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The numerical solution of the eigenvalue problem in periodic thin films

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ABSTRACT

In this study, the eigenvalue problem for one-dimensional thin films made of alternating layers of two dielectric materials with dielectric constants ε1 and ε2 was solved for both transverse electric (TE) and transverse magnetic (TM) modes to determine the allowed and forbidden frequencies in the bandgap. The dispersion relation for the one-dimensional thin films was obtained, and the eigenvalue problems were solved using a MATLAB program. The results show that the photonic band structure for the film in a homogeneous medium (ε1 = ε2) has no forbidden frequencies between the bands due to the continuous translational symmetry. However, when the dielectric constant is changed (ε1 ≠ ε2), gaps and bands appear alternately on the frequency axis. The first nine gaps and ten bands were obtained, and it is possible to determine the forbidden and allowed frequencies through the photonic band structure.

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الحل العددي لمسألة القيمة الذاتية في الأغشية الرقيقة الدورية

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الـــخُـــلاصـــة

في هذه الدراسة، تم حل مسألة القيمة الذاتية للأغشية الرقيقة أحادية البعد المصنوعة من طبقات متناوبة من مادتين عازلتين مع بثابت عزل ε_1 وε_2 لكل من الانماط TE (Transverse Electric)و TM (Transverse Magnetic) لتحديد الترددات المسموح بها والممنوعة في فجوة الطاقة. تم الحصول على علاقة التشتت للأغشية الرقيقة أحادية البعد من خلال حل مسألة القيمة الذاتية باستخدام برنامجMATLAB. وتظهر النتائج أن تركيبة النطاق الفوتوني للفيلم في وسط متجانس ($\varepsilon_1 = \varepsilon_2$) لا تحتوي على ترددات ممنوعة بين النطاقات بسبب التماثل الانتقالي المستمر. ولكن، عندما يتغير ثابت العازل($\varepsilon_1 \neq \varepsilon_2$) ، تظهر فجوات ونطاقات بالتناوب على محور التردد. حيث تم الحصول على أول تسع فجوات وعشرة نطاقات، ومن الممكن تحديد الترددات الممنوعة والمسموح بها من خلال البنية النطاقية الفوتونية.

الكلمات المفتاحية:

الفجوة الفوتونية
علاقة التشتت
مسألة القيمة الذاتية
البلورات الفوتونية

1. INTRODUCTION

Thin films are periodic dielectric structures that are formed by periodically varying the dielectric constant. This is achieved by taking two different dielectric materials with very different refractive indices and repeating them in an alternating fashion to obtain a periodic structure. The purpose of this design is to prevent the propagation of electromagnetic waves in the periodic direction of the thin films, as shown in Figure 1 [1].

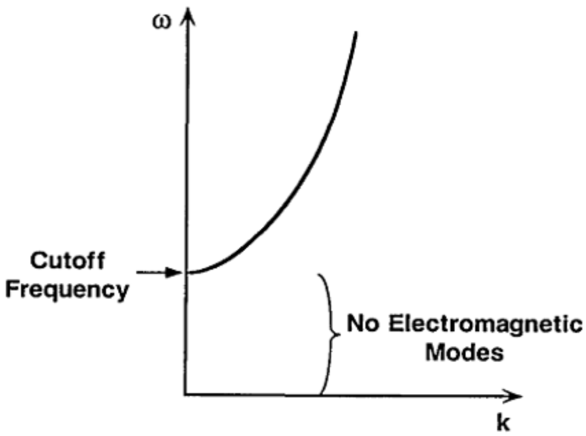

Figure (1): The electroma-gneticmodes of spontaneous emission with frequencies lower than the band gap are forbidden to propagate through the thin film.

The wavelength of electromagnetic waves propagating through periodically alternating layers is partially reflected at each interface, as shown in Figure 2. The multiple reflections interfere constructively and destructively, hindering the forward propagation of the incident waves [2].Since thin films are one-dimensional, the constructive and destructive interferences between the incident and reflected waves determine whether the wave propagates or not.The wave behavior within the forbidden gap has two cases:-

- If the wavelength is within the band gap, partial reflections of the incident waves will be generated at the interfaces of the alternating layers. These reflected waves will be in phase, and will combine with the incident waves to create standing waves that cannot propagate through the crystal.

