High Precision and Accuracy Temperature Sensor Design Using 1 Dimensional Defect Layered Photonics Crystals Composed of Air, TiO_2, InP, and Ta_2O_5 Layers

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A B S T R A C T

First observed by Lord Rayleigh in 1887, the work of Eli Yablonovitch and Sajeev John in 1987 on photonics crystals is truly a revolution in physics. These crystals have many applications in many fields such as nanotechnology, solar cells and color displays in the era of modern civilization. Because these crystals only transmit waves within certain band gaps, they are widely used in electromagnetic applications. With these manipulations over the band gaps and transmittance, full control over electromagnetic waves can be achieved. Similar to other materials, these periodic structures are affected to temperature changes.

Key words: *Photonics Crystals Defect Modules High Sensitivity Temperature Sensor*

1 Introduction

In order to fully understand the characteristics of the periodic structure of photonics crystals formed by dielectric and superconductors, it is beneficial and crucial to examine the foundations of photonics crystals. Based on these foundations, the analysis of band gaps can also be carried out and examined more deeply.

1-1 Photonics Crystals

The dielectric periods, first observed by Lord Rayleigh in 1887, led to a complete revolution in photonics crystals in physics as a result of the work of Eli Yablonovitch and Sajeev John in 1987. In fact, photonics crystals are medians with dielectric properties that are periodically arranged [1].

This means that they are actually made up of dielectric and superconducting layers in an arranged sequence. Made using not only dielectrics, but also superconductors, semiconductors and metals, these periodic systems have crucial features that make them different. Because of these periodic structures, photonics crystals pass only certain frequencies and wavelengths in the electromagnetic spectrum such as light, preventing the spread of other wavelengths. The ranges in which these electromagnetic waves cannot pass are called band gaps.[2] Therefore, with this feature of photonic band gaps, a complete control can be established over electromagnetic spectrum (Fig. 1).

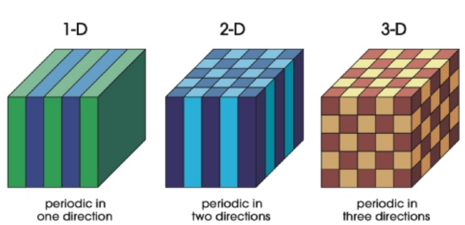

Fig. 1: 1D, 2D and 3D Periodic Photonic Crystal Topologies without Defect Modules [5]

As shown in Figure (1), photonic crystal structures can be created in 1 1D, 2D and 3D. And since only 3D periodic structures of these different topologies contains a versatile and all directional periodic structure, only 3D photonic crystal structures feature band gaps in all 3 directions[2].

1-2 Defect Modules

From the fundamental perspective, not all photonic crystals have to consist of only 2 materials. Essentially, it is possible to transform a perfect photonic crystal into an irregular photonic crystal byinserting or removing a different material called defect layer in certain layers of these dielectric materials that continue periodically.

As illustrated in Figure (2), in fact, there are 2 perfectly periodic dielectric materials in photonic crystals with single defects. On the contrary, a layer of defect is present, which is like a buffer between them. Furthermore, a defective structure can also be obtained by changing the thickness or location of a layer [3] .

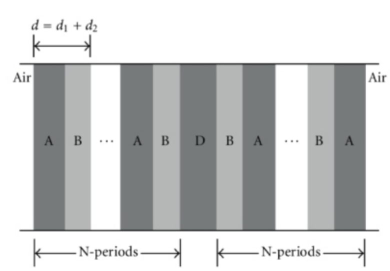

Fig. 2: Single Defect Layered 1D Photonic Crystal Structure [3]

Defect layers also significantly change the bandwidth of a periodic structure and form peak transmission values at certain band gaps where no transmission occurs in normal periodic structures [4]. Moreover, any temperature change in periodic systems can significantly change the band gap ranges in the structure, so that even the smallest temperature changes can be measured.

