

RESEARCH PAPER

Extension of the Transfer Matrix Method for Photonic Band Gap Engineering in Optimized TiO₂ Nanomaterial Bragg Reflectors

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ARTICLE INFO

Article History:

Received 19 May 2026

Accepted 16 July 2026

Published 01 October 2026

Keywords:

Nano-photonics

Nanostructured Bragg Reflector

Photonic Band Gap

TiO₂ Nanoparticles

Transfer Matrix Method

ABSTRACT

XRD confirmed that the TiO₂ nanoparticles were optimized; a multi-layer dielectric mirror was designed using ZEMAX optical simulation software. A high-reflectivity Bragg reflector is presented in the near-infrared spectral range of 1.0-2.0 μm at an incident angle of 89°. The extended Transfer Matrix Method (TMM) analysis of photonic band gap characteristics and optical performance of the proposed structure indicates that the thicknesses of the layers are optimally different from those in the conventional quarter-wave design. The optimized Bragg reflector has reflectivity over a wide wavelength range from 1.3 to 2.0 μm. It is proposed that TiO₂/SiO₂ nanostructured Bragg reflectors may find applications in advanced Nano-photonic devices, optical filters, and near-infrared sensing.

How to cite this article

Katif H., Mahmood Y., Saadoon N., Hamama Y. Extension of the Transfer Matrix Method for Photonic Band Gap Engineering in Optimized TiO₂ Nanomaterial Bragg Reflectors J Nanostruct, 2026; 16(4):4832-4840. DOI: 10.22052/JNS.2026.04.030

INTRODUCTION

At present, Nano-materials stand as the most advanced type of material in scientific knowledge and commercial applications. Inorganic nanoparticles (NPs), including silver, copper, titanium, and zinc, are among the most interesting NPs because of their applications and positive impact against pathogenic microorganisms. Recently, TiO₂ NPs have gained special attention because of their unique optical, electrical, and chemical properties. TiO₂ is an excellent photo catalyst that has been widely used for antibacterial activity due to its high photosensitivity, high efficiency, nontoxic nature, strong oxidizing power, relative cheapness, and chemical stability. In order to enhance the photocatalytic activity, intensive interdisciplinary researches have been made on

TiO₂. It is known that the photocatalytic activity of NPs depends on their crystalline structure, doping, surface area, and hydroxyl group. One of the most significant developments in laser physics was the ultrafast laser technology. The duration of the pulse of the pulse laser is ultra-short, measured in picoseconds (ps) or femtoseconds (fs) [10,11]. An ultrashort pulse optical system reflector needs to have reflection extremely high across the bandwidth of the pulse. Two methods were used to realize an omnidirectional reflector for both normal and oblique light incidents: one was to use thin sheets of gold or silver as mirrors, and the other was to use entirely dielectric materials. Metallic mirrors do not allow light to pass through a dispersive material and maintain the shape of the pulse after reflection; however, their reflection

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is too low for applications that involve ultrashort pulse use [12]. High-intensity, femtosecond pulses can be reflected by metallic reflectors; however, absorption in the metallic reflector leads to damage and eventual destruction of the assembly. Because all-dielectric mirrors have very low losses (less than 0.01%) at optical and infrared wavelengths, they were used over regular metallic mirrors [13]. Most probably Penselin and Steudel used the dielectric high reflection mirror for the first time [14]. They used thicknesses with harmonic progression to make an all-dielectric high-reflecting mirror with reflectivity near 95% and bandwidth of 430–450 nm for Ti: sapphire laser systems [15]. Baumeister and Stone made a basic computer-based method [16], maximize the reflectivity of the multilayer reflector to about 94% over the 1.5–1.6 μm wavelength range. Pelletier et al. [17] reported computer design and improvement of reflectors in 1971. The results showed that ripple appeared in the high reflection zone within 95.5% to 98.8% over a wide spectrum range of 1.0–2.0 μm . Numerical approaches were split into two categories: refinement methods and synthesis methods. The former was said to have better potential in building filter coatings of the specificities complex spectrum, which cannot be designed in the standard ways. The synthesis method used in this paper to arrive at the best

design was ZEMAX optimization operand — Hammer optimization. It is, therefore, the objective of this work to present a design methodology for 1D-photonic wideband omnidirectional reflectors for application in the near-infrared region.

