Numerical Simulation Study of the Influence of the Bragg Mirror's Optical Properties on the Reflection Spectrum

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Abstract

The field of thin films is interesting in the design and manufacture of Bragg mirrors by multilayer, which they must be, sprayed on the substrate on one side only. The working principle of the Bragg mirror is based on the realization at a given wavelength results from the constructive interference of the set of reflections from each mirror interface. The design of a Bragg mirror had based on the schematic formula of the layers, which are adapted to the spectral properties of the chosen mirror. To do this, we have optimized the Bragg mirror's spectral properties by means of numerical simulation, in order to identify the factors, influencing these properties and how, to improve the mirror's reflection. The results obtained show that the increase in the number of pattern the bandwidth decreases and the number of oscillations outside the bandwidth increases. The greater the index contrast between the high index n_H and the low index n_B, the closer the reflection coefficient will be to 1 and the higher the normalized bandwidth width. To obtain a pattern of bilayers with a wide spectral bandwidth, we need to choose a quarter-wave thickness that has not multiplied by λ/4.

Passwords: Bragg mirror, Layer stacking, constructive interference, reflection spectrum,

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I. Introduction

The interaction of light with an interface causes a more known phenomenon, which is reflectivity, due to the change of refractive index during the passage of light through these interfaces [1]. Highly reflective Bragg mirrors play an important role, as they had found in a wide range of applications [2].

A Bragg mirror or quarter-wave mirror is a one-dimensional photonic crystal characterized by alternating layers of two different dielectric media in a single spatial direction [3]. consisting of a periodic stack of high (H) and low (L) index materials, whose thickness are all quarter wave$n(\boldsymbol{\lambda}_0)e = \frac{\lambda_0}{4}$ has a centring wavelength $\boldsymbol{\lambda}_0$, thus the phase shift given by each layer is $\pi/2$, The period or mesh of the Bragg mirror stack is called the q-pattern given by $q = p/2$ with q number of pattern (HL) and p number of layer [4]. They have also called multi dielectric mirrors because of their stacks of quarter-wave dielectric thin films.

The periodic index structure of this mirror allows it to generate constructive interference from reflected light and thus causes maximum reflection at the central wavelength outside the reflection region, reflection becomes zero [5]. The Bragg condition that reflects the constructive interference of reflected waves is to write in the form: [5,6]

$$2d \sin \boldsymbol{\theta} = m\boldsymbol{\lambda} \qquad (1)$$

Where m is odd, positive integer corresponds to layer order, λ: working wavelength, θ is the diffraction angle and d is the distance.

The deposition technique used for the realization of Bragg mirrors is Sputtering. the dielectric materials used to produce a Bragg mirror are:TiO_2 , MgO, CaF_2, SiO_2, Al_2O_3, ZnS, Ta_2O_5, HfO_2, BaF_2, LaF_3, MgF_2, Al_2O_3, Nb_2O_5[7-10].

In a metal mirror, the wave undergoes a phase shift of π, so cannot penetrate the mirror. In a Bragg mirror, on the other hand, the total reflection is the result of interference from the reflections of the different layers [11]. The loss of laser power after reflection has minimized when using dielectric mirrors 5% versus 20%. The multi-layer structure for a suitable period allows any wavelength to be, reflected at any angle, whereas other mirrors are limited to grazing incidence [12]. The stacking of quarter-wave layers generates constructive interference in reflection and destructive interference in transmission. The value reached by the reflection coefficient depends on the number of layers and the index contrast of the materials n_H-n_L [13].

Optimization by simulation, since it follows a mathematical model of the real system, has the advantage of being easy, inexpensive and we can predict the optimal parameters that contribute to the manufacture of a Bragg mirror of a reflection at a chosen wavelength. The objective of this work is to study the spectra of light reflection by Bragg mirrors by different materials and to find the optimal conditions to achieve them.

II. Numerical simulation study

Bragg mirrors are, obtained by depositing thin multilayers on a single side of the substrate. We have simulated a mathematical model using MATLAB.

MATLAB is a digital computing software marketed by Math Works. It was initially developed in the late 1970s by Cleves Moler, professor of mathematics at the University of New Mexico and then at Stanford. The latter is a programming language suitable for scientific problems. It can also, had considered a simple syntax matrix, calculation software, using its specialized functions [14].