1-3 Band Gaps

Fundamentally, photonic band gaps occurs on ranges of values were given Maxwell Equations (1), (2), and (3) have no real solution of ~k wave vectors.

$$\vec{\nabla} \times \frac{1}{\varepsilon}\vec{\nabla} \times \vec{H}(\vec{r}) = \left(\frac{\omega}{c}\right)^2 \vec{H}(\vec{r}) \tag{1}$$

$$\hat{\Theta} = \vec{\nabla} \times \frac{1}{\varepsilon}\vec{\nabla} \tag{2}$$

$$\hat{\Theta}\vec{H}(\vec{r}) = \left(\frac{\omega}{c}\right)^2 \vec{H}(\vec{r}) \tag{3}$$

Furthermore, using the Bloch-Floquet Theorem described in (4), the equation (5) can be derived.

$$\vec{H}\,(\vec{r}) = e^{i\cdot\vec{k}\cdot\vec{r}}\vec{H}_{n,\vec{k}}\,(\vec{r}) \tag{4}$$

$$\left(\vec{\nabla} + i\vec{k}\right) \times \frac{1}{\varepsilon}\left(\vec{\nabla} + i\vec{k}\right) \times \vec{H}_{n,\vec{k}} = \left(\frac{\omega_n\left(\vec{k}\right)}{c}\right)^2 \vec{H}_{n,\vec{k}} \tag{5}$$

The value n in (5) is essentially a positive integer, therefore this indicates discrete eigenvalues of n. In such a case, even though n is a continuous function, when it is plotted with varying n values, the specific separations can be observed where no such eigenvalue for n is obtained. These separations, as stated earlier, are essentially the band gaps of the given ~k wave vectors. These band gaps can be represented as in Figure (3).

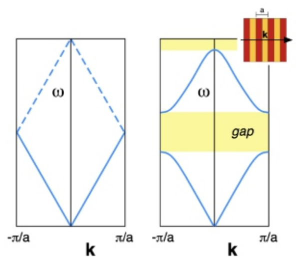

Fig. 3: Band Gap for a 1D Photonic Crystal[2]

2 Purpose and Rationale

This band gap can be manipulated much more effectively with the use of aperiodic and irregular structures obtained by inserting or removing a different superconducting or dielectric material inside the periodic structure, which is fundamentally a defect layer. Because of the thermo optic and thermal expansion effects on defect layers, the structural properties of the defective layers used is highly affected by the environmental temperature differences. The change in temperature changes the refractive index and thickness of the defective layer, resulting in a detectable change in the band gap. By observing this change in the band gap region, temperature change can be measured very precisely with defected photonic crystals. This research project examines the 1D triple defect layered photonic crystal structures of different dielectric and superconducting mixtures and finds the most effective and precise sensor design according to permeability and transmittance in mathematical and simulation-based methods.

3 Literature Review

3.1 Historical Background

In fact, the periodic placement of dielectric materials began to be examined on by Lord Rayleigh in 1887. In Lord Rayleigh's 1917 article "On the Reflection of Light from a Regularly Stratified Medium"[7], he made some determinations on the bandwidth and permeability(transmittance) of 1D dielectric material structures.

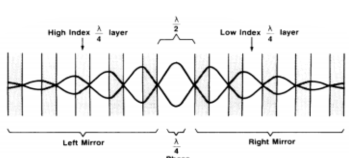

Fig. 4: Fabry-Pérot Interferometer Created with 1D Dialectic Defective Photonic Structure[8]

However, research on photonic crystals did not progress much until Eli Yablonovitch's "Inhibited Spontaneous Emission in Solid-State Physics and Electronics"[8] in 1987 and Sajeev John's "Strong Localization of Photons in Certain Disordered Dielectric Superlattices"[9] in 1987. In these two articles, unlike before, various studies were made in multidimensional geometric topologies. These studies can be illustrated as in Figure 4 and Figure (5).

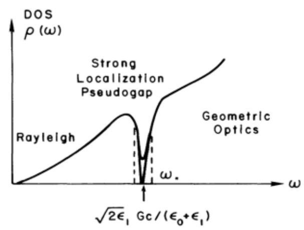

Fig. 5: Photon Density Graph at Low and High Frequencies for An Irregular Super Lattice Structure[9]

3.2 Current State of the Art

The use of photonic crystals in temperature sensor design is actually a subject that has been researched for decades. In 2010, in an article titled "Multicore Photonic Crystal Fiber Thermal Sensors" [10] prepared by a group of researchers at Villanova University in the USA, presented a 1, 2 and 3 core sensor design that can measure the temperature changes with a margin of error of 3.6% for temperatures of <0.2 °C with 0.0036nm K.

