

Photonic Bandgap Expansion and Defect Mode Control in One-Dimensional Graded-Index Si/SiO₂ Photonic Crystals

Ahlam AOUACHIR^{1*}, Khalfallah BENBELGACEM^{1,2}, Abdellatif MAMANOU², Omar BENTOUILA¹

¹ LENREZA Laboratory, Physics Department, University Kasdi Merbah Ouargla, 30000, Ouargla, Algeria

² LRPPS Laboratory, Physics Department, University Kasdi Merbah Ouargla, 30000, Ouargla, Algeria

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One-dimensional photonic crystals (1D-PhCs) have attracted considerable attention owing to their ability to manipulate electromagnetic wave propagation through photonic bandgap (PBG) formation. In conventional structures, the refractive indices of the constituent layers are assumed constant, which limits the flexibility in tailoring their optical response. In this study, a novel 1D-PhC incorporating a layer-to-layer graded refractive index profile and a central defect cavity is proposed and theoretically investigated. The structure consists of alternating silicon dioxide (SiO₂) layers with a fixed refractive index and silicon (Si) layers, whose refractive indices vary discretely according to the layer-to-layer refractive-index grading parameter, Δn . Moreover, a defect layer has been introduced at the center of the structure to generate a localized resonant mode within the PBG. The optical properties of the described structure were analyzed using the Transfer Matrix Method (TMM). The results showed that as Δn increased significantly, the PBG expanded from 393.7 to 747.4 nm, accompanied by a red shift of the defect resonance wavelength from 737.8 to 816.8 nm. However, the resonance line width decreased considerably, which enhanced the quality factor from 10^3 to 5.1×10^4 . It was found that layer-to-layer refractive index grading could be an effective approach for PBG engineering and defect mode control, making the proposed structure a promising candidate for optical filters, resonators, and high-performance photonic devices.

Keywords: photonic crystal, photonic band gap, graded refractive index, defect mode, transfer matrix method.

1. INTRODUCTION

Photonic Crystals (PhCs) are artificial periodic structures designed to control the propagation of electromagnetic radiation [1, 2, 3]. One-dimensional photonic crystals (1D-PhCs) are valued for their simple design and versatility across applications including optical filters, mirrors, and sensors [4, 5, 6]. These structures are characterized by a photonic band gap (PBG), a range of frequencies at which light cannot propagate owing to Bragg interference. The periodicity of the structure is broken by the presence of a defect layer, and localized resonant modes appear in the PBG. These modes are particularly promising for sensing applications due to their strong field confinement and favorable quality factors [6, 7, 8]. Several approaches have been proposed to tailor the optical properties of 1D-PhCs. One approach involves continuous refractive index grading within a layer, described by a spatial function $n(x)$, which significantly affects the photonic band structure [9, 10, 11]. Another approach is to chirp the layer thickness, which can broaden the PBG and improve the omnidirectional reflection [12, 13, 14]. Moreover, graded defect layers were investigated for their application in tuning localized modes within the photonic band gap [15, 16].

Despite these advances, limited attention has been paid to discrete layer-to-layer refractive-index grading, a scheme in which each layer is homogeneous. Still, its refractive

index varies progressively throughout the structure. This approach can be described as follows:

$$n_{2i} = n_2 + i\Delta n, \quad i = 0, 1, 2, \dots, N-1. \quad (1)$$

Such discrete grading provides a practical alternative to continuous gradient profiles while offering enhanced flexibility in PBG engineering.

In this study, we propose a symmetric 1D-PhC with a layer-graded refractive index and a central defect cavity. The structure was analyzed using the Transfer Matrix Method (TMM) to investigate the effect of refractive index grading on PBG and defect modes. The results demonstrate improved tunability and enhanced sensing performance, highlighting the potential of the proposed design for advanced photonic applications.

2. STRUCTURE DESIGN

The proposed one-dimensional photonic crystal (1D-PhC), illustrated in Fig. 1, consists of a symmetric multilayer structure composed of alternating layers of silicon dioxide (SiO₂) and silicon (Si), separated by a central defect cavity. Unlike conventional PhCs, in which the refractive indices of all constituent layers remain constant throughout the structure, the present design introduces discrete layer-to-layer refractive index grading within the silicon layers.