This simple mathematical model based on the reflection of an electromagnetic (EH) wave in a multilayer optical system, enables us to analyse reflectance spectra in a more rigorous way, with the aim of studying the influence of different parameters on the total reflectivity of Bragg mirrors. The conditions of continuity at the interfaces of the E and H field components, imposed by Maxwell's equations, enable us to calculate the relationships linking n and k with the reflectance and transmittance intensities of the light passing through, which have linked to the Fresnel coefficient. We have set up a program to study the variation in reflectance intensity of a single layer deposited on a glass substrate, as a function of wavelength, under the effect of varying the refractive index of the layer material [15].

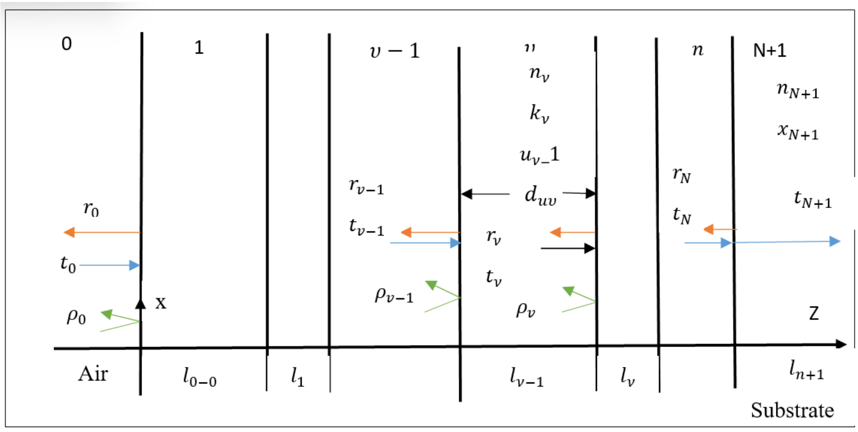


Fig. 1: Reflectance of light at normal incidence for an electric field

The complex reflectance at the υ^{th} layer interface is:

$$\rho_\upsilon = \frac{r_\upsilon}{t_\upsilon} \qquad (2)$$

The simulated mathematical equations are: [15]

-The Fresnel coefficient of reflectance at the interface between the $^{\upsilon\text{-}1}$th than υ^{th} layer have given by:

$$\rho_{\upsilon-1} = \frac{\rho_\upsilon e^{i\beta_\upsilon} + W_\upsilon}{1+\rho_\upsilon e^{i\beta_\upsilon} W_\upsilon} \qquad (3)$$

-In medium (N+1), i.e. the substrate, reflectance $\rho_{(N+1)}=0$ because there is no reflection in the last medium, and for medium N we have :

$$\rho_N = W_{\upsilon+1} = \frac{n_N - n_{N+1}}{n_N + n_{N+1}} \qquad (4)$$

ρ_N is the Fresnel coefficient of the last multilayer interface. When ρ_N have known we can easily calculate ρ_{N-1} using equation (3), this equation has applied consecutively to determineρ_{N-2}, ρ_{N-3}up toρ_0. The reflectance energy of the multilayer stack is then given by: R =$|\rho_0{}^2|$

-The Fresnel coefficient of reflectance for vector E perpendicular from medium n_0 to medium n_1 has obtained by W_1 and given by the relationship:

$$W_1 = \frac{n_0 - n_1}{n_0 + n_1} \quad (5)$$

-We define the phase βυ for a normal incidence:

$$\beta_\upsilon = \frac{4\pi}{\lambda} n_\upsilon d_\upsilon \quad (6)$$

III. Results and discussions

III.1. Variation effect of monolayer thickness λ/4 and λ/2

We have studied two cases; the first case is to deposit a high index layer (TiO_2) on a glass substrate. The second case is to deposit a low index layer (SiO_2) on the same substrate, under the effect of the variation of the layer thickness; once the variation of the pitch of the thickness with quarter wave $d_{\lambda/4}$ and another time with a variation of the thickness with half wave $d_{\lambda/2}$.

