

PHOTONIC BAND-GAP STRUCTURES

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ABSTRACT. In this short talk I will be introducing the concept of Photonic band gap and Photonic band gap structures. Later, I have introduced few applications of PBG's and tried to emphasize on few interesting analogies of these with electronic band gap structures.



1. FEW DEFINITIONS^[1]

1.1. Reciprocal Lattice. *The Reciprocal Lattice of a Bravais Lattice is the set of all vectors \vec{K} such that $e^{i\vec{K}\cdot\vec{R}} = 1$ for all lattice position vectors \vec{R} .* The Reciprocal Lattice is itself a Bravais Lattice and the reciprocal of the reciprocal lattice is the original lattice.

1.2. Brillouin Zone. The first Brillouin zone is defined to be the Wigner-Seitz primitive cell¹ of the reciprocal lattice, or it could be defined as the set of points in k space that can be reached from the origin without crossing any Bragg plane. The second Brillouin zone is the set of points that can be reached from the first zone by crossing only one Bragg plane. The $(n + 1)$ th Brillouin zone is the set of points not in the $(n - 1)$ th zone that can be reached from the n th zone by crossing $n - 1$ Bragg planes.

1.3. Dispersion Relations. *The dispersion relation is the relation between the energy of a system and its corresponding momentum.* In the study of solids, the study of the dispersion relation of electrons is of paramount importance. The periodicity of crystals mean that for a given momentum, many levels of energy are possible, and that some energies might not be available at any momentum. The collection of all possible energies and momenta is known as the band structure of a material. Properties of the band structure define whether the material is an insulator, semiconductor or conductor.

1.4. Bloch wave. A Bloch wave or Bloch state is the wavefunction of a particle (usually, an electron) placed in a periodic potential. It consists of the product of a plane wave and a periodic function (Bloch envelope) $u_{n\vec{k}}(\vec{r})$ which has the same periodicity as the potential:

$$\psi_{n\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} u_{n\vec{k}}(\vec{r}).$$

The result that the eigenfunctions can be written in this form for a periodic system is called Bloch's theorem.

1.5. Band-Gap. In solid state physics and related applied fields, the band gap, also called an energy gap or stop band, is a region where a particle is forbidden from propagating. For insulators and semiconductors, the band gap generally refers to the energy difference between the top of the valence band and the bottom of the conduction band. The mathematical interpretation is:

The probability that a state of energy, E_0 , will be occupied by an electron is derived from Fermi-Dirac statistics. An approximation, called the Boltzmann approximation, is valid if the energy of the state $E_0 \gg E_F$, where E_F is the Fermi energy. The Boltzmann approximation is given by:

$$e^{\left(\frac{-E_g}{kT}\right)}$$

where E_g is the band gap energy, k the Boltzmann's Constant and T is the Temperature.

¹The Wigner-Seitz cell around a lattice point is defined as the locus of points in space, which are closer to that lattice point than to any of the other lattice points.

1.6. Direct-gap semiconductors. The top of the valence band and the bottom of the conduction band might not occur at that same value of k . Materials with this situation, such as silicon and germanium, are known as indirect band gap materials. *Materials in which the band extrema are aligned in k , for example gallium arsenide, are called direct band gap semiconductors. Direct gap semiconductors are particularly important in optoelectronics because they are much more efficient as light emitters than indirect gap materials.*

1.7. Stop Band. A stopband is a band of frequencies, between specified limits, in which a circuit, such as a filter or telephone circuit, does not let signals through. Frequencies between the lower and upper limits are not transmitted.

The limiting frequencies are those at which the transmitted power level increases to a specified level, usually 3 dB below the maximum level, as the frequency is decreased or increased from that at which the transmitted power is a minimum. The difference between the limits is the stopband bandwidth, which is usually expressed in hertz.