In 2015, researchers at Shandong University of Technology published a paper titled "Low-Temperature Sensor Based on One-Dimensional Photonic Crystals with a Dielectric- Superconducting Pair Defect"[11] presenting a temperature sensor design that can measure 0.0096nm K in precision using both dielectric and superconducting defect layers. Similarly, in another article published in 2012, 0.001nm K value of sensitivity was obtained using aperiodic irregular (defective) 1D photonic crystal obtained by removing only one layer from aperiodic system[12].

In a 2018 study titled "Designing a Temperature Sensing Device Using an Defect Based Photonic Crystal"[6] in Turkey, the sensor design obtained using indium antimonite as a defective layer achieved a sensitivity of 0.077nm K.

4 Method

First of all, it is necessary to examine the structure of a perfect 1D photonic crystal before examining the structure of a 1D photonic crystal containing irregularities. Therefore, it is crucial and beneficial to make calculations of the periodic part initially, which is essentially the main element of the whole system. In this process it is necessary to represent each layer in the periodic system through an individual matrix. Therefore, calculations can be made using this Transfer Matrix Method(TMM)[12][16].

By using the different combinations of these matrices with each other, it is possible to obtain different photonic crystal structures. To accomplish these combinations, high and low refractive index layers of the regular periodic structure made of 2 materials can be represented as H (High) and L (Low) respectively. Based on this, a perfect periodic structure with only two layers, it can be shown as a periodic order of H L. If this system contains a total of 2N layers, the expression for this 1D photonic crystal is obtained as in equation (6).

$$(H\cdot L)\,(H\cdot L)\,(H\cdot L)\;...\,(H\cdot L)\;(H\cdot L) = (H\cdot L)^N \tag{6}$$

Similarly, for a 1D photonic crystal with only one defect layer D and 2N + 1 layers the periodic order can be represented as equation (7).

$$(H \cdot L) \ldots (H \cdot L)\ (Defect)\ (H \cdot L) \ldots (H \cdot L) = (H \cdot L)^{\frac{N}{2}}\ (Defect)^{1}\ (H \cdot L)^{\frac{N}{2}} \tag{7}$$

The matrices can be defined for the transfer matrix of layers containing high refractive index as MHigh, low refractive index as MLow, and defect layers as MDefect. From here, transfer matrices can be expressed as multiplication of "D" dynamic and "P" propagation matrices. These expressions
are written as equation (8).

$$\begin{aligned} M_{High} &= D_{High} \cdot P_{High} \cdot D_{High}^{-1} \\ M_{Low} &= D_{Low} \cdot P_{Low} \cdot D_{Low}^{-1} \\ M_{Defect} &= D_{Defect} \cdot P_{Defect} \cdot D_{Defect}^{-1} \end{aligned} \tag{8}$$

Each D dynamic matrices represented as equation (8) can be written as equations described in (9). Furthermore, each P propagation matrix can be represented as equation (10). In equation (10), ~ k refers to the wave vector described in equation (5), n refers to the refractive index of the material selected for the layer, and d refers to the thickness of the layer. Similarly, shows the phase in the selected layer.

$$D_\alpha = \begin{pmatrix} 1 & 1 \\ n_\alpha \cos\Theta_\alpha & -n_\alpha \cos\Theta_\alpha \end{pmatrix} \Rightarrow \text{If } \vec{E} \text{ electric field vector is perpendicular to the propagation}$$

$$D_\alpha = \begin{pmatrix} \cos\Theta_\alpha & \cos\Theta_\alpha \\ n_\alpha & -n_\alpha \end{pmatrix} \Rightarrow \text{If } \vec{H} \text{ magnetic field vector is perpendicular to the propagation}$$

$$\alpha \equiv High,\ Low,\ Defect$$

$$\begin{aligned} P_\alpha &= \begin{pmatrix} e^{i\phi_\alpha} & 0 \\ 0 & e^{-i\phi_\alpha} \end{pmatrix} \\ \phi_\alpha &= k_\alpha d_\alpha \end{aligned} \tag{9}$$

$$\begin{aligned} k_\alpha &= \frac{2\pi n_\alpha}{\lambda} \\ \phi_\alpha &= \frac{2\pi n_\alpha}{\lambda} d_\alpha \end{aligned} \tag{10}$$

