Kingdom of Saudi Arabia
Imam Mohammad Ibn Saud Islamic University (IMSIU)
Faculty of Sciences – Department of Physics

Simulation of one-dimensional photonic crystal

A graduation project submitted to the Department of Physics in partial fulfillment of the requirements for the degree of Bachelor of Science in physics

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بسم الله الرحمن الرحيم

الشكر

أود أن أشكر الله أولاً وقبل كل شيء على بركاته طيلة دراستي وإتمام هذه الرسالة. وصلى الله على سيدنا محمد وعلى آله وصحبه.
كما أود أن أعرب عن خالص امتناني للدكتور عاشور محمد أحمد، مشرفي، على نصيحته المتميزة خلال هذا الجهد الدراسي. كما أود أن أعرب عن خالص امتناني لعائلتي، الذين ألهموني وشجعوني باستمرار. لقد كان تفانيهم وتشجيعهم وإيمانهم الراسخ بي ضروريًا لنجاحي الأكاديمي.

Acknowledgment

I want to thank Allah, first and foremost, for His blessings throughout my studies and the completion of this thesis. May God bless our master Muhammad, his family and all his companions.
I also want to express my sincere gratitude to Dr. Ashour Mohamed Ahmed, my supervisor, for his outstanding advice during this study effort. I also want to express my sincere gratitude to my family, who have continuously inspired and encouraged me. Their devotion, encouragement, and unwavering faith in me have been essential to my academic success.

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الملخص العربي

تلعب البلورات الضوئية حاليًا دورًا مهمًا في العديد من التطبيقات الحديثة. في هذه الدراسة، تم محاكاة انعكاس الضوء في البلورات الضوئية أحادية البعد، والتي تتكون من طبقات متناوبة من السيليكون وأكسيد السيليكون. تم إجراء الحسابات باستخدام طريقة مصفوفة النقل، حيث تم دراسة تأثير عدد الطبقات وسمك المواد على طاقة الفجوة الضوئية. أظهرت النتائج أنه مع زيادة عدد الطبقات، تصبح طاقة الفجوة أكثر وضوحًا وأقل اتساعًا بسبب زيادة تداخل الضوء. كما تبين أنه مع زيادة سمك المواد، تتحرك طاقة الفجوة نحو الأطوال الموجية الأكبر، ويزداد اتساعها وفقًا لقانون براج-سنل. نظرًا لهذه الخصائص الفريدة، يمكن استخدام البلورات الضوئية في تطبيقات متعددة مثل الحساسات الضوئية، والخلايا الشمسية، وغيرها من الأجهزة البصرية المتقدمة.

Abstract

Photonic crystals play a crucial role in various modern applications. In this study, the reflection of light in one-dimensional photonic crystals, composed of alternating layers of silicon and silicon oxide, was simulated. The calculations were conducted using the transfer matrix method to analyze the influence of the number of layers and material thickness on the photonic band gap energy. The results indicated that as the number of layers increased, the band gap energy became more distinct and narrower due to enhanced light interference. Additionally, increasing the material thickness caused the band gap energy to shift toward longer wavelengths while expanding in width, following the Bragg-Snell law. These unique properties make photonic crystals highly suitable for applications in optical sensors, solar cells, and other advanced optical technologies.

Chapter 1

General Introduction

1.1 Electromagnetic spectrum

The electromagnetic wave consists of oscillating electric and magnetic fields that are perpendicular to each other and to the direction of wave propagation. These waves do not require a medium and can travel through a vacuum, which distinguishes them from mechanical waves that need a substance to travel through. Electromagnetic waves are a form of energy propagation through space, and they all travel at the speed of light in a vacuum (approximately 299,792 kilometers per second). The waves vary in wavelength and frequency, and different regions of the spectrum are harnessed for various technologies and applications.

The electromagnetic spectrum encompasses a range of electromagnetic waves categorized by their wavelength or frequency (Figure 1.1):

Radio Waves: These have the longest wavelengths and are primarily used for communication, such as in radio and television broadcasting. They can travel long distances and penetrate through various materials, making them ideal for transmitting information.

Infrared Waves: Associated with heat, infrared waves are emitted by warm objects and are commonly used in applications like remote controls, thermal imaging, and night-vision technology.

Visible Light: This is the range of the electromagnetic spectrum that is visible to the human eye. It spans wavelengths from approximately 400 nanometers (violet) to 700 nanometers (red) as seen in Figure 1.2. Visible light plays a crucial role in various natural processes, such as photosynthesis in plants, and is essential in many technological applications, including lighting and displays.

Ultraviolet Rays: These rays have shorter wavelengths than visible light and are used in sterilization processes, as well as in affecting biological processes, such as the production of vitamin D in the skin. However, excessive exposure to ultraviolet rays can lead to harmful effects, including skin cancer.

X-rays and Gamma Rays: These have very short wavelengths and high frequencies. X-rays are widely used in medical imaging to view the internal structure of the body, while gamma rays are utilized in radiation therapy for cancer treatment due to their ability to kill cancer cells.

