

# Novel Design of a Three-Dimensional Photonic Crystal

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## **Abstract:**

In this paper, we review several proposed designs for three-dimensional photonic crystals and propose a new design that complements a two-dimensional array of holes with a semiconductor/oxide superlattice to create dielectric constant periodicity in all three directions. Common band gaps along the main crystal axes and a negative refractive index within a certain frequency range are achieved based on the novel structure.

## **Introduction:**

For more than a decade, photonic crystals (PhCs) have been investigated as a means of creating a material that manipulates electromagnetic radiation just as electronic crystals manipulate electrons. [1] Both electronic and photonic crystals are governed by the Bloch-Floquet theorem. However, for PhCs, it is Maxwell's equations and not the Schrödinger equation that are used to describe the behavior of the material. And while this fundamental difference does exist, electronic and photonic crystals share many properties due to the periodic nature of both materials. Just as a semiconductor crystal structure gives rise to a periodic electric potential, a PhC is designed to have a periodic dielectric constant. In semiconductors, the periodic potential results in a "forbidden gap" – a range of energies at which an electron propagating in the material cannot exist. Similarly, a PhC's periodic dielectric constant results in a forbidden gap for photons. A photonic band gap is a range of forbidden photon energies in a PhC. This result can be made clearer by recasting Maxwell's equations into an eigenvalue equation.

We start with the source-free Faraday's and Ampere's laws.

$$\vec{\nabla} \times \vec{E} = -\frac{1}{c} \frac{\partial}{\partial t} \vec{H} = i \frac{\omega}{c} \vec{H} \quad (1)$$

$$\vec{\nabla} \times \vec{H} = \epsilon \frac{1}{c} \frac{\partial}{\partial t} \vec{E} + \vec{J} = i \frac{\omega}{c} \epsilon \vec{E} \quad (2)$$

We can combine equations 1 and 2 to obtain an expression that is a function only of magnetic field.

$$\nabla \times \frac{1}{\epsilon} \nabla \times \vec{H} = \left( \frac{\omega}{c} \right)^2 \vec{H} \quad (3)$$

Equation 3 is an eigenvalue equation. The  $(\omega/c)^2$  term is the eigenvalue and the two curls make up the eigen-operator. With Maxwell's equations in the form of an eigenvalue problem, the same techniques applied to the Schrödinger equation in quantum mechanics can now be applied to electromagnetism. Such analysis concludes that for periodic dielectric media, there exists a range of  $\omega$  for which there is no real  $k$  solution. That is, there is no propagating plane-wave solution to Maxwell's equations.

Photonic crystals offer great promise in the areas of optical communications and computation: lossless waveguide bends, optical cavities, photonic transistors, negative refraction and perfect lenses may all be made possible with PhCs. Perhaps the greatest applications have yet to be discovered. The "holy grail" of photonic band gap materials is a three-dimensional photonic crystal. That is, a crystal that exhibits a complete photonic band gap (PBG) in all three directions. For some time, two-dimensional photonic structures have been fabricated with relative ease. [2] However, three-dimensional structures present many obstacles to easy fabrication. [3]

The behavior of electromagnetic (EM) waves in both periodic components of our structure has been extensively studied. The propagation of EM waves in a one-dimensional periodic dielectric material was first studied by Lord Rayleigh in the late 19<sup>th</sup> century. [4] Investigation of EM wave behavior in 2D and 3D structures, however, was not started until 100 years later by Yablonovitch. [1] Since that time, much effort has been put into the creation of a 3D structure that exhibits a PBG in all three directions. In fact, several have created such structures using a variety of materials and techniques such as inverse opals and wire meshes. [3, 5] These are rather difficult structures to create, however, on the length scales necessary to create a forbidden wavelength in the visible spectrum.

Our approach greatly simplifies the fabrication process of a 3D PhC because it combines the atomic-layer control of molecular beam epitaxy (MBE) with the tried-and-true processes of electron beam lithography (EBL) and reactive-ion etching (RIE). Our design for a 3D PBG structure consists of a GaAs/AlO<sub>x</sub> (oxidized AlAs) superlattice grown by MBE and a 2D array of holes that are defined by EBL and etched with RIE. The AlO<sub>x</sub> is created in a furnace after sample growth. [6] A superlattice is a semiconductor “parfait” of sorts. By alternating semiconductor and oxide layers in a periodic fashion, we are able to create an effective lattice constant, one greater in length than that of the bulk materials that compose the superlattice. This concept is frequently used to create materials that exhibit Bloch oscillations. [7] Of course, this larger effective lattice constant is not a requirement of photonic crystals; in fact, the material need not even be crystalline. The only material requirement is a periodic dielectric constant.