* Corresponding author: A. Aouachir
E-mail: aouachir.ahlem@univ-ouargla.dz

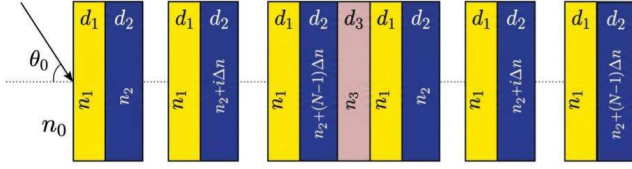


Fig. 1. Schematic illustration of the proposed 1D-PhC with a layer-to-layer graded refractive index and a central defect cavity

The SiO₂ layers possess a constant refractive index, denoted by (n_1), which is calculated using the Sellmeier dispersion relation [17]:

$$n_1 = 1 + \frac{0.6961663 \lambda^2}{\lambda^2 - 684.3^2} + \frac{0.4079426 \lambda^2}{\lambda^2 - 116241.4^2} + \frac{0.8974794 \lambda^2}{\lambda^2 - 9896161^2}. \quad (2)$$

The refractive indices of the silicon layers are discretely graded from one period to another and are denoted by (n_{2i}), according to:

$$n_{2i} = n_2 + i\Delta n, \quad i = 0, 1, 2, \dots, N-1; \quad n_2 = 3.7, \quad (3)$$

where n_{2i} is the refractive index of the (i)-th graded silicon layer; n_2 is the minimum refractive index [18]; Δn is the refractive-index increment between two adjacent silicon layers, and (i) is the sequential index of the graded silicon layers. The parameter (N) denotes the number of graded periods on each side of the central defect cavity, and $n_3 = 1.0003$ denotes the refractive index of the central defect layer.

For constructive Bragg interference to occur at the design wavelength ($\lambda_0 = 800$ nm), the thicknesses of the constituent layers must adhere to the quarter-wave condition.

$$n_i d_i = \lambda_0 / 4, \quad (4)$$

where n_i and d_i denote the refractive index and thickness of the i -th layer, respectively. In this study, the materials of the first and second layers are SiO₂ and Si. Their thicknesses are fixed at: $d_1 = 138$ nm and $d_2 = 54$ nm, respectively. While the defect layer thickness d_3 is designed to satisfy the following conditions:

$$d_3 = d_1 + d_2. \quad (5)$$

to introduce a localized resonant state within the PBG.

In the present theoretical analysis, the refractive indices of the constituent layers are considered in the lossless approximation; therefore, only the real part of the refractive index is used in the calculations. In general, the refractive index of an absorbing material is complex and can be expressed as ($\tilde{n} = n + ik$), where (n) is the real part and (k) is the extinction coefficient associated with optical absorption. The inclusion of the imaginary component would introduce additional optical attenuation within the silicon layers, which may reduce the transmission intensity and affect the resonance linewidth and, consequently, the quality factor. Accordingly, the results presented in this work represent the intrinsic lossless optical response of the proposed graded photonic crystal and are intended to isolate the effect of the discrete layer-to-layer refractive-index grading on the photonic bandgap and defect-mode characteristics.

3. METHODOLOGY

The optical properties of the proposed 1D-PhC were examined using the Transfer Matrix Method (TMM). The theoretical framework and numerical implementation of the TMM were detailed in our previous study [19]; here, only the essential components pertinent to the current structure are summarized.

The global transfer matrix of the structure is represented as:

$$M_{\text{tot}} = \left(\prod_{i=0}^{N-1} M_1 M_{2i} \right) M_3 \left(\prod_{i=0}^{N-1} M_1 M_{2i} \right). \quad (6)$$

The transmission coefficient is calculated as follows:

$$T = 1/|M_{11}|^2. \quad (7)$$

The PBG was discerned from the transmission spectrum as the wavelength range where transmission was significantly suppressed. Furthermore, the characteristics of the defect mode are analyzed with respect to the resonance wavelength, full width at half maximum (FWHM), and the quality factor, which is defined as:

$$Q = \frac{\lambda_r}{FWHM}. \quad (8)$$

All simulations were performed over a predefined wavelength range using a custom numerical code based on the TMM formalism. The effect of the grading parameter (Δn) is systematically investigated to evaluate its influence on the PBG and defect mode properties.

