values of k_y yield different eigenvalues. Consider two modes, one with wave vector k_y and the other with wave vector $k_y + \frac{2\pi}{a}$. A quick insertion into (19) shows that they have the same T_R -eigenvalues. In fact, all of the modes with the wave vectors of the form $k_y + m(\frac{2\pi}{a})$, where m is an integer, form a degenerate set; they all have the same T_R -eigenvalue of $e^{i(k_y la)}$. Augmenting k_y by an integral multiple of $b = \frac{2\pi}{a}$ leaves the state unchanged. Here b is the primitive reciprocal lattice vector.

Since any linear combination of these degenerate eigenfunctions is itself an eigenfunction with the same eigenvalue, we can take linear combinations of our original modes to put them in the form

$$H_{k_x, k_y}(r) = e^{ik_x x} \sum_m c_{k_y, m}(z) e^{i(k_y + mb)y} = e^{ik_x x} \cdot e^{ik_y y} \sum_m c_{k_y, m}(z) e^{imby} = e^{ik_x x} \cdot e^{ik_y y} u_{k_y}(y, z) \quad (20)$$

where the c 's are expansion coefficients to be determined by explicit solution, and $u(y, z)$ is a periodic function in y . By inspection of eqn(20), we can verify that $u(y + la, z) = u(y, z)$.

The discrete periodicity in the y -direction leads to a y -dependence for H that is simply the product of a plane wave with a y -periodic function. We can think of it as a plane wave, as it would be in the free space, but modulated by a periodic function because of the periodic lattice:

$$H(\dots y \dots) \propto e^{ik_y y} u_{k_y}(y, \dots). \quad (21)$$

This result is known as Bloch's theorem. The form of (21) is known as a Bloch state (as in Kittel).

One key fact about Bloch state is that the Bloch state with wave vector k_y and the Bloch state with wave vector $k_y + mb$ are identical. The k_y 's that differ by an integral multiples of $b = \frac{2\pi}{a}$ are not different from a physical point of view. Thus the mode frequencies must also be periodic in k_y : $\omega(k_y) = \omega(k_y + mb)$. In fact, we need only consider k_y to exist in the range $-\frac{\pi}{a} < k_y \leq \frac{\pi}{a}$. This region of important, nonredundant values of k_y is called the Brillouin zone. In three dimension the magnetic field inside the crystal is then:

$$H_k(r) = e^{i(k \cdot r)} u_k(r) \quad (22)$$

where $u_k(r)$ is a periodic function on the lattice: $u_k(r) = u_k(r + R)$ for all lattice vectors R .

The master equation (14) now becomes,

$$\nabla \times \left(\frac{1}{\epsilon(r)} \nabla \times H_k \right) = \left(\frac{\omega(k)}{c} \right)^2 H_k \quad (23)$$

where H_k is given by equation (22).

The mode profiles are determined by the above eigenvalue equation of (23), subject to the condition

$$u_k(r) = u_k(r + R) \quad (24)$$

Because of this periodic boundary condition, we can regard the eigenvalue problem as being restricted to a single unit cell of the photonic crystal. As we remember from electron-in-a-box problems in quantum mechanics, restricting an eigenvalue problem to a finite volume leads to a discrete spectrum of eigenvalues. We can expect to find, for each value of k , an infinite set of modes with discretely spaced frequencies, which we can label with the band index n .

This way we arrive at the description of the modes of a photonic crystal. They are a family of continuous functions, $\omega_n(k)$, indexed in order of increasing frequency by the band number. The information contained in these functions is called the band structure of the photonic crystal.

4 A One-Dimensional Photonic Crystal

The simplest possible photonic crystal, shown in figure: 2, consists of alternating layers of material with different dielectric constants.

