Influence of disorder and deformation on the optical properties of a two-dimensional photonic crystal waveguide*

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We investigate the effect of disorder and mechanical deformation on a two-dimensional photonic crystal waveguide. The dispersion characteristics and transmittance of the waveguide are studied using the finite element method. Results show that the geometric change of the dielectric material perpendicular to the light propagation direction has a larger influence on the waveguide characteristics than that parallel to the light propagation direction. Mechanical deformation has an obvious influence on the performance of the waveguide. In particular, longitudinal deformed structure exhibits distinct optical characteristics from the ideal one. Studies on this work will provide useful guideline to the fabrication and practical applications based on photonic crystal waveguides.

Keywords: photonic crystal waveguide, deformation, disorder, transmittance

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1. Introduction

Over the past two decades, photonic crystals (PCs) characterized by their photonic band gap (PBG) have attracted the increasing interest of many researchers. There are several ways of manufacturing photonic crystals, including interference lithography, photolithographic etching (2D structures), and self-assembling (3D structures).[1–4] In fact, some amount of disorder will be produced in PCs during the manufacturing processes. In the lithographically defined structures, the dielectric interfaces present roughness, and in the self-assembling structures, the spheres forming opals exhibit dispersion in radius and displacement of the feature position in the lattice. Moreover, stresses also cannot be avoided in the complicated structures with many diversified materials due to the fabrication and packaging processes. In addition, an external force may induce changes as well in the refractive index and geometric shape (mechanical deformation) of the PCs. Therefore, the investigation of mechanical deformation and disorder in a PC structure is an important issue for guiding the PC device fabrications and practical applications based on such structures.

In recent years, disorder and mechanical deformation in 2D photonic crystal waveguide (PCW) structures have been investigated extensively. Experimentally, Bayindir *et al.*[5] confirmed that certain PBGs persist despite the existence of a large amount of disorder. Yoshimoto *et al.*[6] studied the PBGs and the refractive index change caused by stress. Theoretically, Frei and Johnson[7] revealed that the waveguide structures in photonic crystals are sensitive to disorder. Jun and Cho[8] explored that strain as an alternative to band structure modifications in the PBG structures just as desired. In this paper, we study the effects of disorder and deformation on the optical characteristics of PCWs in theory, which may provide some useful guidelines for the experimental research of the PC devices.

Up to now, existing works have treated the effect of disorder and mechanical deformation on the PCWs separately, but no investigation considering both disorder and deformation together has been reported yet. In this paper, the effects of both disorder and deformation are discussed simultaneously to explore the optical characteristics of the PCWs. The finite element method (FEM) is employed to simulate the dispersion characteristics and the transmittance of the waveguide. The number of rows, columns, and the mesh density are chosen so that the numerical error of the problem is approximately less than 1%. All analyses are completed with a suitable domain size that meets the calculation requirements.

2. Method and model

The propagation of electromagnetic waves through a PC structure is described by Maxwell's equations. For a two-dimensional (2D) PC, the wave modes can be decoupled into TE and TM modes. For the TE mode, Maxwell's equations reduce to

$$\nabla\left(\frac{\nabla H_z}{\varepsilon_r}\right)+\frac{\omega^2}{c^2}H_z=0, \tag{1}$$

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where $H_z = H_z(\boldsymbol{x})$ is the z component of the magnetic field at position $\boldsymbol{x}$, $\varepsilon_r = \varepsilon_r(\boldsymbol{x})$ is the dielectric constant, c is the light speed in free space, and ω is the frequency. Maxwell's equations are simplified to the scalar Helmholz equation given by

$$\nabla^2 E_z + \frac{\omega^2}{c^2}\varepsilon_r E_z = 0 \tag{2}$$

for the TM mode, where $E_z = E_z(\boldsymbol{x})$ is the z component of the electric field at position $\boldsymbol{x}$.

The FEM[9,10] is commonly used to solve electromagnetic problems and is especially well suited for solving complex geometries. It has been successfully used to study the band structure of the 2D anisotropic PC,[11] the lateral stress-induced propagation characteristics of photonic crystal fiber,[12] the nonreciprocal magneto PCW,[13] and so on. In this paper, the FEM is employed to solve the above equations to obtain the band structure and transmittance of the PCW.

The FEM model of the PCW is shown in Fig. 1. It consists of hexagon-arranged air holes in the GaAs dielectric bulk. The radius of the cylinder r is chosen to be 0.3 a (where a is the lattice constant), and the dielectric constant of the GaAs is 13.1. Only the TE mode is discussed in this work, since the PBG of the TE mode is much larger than that of the TM mode in the above structure. The scattering boundary conditions are applied to the sides of the structure to impose the condition that the plane wave normally incident upon a straight boundary will propagate without reflection. The transmittance of the PCW is defined by the ratio of the Poynting vector integration across the input and output boundaries.