MATERIALS AND METHODS

Design of DBR

It is generally known that a stack of quarter-wave dielectric layers with basic building blocks (HL) or LH that alternately has high and low indices can provide a high reflectivity. This is because the beam reflected from every phase when it reached the front surface, where it combined constructively [18]. The following equation for maximum reflectance and width was presented. The characterize matrix of the basis stack (HL) at an incidence angle of θ in an incident medium of refractive index n_0 is provided by [19] if the refractive index at the thickness of two materials is represented as (n_H, d_H) and (n_L, d_L) respectively.

$$[M] = [M_H] [M_L] \quad (1)$$

At quarter wave length:

$$[M] = \begin{pmatrix} 0 & i\eta_H \\ i\eta_H & 0 \end{pmatrix} \begin{pmatrix} 0 & i\eta_L \\ i\eta_L & 0 \end{pmatrix} = \begin{pmatrix} -\eta_L/\eta_H & 0 \\ 0 & -\eta_H/\eta_L \end{pmatrix} \quad (2)$$

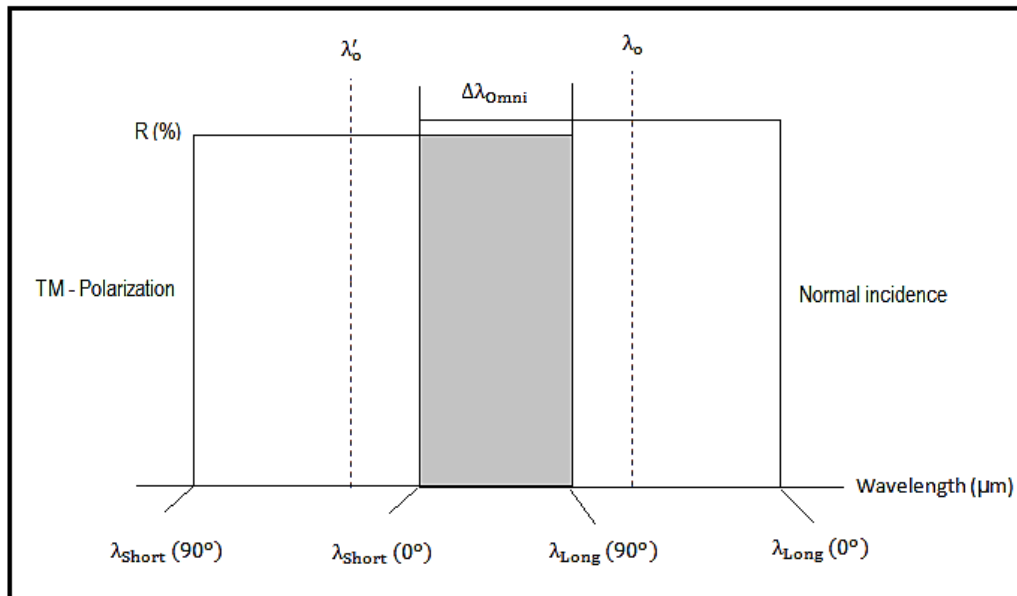


Fig. 1. Omnidirectional optical performance sketch.

Then, the reflectance for TE and TM polarization is:

$$R = \left(\frac{\eta_{0\Lambda} - \eta_{\Lambda}}{\eta_{0\Lambda} + \eta_{\Lambda}} \right) \left(\frac{\eta_{0\Lambda} - \eta_{\Lambda}}{\eta_{0\Lambda} + \eta_{\Lambda}} \right)^* \quad (3)$$

here Λ represents a polarization of TE and TM, ZEMAX, which is based on the elegant transfer matrix approach (TMM) for optical performance analysis, was used in this investigation [20]. As

shown in Fig. 1 and omnidirectional reflection were specified by two factors (Center wavelength λ_c , Omnidirectional bandwidth $\Delta\lambda_{\text{omni}}$).

