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Photonic characteristics and microcavity structure of ZnX (X =S, Se, Te)

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The dielectric photonic band gap materials have received broad attention due to their distinguished performance in optical devices, microwave generation and laser acceleration. We have theoretically studied photonic band structure parameters and defected structures of ZnX (X = S, Se, Te). The cavity was formed by a periodic sequence of holes in a dielectric waveguide, with a defect formed by a larger spacing between one pair of holes. The band structures of TE modes were obtained and the frequency/transmission calculations for different geometric structures were implemented. Then, the quality factor of resonance frequency for ZnX structures were examined. High levels of the quality factor values for these structures were obtained. It is proved that these structures carry the characteristics of photonic crystals.

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Keywords: Photonic band, Microcavity, Quality factor

1. Introduction

The photonic crystals (PCs) are defined as periodic dielectrics, which affect the electromagnetic wave propagation. It is known which they contain regularly repeating regions of high and low dielectric constant. PCs have been studied as an important area of research since 1887 [1], but Yablonovitch [2] and John [3] were first revealed their studies with photonic crystal idea in 1987. These studies concerned high-dimensional periodic optical structures, i.e., PCs, and display a range of frequency where propagation is completely forbidden. This situation is called the photonic band gap (PBG) and is analogous to the electronic band gap that is found in semiconductors. Yablonovitch [4] demonstrated the first three-dimensional photonic band-gap in the microwave regime in 1991. Subsequently, it was presented that PCs were well acknowledged for their capability to control and manipulate the propagation of electromagnetic waves in confined space [5]. Furthermore, in 1996, a two-dimensional photonic crystal at optical wavelengths was obtained [6]. It was observed that studies with PCs are increasing rapidly.

These dielectric materials, with complete band gaps, appear to be promising candidates for next generation optoelectronic devices and a new class of waveguiding [7, 8]. Linewidth, emission energy and momentarily emission rate control can be achieved by the arrangement of 2D PC structures designed as microcavities. Hence, these properties not only represent the designed cavity but also bulk material characteristics. This designed new type of microcavity that exhibit long life time and small modal volume with narrow transmission resonance widths have important application potentials in many different fields including photonics [9, 10], low-threshold lasers [11], nonlinear optics [12], cavity quantum electrodynamics [13-15].

ZnX (X = S, Se, Te) and related II–VI compounds that have wide and direct band gap energies, have attracted much research interest because of their excellent properties of luminescence [16-20]. Their applications in photonic crystal devices operating in the visible and near infrared region due to high indices of refraction and large band gaps make them highly transparent in the visible region [21]. The quality and reliability of microelectronic materials can be dramatically changed by point and linear defects. The control of defect distribution requires a measurement method capable of investigating the defects on a micrometer scale [22] and optical rectification of amplified femtosecond pulses [23]. In this study complete suppression of transmission in the region precisely coincident with the gap in the band structure is given, and the effect of photonic bands on the important characteristics of ZnX is clearly demonstrated.

2. Theory and computational method

In the calculations, dielectric constants of structures are considered to be 5.76 for ZnS, 7.12 for ZnSe and 8.7 for ZnTe, respectively in the spectral range from 0.3 to 1 μm [24, 25]. This structure prohibits propagation of TM light (in-plane magnetic field) in the frequency range 0.3 to 0.4 c/a. We consider two-dimensional structures, which are invariant in z-direction of the Cartesian coordinate system. The two-dimensional view of the designed structure is given in Fig. 1. The dimensions of the structure are given as (x, y, z) coordinates. But, z dimension is considered as unlimited. Blue area of the structure is dielectric slab which its dielectric constant was changed in the studies. In the designed structure, electromagnetic wave transmitted from left side proceeds through slabs and holes. Then, variation of wave and quality factor was examined through the circular gap by changing the length d. In this design, quality factor expresses the lifetime in the structure of the electromagnetic wave. Firstly, we have examined the state d=0, which is non-defect, and then we have created the defect by changing the d.