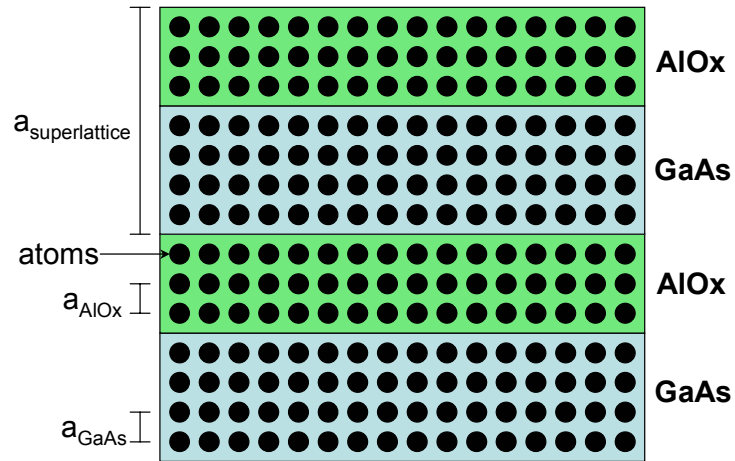


Fig. 1 A GaAs/AlOx superlattice. By alternating two materials, an effective lattice constant can be tailored to that needed for optical wavelengths.

Since our fabrication process uses tools and processes that have been well researched and developed, the real challenge comes in the design of the structure itself. Several design parameters exist; in addition to the choice of semiconductor and oxide materials, there is the hole-radius-to-hole-spacing ratio and semiconductor-to-oxide thickness ratio, as well as the absolute values of these parameters. The choice of these parameters is dictated by the need to create a forbidden wavelength that exists in all three directions and all incidence angles for both transverse electric and transverse magnetic (TE and TM) polarizations. It is the fulfillment of these requirements that defines a complete PBG structure.

**Current work:**

Most 3D structure fabrication relies on inverse opal structures formed by a self-assembly method, which is difficult to engineer precisely with current technology. [3, 5] With lithography and etching, 2D structures are easier to create.

A practical 3D photonic crystal based on 2D structures with an etching process is drawing people's attention. The idea is to etch a triangular array of circular holes through a distributed Bragg reflector (DBR) along the growth direction. [8, 9] The basic structure is shown in Fig. 2. Due to the periodicity of the dielectric constant, band gaps occur both along the growth direction,  $z$ , and in the 2D crystal plane,  $x$ - $y$ . By engineering the structure and material parameters, common band gaps will be formed along the main crystal axes when the frequencies of gaps along the  $z$  direction and in the  $x$ - $y$  plane overlap. The thickness of the DBR layers are denoted by  $l_1$  and  $l_2$  and the dielectric constants are  $\epsilon_1$  and  $\epsilon_2$ .  $L = l_1 + l_2$  is a fixed period determined by the target optical frequency. A large contrast between  $\epsilon_1$  and  $\epsilon_2$  is desired to achieve high reflection over a small number of periods. The following studies are based on GaAs/oxidized AlAs (AlOx) Bragg reflectors with  $\epsilon_1 = 14.44$  (GaAs) and  $\epsilon_2 = 2.25$  (AlOx).

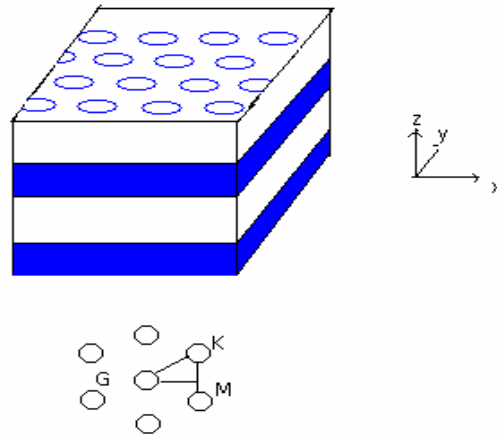


Fig. 2 Schematic structure of a DBR with triangular array of holes

For dielectric materials such as photonic crystals, common approaches of theoretical computation focus on either the frequency domain or the time domain. The time domain method has advantages related to field propagations involving time. [12] Since our major concern is band structures and eigenstates, frequency domain calculations are better suited and more practical. As we addressed in the introduction, Maxwell's equations can be translated to a form similar to the Schrödinger equation. We can expand the H field into plane waves using Bloch's theorem. [10] Thus band structures are obtained only through a periodic, position dependent dielectric constant, which is known as the plane wave expansion method. Both the real space lattice and reciprocal lattice are necessary to make calculations. Fig.3 shows the basic lattices of the  $x$ - $y$  plane in our structure. The Reduced Brillion Zone, shadowed in Fig. 3(b), is the working area for solving the eigenvalue problem.