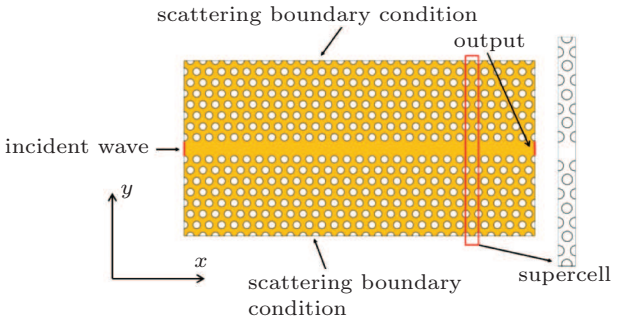


Fig. 1. (color online) Sketch of the PCW. The marked rectangle (red) denotes its supercell.

The disorder is modeled as fluctuations of either radii or positions of the air holes. The degree of disorder is defined by a deviation δ in the hole radius or position. For positional disorder, the relationship between the new position p and the original position p_0 of a hole is

$$p = p_0 + \delta(1 - 2\xi), \tag{3}$$

where ξ is a random variable uniformly distributed between the interval (0, 1). A similar equation for the radial disorder is

$$r = r_0 + \delta(1 - 2\xi), \tag{4}$$

where r is the new hole radius and r_0 is the original one.

Structure mechanics models are established to investigate the strain effects. Longitudinal strain and transversal strain are introduced to the FEM model. For the longitudinal strain case, the bottom edge of the PCW is fixed in the longitudinal direction, and the applied load is uniformly distributed at the top edge in the vertical downward direction. No constraints are applied to the other boundaries of the structure. The transversal strain is employed in the model by the same method. Young's modulus of 85.5 (GPa) and Poisson's ratio of 0.31 are taken for GaAs in this work. The mechanical deformation is expressed by the corresponding displacements (u_x, u_y) along the boundary of the structure. The strain is described as

$$\varepsilon_{ij} = (\partial u_i/\partial x_j + \partial u_j/\partial x_i)/2, \tag{5}$$

where $u_1 = u_x$, $u_2 = u_y$, $x_1 = x$, and $x_2 = y$. The largest ε_{ij} $(i, j = 1, 2)$ is denoted as ε (defomation degree). In this work, our study is restricted to a relatively small deformation of ε=3%. The stress will also cause dielectric constant change in the material. However, the deformation investigated in this paper is small enough to neglect the change.[14]

In this work, the PCW is oriented along the x axis, and a supercell with a size of $a \times 8\sqrt{3}a$ is periodically extended to model the disordered PCW structure. Therefore, the air holes in the same row have the same disorder, which will bring some distinctions between the FEM model and the realistic PCW structure. Thus, our simulation still cannot completely agree with the practical applications. However, the qualitative investigation of this work still can give some useful directions for the future study of PCW devices.

3. Results and discussion

The disordered PCW structure is generated by periodically extending a supercell structure along the x direction. Three typical disorder supercells are shown in Fig. 2. For the transversal disorder supercell, the cylinders move from the initial positions in the x direction. The displacements are controlled by the disorder deviation δ ($\delta = 0.15$ is shown in Fig. 2) and random variable ξ (see Eq. (3) for details). The other two disorder supercells are defined by using the same method. The supercells with sizes of a, $2a$, $4a \times 8\sqrt{3}a$ are all calculated to obtain more accurate simulation results. The study indicates that a supercell with the size of $a \times 8a$ can meet the requirement of qualitative investigation and minimum computational cost. The periodic boundary conditions are applied to both the x and the y directions of the supercell to calculate the corresponding guided bands. The guided modes are hardly affected by the super periodicity along the $y$axis since the length of the supercell is selected large enough

$(8\sqrt{3}a)$. Each guided band $\omega(k)$ is described as

$$\overline{\omega(k_x)} = \frac{1}{10}\sum_{i=1}^{10}\omega_i(k_x), \tag{6}$$

where $\omega_i(k)$ $(i = 1,2,3,\ldots,10)$ is one guided band of ten randomly disordered supercells. Therefore, the results depicted in this work are the average effects.