As a result, the transfer matrix defined for a single layer is written as equation (11).

$$M_\alpha = \begin{pmatrix} \cos\phi_\alpha & \frac{-i}{n_\alpha}\sin\phi_\alpha \\ -in_\alpha \sin\phi_\alpha & \cos\phi_\alpha \end{pmatrix} \tag{11}$$

Since this research project examines 1D photonic crystals made using 3 defective materials, the transfer matrix MT defined for the definition of the whole crystal can be done with equation (12).The coefficient of transmittance can be calculated as equation (13).

$$M_{Total} = (M_{High} \cdot M_{Low})^{\frac{N}{2}} (M_{Defect_1} \cdot M_{High} \cdot M_{Defect_2} \cdot M_{Low} \cdot M_{Defect_1}) \\ (M_{High} \cdot M_{Low})^{\frac{N}{2}} \tag{12}$$

$$T = \frac{4}{(M_{T_{11}} + M_{T_{22}})^2 + (M_{T_{12}} + M_{T_{21}})^2} \tag{13}$$

As shown in equation (12) 4 materials will be used in this research project to calculate the matrix operations. As shown in equation (9) and (10) the thickness d and refractive indices n of these selected materials must be determined in order to calculate the matrices. Finally, the Python programming language, NumPy library, and the Matplotlib library were used to calculate and visualize the expressed matrix operations in this project.

5 Results

As stated in the method section, the sensor design on which this research project is concentrated fundamentally consists of 4 different materials in nanoscale. While 2 of these materials continue periodically, the other 2 are selected only for layers of irregularity, defect layers. Since the selected periodic materials will form a basis over the photonic crystal structure, they are crucial for this project. Therefore, in this perspective, the thickness and refractive index of the selected materials should be taken into account.

Table (1): Determination of Periodic High and Low Index of Refraction Dielectric Layers

Material Name	Chemical Formula	Index of Refraction n_α	Thickness d_α nm	$n_\alpha \cdot d_\alpha$ nm
Air	*N/A*	*1.0*	*1110.7*	*1110.7*
Titanium Dioxide	TiO_2	*3.83*	*290*	*1110.7*

In order for the experiment to function properly and consistently, the two selected materials must have the same result when their thickness and their refractive indices are multiplied. At the same time, the sensor should take up as little space as possible, but in doing so should be able to give the greatest differentiation in the refractive index. Air is preferred for the low refractive index "L" because the air has a low in refractive index, and it is easy to use. Similarly, Titanium Dioxide was preferred for the high refractive index "H" layer because it demonstrates a high refractive index in a thin layer. The total transfer matrix for a 12-layer periodic system consisting only of Air and Titanium Dioxide can be shown with equation (14).

$$M_{Total} = (M_{TiO_2} M_{Air})^6 \tag{14}$$

The refractive indices of the titanium dioxide layer and air layers ($nTiO_2$ and nAir respectively) and the thickness of these layers (nHava and nHava) are given in Table 1. Based on this data, the transmittance versus wavelength graph in for this perfect periodic system can be drawn as in Figure (6).

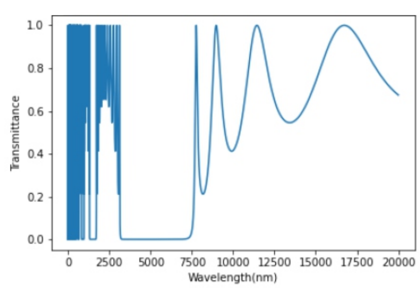

Fig. 6: The Graph of Transmittance VS Wavelength for a Perfect Photonic Crystal with TiO2 and Air Layers

As can be seen from Figure (6), there is a band gap range between approximately 3000 nm and 7500 nm for the perfect 1D photonic crystal with TiO2 and Air layers. No incident electromagnetic wave with the wavelength within the boundaries of this band gap passes through the photonic crystal.