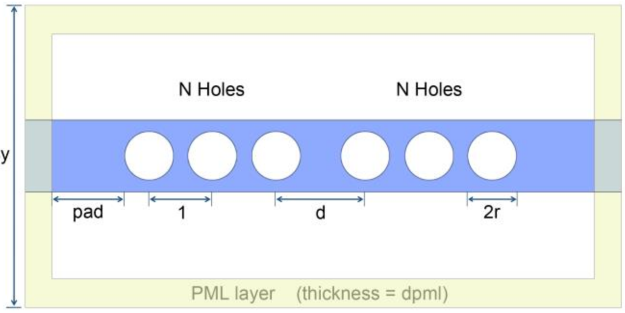

Fig. 1. Design of two-dimensional geometric structure

After the structure is designed, we organized the fields which can be divided into two polarizations by symmetry, i.e., a transverse magnetic (TM), in which the magnetic field is in the *xy* plane and the electric field is perpendicular to *z*; and transverse electric (TE), in which the electric field *E* is in the plane and the magnetic field is perpendicular. In our work we used the MIT Electromagnetic Equation Propagation (MEEP) [26] package program, which is a freely available finite-difference time-domain (FDTD) implementation [27]. FDTD is a numerical analysis technique used for modeling computational electrodynamics and used as an accurate method for determining the interaction of any physical structure with electromagnetic radiation. This calculation technique involves representing the physical structure to be modeled as a 2D and 3D object consisting of materials with known dielectric permittivity and solves Maxwell's equations to determine a nearly exact representation of how the light pulse propagates through the physical structure. The modern FDTD implementations contain a special absorbing, which is called as perfectly matched layer (PML) to implement absorbing boundaries. A PML with a thickness of one lattice constant is the inside wall for the entire simulation area. In addition, the frequencies are expressed as dimensionless, that are wa/2πc and c/a, in the MEEP package program. In simulations, application of PML boundary condition absorbed numerical reflections at the boundary of computational area and consequently provided an accurate solution [28]. In this regard, we calculated the properties of ZnX PCs structures that can be fabricated easily and operated in the microwave region because lattice constant (a) is in the order of microwave wavelengths.

3. Results and discussion

Fig. 2 (a, b, and c) denotes the band structure of TE modes for strip waveguide with air-hole-array for ZnS, ZnSe and ZnTe, respectively. We have used the cylindrical holes for all structures. Upper side of the black line in Fig. 2 is the light cone region ($\omega > ck_x$), which represents the modes extended in the air surrounding the strip waveguide. Lower side of the light cone, discrete guided bands denote field patterns around the waveguide. The band gap between the first two guided modes for ZnX structure is localized from 0.20 to 0.35. Displacement field results from modes in the first band are observed in the dielectric around each air hole. Besides, much of the power of the second band is distributed inside the air holes. Many discrete bands are also observed inside the light cone. These modes are either leaky or resonance modes that are reflected at the imaginary parts of angular frequency (w). Since these modes couple with radiating modes inside the light cone, intrinsic lifetime and losses were observed.

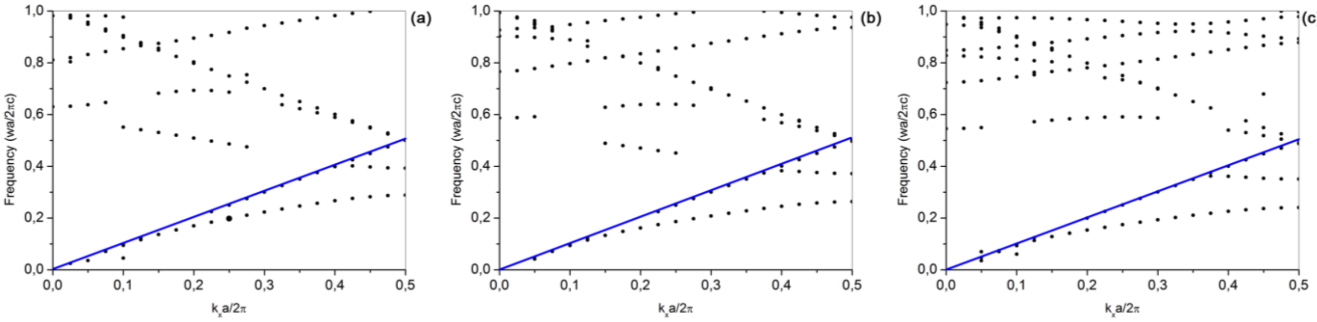

Fig. 2. Band structure of TE modes for air-hole-array strip waveguide. a) Infinite-length air columns (ε = 1) inside a strip of dielectric (ε = 5.76 for ZnS). b) Infinite-length air columns (ε = 1) inside a strip of dielectric (ε = 7.12 for ZnSe). c) Infinite-length air columns (ε = 1) inside a strip of dielectric (ε = 8.7 for ZnTe). The distance between nearest-neighbor air holes defines length unit a. The width of the slab is 1.2a and the radius of each hole is 0.36a