4. RESULTS AND DISCUSSION

The transmission spectra of the proposed 1D-PhC were calculated for $\Delta n = -0.4, -0.3, -0.2, -0.1, 0, 0.1, 0.2, 0.3, 0.4$ to investigate its effect on the PBG and defect-mode characteristics. For the maximum positive grading ($\Delta n = 0.4$) with $n_2 = 3.7$ and $N = 5$, the graded silicon layers exhibit refractive indices of 3.7, 4.1, 4.5, 4.9, and 5.3, giving $n_{\text{max}} = 5.3$. These values are considered within the theoretical framework as an effective engineered refractive index profile for examining the optical effects of discrete layer-to-layer grading.

Fig. 2 shows the transmission spectra of the proposed 1D-PhC for three different values of the refractive index grading, namely $\Delta n = -0.2, 0$, and 0.2 . The case $\Delta n = 0$ corresponds to a conventional structure with uniform silicon layers. Whereas $\Delta n = -0.2$, and $\Delta n = 0.2$ represent negatively and positively graded configurations, respectively. The analysis of structures with and without refractive index grading indicated that the optical behavior of PhC is influenced significantly by the presence of grading. In the standard structure, where $\Delta n = 0$, the PBG width is approximately 611.647 nm. The introduction of a positive grading of $\Delta n = 0.2$ results in an expansion of the PBG, whereas a negative grading of $\Delta n = -0.2$ leads to a reduction in the PBG width. This pattern demonstrates that refractive index grading serves as an effective method for adjusting the spectral width of the forbidden band. The optical parameters extracted from the calculated transmission spectra for different values of the refractive index grading parameter are summarized in Table 1. The table provides the numerical values of the resonance

wavelength, PBG width, full width at half maximum (FWHM), and quality factor, which are subsequently analyzed and illustrated in Fig. 3.

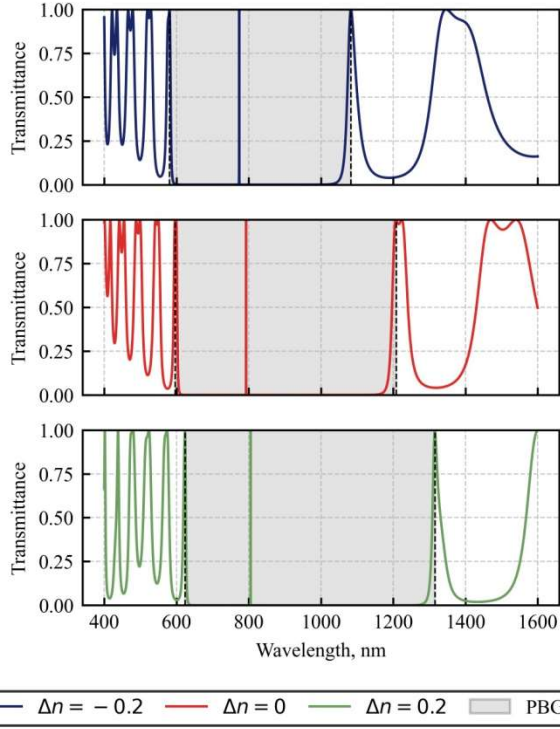


Fig. 2. Influence of the grading parameter Δn on the transmission spectra of the 1D-PhCs

Table 1. Evolution of the optical response parameters with the refractive index grading parameter

Δn	λ_{max} , nm	FWHM, nm	Q factor	PBG, nm
-0.4	737.798	0.7351	1003.73	393.721
-0.3	758.798	0.3302	2297.66	446.007
-0.2	773.627	0.1550	4990.04	502.326
-0.1	784.378	0.0799	9822.91	557.681
0	792.62	0.0460	17232.94	611.647
0.1	799.373	0.0297	26881.16	653.742
0.2	805.321	0.0216	37221.9	691.808
0.3	810.977	0.0176	46093.12	722.89
0.4	816.806	0.0160	50985.29	747.415

A comprehensive assessment of the grading effect is shown in Fig. 3, which summarizes the evolution of the PBG width, resonance wavelength, full width at half maximum (FWHM), and quality factor as a function of Δn . The refractive index grading is an effective tuning parameter for controlling the optical response of the structure.