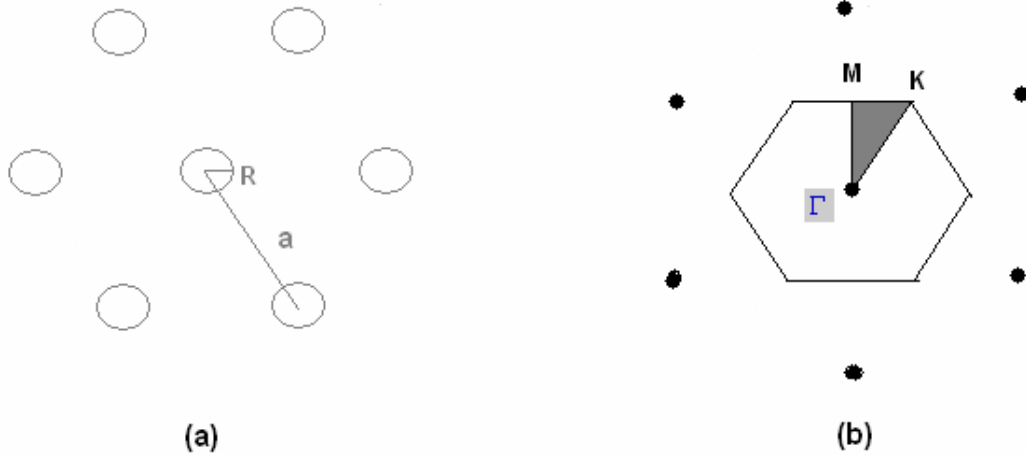


Fig. 3 (a) Real space lattice of 2D triangle structure with size ratio  $R/a$ ; (b) Reciprocal lattice of 2D triangle structure; shadowed area is the reduced Brillion Zone.

Band gaps usually form for TE modes with air-hole type materials while materials made up of rod lattices usually create band gaps for TM polarization. [13] Based on the etched DBR structure, our calculations concentrate only on the TE mode. The dielectric constant for holes is set to be  $\epsilon_0 = 1$  as air. Bloch waves are expanded by 961 plane waves in our calculations. Band structures in the  $x$ - $y$  plane and along the  $z$  direction are shown in Fig. 4 (a) & Fig. 4 (b). Band gaps overlap each other, which indicate common band gaps along the main crystal axes as we expected. To confirm our results, the Photonic Bands (MPB) program developed by MIT was used to get the 2D band diagrams shown in Fig. 5. [11] Both results are consistent with each other.