For optimal reflection (Bragg condition) from a pair of low and high refractive index layers at a specific angle and polarization, the optical thickness at the stop band center must be half wavelength. [21]:

$$\lambda_c/2 = n_L d_L + n_H d_H$$

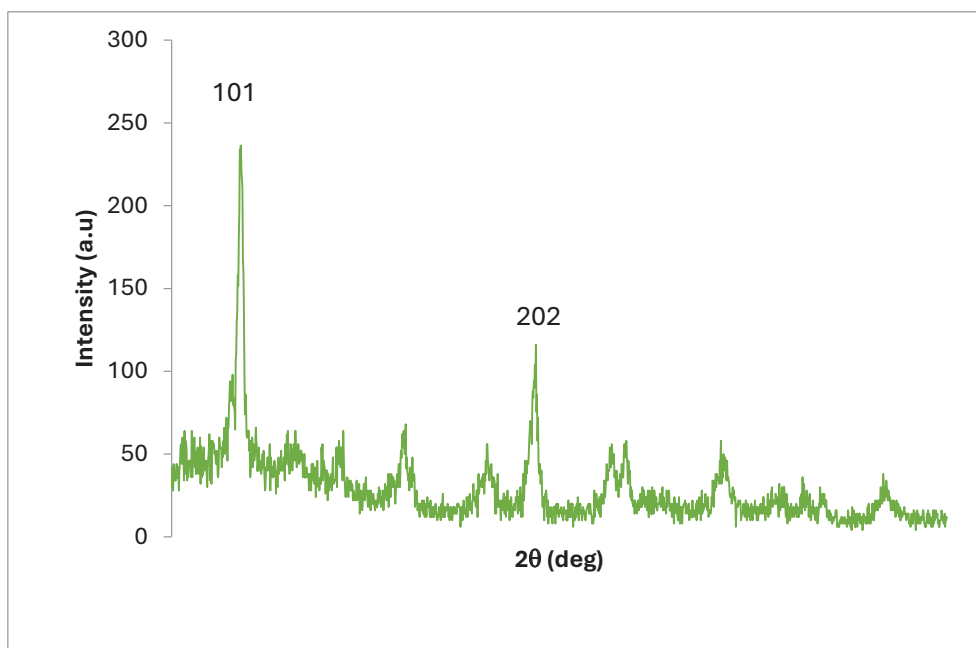


Fig. 2. XRD pattern of TiO₂NPs.

Table 1. The average of the grain size of TiO₂-NPs.

Peak position (2 θ)	Grain size (nm)	Average of grain size (nm)
25.35	14.53	10.45
36.8	16.73	
37.81	9.32	
48.08	11.14	
53.96	9.90	
55.13	6.89	
62.78	7.56	
68.8	8.74	
70.3	9.71	
75.03	10.01	

For TM-polarization light, λ_c is also a very excellent approximation for the reflectance band center [22] in the following:

$$\frac{\Delta\lambda_{\text{Omni}}}{\lambda_c} = 2 \frac{\lambda_{\text{long}}^{\text{TM}}(90^\circ) - \lambda_{\text{short}}^{\text{TM}}(0^\circ)}{\lambda_{\text{long}}^{\text{TM}}(90^\circ) + \lambda_{\text{short}}^{\text{TM}}(0^\circ)} \quad (4)$$

$$\lambda_c = [(1 - \sin^2\theta_0/n_L^2)(1 - \sin^2\theta_0/n_H^2)]^{1/2}$$

Accordingly, the normalized omnidirectional band width $\Delta\lambda_{\text{Omni}}$ with respect to the omnidirectional band's center wavelength λ_c was determined to be [22].

Optimization method

Nearly all numerical techniques for designing optical multilayer coatings rely on the merit function MF, which must reflect the discrepancy between the needed Ti and the calculated spectral characteristic Vi. Merit functions are