The program established in this study, when the vector E is perpendicular to the plane of incidence under an angle of zero incidence, and a specific wavelength at 500nm. Figure 2 shows the monolayer reflection intensity spectra for high and low indices respectively, under the effect of thickness (phase) variation as a function of wavelength.

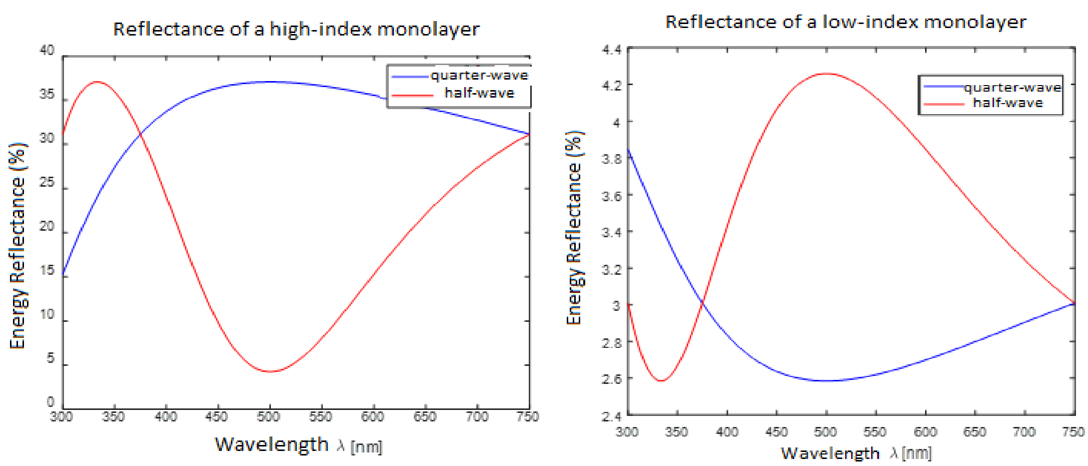


Fig.2: Reflection spectrum for TiO_2 monolayer (high refractive index) and SiO_2 monolayer (low refractive index) respectively under the effect of wavelength variation.

The results show that:

For a high index layer, with a quarter wave thickness (corresponds to a phase π) where the latter is equal to double the optical path, the reflection is maximum at R_{max}=37% for the wavelength λ=500 nm, and vice versa when the thickness is half-wave (for the phase is double the optical path that is 2π), there is a minimum reflection R_{min} = 5% for the same wavelength.

On the other hand, for a low-index layer the reflection is maximum (R_{max}=4.3%) for a wavelength (λ=500 nm) when the thickness is half-wavelength, and vice versa the reflection is minimum (R_{min}=2.6%) when the thickness is quarter-wavelength for the same wavelength.

So choose a thickness of λ/4 for high-index layers, and λ/2 for low-index layers, to ensure good reflection.

III.2. Thickness increase effect

The thickness values chosen must be even for the low-index layer (SiO_2) in order to have a phase of 2π and which corresponds to a half-wave thickness, and odd for the high-index layer (TiO_2) in order to have a quarter-wave thickness and which corresponds to a phase of π.

Figure (3): respectively represent the light reflection spectra for a TiO_2 and SiO_2 monolayer under the effect of increasing the thickness of each layer, as a function of wavelength.