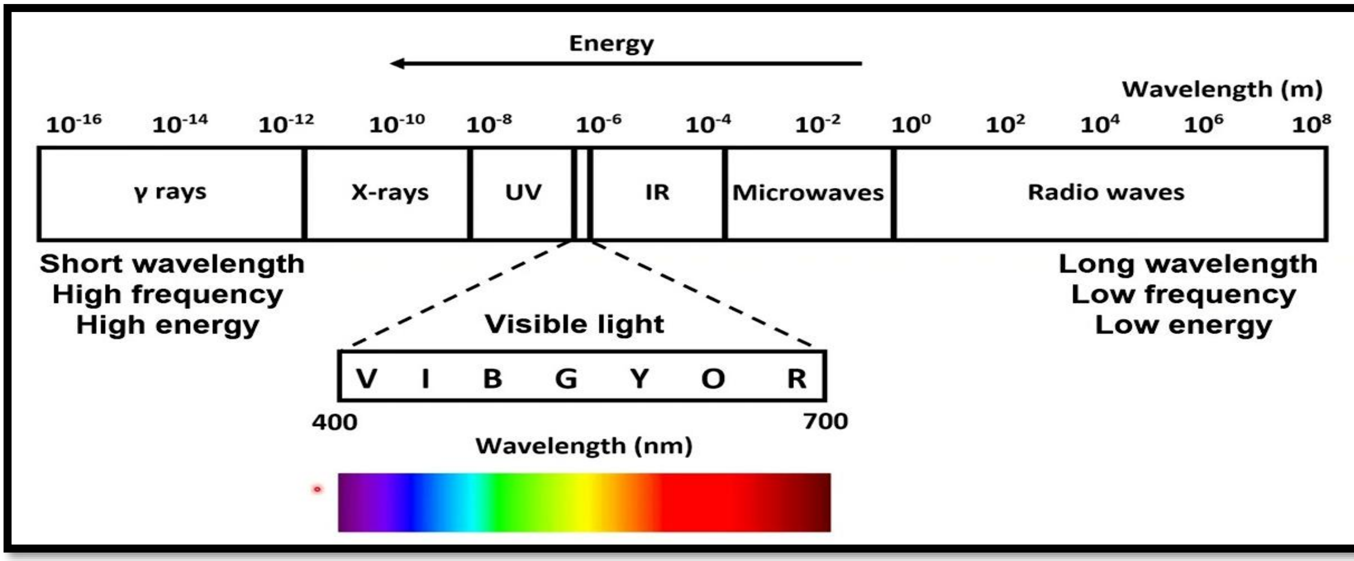
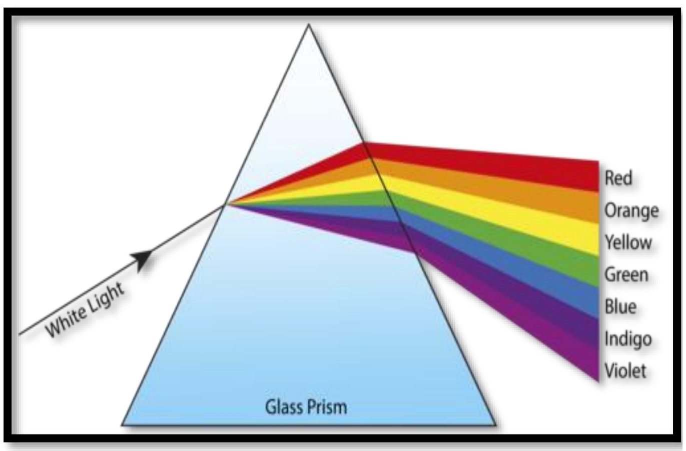


Figure 1.1: Spectrum of electromagnetic waves



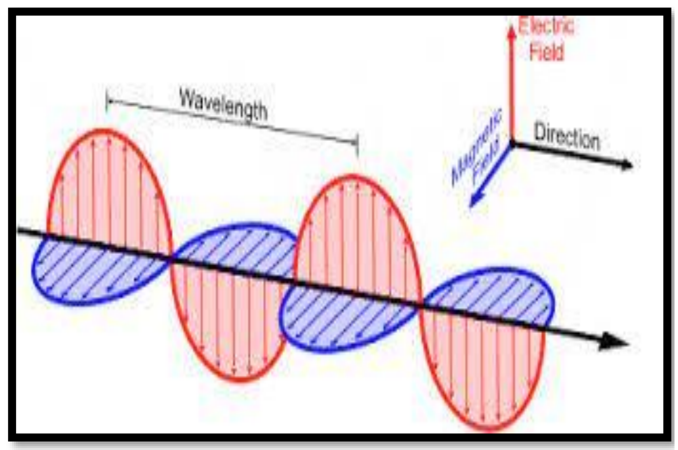


Figure 1.2: (a) Visible light spectrum (b) electromagnetic wave

1.2 Methods of light interaction with matter

Light can interact with matter through various phenomena, as illustrated in Figure 1.3 [1].

Reflection occurs when an electromagnetic wave strikes a surface and bounces back into the same medium instead of passing through. This phenomenon is governed by the Law of Reflection, which states that the angle of incidence equals the angle of reflection.

Example: When light reflects off a mirror, it allows us to see a clear image. The smooth surface of the mirror causes the light waves to reflect uniformly, creating a coherent image.

Refraction is the bending of a wave as it passes from one medium to another with a different density, causing a change in its speed.

Example: A straw in a glass of water appears bent because light changes direction when moving between air and water. The difference in density causes the light to slow down and bend, making the straw look displaced at the water's surface.

This bending is described by Snell's Law, which relates the angles of incidence and refraction to the indices of refraction of the two media:

$$n_1 \cos\Theta_1 = n_1 \cos\Theta_1 \qquad (1.1)$$

where n_1 and n_2 are the refractive indices of the two media, and Θ_1

and Θ_2 are the angles of incidence and refraction, respectively.

Diffraction is the bending of waves around obstacles or through small openings. The degree of diffraction is influenced by the wavelength of the wave and the size of the opening or obstacle.

Example: Hearing sounds around a corner or seeing light spread out when passing through a narrow slit demonstrates diffraction. The wavefronts bend as they encounter obstacles or openings, allowing waves to propagate into regions that would otherwise be shadowed.

Transmission is the process by which a wave passes through a material without being fully absorbed or reflected.

Example: Light passing through clear glass illustrates transmission, as the light waves continue to move through the medium with minimal loss of intensity, allowing us to see through the glass.

Absorption occurs when incoming light interacts with an object, causing its atoms to vibrate and convert the light energy into heat, which is then radiated.

Example: A dark-colored car left in the sun on a hot day will absorb more light energy, resulting in a significant increase in surface temperature. The absorbed light energy is transformed into heat, demonstrating the effect of absorption on the material's temperature.

Scattering occurs when incoming light hits an object and is redirected in various directions. This phenomenon is particularly evident in the scattering of sunlight by gas particles in the atmosphere, which results in the blue color of the sky.

Interference occurs when two or more electromagnetic waves overlap, producing a new wave pattern. This can be categorized into two types:

Constructive Interference: When wave crests align, the amplitude increases, resulting in a brighter or more intense light.

Destructive Interference: When crests align with troughs, the amplitude decreases or cancels out, leading to dimmer or even dark regions.

Example: The colorful patterns observed on soap bubbles are due to the interference of light reflected from different layers of the bubble. The variations in thickness and the wavelength of light cause specific colors to emerge through constructive and destructive interference.

Bragg's Law cite the describes the condition for constructive interference of X-rays scattered by a crystalline material. It is expressed as:

$$n\lambda = d \sin \theta \qquad (1.2)$$

where n is an integer (the order of the reflection), λ is the wavelength of the incident wave, d is the distance between the crystal planes, and θ is the angle of incidence.

