Finite difference time domain method for calculating the band structure of a 2D photonic crystal and simulating the lensing effect

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Abstract. A finite difference time domain method based on regular Yee’s algorithm in an orthogonal coordinate system is utilized to calculate the band structure of a two-dimensional square-lattice photonic crystal comprising dielectric cylinders in air background and to simulate the image formation of mentioned structure incorporating the perfectly matched layer boundary condition. By analyzing the photonic band diagram of this system, we find that the frequency region of effective negative refraction exists in the second band in near-infrared domain. In this case, electromagnetic wave propagates with a negative phase velocity and the evanescent waves can be supported to perform higher image resolution.

1. Introduction
Photonic crystals (PCs) as human-made structures are able to modify the flow of light by means of periodic spatial modulation of the refractive index [1, 2]. These structures exhibit the frequency band gap which eliminates the electromagnetic wave propagation [3]. Currently PCs in the form of metamaterials have attracted a lot of attention due to anomalous behaviour that has potential to develop biomedical imaging, optical communications and optoelectronic technologies. These metamaterials are able to restore both the phase of propagating waves and amplitude of evanescent waves to make perfect lens and as a result can overcome the diffraction limit of conventional convex lenses [4, 5].

Because of strong diffraction and multiple scattering in periodic structure of PCs, Maxwell’s equations need to be numerically solved. Finite difference time domain method (FDTD) has been widely applied in simulating and modelling photonic band gap materials. This method linearly scales with the simulation dimension and can be implemented in a parallel computing environment very efficiently [6].

In this paper, FDTD method based on common Yee’s lattice is implemented for calculating the dispersion band diagram of a 2D photonic crystal made from partitioned cylinders. We use the standard central-difference equations in an orthogonal grid scheme. By analyzing the band structure we show that this model system can be regarded as a superlensing device which can work at near-infrared regime. We also employ the FDTD method with perfectly matched layer (PML) boundary condition for simulating the field pattern of the point source and its image.
2. FDTD method for calculating the band structure

The FDTD method imitates the electromagnetic wave by volumetric sampling of unknown fields [7, 8]. In photonic band structure materials where the dielectric constant is periodically modulated, the electric and magnetic fields of the electromagnetic waves, $\vec{E}(r)$ and $\vec{H}(r)$, through the structure can be described by band index $n$ and a wave vector $k$ in irreducible Brillouin zone due to Bloch’s theorem:

$$
\vec{E}_{n,k}(r) = u_{n,k}(r) \exp(ik \cdot r), \quad \vec{u}_{n,k}(r + \vec{R}) = \vec{u}_{n,k}(r)
$$
$$
\vec{H}_{n,k}(r) = v_{n,k}(r) \exp(ik \cdot r), \quad \vec{v}_{n,k}(r + \vec{R}) = \vec{v}_{n,k}(r)
$$

(1)

where $\vec{R}$ is the lattice constant and $u_{n,k}(r)$ and $v_{n,k}(r)$ are periodic functions related to the Bloch waves. From (1), one can find eigenvalues of the periodic structure for a given periodic boundary condition. In order to compute the eigenmodes of the structure by means of FDTD method, random initial condition is used. Also we need sufficient amount of time to catch enough accuracy. For attaining eigenmodes we choose various low-symmetry locations in the unit cell as probes, in order to record peaks of the Fourier transform of the complex field components in the time domain for a given propagation constant. We should notice that, probes at high-symmetry locations of the unit cell are not able to detect all eigenmodes.

The PC proposed here is a 2D square lattice consisting of periodic arrays of long dielectric partitioned rods of Silica (SiO₂) and Silicon (Si) immersed in air background. It is assumed that the length of cylinders is long enough compare with the lattice constant. Furthermore, the width of the slab in the x direction is limited while in the y direction is unrestricted. Dielectric constants of two substances are $\varepsilon_{\text{SiO}_2} = 2.1$ and $\varepsilon_{\text{Si}} = 12.1$ at $\lambda = 1.55$ μm and the radius of cylinders is $R = 0.45a$, where $a$, is the lattice constant of the PC structure. Here the lattice constant $a$, is set to 460 nm and the TM-polarized electromagnetic wave is considered for calculating the band structure and simulating the electromagnetic wave propagation. Figure 1 displays the band diagram of proposed configuration.

It should be noted that the partitioned cylinders create a complete band gap between second and third bands while there is no band gap within the first five bands of the PC that includes just silicon cylinders.

To achieve the frequency with the negative refractive effect, we should pay attention to some important conditions. First of all, the frequency should be below $0.5 \times 2\pi c/a$ to avoid higher order Bragg diffractions ($c$ is the speed of light in vacuum); secondly, the equifrequency surface (EFS) of the PC around the center of Brillouin zone ($\Gamma$ point), should have an inward gradient leading to negative group velocity; and finally, the PC’s EFS should contain the EFS of the background [9, 10]. We choose the frequency of the intersection point of PC and air band diagrams to evaluate the imaging properties of this structure. The intersection normalized frequency, $\omega a/2\pi c$, is around 0.295. It is apparent from Figure 1, that there is an inward gradient around the $\Gamma$ point. Moreover, for this normalized frequency, the PC can be represented as a nearly isotropic medium and the normalized frequency can be managed by the refractive index of the materials incorporated in the PC [11].

3. Near-infrared imaging

We consider a $4a$-thick PC slab and locate a point source working at 0.295 normalized frequency at distance “$a$” from the left side of the PC structure. Then we utilize FDTD method with PML boundary condition to simulate the propagation of TM-polarized electromagnetic wave. Figure 2 shows the electric field distribution of the point source and its image. Two lines show the boundaries of the PC slab.
Figure 1. Band diagram of corresponding structure composed of Si and SiO$_2$ cylinders in air with the radius of $R=0.45a$. Inset: partitioned cylinder PC made from Si (light parts) and SiO$_2$ (dark parts) with lattice constant $a$.

Figure 2. Electric field distribution of the point source located at the distance “$a$” from the left side of the PC slab and its image in the $x$-$y$ plane.

According to Figure 2 we can easily see the point image of the point source on the right side of the PC slab and far from it. Narrowing behavior of the wave front of electromagnetic wave when transmits through the slab, implies that negative refraction effect is the dominant phenomena in image formation.
4. Conclusion
In this report, we introduced a novel 2D photonic crystal made by Si and SiO₂ partitioned cylinders to investigate the image formation characteristics. We used FDTD method for band diagram calculations and imaging simulation of this system. We found that the band diagram of this structure opens a gap between the second and third bands and satisfies three conditions required to create a PC superlens.

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