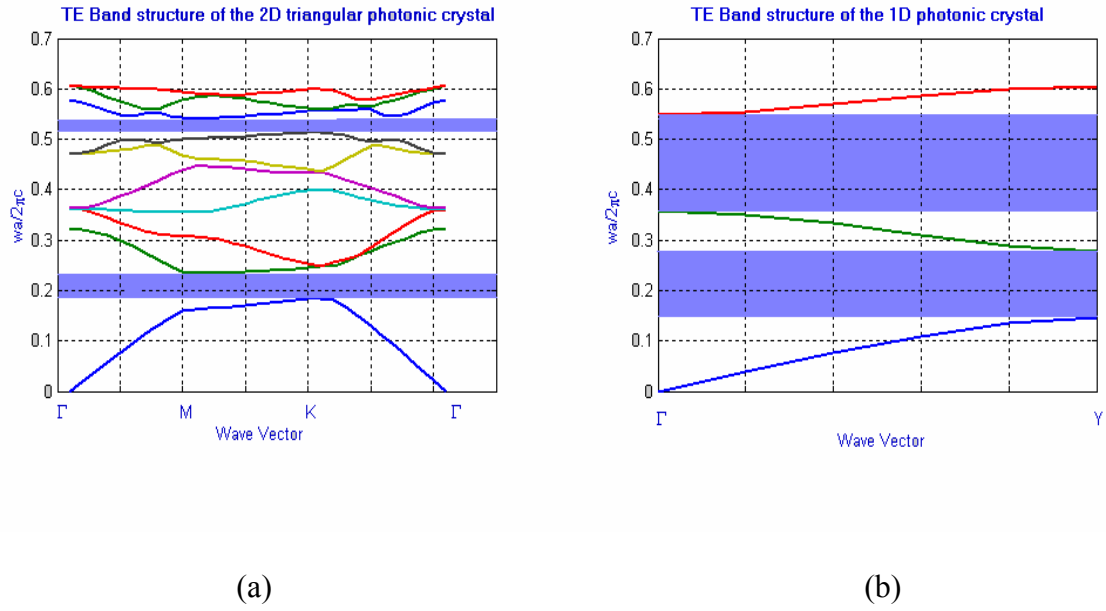


Fig. 4 (a) Bands for  $x$ - $y$  plane made of GaAs with  $r/a = 0.275$  and  $\epsilon = 14.44$ .  
 (b) Bands along  $z$  direction with  $l_1 / l_2 = 1.69$ ,  $l_1$  and  $l_2$  are the thicknesses of AlOx and GaAs, respectively.

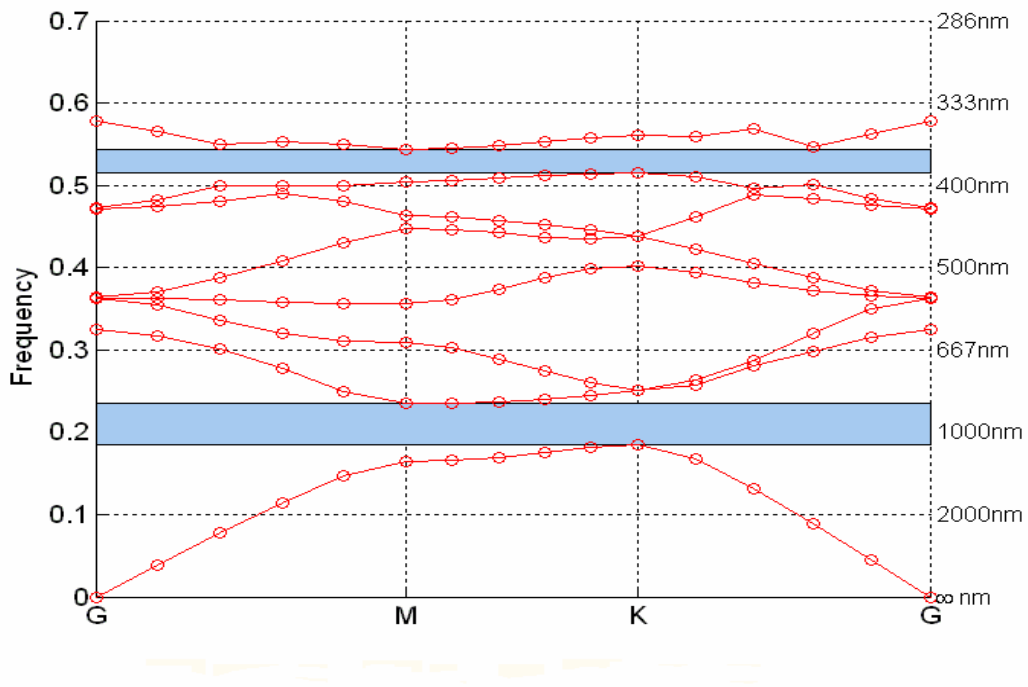


Fig. 5 2D band structure calculated from MPB program

Band structures can give us important information on optical properties, such as refractive index,  $n$ . Photonic crystals are expected to show negative refractive index within a certain frequency range. Negative refractive index is also crucial to implementing a perfect lens. [14] The absolute value of the effective  $n$  is given by  $|n| = c \cdot |k| / \omega$ , a function of frequency  $\omega$ . Here  $k$  is the wave vector. But to determine the sign of the refractive index, we have to consider the relation between phase velocity,  $v_p$ , and group velocity,  $v_g$ . Anti-parallel  $v_p$  and  $v_g$  results in a negative refractive index. [13, 15] Since the direction of the phase velocity is parallel to the wave vector  $k$ , the sign of  $n$  is usually determined by the behavior of the equi-frequency surface (EFS). In Fig. 6, we plot the EFS corresponding to the first and second bands of the band structure. The center of the diamond shape is the center of the first Brillion zone,  $\Gamma$ . As we can see, frequency contours move outwards with increasing frequency for the first band while the EFS of the second band shows an opposite behavior. A general conclusion is that convergent frequency contours always give negative refractive index. To confirm this, we calculated the refractive index according to the band structure; results are shown in Fig. 7 and agree with the prediction.