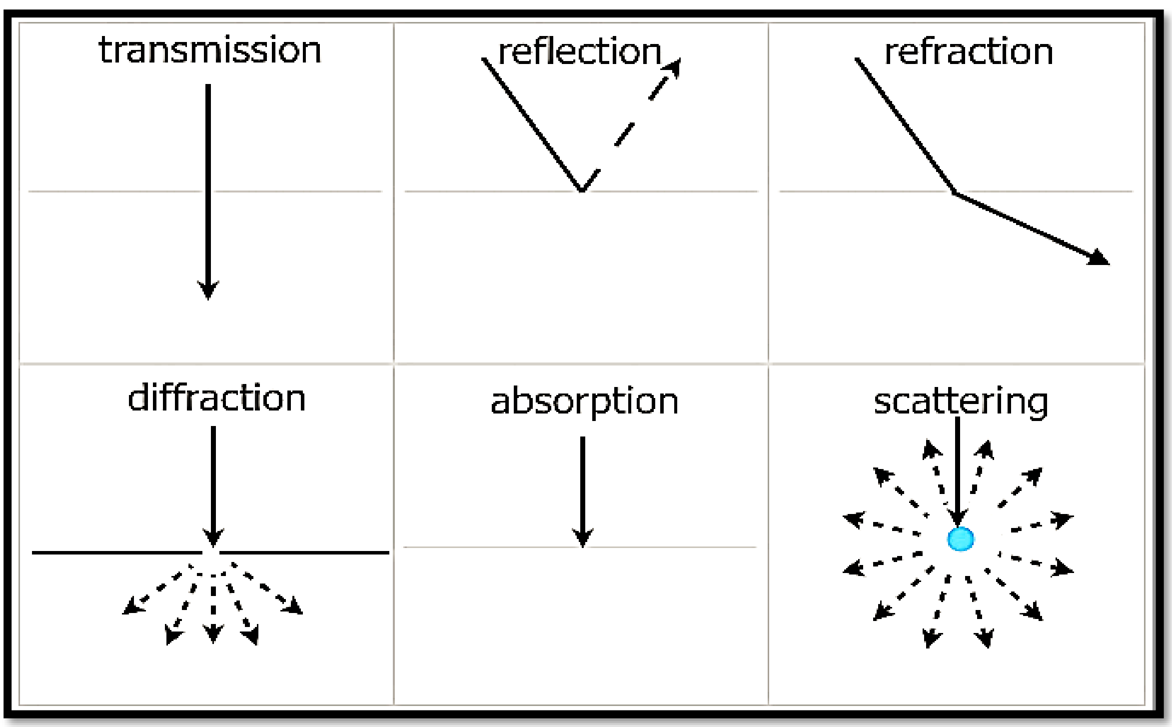


Figure 1.3 : Methods of light interaction with matter

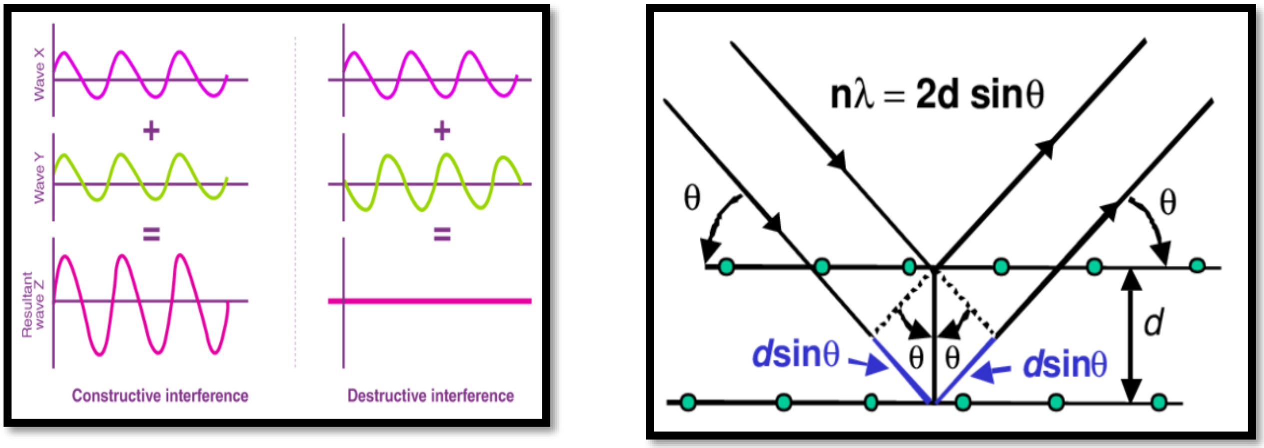


Figure 1.4: (a) light interferences (b) Bragg law condition

1.3 Semiconductors

Semiconductors are materials that have electrical conductivity between that of conductors (like metals) and insulators (like rubber). The most common semiconductor materials include silicon (Si), germanium (Ge), and gallium arsenide (GaAs). Semiconductors have a specific energy band gap that allows them to conduct electricity under certain conditions. The band gap is the energy difference between the valence band (where electrons are present) and the conduction band (where electrons can move freely). This gap allows semiconductors to act as insulators at low temperatures but conduct electricity when energy is provided (e.g., through heat or light).

The electrical and optical properties of semiconductors can be modified through a process called doping, where impurities are added to the material. Doping creates either n-type semiconductors (with extra electrons) or p-type semiconductors (with holes, or positive charge carriers). Semiconductors play a crucial role in a wide range of modern applications and devices due to their good explain properties such as transistors, diodes, integrated circuits, solar cells, and sensor.

1.4 Silicon (Si)

Silicon is a vital element in the fields of electronics and photonics, recognized for its high refractive index and excellent semiconductor properties. It has an atomic number of 14 and can be found in both crystalline and amorphous forms. Figure 1.5 displays some properties of Si. With a melting point of approximately 1414 C° and good thermal conductivity, silicon is well-suited for a variety of applications. In its pure state, silicon exhibits a shiny, metallic appearance, characteristic of many semiconductors. It serves as the foundation for microelectronics, including transistors and integrated circuits, and plays a crucial role in the production of photovoltaic solar cells. Additionally, silicon is frequently alloyed with metals such as aluminum and steel to improve their strength, making it an essential material across multiple industries.