1.8. Refractive-index contrast. Refractive index contrast, in an optical fiber, is a measure of the relative difference in refractive index of the core and cladding. Refractive index contrast, Δ , is given by $\Delta = (n_1^2 - n_2^2)/(2n_1^2)$, where n_1 is the maximum refractive index in the core and n_2 is the refractive index of the homogeneous cladding.

2. INTRODUCTION: DEFINING PHOTONIC BAND-GAPS^[2]

2.1. What is a PBG?. It is a frequency band in three-dimensional dielectric structures in which electromagnetic waves are forbidden irrespective of the propagation direction in space.

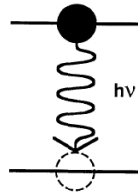
We will create an analogy between the electromagnetic wave propagation in three-dimensionally periodic dielectric structures and electron waves in natural crystals. By creating such an analogy we can use the concepts of real crystals such as Brillouin Zones, reciprocal space, etc. in the case of electromagnetic waves. It then makes sense to speak of Photonic band-gap structure and also a photonic reciprocal lattices¹. Under favourable conditions a photonic band-gap can open up a frequency band which forbids all electromagnetic waves. Inside a photonic band gap optical modes, zero-point fluctuation and spontaneous emission are absent.

2.2. Motivation. Spontaneous emission of light is one of those natural and highly useful phenomenon. To brief upon it, in solar cells, this determines the maximum available output voltage, in semiconductor lasers this is the sink for threshold current and must be surmounted to initiate lasing, this also determines the degree of photon-number-state squeezing, which is useful in the quantum optics of semiconductor lasers, etc..

For understanding the effect of PBG on spontaneous emission let's consider the Fermi's rule² of the transition shown in the figure below

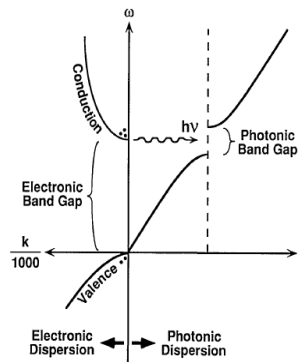
¹The Photonic Reciprocal Lattice has a Brillouin Zone approximately 1000 times smaller than the Brillouin Zone of electrons

² $\omega = \frac{2\pi}{\hbar} \rho(E_k) | \langle u_k | H' | u_m \rangle |^2$ is the Fermi's Golden Rule, where $\rho(E)$ is the density of final states per unit energy and u_k, u_m are states of the system. We can represent $|\langle u_k | H' | u_m \rangle|$ as $|V|$



In spontaneous emission the density of final states is the density of optical modes available to the photon emitted. No optical mode, no spontaneous emission. See *Appendix A* for a brief history of spontaneous emission. Inhibited spontaneous emission was first given by Kleppner from his experiments on Rydberg-atoms¹. As we have previously seen in the class, a pair of metal plates act as waveguide with a cutoff frequency for one of the two polarizations. It had been shown by other scientists that Rydberg atoms in a metallic waveguide could be prevented from undergoing spontaneous decay i.e there is absence of EM modes available below cutoff. The metallic waveguides have been replaced by *Optical Fibres* which are more efficient and hence not giving rise to virtual modes due to losses. **Hence, if such materials with positive dielectric constant which have almost pure dielectric response and low losses, can be arranged into a three-dimensionally periodic structure, there might occur a PBG**

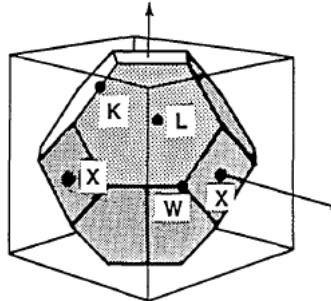
A direct-band semiconductor with a PBG has benefit which can be illustrated by the figure below



The right hand side has a plot of photonic dispersion and the left side is of electronic dispersion except that the electron wave vector is 1000 times smaller than the photon wave vectors, because atomic spacings are 1000 times smaller than optical wavelengths. The dots are holes and electrons. If an electron combines with a hole then a photon will be formed at the electron-band-edge energy. If a PBG were to exist at the electronic band edge, then the photon would have no place to go, hence spontaneous emission would be inhibited. This has deep uses in semiconductor photonic devices.