In order to investigate the effects of transmission for these structures, we have performed the frequency/transmission calculations and focused on typical monorail photonic crystal microcavity [29] as shown in the inset of Fig. 3. The microcavity of proposed structures include periodically arranged corrugate waveguide and was realized by assigning a defect in to the periodic structure. The signal used for structures is applied from the left side that is used as input channel, it couples through tunneling into the cavity, from where it decays into the radiation modes, and also into the waveguide on the left, and the waveguide on the right that behave as the output channel. At the same time, the magnetic field of the high-*Q* TE defect mode is shown in Fig. 3. We show that the dielectric region of the defect includes the largest peak in the magnetic field, the circular air regions of the waveguide also includes the other peaks. The model profile of the resonant mode is shown in the bottom panel of Fig. 3. According to the results of these calculations, the band gap extends from (0.20-0.35) $wa/2\pi c$ for all ZnX structures. The resonant frequency of the cavity occurs at 0.33 $wa/2\pi c$, quality factor Q= 81 for ZnS; 0.31 $wa/2\pi c$ Q= 133 for ZnSe; 0.28 $wa/2\pi c$, Q= 200 for ZnTe. When we examine the band structure of these three structures, it can be seen that the refractive indexes of the structures are increasing. In this case, the guidance resonance mode for especially ZnTe has shifted to lower frequency values. In this manner, the obtained transmission rate and quality factor is higher than for ZnTe. This result means that the losses incurred in ZnTe are less due to the high quality factor.

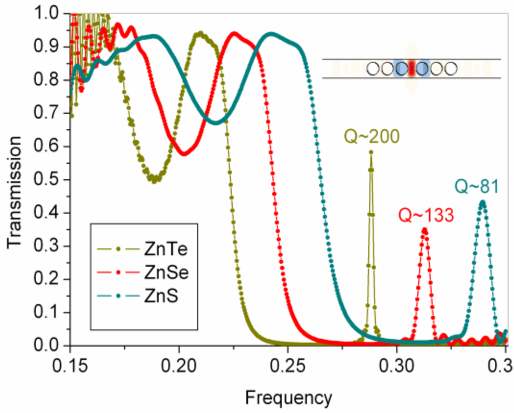

Fig. 3. TE transmission through a cavity formed by a periodic sequence of holes in a dielectric waveguide, with a defect formed by a larger spacing between one pair of holes

As the observation of the photonic band gap of structures is required, we have established 1D cylindrical holes for finite structure on PCs and investigated the transmission spectrum (Fig. 4). In these calculations, the defect is removed for all ZnX structures. We obtained that the band gap was between the (0.20-0.35) $wa/2\pi c$ for ZnX structures. According to the chart results, we observed that the photonic band gap of ZnTe was wider. The most important reason of these results has originated from the fact that the dielectric constant of ZnTe was greater than the other structures. When the transmission is zero, which is the photonic band gap, the reflected light in the structure leads to the fading of the progressive light by merging with incident light. As shown in Fig. 4, the dielectric constant of ZnTe is large as well, which have provided the shift to lower the values of frequency forming the photonic band gap.

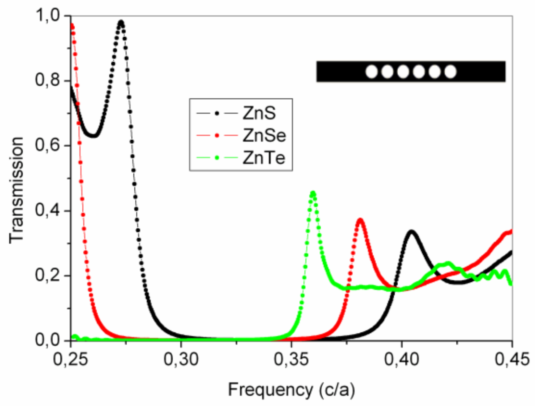

Fig. 4. Transmission spectra graph of ZnX structures when the defect is removed

It is known that many photonic materials exhibit different properties at different geometric conditions. Therefore, we have used spherical and ellipsoid holes instead of the cylindrical holes in the continuation of study. After changing the geometric conditions, we have made new calculations for ZnX structures and obtained transmission results in Fig. 5. Then, we have evaluated the transmission according to the structural features and investigated the variation of resonance frequency in the transmission spectrums. The resonance frequency shifts lower frequency value when we use spherical holes and higher value when we use ellipsoid holes as seen in Fig. 5a and 5b. According to these results, while the finite spherical gaps increase the effective refractive index of environment, ellipsoid geometric structure reduces the effective refractive index. It is obtained the better results in respect of the transmission values when the spherical and ellipsoid gaps were used instead of the cylindrical holes. In other words, the transmission value is approximately 80% for sphere structure of ZnTe.