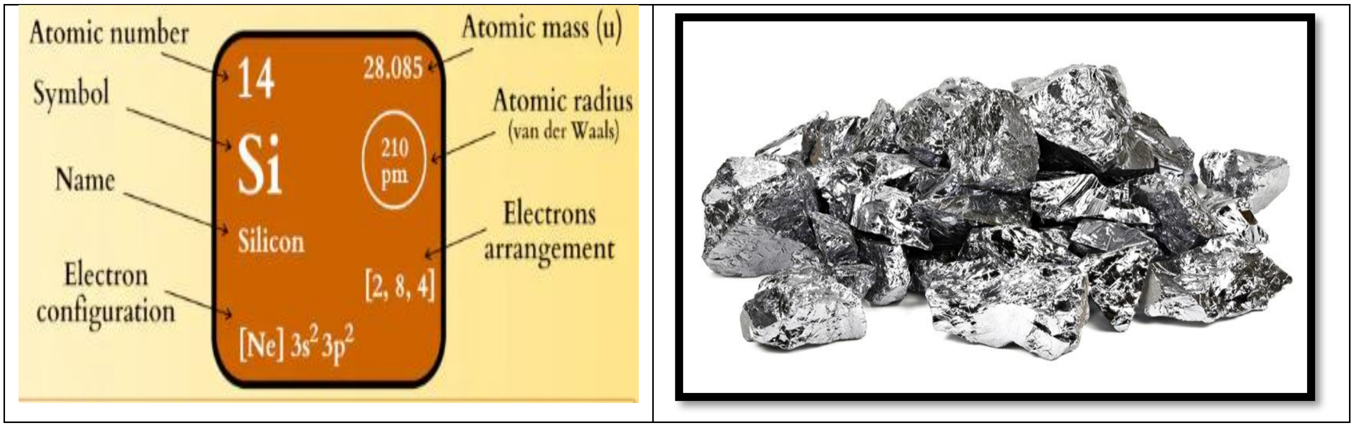


Figure 1.5: (a) Silicon atom properties (b) Si metal

1.5 Dielectric Materials

Dielectric materials are insulating substances that do not conduct electricity but can support an electric field. These materials are distinguished by their capacity to store electrical energy when subjected to an electric field. Typically, the energy level gap in dielectric materials is wide, often exceeding 3 electron volts (eV). This significant gap indicates that electrons cannot easily acquire enough energy to transition from the valence band to the conduction band, which is essential for electrical conduction. Consequently, materials with a wide band gap frequently exhibit transparency to visible light, making them ideal for use in optical devices and coatings. The dielectric constant, or relative permittivity, quantifies a material's ability to store electrical energy in an electric field in comparison to a vacuum. A higher dielectric constant signifies enhanced energy storage capabilities. Additionally, the maximum electric field that a dielectric material can endure without breaking down or becoming conductive is referred to as electrical strength. High electrical strength is crucial for ensuring that dielectric materials can safely operate in high-voltage applications. Common types of dielectric materials include ceramics, polymers, glass, and air. Dielectric materials play a vital role in modern technology due to their insulating properties, finding applications in microwave components, energy storage in capacitors, and dielectric resonator oscillators.

1.6 Silicon Oxide (SiO_2)

Silicon dioxide, commonly known as silica, is an oxide of silicon represented by the chemical formula SiO_2 (Figure 1.6). It is primarily found in nature as quartz and is a major component of sand in various regions around the globe. Silica belongs to one of the most abundant material families, existing both as a natural compound in several minerals and as a synthetic product. Silicon dioxide (SiO_2) is extensively utilized as a dielectric material. Its dielectric constant is approximately 3.9, and it possesses a high electrical breakdown strength, typically around 10 MV/cm. Additionally, silicon dioxide is characterized by its low refractive index and high transparency. It has a high melting point of about 1600 °C, which allows it to remain durable under high-temperature conditions. Silica is also chemically inert and stable, contributing to its longevity and reliability. As an excellent electrical insulator, it is particularly valuable in electronic components. Furthermore, silicon dioxide exhibits resistance to thermal shock, enabling it to endure rapid temperature fluctuations without fracturing. Silicon dioxide (SiO_2) is an adaptable material employed in numerous applications across diverse industries, including glass manufacturing, fiber optics, protective layers, fillers in rubber and plastics, and the construction industry.

Figure 1.6: SiO_2 powder

1.7 Photonic Crystals

A photonic crystal (PC) is an optical nanostructure distinguished by a periodic variation in refractive index, comprising alternating regions of high and low refractive index. Introduced by Eli Yablonovitch and Sajeev John in 1987 [2][3]. This unique configuration of PC enables the manipulation of photon (light) propagation in a way similar to how semiconductor crystals control electrons, establishing allowed and forbidden electronic energy bands. Depending on their wavelength, light waves may either propagate through the structure or encounter restrictions. Wavelengths that can propagate in a specific direction are referred to as modes, while the ranges of wavelengths that are not allowed to propagate are known as photonic band gaps (PBG), indicating that light cannot pass through certain frequency ranges.

Photonic crystals can be fabricated in one, two, or three dimensions (1D, 2D, and 3D). One-dimensional photonic crystals are usually created by the successive deposition of thin film layers as seen in Figure 1.7. Two-dimensional photonic crystals can be fabricated using techniques such as photolithography or by drilling holes into an appropriate substrate. For three-dimensional photonic crystals, fabrication methods include drilling at various angles, stacking multiple two-dimensional layers, direct laser writing, or promoting the self-assembly of spheres within a matrix, followed by the dissolution of the spheres. Figure 1.8 present the applications of photonic crystals.

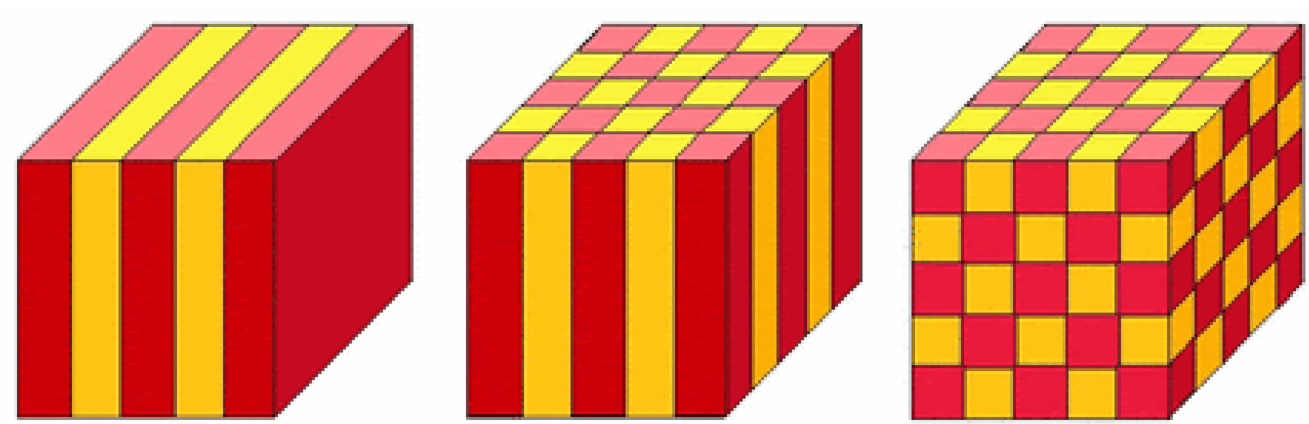


Figure 1.7:

Geometrical shapes of photonic crystals (a) 1D (b) 2D and c) 3D

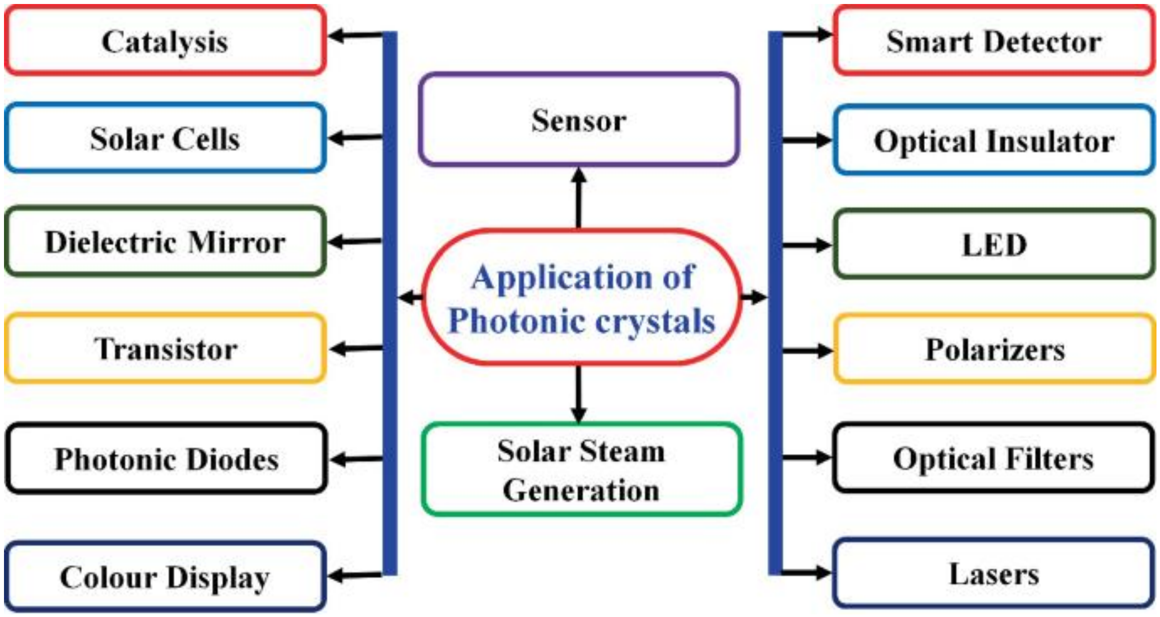


Figure 1.8: Applications of photonic crystal

Chapter 2

Theoretical analysis

2.1 Maxwell's equations

Maxwell's equations consist of four fundamental equations in electromagnetism that describe the behavior of electric and magnetic fields and their interactions with charges and currents. They provide the foundation for classical electrodynamics, optics, and electrical circuits. Formulated by James Clerk Maxwell in the 19th century, these equations are essential for understanding classical physics. They are fundamental to our understanding of various physical phenomena, including light propagation and electromagnetic waves.

Gauss's Law for Electricity: This law states that the electric flux through a closed surface is proportional to the charge enclosed within that surface.

Gauss's Law for Magnetism: This law asserts that there are no magnetic monopoles; the total magnetic flux through a closed surface is zero.

Faraday's Law of Induction: This law states that a changing magnetic field linked with a conductor can induce an electromotive force (EMF) in the conductor.

Ampère-Maxwell Law: This law describes the magnetic fields that result from changing electric fields and electric currents.

$$\vec{\nabla}.\vec{D} = \sigma \qquad ...(1)$$

$$\vec{\nabla}.\vec{B} = 0 \qquad ...(2)$$

$$\vec{\nabla} \times \vec{E} + \frac{\partial B}{\partial t} = 0 \qquad ...(3)$$

$$\vec{\nabla} \times \vec{H} = \vec{J} + \frac{\partial \vec{D}}{\partial E} \qquad ..(4)$$

Symbol	Meaning
E	Electric field
D	Electrical displacement
H	Magnetic field stength
B	Magnetic field
σ	Charge density
$\boldsymbol{\varepsilon}_0$	Permittivity of free space
$\boldsymbol{\mu}_0$	Permeability of free space
J	Current density
∇ ·	Divergence operator
∇ ×	Curl operator

2.2 Transfer Matrix Method:

The Transfer Matrix Method (TMM) is a mathematical technique employed to compute the reflection and transmission spectra of multi-layered optical structures [4]. It serves as a numerical approach to solve Maxwell's equations in one-dimensional systems. In TMM, the optical properties of each layer in the structure are represented using matrices. For any given layer in the multilayer structure, the transfer matrix can be expressed as follows:

$$m = \begin{pmatrix} \cos\delta & \frac{i \sin\delta}{p_1} \\ i\ p_1 \sin\delta & \cos\delta \end{pmatrix} \qquad (2.1)$$

For normal incident

$$p_j = n_j \cos(\theta_j) \qquad (2.2)$$

The phase difference for any layer is defined as

$$\delta_j = \frac{2\pi}{\lambda} d_j n_j \cos(\theta_j) \qquad (2.3)$$

Where j indicates to the matrix for specific layer in the structure, which can be Si or SiO2. The variables θ_j , d_j , n_j denote the angle of incidence, thickness, and refractive index for layer j. The term λ represents the wavelength of the incident wave.

The total characteristic matrix M for the entire multilayer structure is given by

$$M = m_1\ m_2\ m_3 \dots\dots\dots\ m_N = \begin{pmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{pmatrix} \qquad (2.5)$$

Finally, the reflection (R) of the suggested multilayer structure is given by

$$R = \left| \frac{p_0 X_{11} + p_0\ p_s X_{12} - X_{21} - p_s X_{22}}{p_0 X_{11} + p_0\ p_s X_{12} + X_{21} + p_s X_{22}} \right|^2 \qquad (2.6)$$

where $p_0 = n_0 \cos\theta_0$ and $q_s = n_s \cos\theta_s$ for air and the glass substrate, respectively.