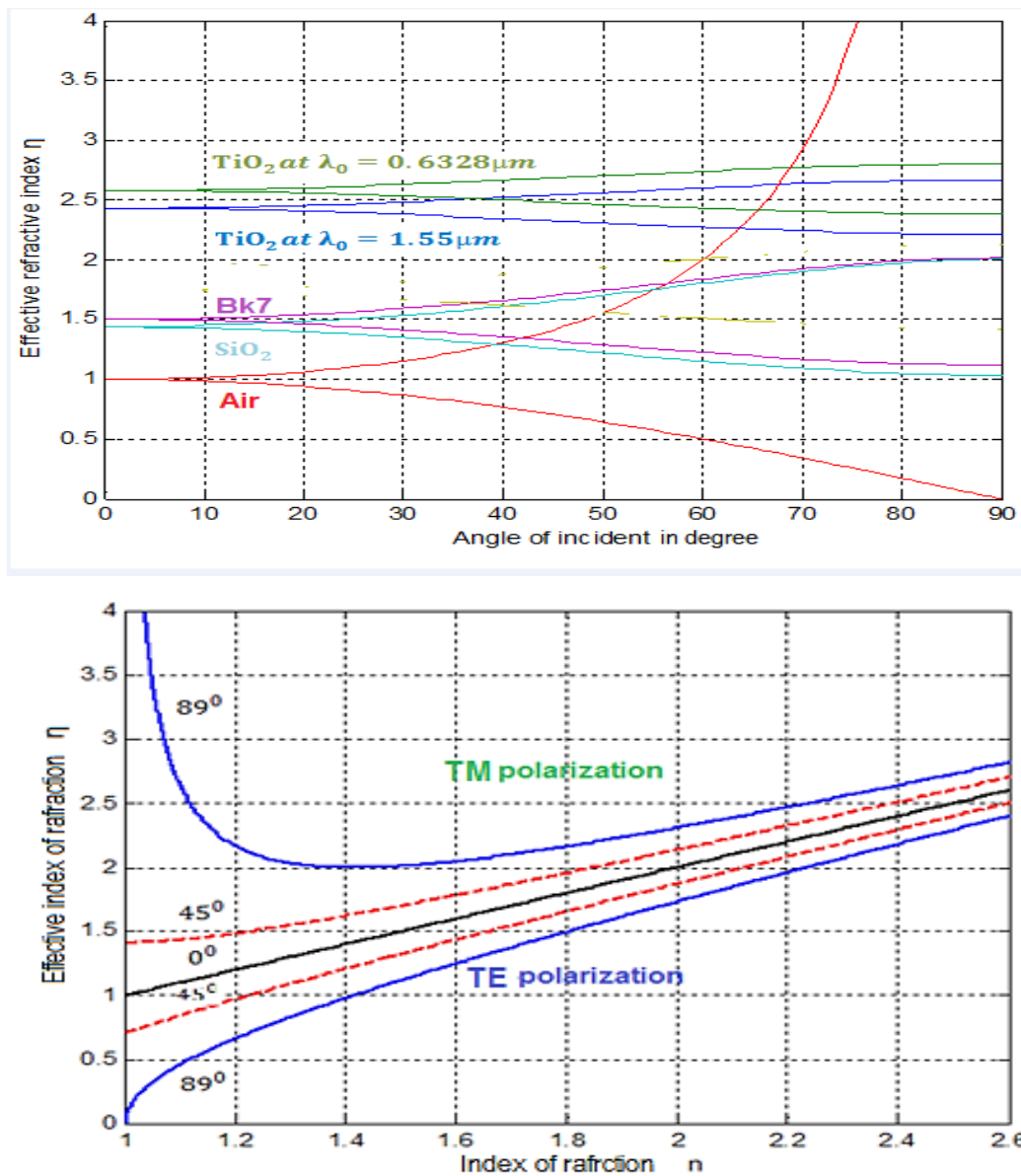


Fig. 3. (a) Effective index η_{TM} and η_{TE} of specific materials (TiO₂, SiO₂) in relation to the light's incident angle. (b) The material refractive indices at various angles of incidence in air are represented by the effective refractive index η_{TM} and η_{TE} .