Therefore, there is no transmittance in this region. To more effectively analyze values between 1 nm and 2000 nm, Figure (7) can be used. As can be seen from Figure 7, this 12-layer crystal structure can form repeated band gaps where no transmittance occurs.

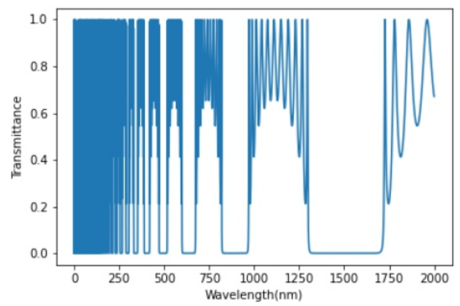

Fig.7: The Zoomed Graph of Transmittance VS Wavelength for a Perfect Photonic Crystal with TiO2 and Air Layers

As mentioned earlier, Figures (6) and (7) are designed for a non-defected periodic crystal. To achieve the structure in equation (12) two defect layers must be selected. This selection will be made from the materials specified in Tables (2)and (3).

Table (2): Determination of Two Defect Layers for the Photonic Crystal

Material Name	Chemical Formula	Index of Refraction n_α	Thickness d_α nm
Silicon Dioxide	SiO_2	1.46	500
Tantalum Pentoxide	Ta_2O_5	2.16	500
Indium Phosphide	InP	3.80	500

Table (3): Thermal Expansion and Thermo-optic Effect Coefficients of Materials on Table (2)

Material Name	Chemical Formula	Thermal Expansion Coefficient α $(\frac{1}{K})$	Thermo-optic Coefficient β $(\frac{1}{K})$
Silicon Dioxide	SiO_2	1.46	500
Tantalum Pentoxide	Ta_2O_5	2.16	500
Indium Phosphide	InP	3.80	500

The materials contained in Tables (2) and (3) which has a high thermal expansion coefficient show a much greater expansion when exposed to the same temperature change as others. Therefore, since the refractive index of Tantalum Pentoxide, Ta2O5, at 500 nm thickness is higher and the thermal expansion coefficient is much higher than other materials, it has been selected for the defect layer Defect2. Similarly, due to its high refractive index and thermo-optical coefficient, Indium Phosphide InP, it was selected for the Defect1 defect layer. As a result, the transfer matrix shown in equation (15) was obtained.

$$M_T = (M_{TiO_2} \cdot M_{Air})^3 (M_{InP} \cdot M_{TiO_2} \cdot M_{Ta_2O_5} \cdot M_{Air} \cdot M_{InP}) (M_{TiO_2} \cdot M_{Air})^3 \quad (15)$$

Based on the matrix shown in the equation (15), the graph in Figure (8) can be calculated. Compared to Figure (6), it can be understood that there is transmittance between 3000-7500 nm, which was the band gap for Figure 6. Moreover, Figure 9 is obtained for the range of 3000-7500 nm to further analyze the transmittance values.

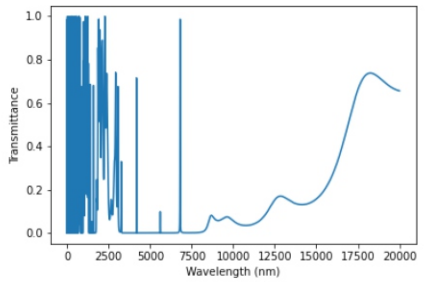

Fig. 8: The Graph of Transmittance VS Wavelength for a Defected Photonic Crystal With TiO2 and Air Periodic and InP and Ta2O5 Defective Layers

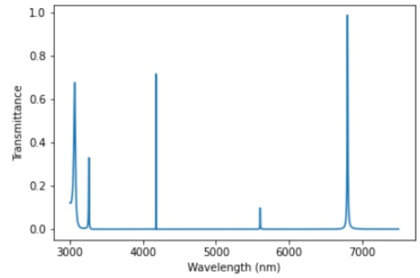

Fig. 9: The Zoomed Graph of Transmittance VS Wavelength for a Defected Photonic Crystal with TiO2 and Air Periodic and InP and Ta2O5 Defective Layers