- If the wavelength is not within the band gap, the reflected waves will not be in phase, and will cancel each other out. Consequently, the incident waves will propagate without losing any energy [3].

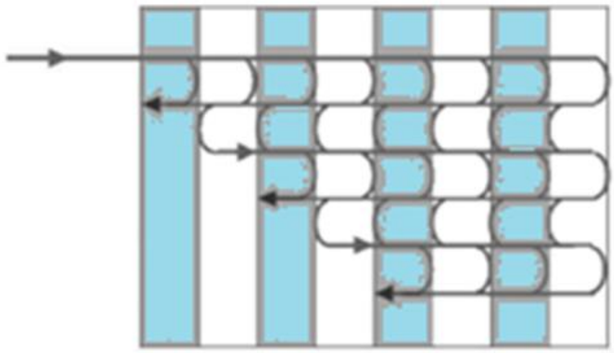

Figure (2): Partial reflection of waves at the interfaces of alternating layers in a Bragg reflector.

This research aims to study the effect of changing the film thickness on its optical properties. The plane wave extension method will be used to solve the Bloch equation to obtain the photonic band structure of the film. The effect of changing the film thickness on the photonic bandwidth and photon capture characteristics will be analyzed. The results will be used to design thin films with desired optical properties.

2. Mathematical model

a- Maxwell's equations in periodic media:

We will discuss Maxwell's equations in detail and analyze them, as they represent an important role in the study of periodic media. The propagation of electromagnetic waves in thin films is subject to the four Maxwell equations [4].

Before formulating Maxwell's equations for the medium, we will make some approximations that will facilitate the mathematical processing in this research. These are: -

- The field intensities are small, so we will deal with a linear system.
- The dielectric constant does not depend on the frequency.
- The material is isotropic, so the vectors $\boldsymbol{E}$Electric Field, and, $\boldsymbol{D}$ Electric Displacement are related to the dielectric constant $\varepsilon_{\circ}$ multiplied by the standard dielectric function$\varepsilon(\boldsymbol{r})$.
- In dealing with transparent materials, it is possible to treat $\varepsilon(\boldsymbol{r})$ as a positive real quantity.
- The magnetic permeability $\mu(\mathbf{r})$ of thin films is very close to unity.
- Finally, there are no free charges ρ or current density $\boldsymbol{J}$, so there are no

sources or sinks. Therefore, $\rho = 0$ and $\boldsymbol{J} = 0$should be set.

Under these approximations, it is possible to set $\boldsymbol{B} = \mu_\circ \boldsymbol{H}$and $\boldsymbol{D}(\boldsymbol{r}) = \varepsilon_\circ \varepsilon(\boldsymbol{r})\boldsymbol{E}(\boldsymbol{r})$. Therefore, Maxwell's equations are formulated as follows:

Gauss's law for electric field:

$$\nabla \cdot [\varepsilon(\boldsymbol{r})\boldsymbol{E}(\boldsymbol{r},t)] = 0 \quad (1)$$

Gauss's law for magnetic field:

$$\nabla \cdot \boldsymbol{H}(\boldsymbol{r},t) = 0 \quad (2)$$

Faraday's law of induction:

$$\nabla \times \boldsymbol{E}(\boldsymbol{r},t) = -\mu_\circ \frac{\partial}{\partial t}\boldsymbol{H}(\boldsymbol{r},t) \quad (3)$$

Ampere's circuital law with Maxwell's addition:

$$\nabla \times \boldsymbol{H}(\boldsymbol{r},t) = \varepsilon_\circ \varepsilon(\boldsymbol{r}) \frac{\partial}{\partial t}\boldsymbol{E}(\boldsymbol{r},t) \quad (4)$$

Were, **B** **Magnetic flux**, **E** Electric Field, **H** Magnetic Field, **D** Electric Displacement, $\varepsilon(\boldsymbol{r})$Dielectric Function, $\varepsilon_\circ$Dielectric Constant, $\mu_\circ$ Magnetic Permeability.