one-value representations of the system's current performance that guide the course of upcoming computations [23-24]. The square root of the weighted sum of the squares of the difference between each operand's actual and target value for coating determines the merit function. Since this is how the merit function is defined, zero is the ideal value. Because the optimization method will try to minimize the value of this function, the merit function should reflect the desired outcome of the system. The default merit function is not required. Dobrowolski's [25] merit function form is the one that is most commonly used:

$$MF2 = \frac{\sum W_i (V_i - T_i)^2}{\sum W_i} \quad (5)$$

where the operand number (or spreadsheet row number) is indicated by the subscript "i" and "W", "V", and "T" stand for the operand's weight, current value, and target value, respectively [26]. The aforementioned formula makes it very evident that the closer the system performs to the aim, the smaller the MF value. Additionally, all of the layer systems' construction factors affect MF [17], i.e. $MF = MF[n_s, k_s, n_o, (n_r, k_r, d_r), i:1,2,q]$. By using ZEMAX, the optimization method computes but disregards the operand when the weight is zero. This is especially helpful if the value is used as a

check or monitored parameter, or if the result is calculated without a defined objective but may be used elsewhere in the merit function [27]. In this work Hammer Optimization was used. It was a customized algorithm made to look for different designs that are based on the first design. The main purposes of the Hammer method are to avoid local minimum or to confirm that there isn't a better design in the vicinity of the solution space.

RESULTS AND DISCUSSION

XRD Result for TiO₂ Nano-layer

Fig. 2 shows the XRD pattern for TiO₂. The diffraction peaks at 25,50°, 37,89°, 48,40°, 53,98°, 55,29°, 62,65°, 68,47°, 70,57° were indexed to (101), (004), (200), (105), (211), (204), (220), (220) and (215) crystalline planes respectively. This corresponded to the anatase phase of TiO₂ according to JCPDS Card No. (21-1272). The anatase phase of TiO₂ is preferred over rutile and brookite for photocatalytic degradation of organic compounds [28]. Table 1 is shown the average of the grain size of TiO₂-NPs.

Effective index η

Fresnel equations are the main cause of coating polarization dependency at oblique incidence. It is possible to think of each polarization behavior mode as a normal incidence performance of two

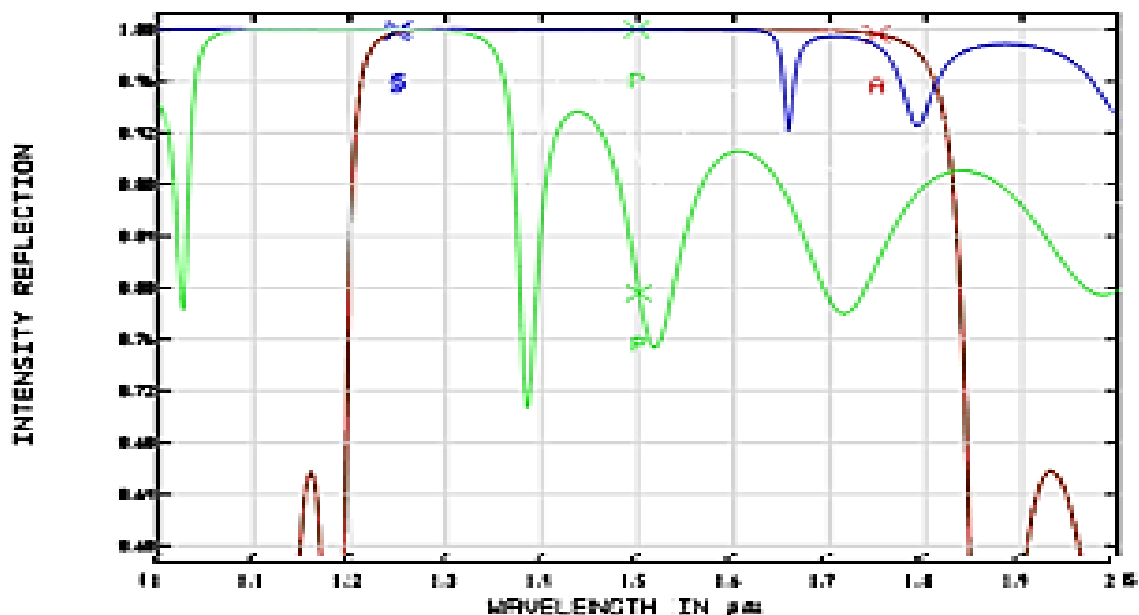


Fig. 4. Reflection vs. wavelength for quarter wave stack for design Air | [LH]10 | glass where $\lambda_0 = 1.55 \mu\text{m}$ at incident angle $\theta_0 = 89^\circ$.

designs. The effective index η was the cause of this. The behavior of η_{TE} and η_{TM} as a function of incidence angle and material refractive indices was shown in Fig. 3. Effective indices for TM and TE polarization are consistently higher or lower (in

the comparable design) than in the actual coating, as seen in Fig. 3. The behavior were shown for three optical commonly used nano- materials (TiO_2 , SiO_2) with indice 2.45,1.44 deposited on glass of index 1.50 at 1.55 μm .

