Blue shift effect on the reflectance in two-dimensional Si-ZnO photonic structure with patterned coupled optical micro-cavities

J A Medina Vázquez, E Y González Ramírez, J G Murillo-Ramírez*, V M Carrillo-Vázquez, G Herrera, A Duarte-Moller

1Centro de Investigación en Materiales Avanzados S.C.
Miguel de Cervantes 120, Complejo Industrial Chihuahua, C. P. 31136, Chihuahua, Chih. México.
2 Catedra CONACYT Assigned to Department of Physics of Materials, Centro de Investigación en Materiales Avanzados S. C., Miguel de Cervantes 120, Chihuahua 31136, Chihuahua, Mexico

E-mail: jose.murillo@cimav.edu.mx

Abstract. This research has revealed the possibility to induce a shift towards short wavelengths on the optical reflectance properties of a two-dimensional photonic crystal which include an embedded array of optical micro-cavities. This ability was attributed to the resonant effect produced by the micro-cavities array embedded in the regular photonic crystal and by the variation on the structural parameters that defined the photonic crystal under research. These results can be useful in future applications of solar cell systems and telecommunications, among others, which can be of great help to increase technological developments.

1. Introduction
A photonic crystal (PhC) is a material that exhibits a periodic modulation of the refractive index induced by the inclusion of structural defects. The purpose of this type of material is to control the reflection and transmission of light through its structure through the phenomenon of diffraction. The control of flow light is a beneficial phenomenon which can help to improve the efficiency of photovoltaic cells and smart windows to mention some examples [1]. Nowadays, the enormous growth in technology demands a greater variety of alternatives for the generation of new devices with capabilities to replace or improve specific electronic devices extensively used in many needs of everyday life; this is where photonics and photonic crystals (PhC) can be very useful. The interest in the PhCs has grown over the past few years because they can be a viable solution to problems in the field of telecommunications [2-5] light extractors in light emission diodes (LEDs) among many others possible applications [6]. Two-dimensional (2D) PhC’s are of particular interest because their manufacture is relatively simple and can be built using techniques developed and well established for electronic industry, including chemical assisted ion beam etching (CAIBE), reactive ion etching (RIE) and focused ion beam (FIB) milling among others [7,8].

* jose.murillo@cimav.edu.mx
In this work, we report measurements of the optical reflectance as a function of wavelength of incident radiation in the ranges of visible (Vis) and near-infrared (NIR) of the electromagnetic spectrum of a two-dimensional photonic crystal built on a silicon substrate containing a ZnO thin film, including an array of optical micro-cavities embedded in a regular square lattice. Also, it was performed a numerical simulation of the optical reflectance and the photonic band structure of a PhC similar to that built, using the “PWE band solver of the software package optiFDTD” in order to compare these results with the measurements performed. Furthermore, in the numerical simulations of the optical properties of the PhC similar to that fabricated were considered variations of their structural parameters such as the diameter of the hole of the regular square structure defining the PhC and the lattice constant of the optical micro-cavities array embedded in the regular square structure. The results of these numerical simulations were extraordinary due to these revealed a blue shift of the reflectance peak as a function of the specific structural parameters that defined the PhC considered.

2. Experimental details

2.1 Sample preparation

The PhC studied was fabricated on a silicon substrate [0 0 1] in which previously has been deposited a ZnO thin film of approximately 240 nm thickness by Assisted Chemical Vapor Deposition (AACVD) method [9]. The PhC was milled directly on the Si-ZnO hetero-structure in an area of 84 x 84 μm² using a Focused Ion Beam (FIB) system JEOL JEM 9320-FIB with Ga+ ion source operated at 26.5 kV. The original purpose of the deposition of ZnO film onto the silicon substrate was to control and prevent excessive damage to the silicon substrate during the irradiation with gallium ions from the FIB system. The specific thickness of the ZnO thin film considered was selected by trial and error, and at the beginning of this research, we had planned to remove it from the silicon substrate after the PhC milling. The structural parameters that defined the PhC with a regular square periodicity were a lattice constant \(a = 1.05 \mu\text{m}\) and circular columns of air with a radius \(r = 0.57a\) and a depth around 1 μm. These structural parameters defining the morphology of the PhC built have similar values such as that generally used in PhC’s reported in the literature, were achieved using a dose of 200 nC/μm² and 1000 pA of irradiated current for 15 seconds per hole using the spot milling shape [10]. Also, a pattern of nine quasi-circular cavities of approximately 10 μm in diameter and a lattice constant of approximately 20 μm, describing a second square lattice, was embedded into the regular PhC as shown in Figure 1. These cavities are regions where no holes of air were milled. Nevertheless, we called cavities to these regions in the sense that they can be coupled and present resonance effects via the illumination to the PhC with coherent light beams. The cavities pattern was introduced into the regular lattice defining the PhC with square periodicity in order to investigate its effect on the optical properties of the new photonic structure.
In the numerical simulation of the PhC sample using the OptiFDTD software, the same geometrical parameters as in the PhC built were used. In these calculations, the dependence of the refractive index on the wavelength for both the ZnO thin film and the silicon substrate was taken into account. The experimentally milled PhC and the structure considered in the simulation are shown in Figures 1 and 2, respectively.