These equations are called Maxwell's equations for periodic media. It is worth noting that the above equations are valid for both uniform and periodic media. However, in the case of periodic media, the field intensities and the dielectric constant are periodic functions of space. This leads to the emergence of new phenomena, such as the band gap, which is a region of frequencies in which electromagnetic waves cannot propagate [3].

b- Wave equations and eigenvalue problems:

One of the vectors $\boldsymbol{E}(\boldsymbol{r},t)$ or $\boldsymbol{H}(\boldsymbol{r},t)$now can be eliminated from the Maxwell equations for a periodic medium to obtain the wave equation for the electric or magnetic field:

$$\frac{1}{\varepsilon(\boldsymbol{r})}\nabla \times \left(\nabla \times \boldsymbol{E}(\boldsymbol{r})\right) = \frac{\omega^2}{C^2}\boldsymbol{E}(\boldsymbol{r}) \quad (5)$$

This is called the wave equation for the electric field.

$$\nabla \times \left(\frac{1}{\varepsilon(\boldsymbol{r})}\nabla \times \boldsymbol{H}(\boldsymbol{r})\right) = \frac{\omega^2}{C^2}\boldsymbol{H}(\boldsymbol{r}) \quad (6)$$

This is called the wave equation for the magnetic field.

The wave solutions of equations (5) and (6) can be written in the form of a spatial pattern multiplied by the complex exponential function as follows:

$$\boldsymbol{E}(\boldsymbol{r},t) = \boldsymbol{E}(\boldsymbol{r}) \exp(-i\omega t)$$

$$\boldsymbol{H}(\boldsymbol{r},t) = \boldsymbol{H}(\boldsymbol{r})\exp(-i\omega t)$$

Where, ω represents the eigenfrequency and $\boldsymbol{E}(\boldsymbol{r})$ and $\boldsymbol{H}(\boldsymbol{r})$ represent the eigenvectors of the wave equations [5].

c- Solving the eigenvalue problem for the electric field in one dimension:

In the case of a periodic arrangement in one dimension, a thin multi-layered film made of two dielectric materials will be considered, with the dielectric constant of the first layer being ε_1 and the second layer being ε_2 which are have the same thickness b with total thickness$a$ of each periodic layer. The two layers are then arranged in a periodic alternating form to infinity in one dimension as shown in Figure 3, while the electromagnetic waves propagate in the *x*-direction.

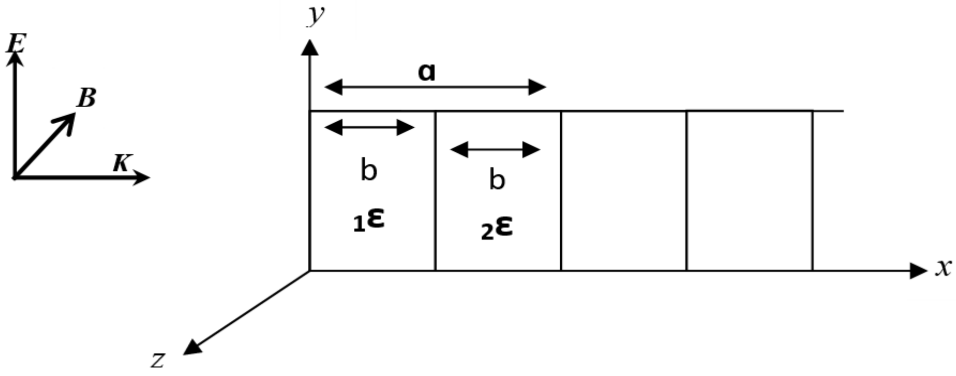

Figure (3). The infinite multi-layered thin films.

The periodicity of the layers is infinite in the x-direction as shown in Figure (3) (The number of layers is infinite) also, clarify the coordinate of electric field which has a component of *y*- axis while the magnetic field has a component of z- axis, while the wave vector will have x-axis$\boldsymbol{k} = k_x\hat{x}$.