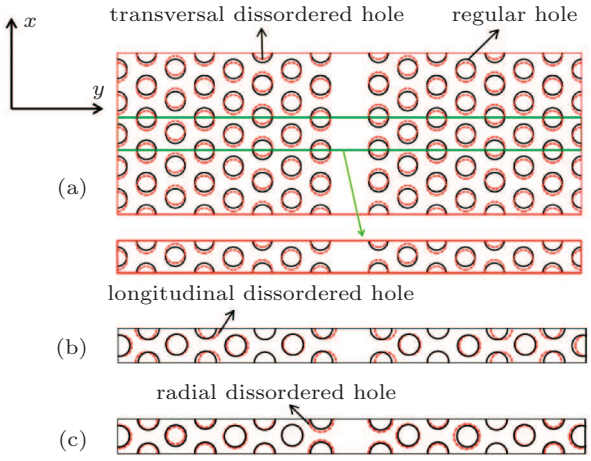


Fig. 2. (color online) Illustrations of typical disorder supercells investigated in this work: (a) transversal disorder cell ($\delta = 0.15$), (b) longitudinal disorder cell ($\delta = 0.15$), and (c) radial disorder cell ($\delta = 0.15$). The full (black) and dashed (red) circles indicate holes of the regular and disordered structures respectively.

The guided modes and transmission spectra of typical positional disordered PCW are exhibited in Fig. 3. It indicates that the optical characteristics of the waveguide are quite robust against transversal disorder. However, a longitudinal disorder structure experiences a larger influence, because the longitudinal disorder causes more geometric change of the dielectric material along the y direction than the transversal disorder. The geometric change of the dielectric material along the y direction affects the propagation bands in the k_x direction. Therefore, the structure performance is more sensitive to the longitudinal disorder than to the transversal disorder.

In the case of radial disorder, the guided modes are moved more closely to the increasing radial disorder (see Fig. 4(a)). The slightly interacting radial defects create more guided modes with higher frequencies, so the transmission range shifts to higher frequencies with this type of disorder (see Fig. 4(b)). In a word, the optical characteristics of the waveguide are obviously affected by radial disorder. Compared with the positional disorder case, the waveguide performance is severely influenced by radial disorder than by positional disorder, because the dielectric constant distributions are changed along both the x and the y directions.

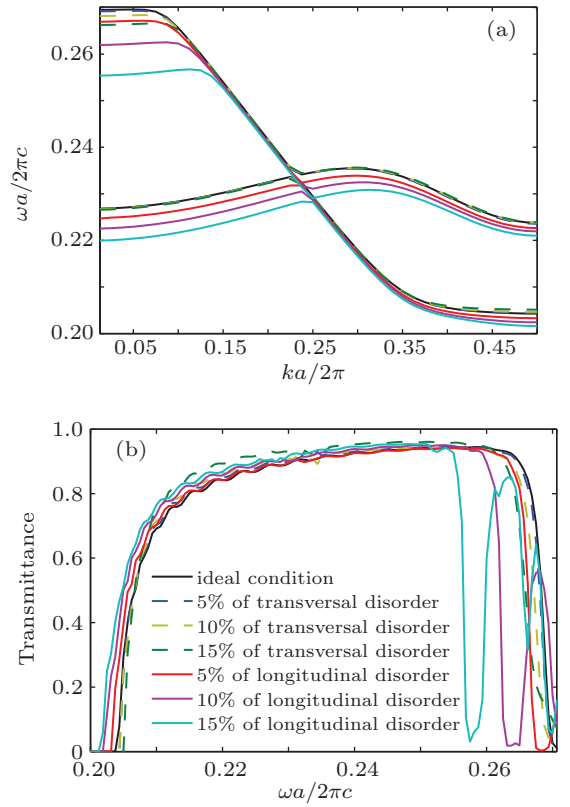


Fig. 3. (color online) Guided modes and transmission spectra of the disordered PCW: (a) guided modes of the PCW with different positional disorders, (b) transmission spectra of the PCW with different positional disorders.