As shown in Fig. 3 a, the resonance wavelength exhibits a monotonic increase with the grading parameter Δn , indicating a continuous red shift of the defect mode. Particularly, the resonance peak shifts from 737.798 nm for $\Delta n = -0.4$ to 816.806 nm for $\Delta n = 0.4$, corresponding to a total shift of approximately 79 nm. This behavior is attributed to the increase in the effective optical path length of the multilayer structure as the refractive indices of the Si layers progressively increase. Consequently, the phase accumulation within the structure increases, leading to resonance at longer wavelengths. The nearly monotonic dependence of the resonance wavelength confirms the

effectiveness of layer-to-layer refractive index grading for precise spectral tuning of defect modes.

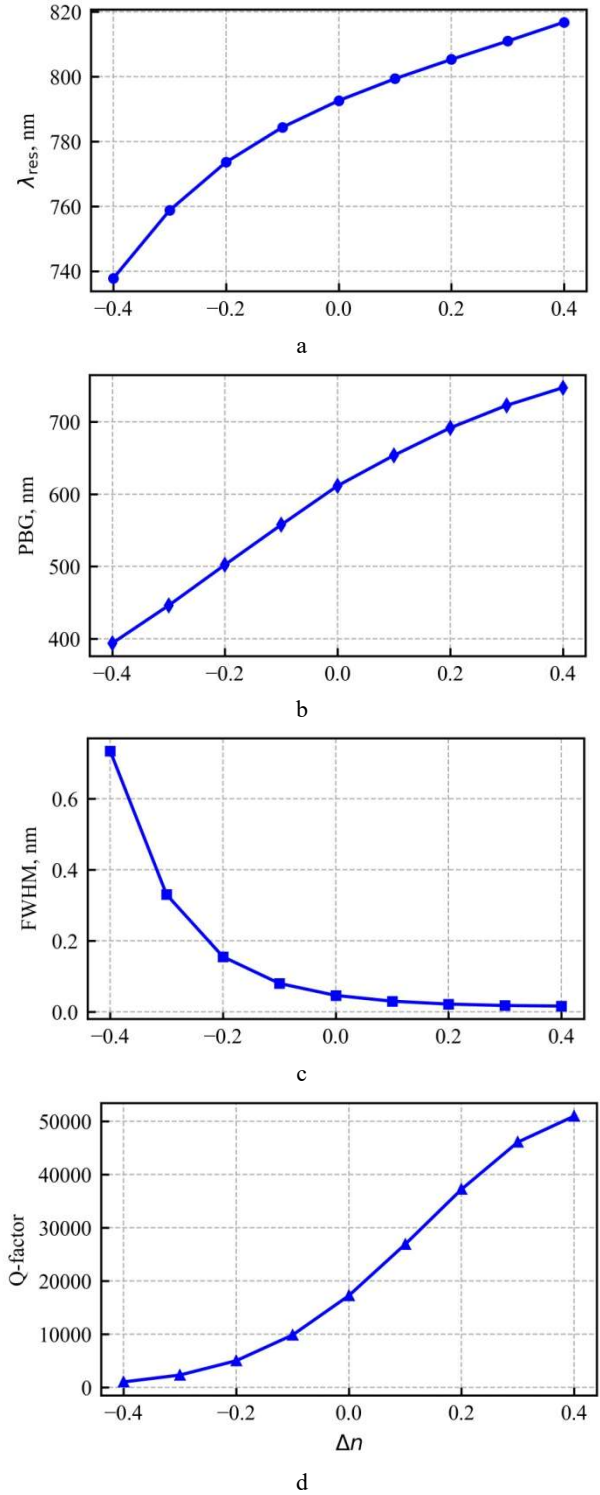


Fig. 3. Optical response width as a function of the refractive index grading parameter