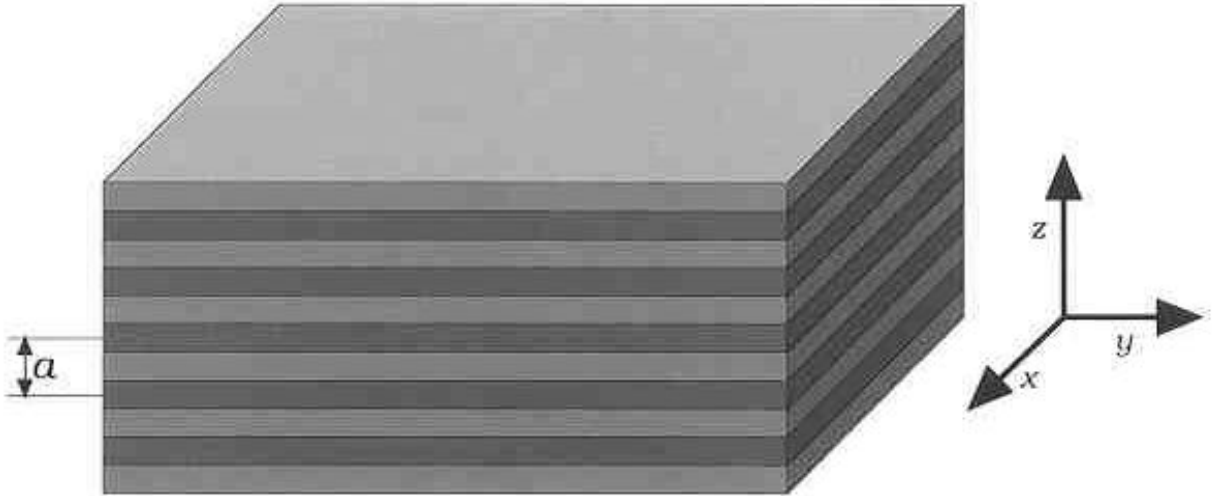


Figure 2: A one dimensional photonic crystal.

Using the prescription of previous section, if primitive lattice vector is a , along z -axis, then the primitive reciprocal lattice vector is $\frac{2\pi}{a}$, in z -axis and the Brillouin zone is $-\frac{\pi}{a} < k_z \leq \frac{\pi}{a}$. Let's consider the light happens to propagate in the z -direction, crossing the sheets of dielectric at normal incidence.

In figure: 3, the plot $\omega_n(k)$ for three different multilayer films is shown (as in Joannopoulos). The leftmost plot is for a uniform dielectric medium, to which an artificial periodicity of a is introduced. The frequency spectrum is just the light line given by

$$\omega(k) = \frac{ck}{\sqrt{\epsilon}} \quad (25)$$

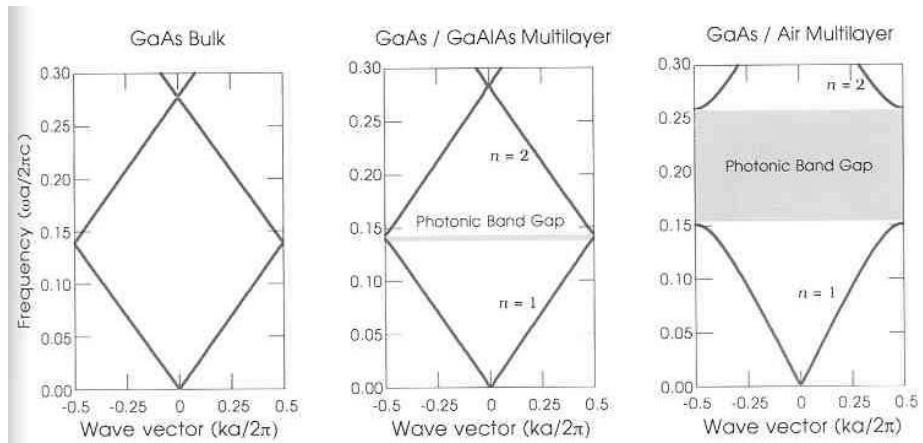


Figure 2 The photonic band structures for on-axis propagation, shown for three different multilayer films, all of which have layers of width $0.5a$. *Left*: each layer has the same dielectric constant $\epsilon = 13$. *Center*: layers alternate between $\epsilon = 13$ and $\epsilon = 12$. *Right*: layers alternate between $\epsilon = 13$ and $\epsilon = 1$.

Because k repeats itself outside the Brillouin zone, the lines fold back into the zone when they reach the edges. The center plot looks like the light-lines with one important difference. There is a gap in frequency between the upper and lower branches of the lines- a frequency gap in which no mode, regardless of k , can exist in the crystal. We call such a gap, a photonic band gap. As we can see on the right, as the dielectric contrast is increased, the gap widens considerably.

The gap between bands $n = 1$ and $n = 2$ occurs at the edge of Brillouin zone, at $k = \frac{\pi}{a}$. For $k = \frac{\pi}{a}$, the modes are standing waves with a wavelength of $2a$, twice the crystal's lattice constant. From the study of electromagnetic variational theorem (as in Joannopoulos), it's found that the low frequency modes concentrate their energy in the high- ϵ regions and the high frequency modes concentrate their energy in the low- ϵ regions. The mode just under the gap has its power concentrated in $\epsilon = 13$ regions, giving it a lower frequency. Meanwhile, the mode just above the gap has most of its power in lower $\epsilon = 12$ regions, so its frequency is raised a bit. This way it creates a frequency gap.

5 Conclusion

The field of photonic crystals is a combination of solid state physics and electromagnetism. Crystal structures are citizens of solid-state physics, but in photonic crystals the electrons are replaced by electromagnetic waves. We have discussed only one-dimensional photonic crystals which offers band gap in one-direction (z -axis). Electromagnetic waves entering from x - and y -directions will not see any band gap. Three-dimensional photonic crystals, which are periodic along 3-axes can be formed. Such a system can have a complete band gap, so that no propagating states would be allowed in any direction in the crystal.

References

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