As we addressed before, our structure with holes drilled through has a band gap dominated by the TE mode. An idea was inspired by high- $\epsilon$ -rod type materials to generate a band gap for the TM mode. Holes could be filled with medium- $\epsilon$  materials to form a connected lattice of high- $\epsilon$  embedded in a low- $\epsilon$  background. [8] In addition to these theoretical pursuits, a fabrication procedure first proposed by Doug Hall can be used to create such a structure. A more balanced refractive index contrast in the three dimensions can be achieved.

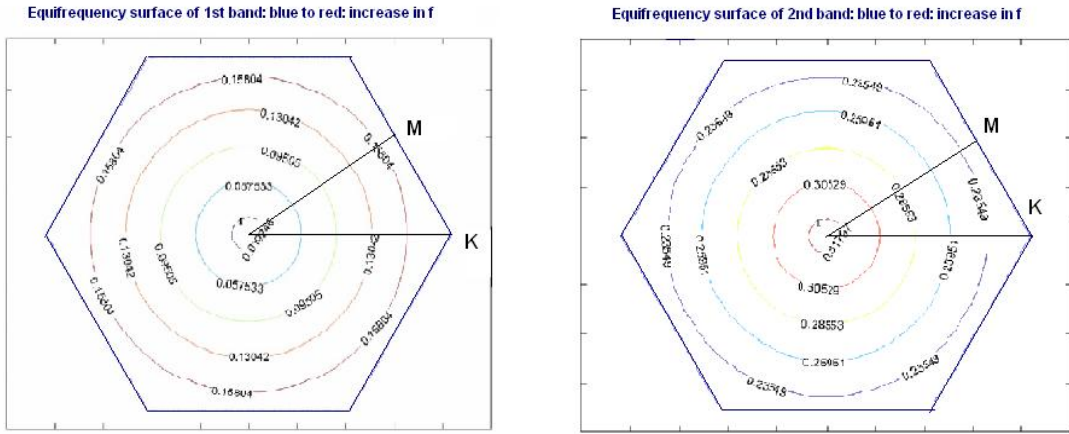


Fig. 6 Equipfrequency surfaces from 1<sup>st</sup> and 2<sup>nd</sup> band of the 2D band structure.

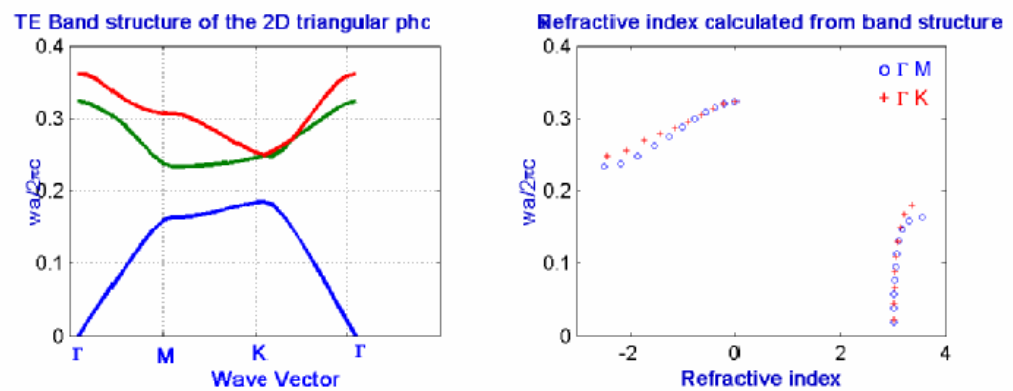


Fig. 7 Refractive index as a function of frequency with corresponding 2D band structure.

## Conclusion:

In conclusion, our work focuses on the combination of a 2D photonic crystal with a 1D super lattice. Based on modified Maxwell's equations, we performed calculations with the frequency domain plane wave expansion method. Results indicate a feasible 3D photonic crystal with overlapping band gaps along the main crystal axes is possible. Within a certain frequency range, the calculated convergent frequency contour results in a negative refractive index.

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