The influence of the grading parameter on the PBG width is illustrated in Fig. 3 b. A significant widening of the PBG was observed as Δn increased from -0.4 to 0.4. Quantitatively, the PBG width increased from 393.721 nm, to 747.415 nm corresponding to an enhancement of approximately 89.8%. This pronounced expansion is attributed to the increased refractive index contrast induced by layer-to-layer grading, which strengthens the Bragg

reflection mechanism within the periodic structure. Consequently, the optical impedance mismatch between the adjacent layers becomes more pronounced, enhancing the multiple-wave interference and improving the confinement of the electromagnetic waves. Consequently, the forbidden spectral region was substantially broadened.

In Fig. 3 c, we observe a marked decrease in the half-height width (FWHM) of the defect resonance with increasing Δn , indicating a gradual improvement in spectral selectivity. The FWHM dropped from 0.7351 to 0.0160 nm, when Δn varied from -0.4 to 0.4. This marked narrowing of the resonance peak results from stronger optical confinement within the defect cavity caused by the refractive-index gradient. The enhanced Bragg mirrors surrounding the cavity reduce radiative losses and suppress energy leakage, leading to a sharper and more focused resonance pattern.

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Consequently, as shown in Fig. 3 d, the quality factor exhibits a strong dependence on the grading parameter, increasing significantly as Δn increases. The calculated Q-factor increased from the order of 10^3 for low grading values to approximately 5.1×10^4 at $\Delta n = -0.4$, demonstrating a remarkable enhancement in the resonant performance of the proposed structure. This enhancement was a direct consequence of the reduced line width and improved energy confinement inside the defect layer. The increasing refractive index contrast strengthens the PBG mirrors, thereby increasing the storage time of electromagnetic energy and producing highly stable resonant modes.

Overall, the obtained results clearly demonstrate that layer-to-layer refractive index grading provides an additional powerful degree of freedom for PBG engineering and defect mode optimization. By appropriately tuning Δn , it is possible to simultaneously control the resonance wavelength, broaden the PBG, suppress the resonance line width, and significantly enhance the quality factor. These combined effects highlight the strong potential of the proposed structure for high-performance optical filters, resonators, and photonic-device applications.

4. CONCLUSIONS

In this work, a one-dimensional photonic crystal (1D-PhC) incorporating a layer-to-layer graded refractive-index profile and a central defect cavity was proposed and analyzed using the Transfer Matrix Method (TMM). The influence of the refractive-index grading parameter (Δn) on the photonic band gap (PBG) and defect-mode characteristics was systematically investigated.

Compared with previously reported graded one-dimensional photonic crystals, which mainly rely on chirped thickness modulation [10] or continuous refractive-index grading within individual layers [15], the proposed structure employs a discrete layer-to-layer refractive-index grading while maintaining constant layer thicknesses throughout the multilayer stack. This design strategy provides an additional

degree of freedom for tailoring the optical response without altering the structural geometry, demonstrating that efficient PBG engineering and defect-mode optimization can be achieved solely through refractive-index modulation between successive layers.

The results reveal that increasing the grading parameter Δn significantly alters the optical characteristics of the proposed structure. Specifically, the PBG broadens as Δn increases, indicating enhanced Bragg reflection and stronger optical confinement, while the defect resonance undergoes a continuous redshift, providing an effective mechanism for spectral tuning. In addition, the resonance linewidth decreases remarkably, resulting in a substantial enhancement of the quality factor from 10^3 to 5.1×10^4 . Meanwhile, the transmission peak remains close to unity for all investigated grading conditions, confirming that high transmission efficiency is preserved despite the introduction of refractive-index grading.

Overall, the proposed layer-graded photonic crystal combines a broadened photonic band gap, excellent optical confinement, a narrow resonance linewidth, and a remarkably high quality factor. These results demonstrate that discrete layer-to-layer refractive-index grading represents an effective and versatile approach for engineering the optical response of one-dimensional photonic crystals, making the proposed structure a promising platform for high-performance optical filters, resonators, and photonic sensing devices.

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