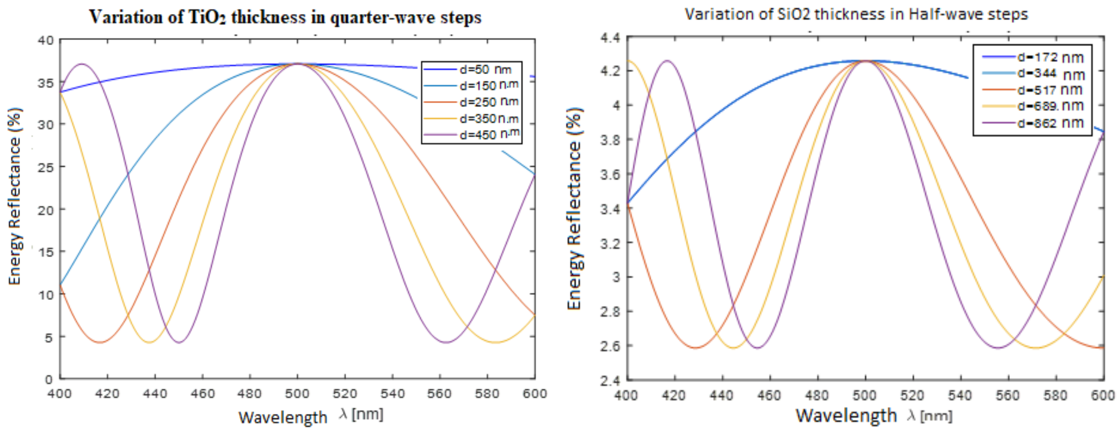


Fig. 3: reflection spectrum respectively of TiO_2 and SiO_2 monolayer as thickness increases.

According to Figure (3), when the thickness has increased for either the TiO_2 or SiO_2 layer, the value of the maximum reflection intensity always remains constant, but we find that there is a change in the width of the spectral band. As the thickness decreases, the spectral width increases.

Therefore, to obtain a wide spectral band you must choose the smallest thicknesses either for a quarter-wave thickness for a high index layer or for a half wave thickness for a low index layer.

III.3. Effect of high-low and low-high refractive index patterns

We studied three effect cases for the two high-low (TiO_2 and SiO_2) and low-high (SiO_2 and TiO_2) patterns respectively:

1. The first case both pairs suffered the same quarter wave delay.
2. The second case the high index layer suffers a delay of λ/4, and the low index layer a delay of λ/2.
3. The third case the two couples suffered the same half-wave delay.

For a wavelength specified at λ=500 nm. Figure (4) represent respectively reflection intensity spectra for a high (TiO_2) low (SiO_2) index pair and a low (SiO_2) high (TiO_2) pair, as a function of wavelength.

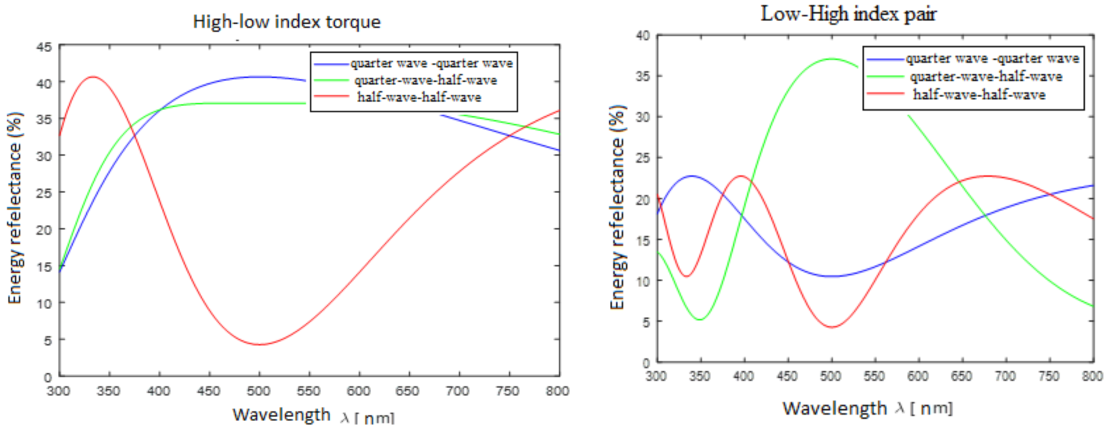


Fig. 4: High low and low high index torque reflection spectrum respectively under the effect of thickness variation of each layer.

From both figures, it can be, seen that:

-The high-low index pattern reaches, a maximum reflectance energy (R_{max}=40%) for the same quarter wave delay for both layers. and when the high index layer undergoes a quarter wave delay and the low index layer undergoes a half wave delay the reflectance energy becomes (R = 37%), so for the case of the same half wave delay for both layers of the low high index pattern, reflectance energy takes a minimum value (R_{min}=5%), for a wavelength λ=500 nm.