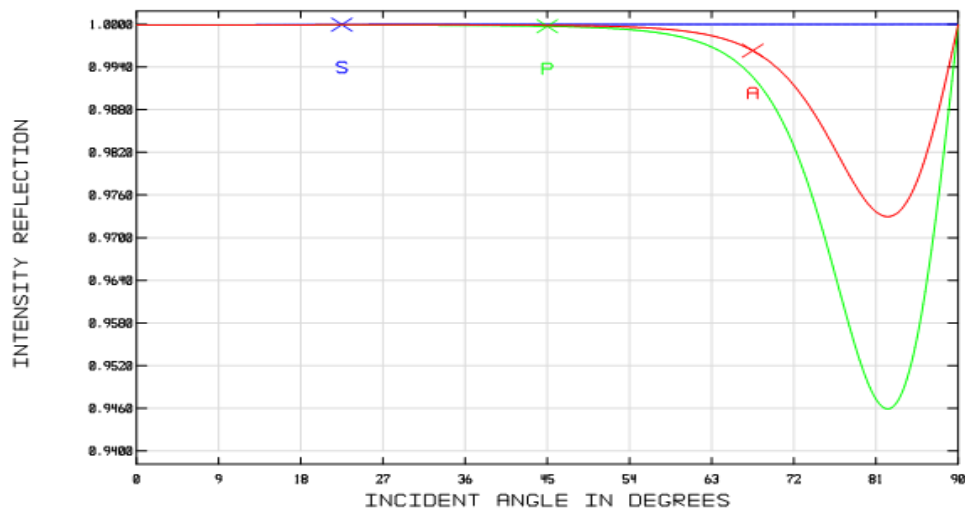


Fig. 5. Reflectance with angle of incident.