¹A Rydberg atom is an excited atom with one or more electrons that have a very high principal quantum number. These atoms have a number of peculiar properties including an exaggerated response to electric and magnetic fields, long decay periods and electron wavefunctions that approximate under some conditions classical orbits of electrons about the nuclei.

3. PHOTONIC BAND-GAP STRUCTURES

3.1. A Mathematical Formulation^[3].

The FCC Brillouin Zone

Before this full vector wave calculation of PBG in FCC dielectric media was given by K. M. Leung and Y. F. Liu the only information that was known was that the dielectric contrast should be large and the Brillouin zone should be as close to spherical as possible which is why which FCC was chosen over BCC (has sharper edges). So the experimentalists made a try at all the feasible samples (amounted to 21 in number) and of which only one exhibited a true PBG. We try to show that the plane wave method can be used to calculate photonic bands in three-dimensionally periodic dielectric media. The structure consists of a FCC lattice of spheres of refractive index n_a embedded in a homogeneous transparent host medium of refractive index n_b . Then, photonic bands were studied for various values of volume filling fraction and relative refractive index, $r = n_a/n_b$. *An interesting situation occurred when the spheres are actually air atoms which are so closely packed that they actually overlap. It was found experimentally to have a common photonic band gap throughout the entire Brillouin zone.* This method which is given works fine for many cases but suggests that a gap does not exist because of symmetry at the W point, where actually a gap does exist. An also, in W to K direction away from the W point, the gap is much feebler than is observed.

We see that the scalar waves are inadequate in predicting a band gap to open up at a refractive-index at 1.7. We find that the convergence is much more slower than in scalar case, but is good enough for obtaining accurate band structures.

We start with Maxwell's equations and eliminate magnetic field in favor of electric field \mathbf{E} to obtain for monochromatic waves of frequency ω , we have

$$\nabla_{\mathbf{x}}(\nabla_{\mathbf{x}}\mathbf{E}) + k_b^2 V \mathbf{E} = k_b^2 \mathbf{E}$$

where $V = 1 - (n/n_b)^2$, $k_b = \mu\omega n_b/c_0$ and $n = n_a$.

This equation has a vector character, owing to the spin-1 nature of the photon, and the potential is proportional to ω^2 , hence vanishing in the long-wavelength limit. In plane-wave method, one works with the Fourier coefficients

$$(1) \quad \mathbf{E}_{\mathbf{k}} = \int d\mathbf{r} f(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} \mathbf{E}(\mathbf{r})$$

$$(2) \quad V_{\mathbf{K}} = \frac{1}{\Omega} \int d\mathbf{r} e^{-i\mathbf{K}\cdot\mathbf{r}} V(\mathbf{r})$$

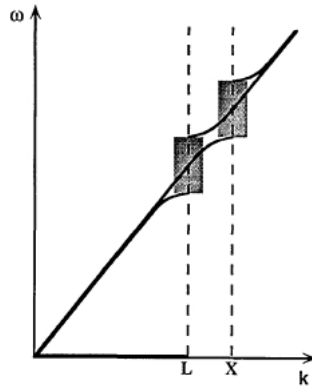
where \mathbf{K} are the reciprocal-lattice vectors. and Ω is the volume of the fcc primitive cell. Hence, the previous equation can be expressed using these. The equation that follows is a infinite-order determinantal equation that can only be solved by truncation. If N reciprocal-lattice points are included, then a $3N \times 3N$ matrix equation has to be solved. But, if we set $k_b = 0$ and work in a coordinate frame in $\mathbf{k} - \mathbf{K}$, then the resulting determinant is zero and eigen vectors corresponding to zero eigenvalue modes have $(\mathbf{k} - \mathbf{K})^x = (\mathbf{k} - \mathbf{K})^y = 0; (\mathbf{k} - \mathbf{K})^z \neq 0$. This is embedded by putting in the condition that $\nabla \cdot \mathbf{D} = 0$.