Chapter 3

Results and discussion

3.1. Design photonic crystal:

The proposed photonic crystal (PC) structure is designed with a periodic arrangement of silicon (Si) and silicon dioxide (SiO2) layers. The refractive indices for these materials are n_1 = 3.5 for silicon and n_2 = 1.45 for silicon dioxide. The thicknesses of the silicon and silicon dioxide layers are denoted as d1 and d2, respectively. The layers repeated N times. The overall configuration of the structure can be represented as air / $(Si / SiO_2)^N$ / glass substrate as in Figure 3.1.

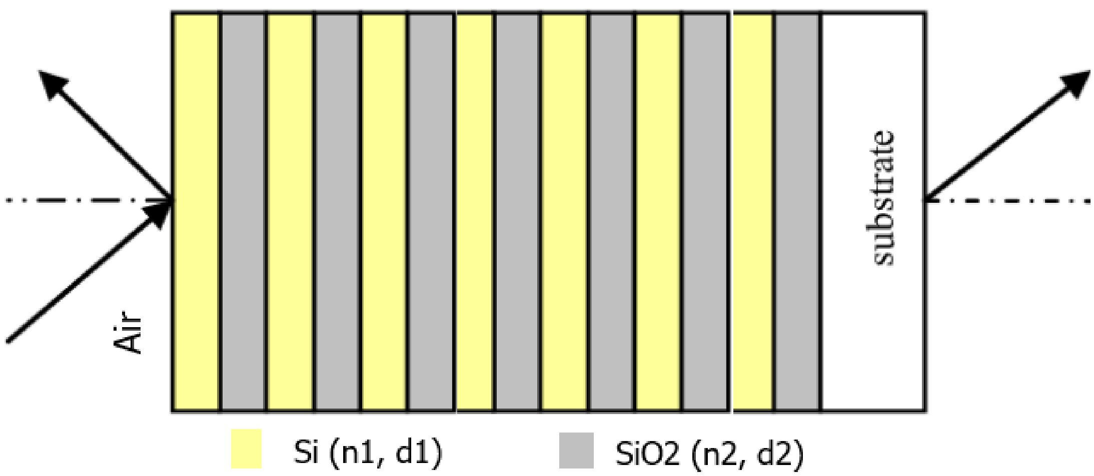


Figure 3.1: The proposed photonic crystal (PC) structure represented as air / $(Si / SiO_2)^N$ / glass substrate

3.2-Effect of number of periods on the reflection spectra

The reflection spectra of the photonic crystal (PC) structure provide essential insights into its photonic properties, particularly in how it interacts with incident light. In this scenario, the thickness of the silicon (Si) layer is set to300 nm, while the thickness of the silicon dioxide (SiO_2) layer is set to100 nm. Light is incident normally on the top surface of the structure from air, and the wavelengths of interest range from 1500 nm to 5000 nm. The number of periods N varies and is set at 1, 3, 5, and 7 as seen in figure 3.2.

As the number of periods N increases in the photonic crystal structure, the overall complexity enhances the formation of photonic band gaps (PBG) and leads to improved reflection at specific wavelengths. For N = 1, the reflection spectrum displays a relatively simple pattern with high reflection across the wavelength range. This indicating minimal interference effects and less effective PBG formation. However, at N = 3, the spectra reveal potentially wider PBGs, with 100% reflection observed from approximately 1790.08 nm to 3339.36 nm, resulting in a width of about 1549.31 nm. The wide PBG attributed to the high contrast in refractive indices between silicon and silicon dioxide. Additional ripples outside the PBG arise from interference effects. As N increases further to 5 and 7, the PBGs become more defined, with sharper edges and decreased widths of 1423.71 nm and 1360.71 nm, respectively. This demonstrating the effective optical manipulation capabilities of the multilayer structure.

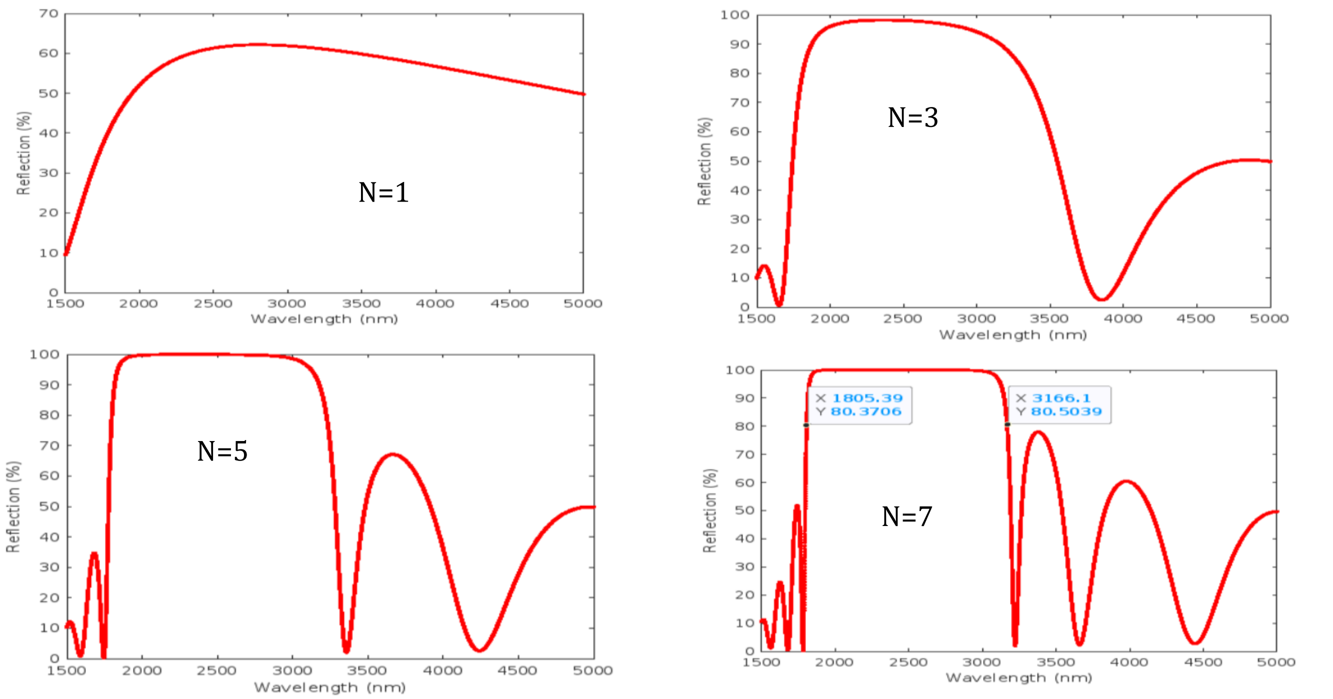


Figure 3.2: Refleation spectra of photonic crystal for diferent number of periods (N=1, 3, 5, and 7) **(by using MATLAB software)**

3.3- Effect of Si layer thickness on the reflection spectra:

Figure 3.3 illustrates the effect of varying silicon (Si) layer thicknesses of 100, 200, 250, and 300 nm on the reflection spectra of a photonic crystal structure, with the silicon dioxide (SiO_2) layer thickness fixed at 100 nm. Light is incident normally on the top surface, covering a wavelength range from 1500 nm to 5000 nm, with the number of periods N set at 7.