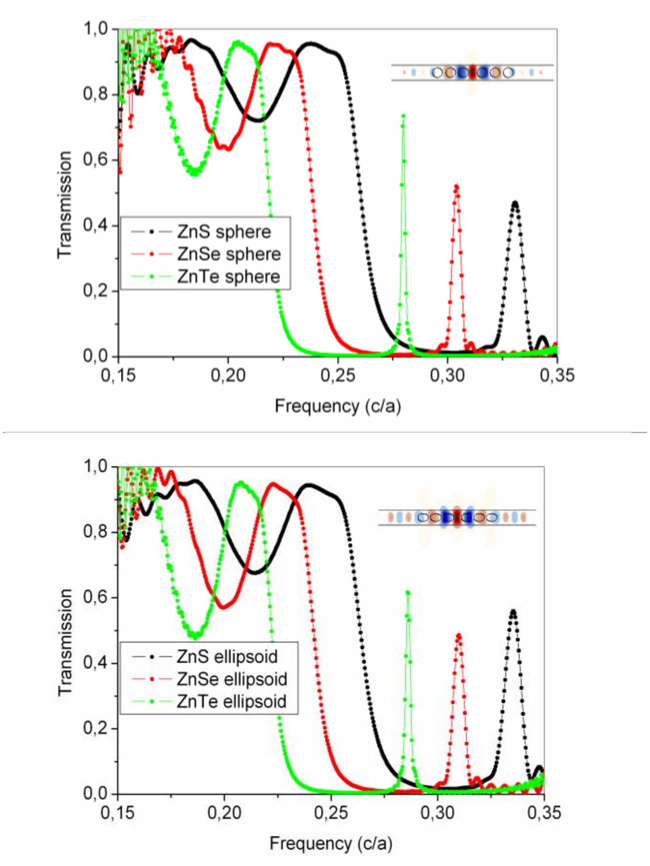

Fig. 5. TE transmission through a cavity formed by a periodic sequence of holes in a dielectric waveguide, with a defect formed by a larger spacing between one pair of holes. a) spherical holes, b) ellipsoidal holes

For different geometric conditions of all structures, the quality factor results of resonance frequency are given Table 1. As we see from table, the quality factor increases for ZnX in each symmetry for X=S, Se and Te, respectively. The reason of this increment can be increase in the dielectric constant while going through S to Te. These resonances can have high quality factors (*Q*). This shows that by changing the geometry of the defect, the cavity properties can be changed, enabling control over the emission color and luminensce properties. When ellipsoid structure is used instead of sphere structure, we show that the quality factor of structures decreases as shown in Table 1.

Table 1. The quality factor of resonance frequency is for ZnX defect structures

Material	Q (Quality Factor)
ZnS sphere	81
ZnS ellipsoid	59
ZnSe sphere	132
ZnSe ellipsoid	96
ZnTe sphere	198
ZnTe ellipsoid	146

If we evaluate the ZnX structures in terms of band structure, transmission (defect and non-defect), we can say that these structures carry the characteristics of photonic crystals, which can be used to the thin-film optics for lenses and in nonlinear devices as fibers.

4. Conclusion

In this paper, a detailed numerical study was performed for ZnS, ZnSe and ZnTe photonic structures. Firstly, the band structure of TE modes for strip waveguide with air-hole-array were obtained and the band gap results for all photonic structures were evaluated. Then, the frequency/transmission calculations were implemented and we have focused on typical monorail PC microcavity to investigate the effects of transmission. In addition, the defect was removed to show the photonic band gap, the transmission spectrum for 1D cylindrical holes were investigated. Finally, the spherical and ellipsoid holes were used for these ZnX structures and the transmission features according to structure modifications were observed. For all geometric conditions, the quality factor of resonance frequencies was obtained. More advanced photonic band engineering can be achieved by introducing a photonic defect state within the band gap to create an optical cavity. By changing the geometry of the defect, the cavity properties can be changed, enabling control over the emission color and luminensce properties. According to the results obtained, it can be seen that quality factor of structures has high values. This means that the time spent in the structure of the electromagnetic wave is rather short. In this case, the energy loss of the structures is very low, which is very important for photonic-based structures. These calculations prove that proposed structures carry the characteristics of PCs. ZnX photonic structures might prove useful in optoelectronic devices, in particular LEDs and low-threshold lasers.

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