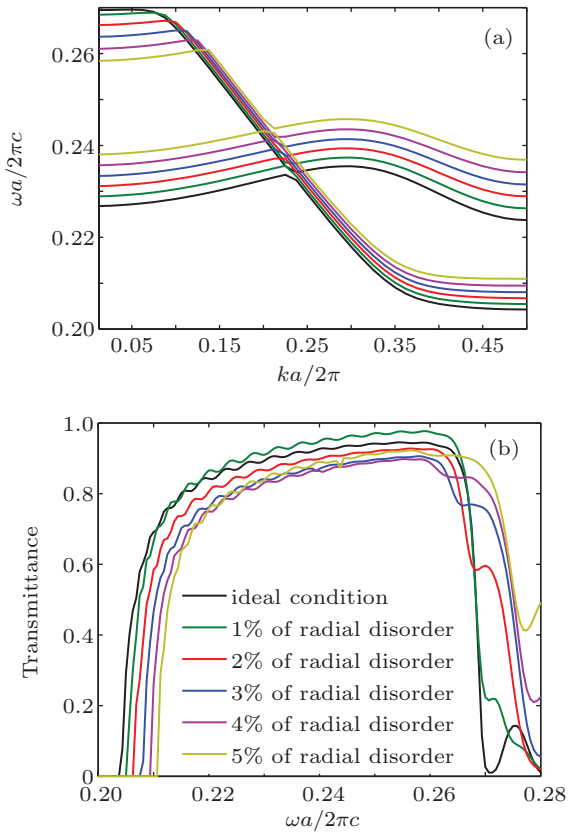


Fig. 4. (color online) Guided modes and transmission spectra of the disordered PCW: (a) guided modes of the PCW with different radial disorders, (b) transmission spectra of the PCW with different radial disorders.

In practice, the strain-induced mechanical deformation will also influence the performance of the PCW besides the disorder effects. Figure 5 illustrates the transversally and longitudinally deformed supercell models of the PCW respectively. The effect of different transversal deformations on the optical characteristics of the PCW is shown in Fig. 6. The transversal deformation brings very little effect to the guided modes and transmission spectra of the PCW. In contrast, the guided modes of the PCW with different longitudinal deformations are shown in Fig. 7. It demonstrates that more guided modes appear with the increase of the longitudinal deformation, this means a large longitudinal strain will destroy the band structure of the PCW, which seriously influences the optical performance.

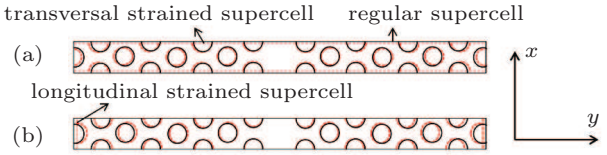


Fig. 5. (color online) Illustrations of typical strain supercells investigated in this work: (a) transversal strain cell ($\varepsilon = 0.03$), and (b) longitudinal strain cell ($\varepsilon = 0.03$). The full (black) and dashed (red) geometries indicate shapes of the regular and deformed structures respectively.

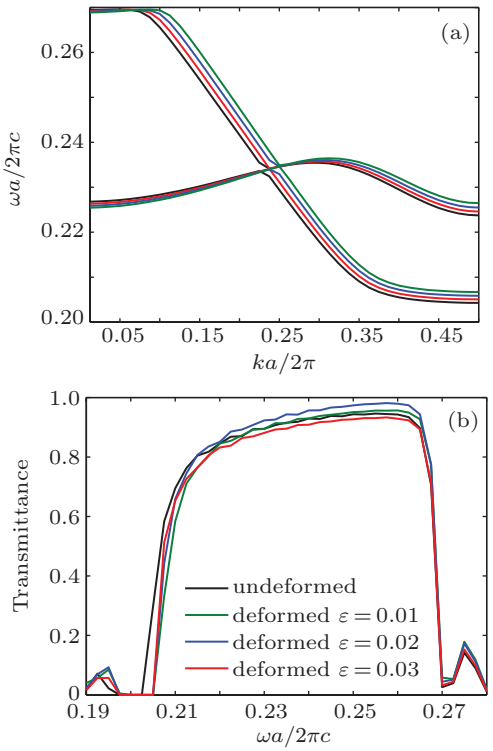


Fig. 6. (color online) Guided modes and transmission spectra of the deformed PCW: (a) guided modes of the PCW with different transversal deformations, (b) transmission spectra of the PCW with different transversal deformations.

