Study of 2D and 3D photonic band-gap structures in Zinc Oxide (ZnO)

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Abstract— **In this paper, we focus on a theoretical study at visible wavelengths of band gap structures in ZnO as a function of the geometry and the features of the grating. Both 2D and 3D photonic crystals are considered. The frequency was also analyzed via this work by computing the resonant mode in two-dimensional photonic crystal cavities. Results of photonic band gap for both transverse magnetic (TM) and transverse electric (TE) polarizations show the existence of a complete 2D photonic band gap (PBG) for an hexagonal structure with a ratio r/a (radius of the holes over the period of the structure) about of 0.42. For 3D PBG, the face centred cubic (fcc) structure allows the obtaining of a PBG with a ratio r/a equal to 0.23 highlighting the great potential of ZnO as a promising material for photonic crystals applications.**

Keywords- Photonic crystal; ZnO; bandgap; cavity; FDTD; PWE.

I. Introduction

In last decades photonic crystal (PhC) structures have been deeply studied for applications in many fields of integrated optics with high scale of integration [1]. The most important property of photonic crystals is the presence of a frequency range (bandgap) where the propagation is forbidden due to the periodic modulation of the refractive index. The edges of the bandgap at specific wavelengths are defined through the design of both physical and geometrical parameters of the structure [2]. When a point defect is introduced into a photonic crystal, a cavity is formed and the energy of light is trapped into a small area around the defect.

Due to its interesting properties such as a wide direct band-gap of ~ 3.37 eV, high refractive index of 2.08 at visible wavelengths, and a large exciton binding energy of 60 meV, Zinc oxide (ZnO) is a an interesting material for photonic crystal cavity devices. It is also a promising material for UV detection, and Photonic crystal cavities with moderate and high quality factors (Q). It is, however, very important to obtain high quality ZnO films in order to effectively utilize its optical and electronic properties [3].

In this work, we used a numerical approach to investigate both the existence and the size of PBG by considering 2D and 3D PC in ZnO according to the geometrical parameters and the features of grating. We analyzed the resonant modes of cavities formed by a point defect on a two-dimensional photonic crystal.

II. Band structure calculations

Using Plane Wave Method (PWM) and Finite Difference Time Domain (FDTD) method [4,5], we calculated the photonic band structures for electromagnetic waves periodic arrays of holes in ZnO: in 2D (square and hexagonal), and in 3D (face centred cubic fcc) by varying the ratio of r/a (radius of the holes over the period of the structure).

To investigate the properties of defect states in photonic crystals, the two computational approaches are used (PWE and FDTD). These two methods reveal different information about the cavity [6]. Indeed, the evolution of the field in time allows to determine the resonant wavelength and the quality factor of the cavity.

In our computations we calculate the refractive index of ZnO by using the Sellmeier equation and the magnetic field formalism. Thus, the photonic band structure for anisotropic material can be obtained [7, 8].

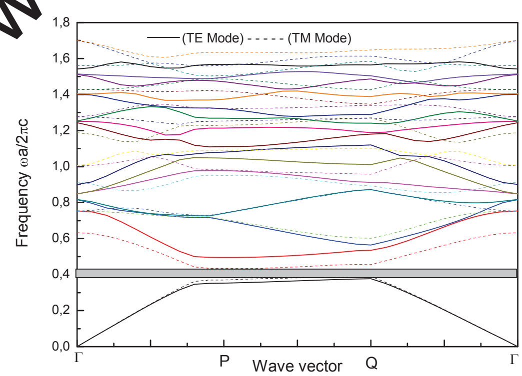

Figure 1. 2D photonic band gap in ZnO, hexagonal structure for TE and TM modes.

Figure 1 shows the band structure for the 2D hexagonal lattice of circular air holes in ZnO without point defect. We note that preliminary calculation of PBG evolution as a function of the ratio r/a, was done in order to determine the optimal ratio permitting to obtain the largest PBG. In the 2D configurations, we clearly observe a complete band gap for TE and TM modes for hexagonal structure with a ratio r/a of 0.42. However, in the case of the square lattice, the PBG was found only for the TM modes. The optimal technological parameters deduced from the 2D hexagonal PBG calculation are summarized in table 1.

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TABLE I. OPTIMAL STRUCTURE PARAMETERS OF THE 2D HEXAGONAL STRUCTURE IN ZNO

Mode	Optimal structure parameters	
	Periodicity a (nm)	*Radius r (nm)*
TE	210	90
TM	200	85

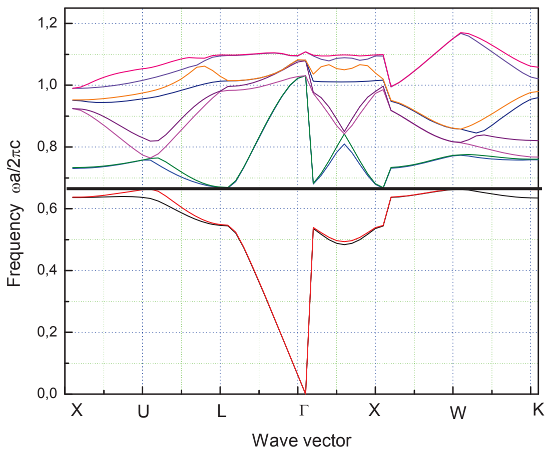

Figure 2. 3D fcc Photonic band gap in ZnO with r/a=0.23.