As the silicon layer thickness increases, the reflection spectra display more pronounced peaks and deeper troughs, indicating enhanced interference effects and sharper photonic band gaps. Both $\lambda 1$ and $\lambda 2$ shift to longer wavelengths, suggesting that thicker Si layers improve the interaction of light within the structure.

The width of the photonic band gap $\Delta\lambda$ also increases, ranging from 1277.58 nm to 1551.91 nm as d1 increases from 100 nm to 300 nm. This shift to longer wavelengths and the widening of the PBG can be attributed to the Bragg-Snell law: $2\,d\sqrt{n_{eff} - \sin\theta^2} = n\lambda$

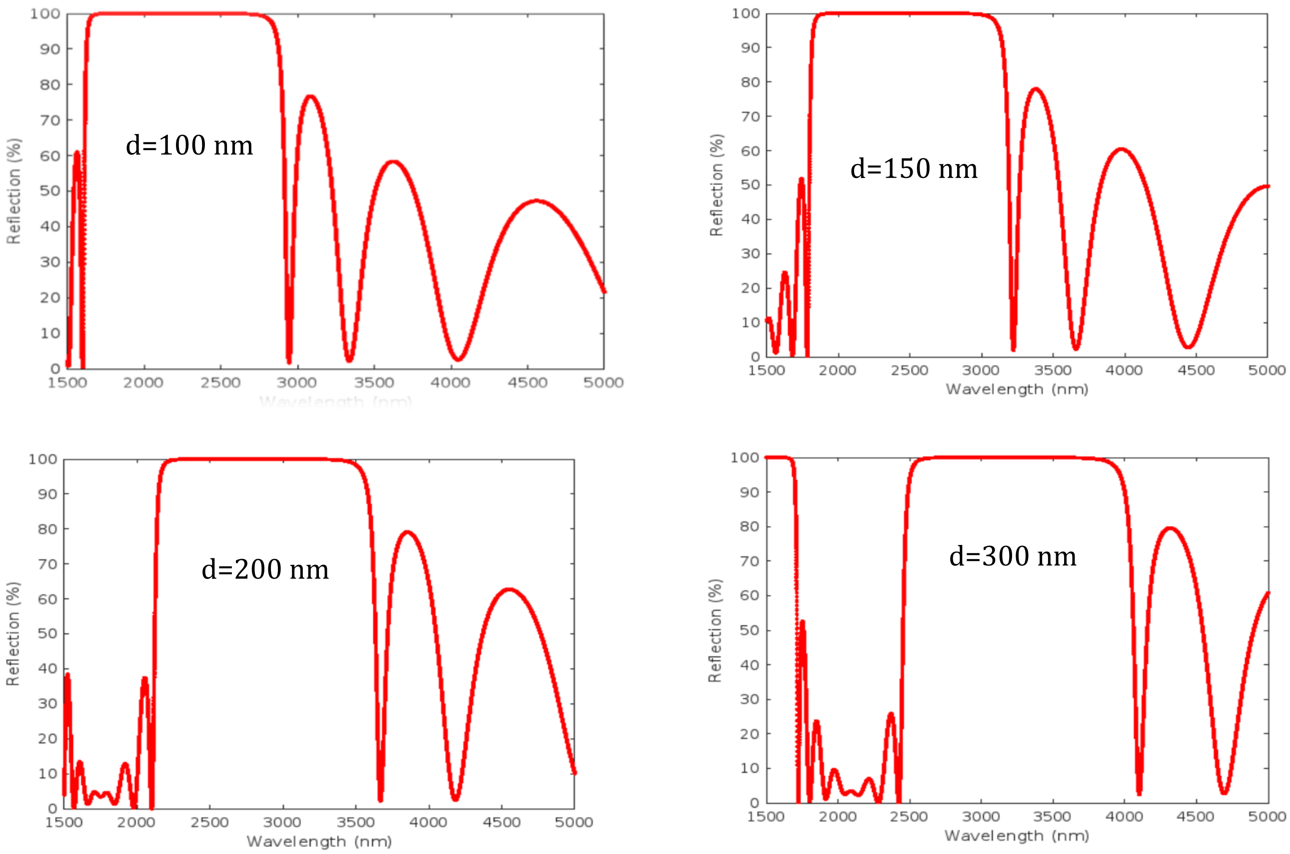


Figure 3.3. Refleation spectro of photonic crystal for diferent number Si layer (d_1= 100, 200, 250, and 300 nm) **(by using MATLAB software)**

3.4 -Effect of SiO_2 layer thickness on the reflection spectra

Figure 3.4 illustrates the impact of varying silicon dioxide (SiO_2) layer thicknesses on the reflection spectra of a photonic crystal structure. The SiO_2 thicknesses examined are 200 nm, 250 nm, 300 nm, and 400 nm, while the silicon (Si) layer thickness is fixed at 300 nm. Light is incident normally on the photonic crystal (PC) with the number of periods N set at 7.

As the SiO_2 thickness increases, both λ_1 and λ_2 shift to longer wavelengths, indicating enhanced light interaction within the structure, while the width of the photonic band gap $\Delta\lambda$ widens from 1034.97 nm to 1613.6 nm as the thickness of SiO2 increases from 200 nm to 400 nm. This increase in thickness leads to more pronounced interference effects, evidenced by sharper peaks and deeper troughs in the spectra, suggesting that thicker layers enhance the photonic crystal's capacity to manipulate light effectively.

