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Topology optimization of photonic structures for all-angle negative refraction

Fei Meng [a,c], Shuo Li [b], Han Lin [b], Baohua Jia [b], Xiaodong Huang [a,*]

[a] Centre for Innovative Structures and Materials, School of Engineering, RMIT University, GPO Box 2476, Melbourne, VIC 3001, Australia
[b] Centre for Micro-Photonics, Faculty of Science, Engineering and Technology, Swinburne University of Technology, PO Box 218, Hawthorn, VIC 3122, Australia
[c] School of Civil Engineering, Central South University, Changsha 410075, China

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ABSTRACT

This paper proposes a new topology optimization algorithm based on the bi-directional evolutionary structural optimization (BESO) method to design photonic crystals with broad all-angle negative refraction (AANR) frequency range. The photonic crystals are assumed to be two-dimensional periodical structures, which consist of dielectric materials and air. The conditions for the occurrence of AANR are identified and the design objective is to enlarge the AANR frequency range. The BESO algorithm is proposed based on finite element analysis for band diagrams of photonic crystals and the derived sensitivity numbers. Starting from a simple initial design without any AANR, BESO gradually re-distributes the dielectric materials within the periodical unit cell so that the AANR property emerges and its frequency range is enlarged accordingly. The numerical results show that the proposed BESO algorithm can effectively obtain AANR photonic crystals with novel patterns. The effects of dielectric permittivity contrast of two constituent materials, mesh-refinement and filter are discussed.

1. Introduction

Negative refraction of electromagnetic waves has attracted a lot of attention in recent years. It refers to the phenomenon that, when light beams travel to the interface of two materials, they refract to the same side of the surface normal. Theoretical analysis of negative refraction originates from the investigation on "left-handed material" which has negative permittivity and negative permeability simultaneously. This kind of material was predicted by Veselago in 1960s [1]. Its unique property gives rise to some interesting applications such as superlensing [2]. Although materials that having negative refractive indices do not exist in nature, some early researchers like Pendry [3], Smith [4] and Shelby [5] have successfully constructed negative refractive metamaterials constituted by periodic metallic resonant structures. These composites are capable of working at microwave region, which has a wavelength much larger than the periodicity of the structure. In recent years, the available frequency of metamaterials has been expanded to visible or higher frequency regions [6–9]. However, the high loss caused by resonance and the intrinsic fabrication limitations are still significant difficulties in the design of metamaterials. Therefore, many researchers have turned to achieve negative refraction through photonic crystals.

Photonic crystals are periodic structures consisting of two or more materials, which could be metal, dielectric material or air/vacuum. The diffraction in photonic crystals may result in one of the components of the group velocity propagating the opposite direction of the wave vector **k**, which will induce negative refraction. Compared with metamaterials, photonic crystals can interfere with light with wavelength comparable to its lattice constant, which mean they can work at higher frequencies like optical or infrared regions. Thus, photonic crystals can take advantage of the unique dispersion properties and generate negative refraction even without negative indices. Furthermore, typical photonic crystals composed of dielectric materials have lower absorption in high frequency regions [10]. Many researchers have investigated the negative refraction in photonic crystals [11–15]. So far, most researches focused on the mechanisms and experiments of photonic crystals. The systematic design of photonic crystals has not been reported yet.

The property of photonic crystals stems from their constituent materials and their spatial distribution. The negative refraction possibly occurs by rationally designing the structures of photonic crystals. In practice, negative refraction for all incident angles is essential for superlensing of near-field images. It is of significant importance to design low-absorption photonic crystals with broad AANR frequency range, which can give rise to a large available

* Corresponding author. Tel.: +61 3 99253320; fax: +61 3 96390138.
E-mail address: huang.xiaodong@rmit.edu.au (X. Huang).

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bandwidth, or lower the monochromaticity requirement of light sources. Furthermore, the diffraction effects should be avoided to ensure all the optical energy is negatively refracted.

Topology optimization is an efficient way to acquire the optimal design of structures based on the mathematical formulation of design objectives and constraints. Topology optimization methods were often employed to find the best or most economic material arrangement of structures in a given design domain. The most commonly used topology optimization methods include Solid Isotropic Material with Penalization (SIMP) method [16–18], level-set method [19,20], Evolutionary Structural Optimization (ESO) [21,22] and its later version Bidirectional Evolutionary Structural Optimization (BESO) [23,24]. Meanwhile, topology optimization methods have been successfully implemented in the design of optical devices [25–27], electromagnetic metamaterials [28–31] and photonic crystals [32–34]. The past research has demonstrated that topology optimization methods possess a powerful capability to find novel designs with extreme or exotic properties which were hardly obtained from physical intuitions.

In order to create novel photonic crystals with broad AANR frequency range, this paper proposes a new topology optimization algorithm based on BESO. The fundamental idea of BESO is to remove low-efficiency materials from and add high-efficiency materials to the design domain simultaneously. Thus, the resulting topology of a structure evolves to an optimum. Although BESO was established based on this simple concept, it has been proven to be effective and reliable for various structural optimization problems [35–37]. In recent years, the BESO algorithm has been further extended to design the microstructures of materials with extreme mechanical properties [38,39], electromagnetic properties [30], and photonic crystals with large band gaps [40].