Figure 2 reports the band structure for the 3D fcc lattice of spherical air holes in ZnO. A complete PBG is obtained for an r/a ratio equal to 0.23 corresponding to an accessible dimensions for a fabrication of photonic structures i.e. radius of the holes r = 80 nm and the period of the structure a = 350 nm.

III. ANALYSIS OF MICROCAVITIES

A. *Square cavity*

The first structure analyzed has been a photonic crystal cavity consisting of a 5x5 square lattice of ZnO rods with refractive index $n_{rods} = n_e = 2.122$ in air (n=1). The wavelength of light is 450 nm. The defect of the cavity consists of a missing rod in the centre of a crystal pattern, as shown in fig 1.

In order to obtain the defect modes in 2D PCs, we use the supercell method which is applied successfully in the study of point defects in 2D photonic structure. The PWE method with 121 plane waves was carried out to construct dispersion curves for along the Brillouin zone as shown in the inset of Figure 3. It can be seen from Figure 4 that a relatively large band gap exists in the normalized frequency range of 0.3993 - 0.4499 $(a/\lambda = \omega a/2\pi c)$ for TM mode. Then the ratio of the rod radius to the lattice constant which gives the large gap band is r/a = 0.26. The lattice constant of the structure a = 190 nm and the rod radius r = 50 nm. A similar PBG for TE mode does not found. However the rod in a center of a cavity is removed, a resonant mode appears at the band gap. The Figure 4.b shows the bands structure of the cavity.

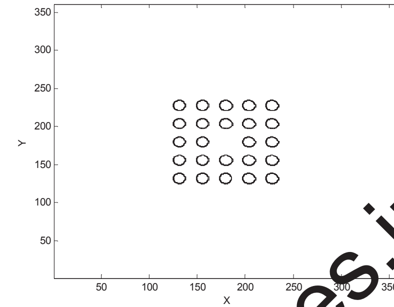

Figure 3. Cavity structure consisting of a single defect (produced by romoving a single rod in a centre of the structure)

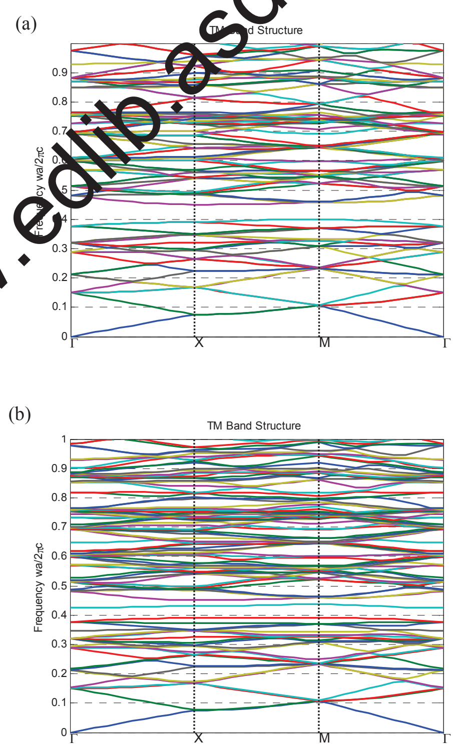

Figure 4. (a) 2-D band structure of the photonic crystal structure without defect, (b) Band structure of the photonic crystal structure used in Fig.1

In our case, in order to excite the structure a Gaussian source with high frequency, localized in the center of the cavity was used. The field distribution as well as the resonant frequency of the cavity mode is calculated by FDTD simulations. For all simulations, a detector was inserted at the center of the PhC cavity in order to store the time domain evolution of the electric field component from which resonant wavelength λ_{res}, has been calculated [6].

The Normalized transmission through the square cavity is shown in figure 5.

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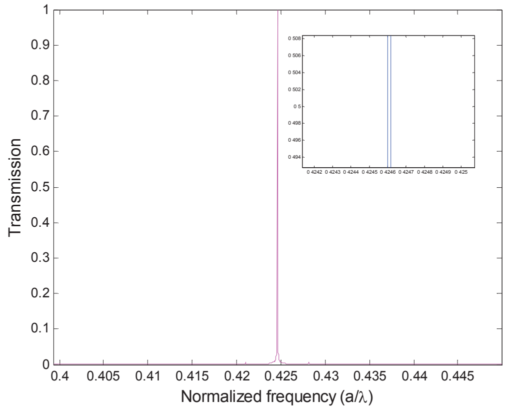

Figure 5. Transmission spectra for the cavity computed by the FFT of temporal response.