Hence, we need to solve a $2N \times 2N$ matrix now. *The photon band structure is then obtained by finding the eigenvalues k_b^2 of the resulting matrix for each value of \mathbf{k} .*

Here I have just outlined the method and have not gone into the calculation of any particular structures. For detailed analysis please refer to "Full Vector Wave Calculation of Photonic Band Structures in Face-Centred-Cubic Dielectric Media" by K. M. Keung and Y. F. Liu. Physical Review Letters, Volume 65, page 2646.

3.2. The Search for Photonic Band Gap and the Construction of a Photonic Band Gap structure. We have naturally occurring crystals for electron waves but for photons we need to artificially manufacture crystals. As I stated above, FCC seemed to be the most favourable structure. Let us consider the previous figure showing the FCC BZ with many special points marked on it. Closest to the center is the L point, oriented towards the body diagonal of the cube. Farthest away is the W point, a vertex where four plane waves are degenerate. In the cubic directions are the X points, K, middle of an edge joining two hexagonal faces and Γ , the center of the Brillouin zone(not shown in figure).

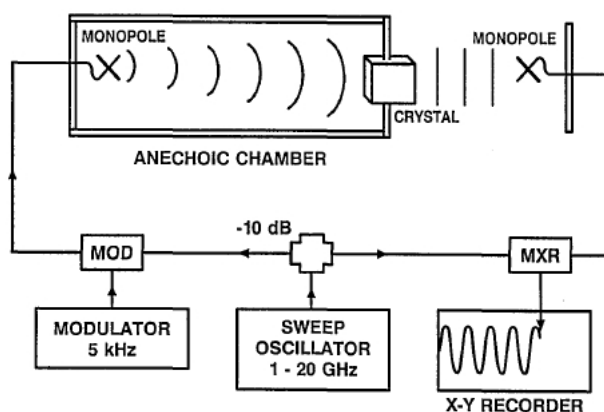
Consider a plane wave in the X direction. It will sense periodicity in the cubic direction, forming a standing wave and opening a forbidden gap as indicated by the shading in Figure below. Suppose, on the other hand, that the plane wave is going in the L direction. It will sense periodicity along the cubic-body diagonal, and a gap will form in that direction as well. But the wave vector to the L point is 14% smaller than the wave vector to the X point. Therefore the gap at L is likely to be centered at a 14% smaller frequency than the gap at X. If the two gaps are not wide enough, they will not overlap in frequency. As shown in the figure, the two gaps barely overlap. This is the main problem in achieving a photonic band gap. It is difficult to ensure that a frequency overlap is ensured for all possible directions in reciprocal space.



Hence, we get motivated that the BZ should be very close to sphere in order to increase the likelihood of a frequency overlap in all directions of space. The photonic band gap can be considered as a stop band with a frequency overlap in all of the $4\pi - sr$ space. The earliest antecedent of PBG is the theory of x-ray diffraction.

The refractive-index contrast for X-rays is small. The forbidden X-ray stop bands form extremely narrow rings on the facets of BZ. As the index contrast is increased, they open up covering the entire facet of BZ and finally the whole of reciprocal space. The high index contrast is the main feature of PBS beyond X-ray diffraction. In addition to which there is the effect of EM wave polarization.

The way a photonic crystal was constructed was by making photonic crystals on the scale of microwaves and then tested using the Mach-Zehnder Interferometer (measures phase and amplitude in transmission through the microwave scale photonic crystal) and then searched for Photonic band gaps. The construction of this is given below



What is the material of Photonic Crystal? We know that larger the refractive index contrast, the easier it is to find a photonic band gap. Largest practical contrast is between Si and GaAs which is 3.6.