This paper is organized as follows. Section 2 describes the mechanism of AANR in two-dimensional dielectric photonic crystals and the calculation of AANR frequency range. Section 3 introduces the finite element analysis formulation which is used to calculate the equi-frequency contours of the photonic crystal. Section 4 depicts the optimization problem, sensitivity analysis and the implement of BESO method. Numerical results are presented and discussed in Section 5. Finally, some conclusions are drawn in Section 6.

2. AANR frequency range

Negative refraction of electromagnetic waves for metamaterials requires its effective permittivity and permeability to be negative simultaneously. However, the mechanism of negative refraction for photonic crystals is totally different. It arises due to the dispersion characteristics of waves in a periodic medium. The band diagram along the boundary of the irreducible Brillouin zone and the equi-frequency contours (EFC) in **k**-space can be employed to identify the possibility of AANR. AANR in a photonic crystal may happen in different frequency ranges, but AANR at lower frequencies is more meaningful in superlensing, because high order diffractions can be suppressed and all the optical energy is negatively refracted [12,41]. Therefore, this paper focuses on the AANR on the first photonic band.

To illustrate the mechanism of AANR on the first band, an example from Ref. [12] is demonstrated in Fig. 1. The two-dimensional square-lattice photonic crystal is composed of air holes in dielectric materials with a relative permittivity of 12. As shown in Fig. 1(a), the lattice constant is a, and the radius of air holes are $0.35a$. The normal of the air-photonic crystal surface is arranged to be parallel to the Γ–M direction. The EFC of the first TE band is shown in Fig. 1(b). For wave vectors **k** on the Γ–M edge, the eigenfrequency increases monotonically, while the curvature of the equal-frequency contours gradually changes from concave to convex. As demonstrated in Fig. 1(c), for an incident beam from air with frequency ω, wave vector $\mathbf{k}_1$ and group velocity $\boldsymbol{v}_{g1}$, if there is a convex EFC on the first band of photonic crystal and the contour intersects with the surface normal, a negative refracted beam with wave vector $\mathbf{k}_2$ and group velocity $\boldsymbol{v}_{g2}$ will arise.

The AANR frequency range is illustrated in Fig. 2. The black curve is the first photonic band in Γ-M direction and the red line is the light line $\omega = ck$ which is shifted to M point [10]. The modes at the first photonic band below the light line can exist and propagate inside photonic crystals to generate negative refraction. Light above the light line cannot be confined in photonic crystals thus the upper limit of AANR ω_u can be obtained by finding the intersection of light line and the first band. The corresponding frequency of the intersection is the upper limit, ω_u, of the AANR frequency range. The relationship between the radius of EFC curvature and wave number |k| along Γ–M is the blue curve depicted in Fig. 2. As illustrated in [10], AANR can only be generated when EFC curvature becomes convex. The lower limit, ω_l, of AANR is therefore determined by the point where the concave EFC changes to a convex one. In other words, the radius of EFC curvature changes from a positive infinity to a negative infinity at the lower limit ω_l of AANR frequency range. An incident light from any angle within the range between ω_u and ω_l will result in a negative refraction beam.

3. Finite element analysis for photonic crystals

To identify the lower and upper limit of AANR frequency range, the first photonic band and the radius of EFC curvature along Γ-M should be obtained. In this paper, they are calculated by using the finite element method.

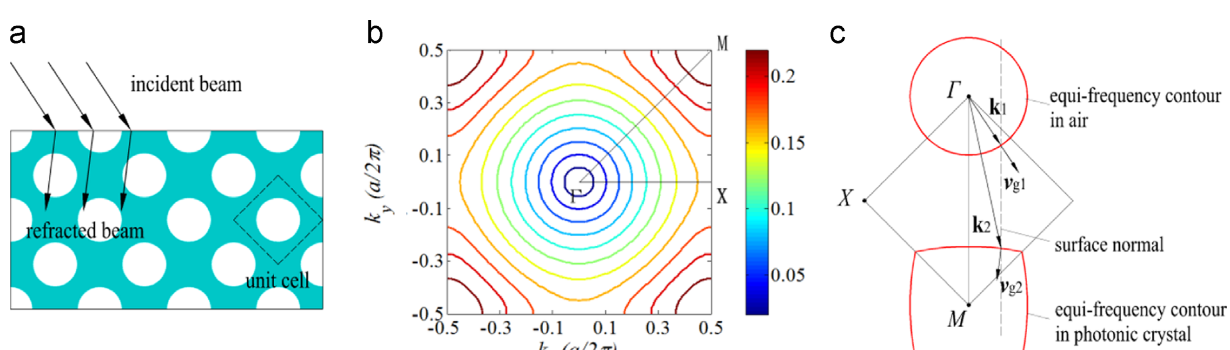

Fig. 1. (a) Structure of the photonic crystal; (b) EFC of the first photonic band (unit of frequency is $2\pi c/a$); (c) Negative refraction of a light beam. $\mathbf{k}_1$ and $\boldsymbol{v}_{g1}$ are the wave vector and group velocity of the incident beam, while $\mathbf{k}_2$ and $\boldsymbol{v}_{g2}$ are the wave vector and group velocity of the refracted beam.