B. Hexagonal cavity

The next structure has been a photonic crystal cavity consisting of a 5x5 triangular lattice of dielectric rods (ZnO) with refractive index $n_{rods} = n_e = 1.942$ in air (n=1). The defect of the cavity consists of a missing rod in the centre of a crystal pattern, as shown in figure 6. The r/a ratio which gives the large gap band is r/a = 0.23. The lattice constant of the structure a = 210 nm and the rod radius r = 50 nm. We begin with a perfect crystal where every rod has a radius of 0.23 a.

A large gap for TM mode is found between a normalized frequency 0.409 and 0.522 as shown in figure.6. A similar gap for TE mode does not found.

The figure 7 shows the bands structure of the cavity. Applying a Gaussian source to the center of the hexagonal cavity, one can measure the wavelength of resonance by the FDTD method.

The time domain parameters of the source were fixed to the same values used for the previous examples. From figure 8, it can be observed the profile of the resonant mode. Furthermore, from the time domain evolution of the electric field the resonant wavelength has been computed to $\lambda_{res} = 451.50\ nm$.

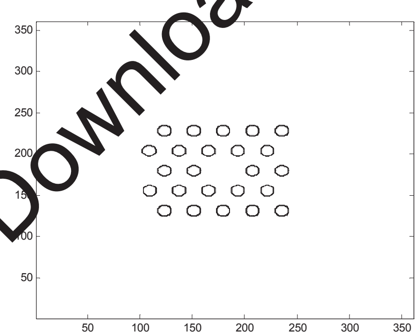

Figure 6. Cavity formed by a point defect in a two-dimensional photonic crystal of 5x5 triangular lattice.

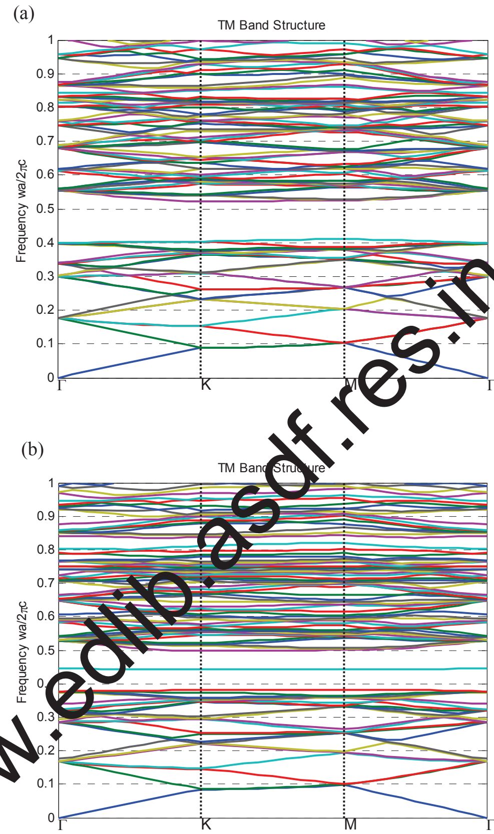

Figure 7. (a) Photonic band structure of a 5x5 triangular lattice computed by a supercell method. (b) Band structure of the photonic crystal structure used in Fig.5

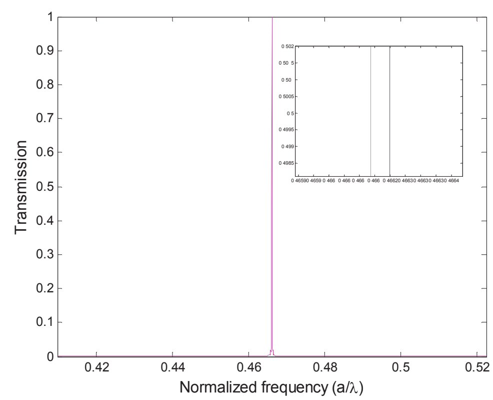

Figure 8. Normalized transmission through the hexagonal cavity.

IV. CONCLUSION

We reported 2D and 3D photonic band gap calculations in ZnO in the visible range. Results show the existence of a complete photonic band gap in hexagonal lattice for TE and TM modes and a photonic band gap in square lattice only for

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TM mode. The calculation of PBG in 3D face centred cubic structure reveals the existence of PBG in ZnO. The values of the optimal technological parameters deduced from the PBG modelling, show the great potentialities of ZnO in photonic crystals cavities applications both for 2D and 3D structures. Two types of 2D cavities have been studied, i.e. square and hexagonal structures. Results showed that the two cavities present a resonant mode in the visible wavelengths.

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