-The low-high index pattern reaches a maximum reflectance energy (R_{max}=37%) for a quarter-wave delay of the high index layer and a half-wave delay of the low index layer. The reflectance energy becomes (R = 10%) when the pair of two high-low layers undergo the same quarter-wave delay, and takes on a minimal value (R_{min}=5%) for the case of the same h So, to obtain a highly reflective pattern, you need to choose the high-low couple (HB) of two different materials; for example TiO_2 and SiO_2 respectively with quarter-wave retardation for the two layers. half-wave delay for both high-low index pattern layers, for a wavelength λ=500 nm.

III.4. The effect of increasing layer thickness of the HB pattern

We studied the effect of increasing the thickness of the high-low pattern, the first case undergoing a quarter-wave delay (an odd multiple) and the second case undergoing a half-wave delay (an even multiple), and for the last case undergoing a quarter-wave delay (an odd multiple) for the high index and a half-wave delay (an even multiple) for the low index, for the wavelength (λ=500 nm).

Figures (5): show the reflection intensity spectra for a high-low bilayer under the effect of increasing thickness for the three cases cited above, as a function of wavelength.

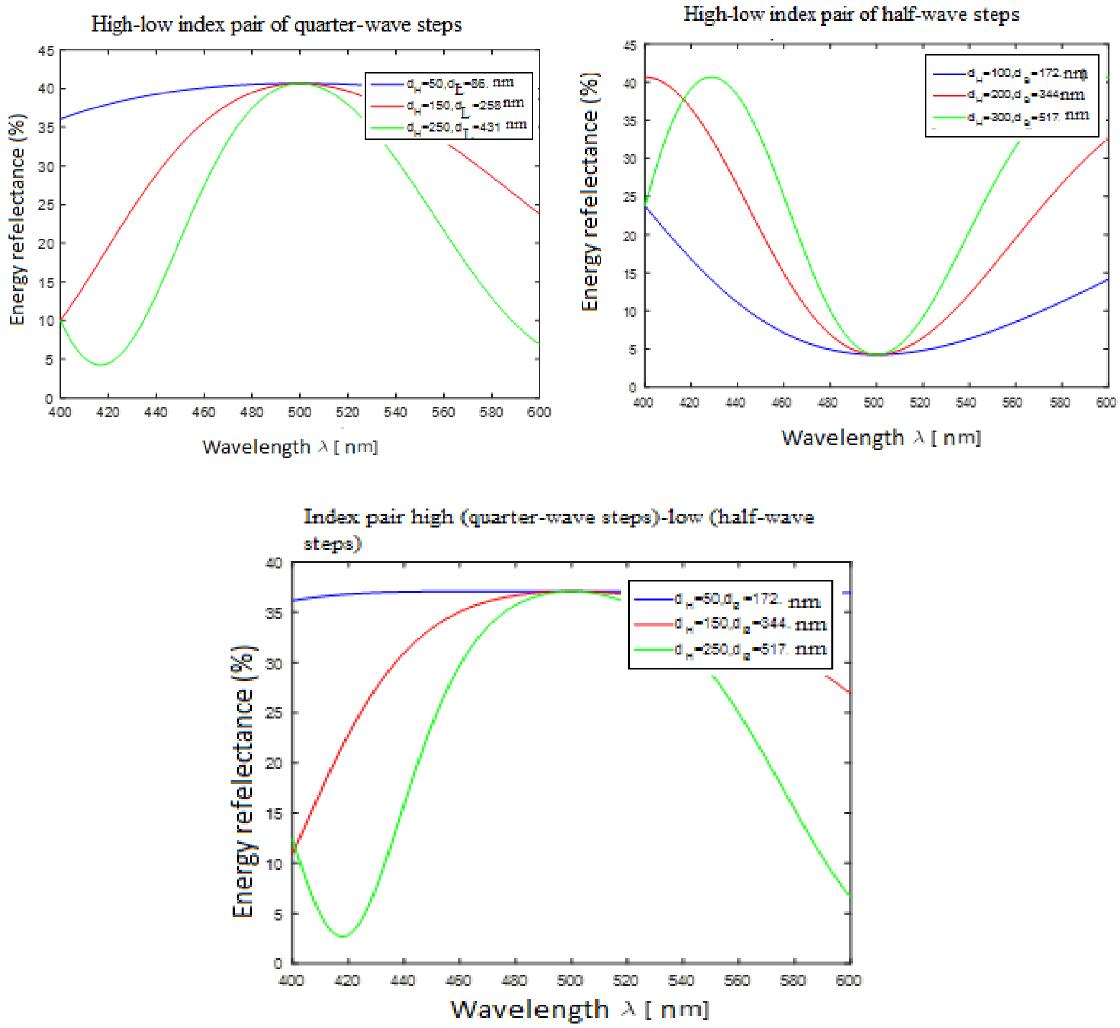


Fig. 5: Reflection spectra of high-low index pair under the effect of increasing thickness for each layer

From the figures, it can be, seen that increasing thickness influences spectral bandwidth in all three cases.