Geometry? There are lots of structures available. We chose our FCC BZ. FCC BZ is composed of primitive cells which are given in the next figure. Now the problem is reduced to filling the space with these primitive cells. Now the decision before us is to what to put inside the unit cells. There are a huge number of possibilities. The first suggestion was to make a three-dimensional checkerboard, in which cubes were inscribed inside the fcc WS real-space cells in the the following figure

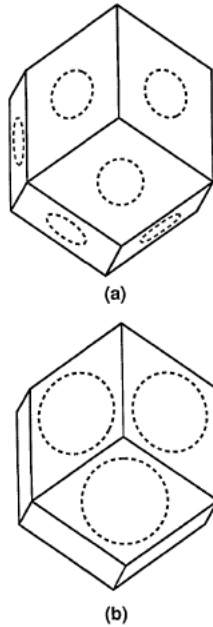


Fig. 10. WS real-space unit cell of the fcc lattice, a rhombic dodecahedron. (a) Slightly oversized spherical voids are inscribed into the unit cell, breaking through the faces as illustrated. This is the WS cell, corresponding to the photograph in Plate II. (b) WS cell structure with a photonic band gap. Cylindrical holes are drilled through the top three facets of the rhombic dodecahedron and pass through the bottom three facets. The resulting atoms are roughly cylindrical and have a preferred axis in the vertical direction. This WS cell corresponds to the photograph in Plate III.

Later the experiments" adopted spherical "atoms" centered inside the fcc WS cell. Plate I is a photograph of such a structure in which the atoms are precision Al_2O_3 spheres, n appx. 3.06, each appx. 6 mm in diameter. The spheres are supported by a thermal-compression-molded blue foam material of dielectric constant near unity. There are roughly 8000 atoms in Plate I. This structure was tested at a number of filling ratios, from close packing to highly dilute. Nevertheless, it always failed to produce a photonic band gap.

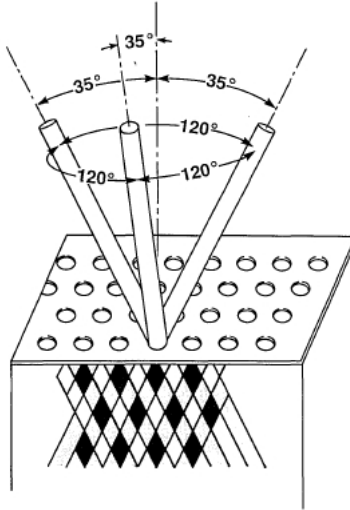
Then we tested the inverse structure, in which spherical voids were inscribed inside the fcc WS real space cell. These could be easily fabricated by drilling hemispheres onto the opposite faces of a dielectric sheet with a spherical drill bit. When the sheets were stacked so that the hemispheres faced one another, the result was an fcc array of spherical voids inside a dielectric block. These blocks were also tested over a wide range of filling ratios by progressively increasing the diameter of the hemispheres. These also failed to produce a photonic band gap.

The success came with the testing of the construction as in Plate II. This is the spherical-void structure, with oversized voids breaking through the walls of the unit cell. There appeared a narrow gap at 15 Ghz. But, there exists a pseudo gap at W instead of a valid one due to the crossing of the conduction and valence bands. The error was due to the size of the sample which was very small limiting the wave-vector resolution.

This can be corrected by lowering the symmetry by filling the unit cell by not single spherical atom but by two atoms positioned along the $\langle 111 \rangle$ direction, just

like the diamond structure. This results in a full opening of the band gap even at refractive-index contrast at 1.87.

The easier way to lower symmetry is by distorting the spheres along the $\langle 111 \rangle$, removing the degeneracy at W. The construction can be seen in the figure below



In spite of the non-spherical atoms the BZ is the same as that we saw at first except that the perspective changes. Instead of having FCC BZ resting on one of its diamond-facet it rests on its hexagonal face. As there is a preferred axis for atoms, the distinctive L points centered in the top and bottom hexagons are threefold symmetry axes, hence labelled L_3 . The other L points in have only 360 degree symmetry hence labelled L_1 .