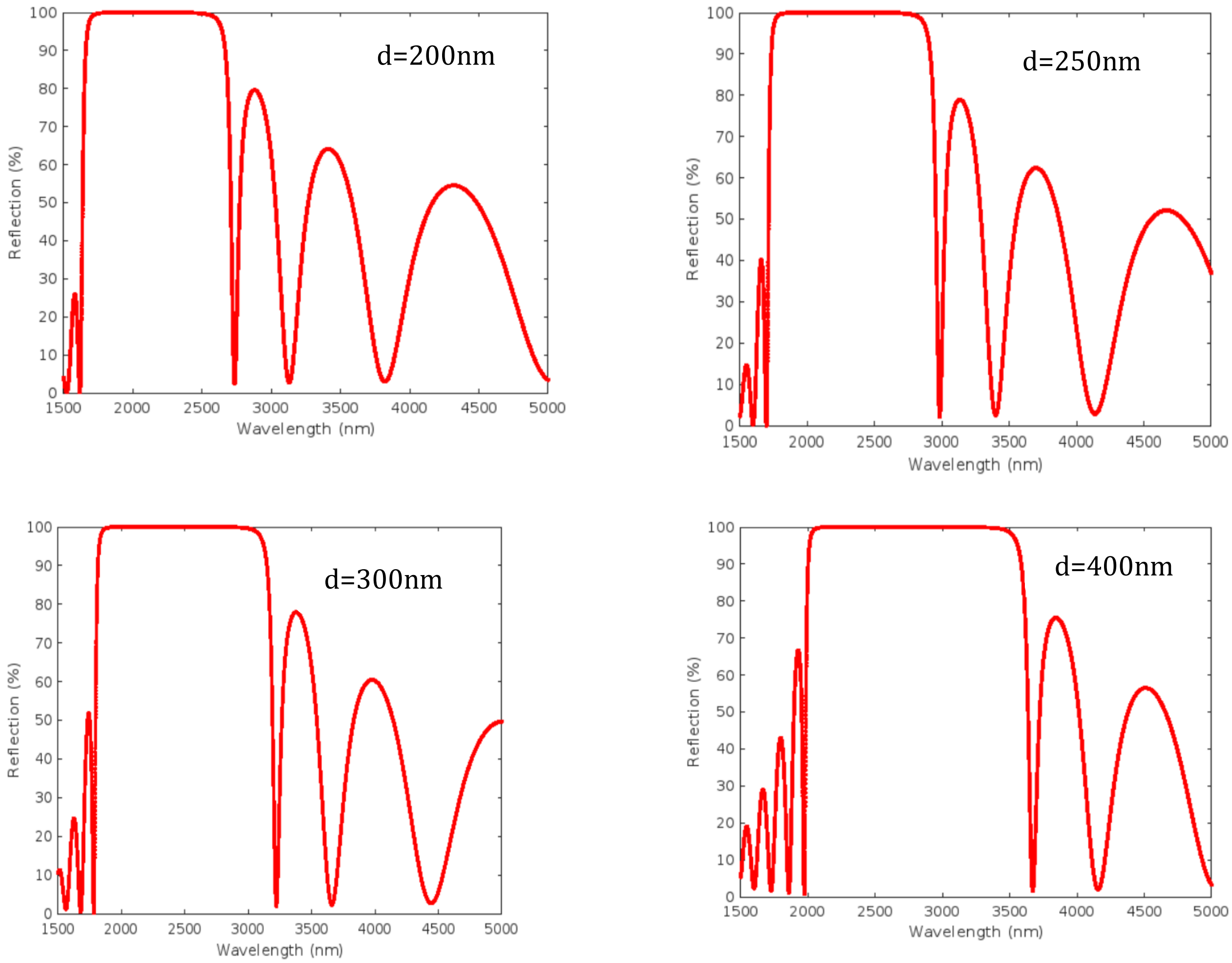


Figure 3.4: Refleation of the photonic crystal change the thickness of SiO2 layer (d_2 = 200, 250, 300, and 400 nm) **(by using MATLAB software)**

Conclusion

The transfer matrix method was utilized to simulate light reflection in a one-dimensional photonic crystal (PC). The PC composed of alternating silicon and silicon oxide layers. The results revealed that increasing the number of layers enhanced light interference, making the photonic bandgap more distinct and narrow this was to increasing interference.

Furthermore, increasing the thickness of the layers resulted in a shift of the bandgap toward longer wavelengths due to the increase in optical path length.

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Appendix: MATLAB Code

```
clear all
close all
clc

% this program calculates and plots Reflection
% in a 1D photonic crystal (PC) for both "s" (TE) and "p" (TM) polarization states;
% the 1D-PhC has a unit cell made of two different  materials;
% the wavelength in one medium is taken as input.
% materials are Si and SiO2
% ========================================

%  Air / PC /Glass
% PC (n1, n2)
lamda=linspace(1500,6000,16000);   % range of wavelength (nm)
gi=0;    % Angle of incidence
Na=7;   % Period (number of unit cells)

% thickness
d1=200;      % first layer nm
d2=300;      % second layer;  nm

% Refractive index
n1=3.5;             % first layer
n2=1.45;            % second layer
n0=1.0;             % air
ns=1.45;             % substrate

% Snells law
g0=gi*pi/180;
g1=asin(n0.*sin(g0)./n1);
g2=asin(n0.*sin(g0)./n2);
gs=asin(n0.*sin(g0)./ns);
```

```
% type plarization
p0=n0.*cos(g0);
p1=n1.*cos(g1);
p2=n2.*cos(g2);
ps=ns.*cos(gs);

% wave vector
k1=(2*pi./lamda).*n1.*cos(g1);
k2=(2*pi./lamda).*n2.*cos(g2);
B1=k1.*d1;
B2=k2.*d2;

% Transfer matrix X= n1/n2
aa11=cos(B1).*cos(B2)-(p2./p1).*sin(B1).*sin(B2);
aa12=-(i./p2).*cos(B1).*sin(B2)-(i./p1).*sin(B1).*cos(B2);
aa21=-i.*p1.*sin(B1).*cos(B2)-i.*p2.*cos(B1).*sin(B2);
aa22=cos(B1).*cos(B2)-(p1./p2).*sin(B1).*sin(B2);
qa=0.5.*(aa11+aa22);

% Chebyshev function
Una1=sin(Na.*acos(qa))./sqrt(1-qa.^2);
Una2=sin((Na-1).*acos(qa))./sqrt(1-qa.^2);
AA11=aa11.*Una1-Una2;
AA22=aa22.*Una1-Una2;
AA12=aa12.*Una1;
AA21=aa21.*Una1;

% Reflection
r=((AA11+AA12.*ps).*p0-(AA21+AA22.*ps))./((AA11+AA12.*ps).*p0+(AA21+AA22.*ps));
R=abs(r).^2;

% Axis
X=lamda;
Y=R*100;
% Graph the solution
plot(X,Y,'r.-');
```