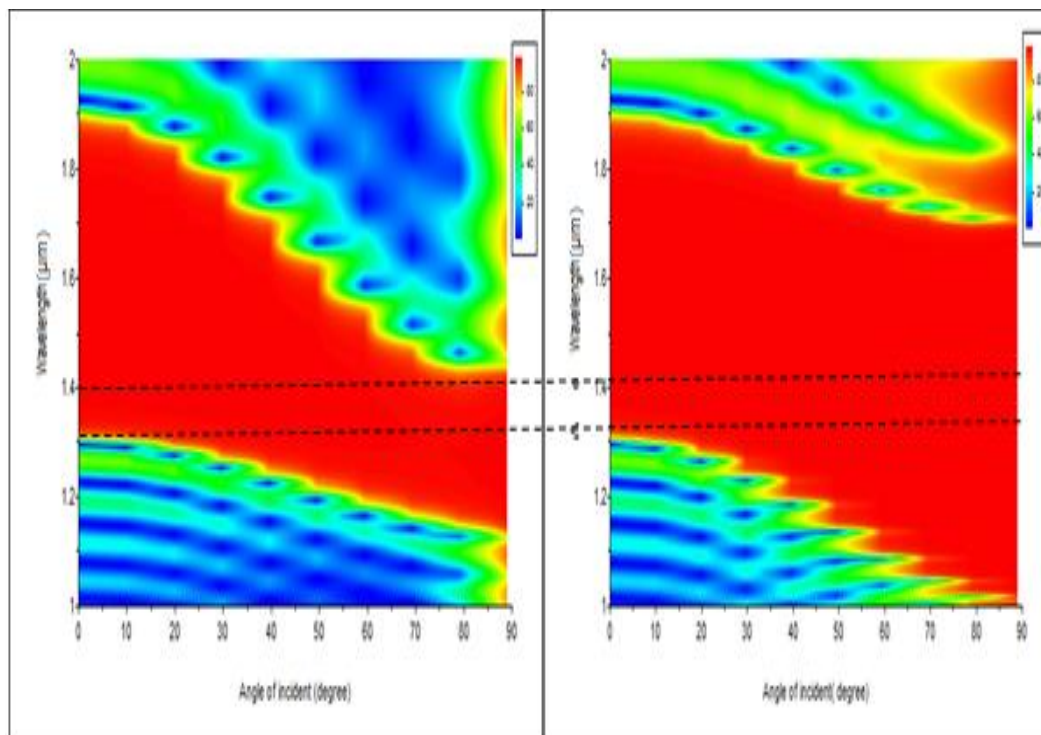


Fig.6. Photonic band gap structure (TODR) of ten pair $\text{SiO}_2/\text{TiO}_2$ for 1.55 μm .

Design Bragg reflector for dielectric material

The two alternating layers with refractive indices $n(\text{TiO}_2)$ and $n(\text{SiO}_2)$ that make up our multilayer, one-dimensional photonic crystal were chosen because they are non-absorbing, isotropic, and homogenous dielectric materials. The reflectance

of TM-polarization light at $\theta=89^\circ$ is greater than 97%, according to the study of the initial design Air | [LH]10 | glass period. The reflectance was plotted against wavelength in Fig. 4. The reflectance 84.8% reflection drop that appears in the near-infrared areas can be interpreted as either “noise”