Therefore, to obtain a pattern of bilayers with a wide spectral bandwidth, we need to choose a quarter-wave thickness that has not multiplied by λ/4.

III.5. Study a mirror of Bragg

1. Effect of increasing the number of patterns

The number of Bragg mirror patterns has been increased q=3, 5, 10 and 18. Figure (6) shows the reflectance for several Bragg mirror patterns.

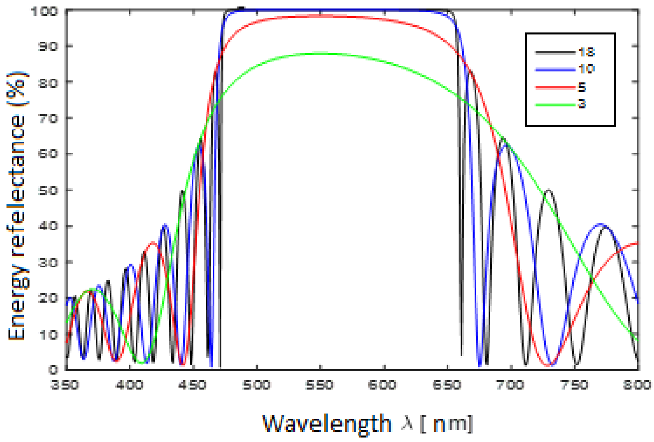


Fig. 6: Reflection spectrum by increasing the number of patterns of a Bragg mirror

From the reflection spectra shown in figure (6), we can see that increasing the number of patterns have indeed accompanied by an increase in the maximum reflectance, and at a certain number of patterns increases the maximum reflectance remains constant. A 3-pattern mirror has 87% maximum reflectance, while a 5-pattern mirror has 98% maximum reflectance. A 10-pattern and 18-pattern mirror with the same maximum reflectance (99%) centred at 550 nm.

We also note that if we increase the number of patterns, the bandwidth decreases, and we also observe an increase in the number of oscillations outside the bandwidth.

2. Effect of increasing layer thicknesses

We want to study the reflectivity of a 10-pattern Bragg mirror under the effect of increasing the thickness of the layers (an odd multiple). Figure (7) shows the reflectance energy of the Bragg mirror, the first undergoing a π phase, the second a 3π phase and the last a 5π phase.

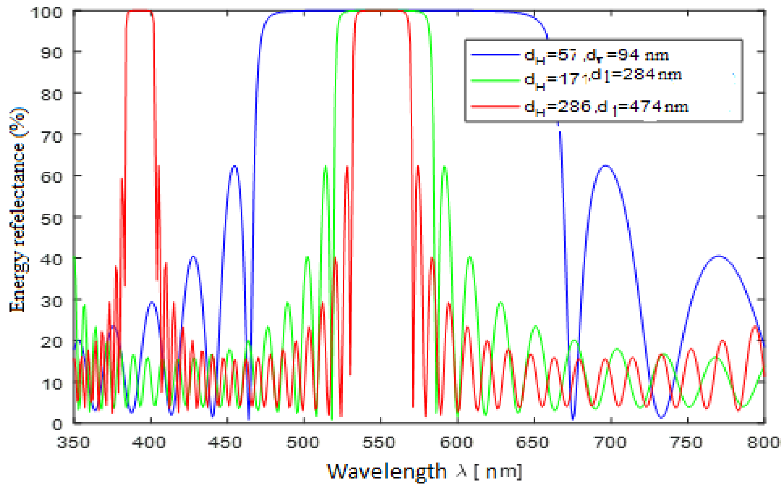


Fig. 7: Reflection spectrum of a 10-pattern Bragg mirror centred at 550 nm as a function of increasing layer thickness.