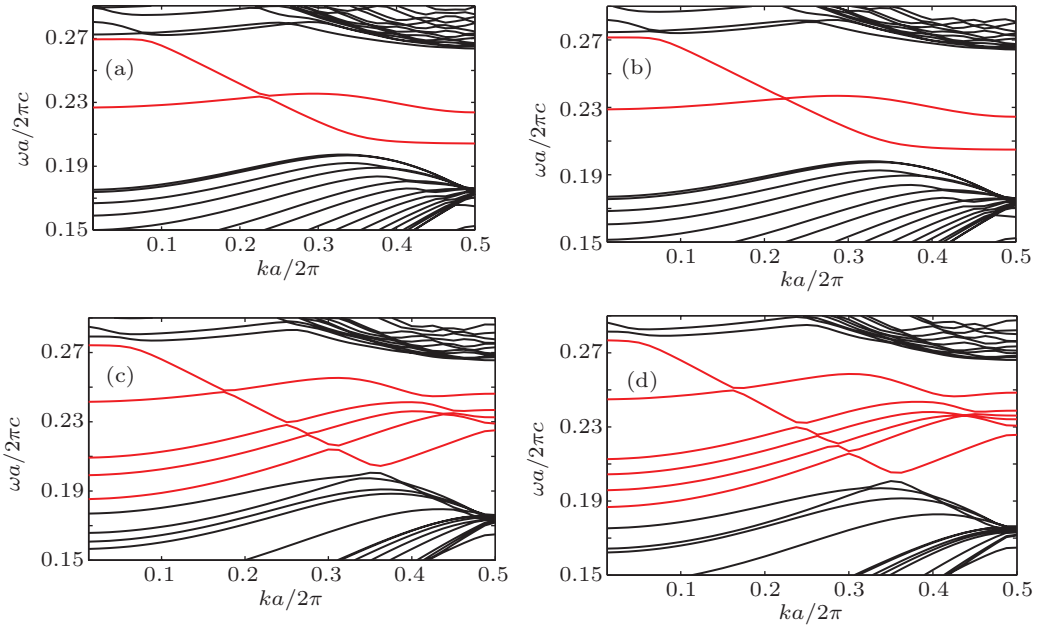


Fig. 7. (color online) Guided modes (red lines) of longitudinal deformed waveguides: (a) $\varepsilon = 0$, (b) $\varepsilon = 0.01$, (c) $\varepsilon = 0.02$, and (d) $\varepsilon = 0.03$.

As discussed above, large radial disorder and longitudinal strain can influence the optical characteristics of the PCW seriously. The slightly interacting radial defects create more higher-guided modes in the band gap. A large longitudinal deformation leads to the emergence of more lower-guided modes. In practice, a photonic crystal structure may be influenced by both mechanical deformation and disorder in some harsh environments, so it is significant to investigate their influence on the structure. Here, a structure undergoing both 5% of radial disorder and 3% of longitudinal strain is investigated in order to find the combined effects. As shown in Fig. 8, some higher guide modes appear in the band gap of the ideal PC. And it indicates that the radial disorder effect is more obvious when the PCW is undergoing both radial disorder and

longitudinal deformation.

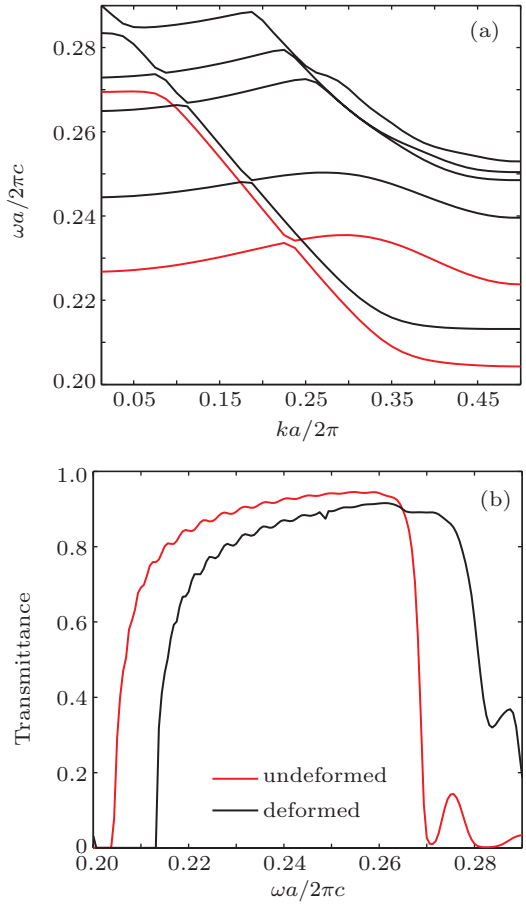


Fig. 8. (color online) Guided modes and transmission spectra of the disordered and deformed PCW: (a) guided modes of the PCW with longitudinal deformation and radial disorder, (b) transmission spectra of the PCW with longitudinal deformation and radial disorder.

4. Conclusion

In summary, we have investigated the influence of disorder and mechanical deformation on the optical characteristics of the 2D PCW. Our investigation indicates that transversal deformation and disorder have a less obvious effect on the PCW's performance. However, longitudinal disorder, radial disorder, and longitudinal deformation can affect the optical properties of the PCW seriously by inducing geometric changes of the dielectric material that is perpendicular to the light propagation direction. In addition, the radial disorder effect is more obvious when the PWC is undergoing both radial disorder and longitudinal deformation. All the analyses in our work are based on a simplified FEM model, and the rigorous study still does not completely agree with the practical applications. However, it can provide some useful guidelines for device fabrications and practical applications based on PCWs.

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