incidence

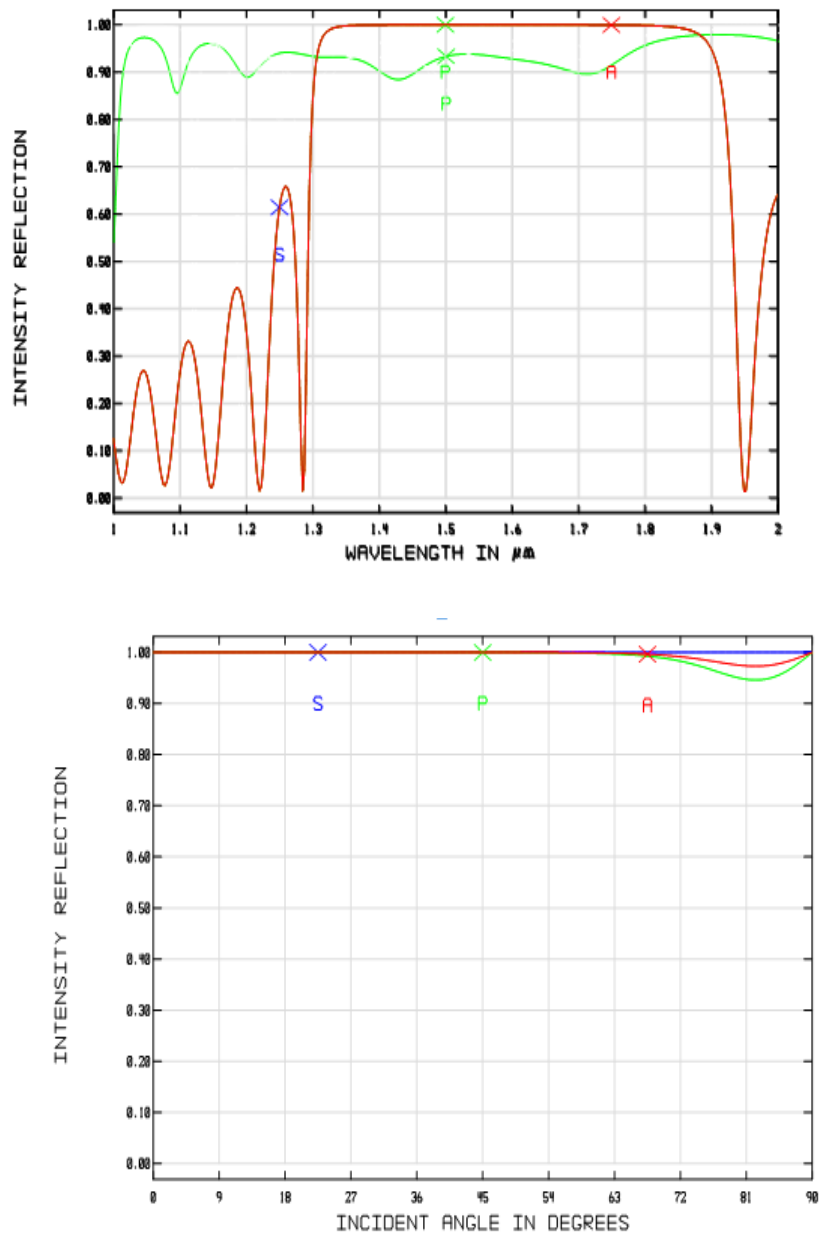


Fig 7. Optimum design for omnidirectional high reflector of infrared region at 89° for: (a) R vs. λ (b) R vs. θ .

or as a narrow photonic bandgap function acting as an omnidirectional narrow band filter

The Fig. 5 is shown between the reflectance and angle of incident ($0^\circ - 90^\circ$) for the design Air | [LH]10 | glass at wave length design $1.55 \mu\text{m}$ in the following.

Infrared region

Fig. 6 represent the conventional photonic band structure for TE and TM polarizations of both design structures:

$$\text{Air}[\text{LH}]^{10}\text{glass} \quad (6)$$

using Teraplot program, the wavelength design $\lambda_0 = 1.55 \mu\text{m}$, which can be obtained by the projection of $R \approx 1$ the spectra are plotted in terms of wavelength and for incident angle θ_0 . The red region represents the forbidden band and the other colored regions the allowed. The area between the two horizontal lines gives the TODR band.

Optimum design Bragg reflector

Numerical approaches were separated into two categories: refinement methods and synthesis methods. The former was described as having a high potential to construct filter coatings of the specificities complex spectrum that cannot be designed in the standard ways [29]. To get to the best design, the ZEMAX optimization operand (Hammer optimization) is used as a synthesis approach in this work. The RTM of the photonic band gap of the original design was extended and improved using ZEMAX optimization operands of coating at (89°) angle of incidence for Air|[LH] 10|Glass. The optimal choice of target, numeric merit function, and operand coating were necessary to achieve such goals like TM-polarization mode with normal incidence curves. Only "thickness multipliers" are discussed as a variable in this section. With design construction, we were able to meet our goal for NIR:

Design #			
Air 0.239322L	0.222700H	0.477447L	
0.197263H	0.044163L	0.220264H	0.153981L
0.555462H	0.126097L	0.550452H	0.255334L
0.067249H	0.161282L	0.169167H	0.537156L
0.213032H	0.081301L	0.149266H	0.234298L
0.534108H	glass		

Shown in Fig. 7 when the reflectance in infrared region behavior was plotted as a function of

wavelength and angle of incidence

It was found that TODR were arrived for NIR regions with photonic band gap ($0.625 \mu\text{m}$). The total optical thickness for before optimization is equal ($5 \mu\text{m}$), then after optimization the total optical thickness for infrared region of design # is ($5.189344 \mu\text{m}$). The Hammer optimization was made cancellation some stack at optimization work for get to optimum design and thus reduced for number of layers, this process needed a high weight to reach the required target. The reflectance versus angle of incidence, for the infrared region where R is approximation $\sim 0.94\%$ at angle of incidence $2\theta = 89^\circ$. Therefore, a remarkable improvement in the performance of omnidirectional reflector for both grazing angle and TM mode of polarization, where the reflected rays from the stack nearly in phase thus, a constructive interference yield within the wavelength infrared range ($1-2 \mu\text{m}$).

CONCLUSION

An omnidirectional 1D-photonic bandgap is very well provided by quarter-wave stacks. When the matching layer thickness was used as the initial design in the optimization process, the omnidirectional reflection band was broadening. Furthermore, the results demonstrate that the suggested optimal approach is not dependent on the specific example being studied and, in certain situations, results in designs that are difficult to solve using other established methods. This technique predicts the ideal thickness that can deviate from the typical quarter-wave design to provide a high performance 1D-photonic band gap, and it is readily adaptable to other materials and wavelengths.

CONFLICT OF INTEREST

The authors declare that there is no conflict of interests regarding the publication of this manuscript.

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