4. APPLICATIONS

- (1) The reflectivity of photonic crystals derives from their geometry and periodicity, not a complicated atomic-scale property (unlike metallic components mirror). The only demand we make on our materials is that for the frequency range of interest, they should be essentially lossless. Such materials are widely available all the way from the ultraviolet regime to the microwave.
- (2) Using of the materials with non-linear properties for construction of photonic crystal lattices open new possibilities for molding the flow of light. In this case the dielectric constant is additionally depend on intensity of incident electromagnetic radiation and any non-linear optics phenomena can appeared.
- (3) SMLED(Single Mode Light Emitting Diode):
The forthcoming availability of single-mode microcavities at optical frequencies will lead to a new situation in quantum electronics. Of course microwave cavities that contain a single electromagnetic mode have been known for a long time. At microwave frequencies, however, spontaneous emission of electromagnetic radiation is a weak and unimportant process. At optical frequencies spontaneous emission comes into its own. Now we can combine the physics and technology of spontaneous emission with the

capability for single-mode microcavities at optical frequencies, where spontaneous emission is important. This combination is fundamentally a new regime in quantum electronics.

The example of such a thing is this SMLED which has all the coherence properties of a LASER while being a more reliable and thresholdless device like the LED. Progress in electromagnetic microcavities permits all the spontaneous emission of an LED to be funneled into a single electromagnetic mode. In this new form LED is surrounded by an optical cavity. The idea is for the optical cavity to make available only a single electromagnetic mode for the output spontaneous emission from the semiconductor diode. In fact the figure of merit for such a cavity is β , the fraction of spontaneous emission that is funnelled in to the desired mode. What is new for this application is the prospective ability to make high- β , cavities at optical frequencies that employ photonic crystals. The three-dimensional character of the cavities ensures that spontaneous emission will not seek out those neglected modes that are found propagating in a direction where this is no optical confinement.

With all the spontaneous emission funneled into a single optical mode, the SM-LED can begin to have many of the coherence and statistical properties normally associated with above-threshold lasing. The essential point is that the spontaneous-emission factor β should approach unity.

5. APPENDIX A : A HISTORY OF SPONTANEOUS EMISSION

Before the 1980's spontaneous emission was often regarded as a natural and inescapable phenomenon, one over which no control was possible. In spectroscopy it gave rise to the term natural linewidth. However, in 1946, an overlooked note by Purcell [4] on nuclear spin-levels already indicated that spontaneous emission could be controlled. In the early 1970's interest in this phenomenon was reawakened by the surface-adsorbed dye molecule fluorescence studies of Drexhage.⁷ Indeed, during the mid-1970's Bykov proposed that one-dimensional periodicity inside a coaxial line could influence spontaneous emission. The modern era of inhibited spontaneous emission dates from the Rydberg-atom experiments of Kleppner. A pair of metal plates acts as a waveguide with a cutoff frequency for one of the two polarizations. Rydberg atoms are atoms in high-lying principal quantum-number states, which can spontaneously emit in the microwave region of wavelengths. Hulet et al. shows that Rydberg atoms in a metallic waveguide could be prevented from undergoing spontaneous decay. There were no electromagnetic modes available below the waveguide cutoff.

REFERENCES

- [1] All definitions are from "Structure and Dynamics" by Martin T. Dove.
- [2] The Theory part of the Photonic Band gap structures including their construction and introduction are from the paper "Photonic Band Gap Structures" by Eli Yablonovitch, Vol.10 No.2/February 1993/J.Opt. Soc. Am. B.
- [3] The mathematical formulation is a briefing of "Full Vector Wave Calculation of Photonic Band Structures in Face-Centred-Cubic Dielectric Media" by K. M. Keung and Y. F. Liu. Physical Review Letters, Volume 65, page 2646"