Considering Maxwell's equations, which can be written in the complex form, this allows the wave function to be written in the form of a spatial pattern multiplied by the complex exponential function:

$$\mathbf{E}(\boldsymbol{x},t) = \boldsymbol{E}(\boldsymbol{x})e^{-i\omega t}, \boldsymbol{H}(\boldsymbol{x},t) = H(\boldsymbol{x})e^{-i\omega t}$$

By substituting these functions in Maxwell's equations (5 and 6), and then taking the temporal derivative of those functions, the eigenvalue problem for the one-dimensional photonic crystal is derived:

$$\frac{1}{\varepsilon(x)}\frac{\partial^2\boldsymbol{E}(\boldsymbol{x})}{\partial x^2} = -\lambda_E^2\boldsymbol{E}(\boldsymbol{x}) \qquad (\mathbf{7})$$

Where: $\lambda_E^2 = \frac{\omega^2}{c^2}$ is the derived formula, which is known as the wave equation for the electric field in the periodic medium.

Since the medium is periodic, it is possible to use Bloch's theorem [6].To rewrite the wave equation (7) in the following mathematical forms:

$$\sum_m \kappa_m E_{j-m}\left(k + \frac{2\pi}{a}(j-m)\right)^2 = \lambda_E^2 E_j \qquad (8)$$

This equation is known as the eigenvalue problem for the electric field in the one-dimensional photonic crystal [7].

d- Solving the eigenvalue problem for the magnetic field in one dimension:

The wave equation for the magnetic field can be easily derived from Maxwell's equations and by setting: $\lambda_H^2 = \frac{\omega^2}{c^2}$, we get the following equation:

$$-\frac{\partial}{\partial x}\frac{1}{\varepsilon(\boldsymbol{x})}\frac{\partial}{\partial x}\boldsymbol{H}(\boldsymbol{x}) = \lambda_H^2\boldsymbol{H}(\boldsymbol{x}) \qquad (9)$$

By rewriting the wave equation (9) for the magnetic field in the periodic medium using Bloch's theorem [11], the equation (9) becomes the following equation:

$$-\sum_{\boldsymbol{G}'}\kappa(\boldsymbol{G}-\boldsymbol{G}')\,[(\boldsymbol{k}+\boldsymbol{G}')\cdot(\boldsymbol{k}+\boldsymbol{G})]\boldsymbol{u}_{\boldsymbol{G}'} = \lambda_H^2\boldsymbol{u}_{\boldsymbol{G}} \qquad \mathbf{(10)}$$

This equation is known as the eigenvalue problem for the magnetic field in a one-dimensional photonic crystal [8].

3 . Results:

The eigenvalue problem for the one-dimensional thin films was solved for the transverse electric (TE) and transverse magnetic (TM) modes to determine the allowed and forbidden frequencies in the gap by obtaining the dispersion relation for the one-dimensional thin films. The eigenvalue problems (8) and (10) were solved by writing the differential operator matrix using the MATLAB program to calculate the eigenvalues. The following values were entered into the program: N=50, $\varepsilon_1 = \varepsilon_2 = 12$,represent$\varepsilon_1, \varepsilon_2$the dielectric constants for the first layer and the second layer,and f where $f = \frac{b}{a}$ represents the filling factor and is related to the thickness of the layer, b , and the crystal constant, a, which represents the thickness of two layers. A two-dimensional plot, Figure 4, was obtained, which shows the relationship between the normalized frequency on the vertical axis and the wave vector on the horizontal axis. This plot shows the dispersion relation, (photonic band structure), for the film moving in a homogeneous medium. This plot indicates that there are no forbidden frequencies between the bands due to the continuous translational symmetry.