Based on Figure (9), it is possible to design a temperature sensor that can operate within wavelengths of 5600-7500 nm. For this temperature sensor, the defect layers of InP and Ta2O5 are used. Furthermore, it would be possible to calculate the precision value from the Figure (9). To calculate this, it is needed to model how thickness and refractive index of the material changes under a temperature change. Finally, because the refractive index and thickness is changing, the transmittance changes. To calculate the precision, the shift in transmittance due to the temperature change should be modeled. In order to model this change, it is first necessary to use the Thermal Expansion Coefficient() and Thermo-Optical Coefficient() in Table 3. To model the change, the equations (16) and (17) are used for this.

$$d = d_0 (1 + \alpha \Delta T) \quad (16)$$

$$n = n_0 + \beta \Delta T \quad (17)$$

The new graphic representing the temperature change using the equations in (16) and (17) is shown in Figure (10).

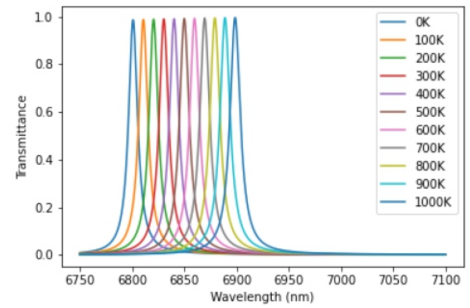

Fig. 10: The Graph of Transmittance VS Wavelength for a Defected Photonic Crystal with TiO2 and Air Periodic and InP and Ta2O5 Defective Layers With Varying Temperature

The sensitivity of the sensor proposed in this article can be found by calculating the temperature dependent change of peak wavelengths in the graph in Figure (10). The temperature-related change of peak wavelengths is shown in Figure (11). By calculating the slope of the graph in Figure (11), a precision value of the sensor is obtained as 0.0978 nm K , which is a more precise value than the sensors presented in all research mentioned at the current level. This proposed state-of-the-art sensor design presented with this research project is given in Figure 12. Considering the melting temperatures of solids used(TiO2, InP, and Ta2O5 respectively), this proposed sensor has can work up to 1335.15 K which is the melting point of InP.

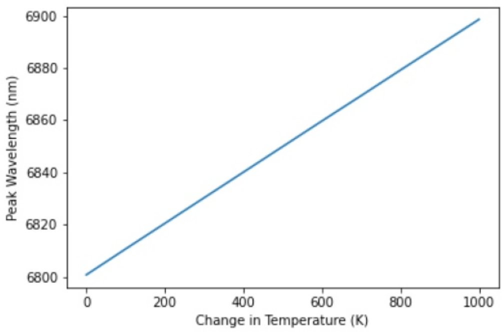

Fig.11: The Graph of the Proposed Sensor's Peak Wavelength VS TemperatureChange

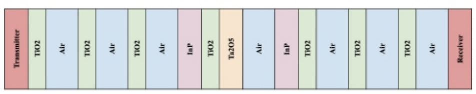

Fig. 12: Proposed Sensor Structure with 0.0978 nm/K Precision

6 Conclusion

The new state-of-the-art crystal proposed by this research article consists of Air, TiO2, InP, and Ta2O5 layers. It has a sensitivity value of 0.0978 nm/K , which is the most precise and wide measurement ranges ever calculated. This value is a sensitivity far beyond the other values specified at the current level. Moreover, it has a much wider working range with a maximum operating temperature of 1335.15 K. This proposed sensor has a width of 11.3 m which can be used for temperature monitoring on patients for intelligent diagnostics.

In this research project, a 1D photonic crystal temperature sensor with 3 defect layers was designed using mathematical calculations. However, due to the Covid-19 pandemic, calculations were made using only computer simulations. Therefore, this project was developed with mathematical simulations. Its performance in the real laboratory environment is an important topic of discussion. The production and testing of this sensor proposed in this research project will prove firsthand evidence on the accuracy of the project's thesis. For this reason, it is very important to test this sensor in a laboratory environment. Similarly, calculations were made on a 1D photonic crystal in this project. However, the precision of photonic crystals of 2D and 3D shapes can be calculated, produced, and tested for further investigation.

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