3. Results and Discussion

The optical characterization of the physical milled PhC was performed by measuring the reflectance at normal incidence for transverse magnetic polarization mode (TM) using as a light source, several single-mode laser diodes coupled to a fiber, a laser source coupled to a multichannel fiber and two resonant cavities. The corresponding wavelengths to these light sources were 633, 750, 785, 852, 1308, 1392, 1547 and 1594 nm. These sources were chosen in order to characterize the optical properties of the hybrid PhC in a broad interval of the Vis-NIR range of the electromagnetic spectrum.

Although at the beginning of this research it was planned to remove the ZnO thin film from the silicon substrate once the PhC had been built, it was decided not removing it in order to research its effect on the optical properties of the hybrid PhC. For this reason, the measurements of the optical reflectance were performed maintaining the ZnO thin film in the hetero-structure that defined the PhC fabricated.

On the other hand, the numerical calculations of the reflectance of the PhC containing the micro-cavities were performed considering a parametric sweep of wavelengths in the Vis-NIR range of the electromagnetic spectrum. Figure 3 shows a comparison of the optical reflectance obtained from the numerical simulations and the experimental measurements performed in the PhC fabricated.
Figure 3. Comparison of the optical reflectance for TM polarization mode obtained from the measurements on the PhC built and studied in this work represented by the solid red line, and the results obtained from the numerical simulations described by the solid black line.

As can be observed in Figure 3, the reflectance as a function of wavelength numerically calculated is very similar to the optical reflectance measured in the PhC built. It is interesting to note how both, the experimental and numerical results reveal a significant improvement of reflectance for wavelengths near the border of Vis-NIR range. Figure 3 shows clearly an excellent agreement among the measurements and numerical calculations; this given the fact both results show a peak with a maximum amplitude of the optical reflectance precisely at the same wavelength of 750 nm.

In order to investigate the effect of inducing variations in the structural parameters defining the hybrid PhC under study, additional numerical simulations modifying the lattice constant and the diameters of the air holes were made. Figure 4 shows the calculation of the optical reflectance of a hybrid PhC similar to the structure built and studied in this work and the reflectance calculated for a new PhC whose structural parameters were modified multiplying the original parameters by a factor of 0.5. In other words, calculations for the new photonic structure were accomplished reducing them by half such that now the lattice constant assumed for the regular square pattern of air holes was $a = 0.525 \, \mu m$ and every circular hole had a radius $r = 0.57a$. The array of the optical micro-cavities organized in a second square lattice embedded in the regular PhC had now a lattice constant of 10 $\mu m$ and the diameter of each circular micro-cavity was 10 $\mu m$. As can be observed in Figure 4 the results obtained revealed a blue shift on the maximum reflectance of the hybrid photonic structure as a function of wavelength, such that the reflectance was selectively improved at smaller wavelengths. In particular, for the PhC with structural parameters reduced regarding the characteristics of the original PhC, the maximum reflectance appears now at a wavelength of 660 nm while before for the original PhC the maximum reflectance was obtained at 750 nm. Figures 5 and 6 show the photonic bands structure numerically calculated for both PhCs considered in this work.
Figure 4. Comparison between the optical reflectance numerically simulated for TM polarization mode, at normal incidence, of the PhC fabricated, represented by the solid black line and the corresponding to the PhC with structural parameters reduced by a factor of 0.5 regarding the structural parameters used in the PhC fabricated, represented by the blue line.

Figure 5. Band structure for TM polarization mode of the PhC with the initial structural parameters, a lattice constant $a = 1.05 \, \mu\text{m}$, and a circular hole radius $r = 0.57a$. The array of the optical micro-cavities embedded in the regular PhC has a lattice constant of 10 $\mu\text{m}$ and the diameter of circular micro-cavity equal to 10 $\mu\text{m}$.

Figure 6. Band structure for TM polarization mode for the PhC with the structural parameters reduced by a factor of 0.5

As in the case of reflectance study, it can be observed in the right axis of Figs. 5 and 6 that the photonic band structure shows a shift towards shorter wavelengths as the lattice parameter, the diameters of the air holes of the regular PhC and the structural parameters of the optical micro-cavities...
array decrease. This shift in the photonic bands towards shorter wavelengths or higher frequencies confirms the results before obtained for the optical reflectance that also showed a shift toward shorter wavelengths. Also, it is important to note how both band structures presented in Fig. 5 and 6 show partial photonic band gaps.

The shift effect toward short wavelengths of the optical reflectance of the PhC studied in this work indeed is a remarkable result because it can be used in applications in general in integrated optics. Some of these possible applications include tunable resonant cavities for lasers development, instrumentation for nonlinear optical devices and optical reflectors in selected ranges of the electromagnetic spectrum.

4. Conclusions
The results of this research have revealed that a variation, specifically a reduction, of the structural parameters of a two-dimensional photonic crystal with an embedded array of optical micro-cavities induces a shift towards blue on the maximum peak of the optical reflectance and the photonics band localization in the frequencies domain. The selectively improving the reflectance of the PhC studied, towards shorter wavelengths we believe has its origin in the introduction of the optical micro-cavities array embedded into the PhC with regular structure and in the variation of the structural parameters that defined the PhC. These results can be useful in future applications of solar cell systems and telecommunications, among others, which can be of great help to increase technological developments.

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