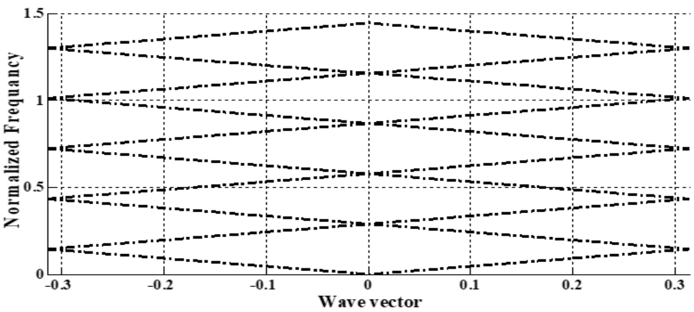

Figure (4): Photonic band structure of the homogeneous medium $a = 10$ ،with $\varepsilon_1 = \varepsilon_2$

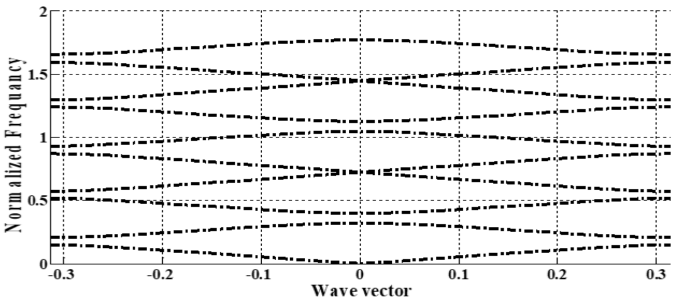

Figure (5): Photonic band structure of the transverse electric (TE) and transverse magnetic (TM) modes for a one-dimensional photonic crystal: $\varepsilon_1 = \frac{\varepsilon_2}{4}$.

By changing the value of the dielectric constant, and entering the following values into the program: N=50 is plane wave number, $\varepsilon_1 = 3$, $\varepsilon_2 = 12$, and f=0.5, the Figure 5 was obtained. The gaps and bands appear alternately on the frequency axis. This diagram gives the first nine gaps and ten bands. It is possible to determine the forbidden and allowed frequencies through the photonic band structure. We note that the transverse electric and transverse magnetic modes have the same photonic band structure in one dimension. The width of each band gap is determined by the quantity ω_r, which is known as the relative gap width, where $\omega_r = \frac{\Delta\omega}{\omega_m}$. The quantity $\Delta\omega$ is the difference between the frequencies of the upper and lower bands of each band gap, while the quantity ω_m is the average of the frequencies of the upper and lower bands. Table (1) shows the effect of changing the value of the dielectric constant between two layers on the width of the photonic band gap. This is consistent with the results of the study described in Reference [9].

Table(1):- shows the effect of changing the value of the dielectric constant between two layers on relative gap width

ε_1	ε_2	Filling Factor(f)	relative gap width ω_r	**Figure**
12	12	1	zero	4
3	12	0.5	0.25	**5**

4. Discussion:

The photonic band structure of multilayer thin films was found to depend on the film thickness, dielectric constant, and refractive indices of the layers. With increasing film thickness, the photonic band gap decreases. With increasing dielectric constant, the photonic band gap shifts to higher frequencies. With increasing refractive index of the first layer, the photonic band gap shifts to higher, these results are consistent with previous studies. In 2010, a study found that the photonic band gap of multilayer thin films depends on the film thickness, dielectric constant, and refractive indices of the layers. In 2011, another study found that the photonic band structure of multilayer thin films can be used to create new light sources [3].

This can be achieved by creating a photonic band gap in the photonic band structure. A photonic band gap is a region in frequency where light cannot propagate. This can be used to reflect or absorb light. For example, a reflective thin film can be used to reduce light loss in optical fibers. A reflective thin film can also be used to create a highly reflective mirror. A reflective thin film can also be used to create a light filter that allows only certain wavelengths of light to pass through [10].

They can also be used to design thin films that allow only certain wavelengths of light to pass through, such as light filters. They can also be used to design thin films that produce light at certain frequencies, such as light sources.

5. Conclusion

The previous results demonstrated the influence of the material's dielectric constant and the number of plane waves on the photonic band structure of one-dimensional thin films. As the dielectric constant increases and the number of plane waves increases, the width of each band gap decreases. This observation highlights the potential for tailoring the photonic band structure by manipulating these parameters. This study provides valuable insights into the behavior of one-dimensional thin films and their potential applications in photonic devices. Further research is encouraged to investigate the effects of additional parameters, such as film thickness and temperature, on the photonic band structure, enabling the design of photonic devices with even more refined properties.

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