According to Figure; the same remarks as seen for a single layer and for a couple of HL index, the increase in thickness does not influence the maximum reflectivity of the mirror but it affects the width of the mirror spectral band.

The width of the spectral band decreases depending on the increase of the thickness of the layers and can have a narrow band of the centring wavelength at λ=550 nm and there is an increase in the number of oscillations.

Increase in thickness causes the appearance of another strip.

Therefore, to obtain a broad spectral band of reflection from a Bragg wavelength we choose a quarter-wave thickness corresponds to a phase of π.

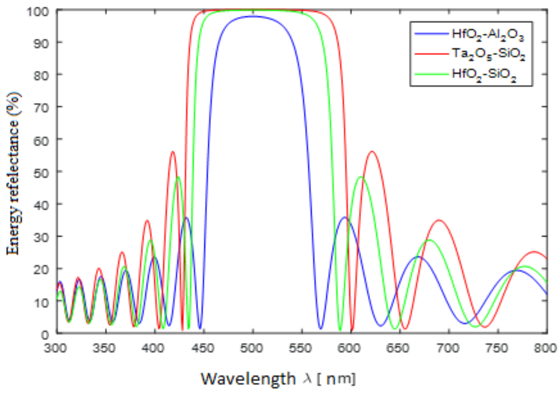
3. Effect of material change

We want to study several cases of Bragg mirrors by different couple of materials in order to obtain a maximum reflection and a wide spectral band.

For a wavelength λ = 500nm uses the following couples: HfO_2 (n_H = 2.1) and Al_2O_3 (n_L = 1.65); Ta_2O_5 (n_H = 2.25) and SiO_2 (n_L = 1.45); HfO_2 (n_H = 2.1) and SiO_2 (n_L = 1.45); HfO2 (n_H = 2.1) and SiO_2 (n_L = 1.45).

For a wavelength λ = 980 nm the couples used are: HfO_2 (n_H = 2.0840) and SiO_2 (nB = 1.4676); a Si (n_H = 3.6568) and SiO2 (n_L = 1.4676);TiO_2 (n_H = 2.4880) and SiO_2 (n_L = 1.4676)

Figure (8) represents the reflectance of several Bragg mirrors centred at a wavelength λ = 500 nm and λ = 980 nm respectively for couples of different materials.



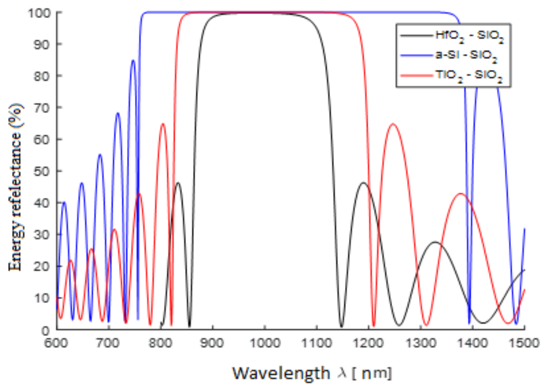


Fig. 8: reflection spectrum of Bragg mirrors centred respectively at 500 and 980nm as a function of different material torques.

Table 1 shows the decrease in the spectral bandwidth value on the index contrast function for a centring wavelength λ_B=500 nm.

Table1: Spectral bandwidth as a function of high-low index couples at λ_B=500 nm.

high index n_H	2.5	2.25	2.1

low indexn_L	1.45	1.45	1.65
the width of the spectral band $\Delta\lambda$	169 nm	137 nm	76nm

Table 2 shows the decrease in the value the spectral band width when the value of the high index for a centring wavelength λ_B=980 nm is decreased

Table 2: Spectral Band Width as a Function of High Low index pairs at λ_B=980 nm.

high index n_H	**3.6568**	**2.4880**	**2 .0804**
low indexn_L	1.46	1.46	1.46
the width of the spectral band $\Delta\lambda$	533nm	321 nm	215nm

Therefore, to obtain a better reflectance energy value and a wide spectral band with fewer layers, you must choose the highest possible high index value and the lowest possible low index value.

IV. Conclusion

The use of a simple mathematical model, based on the reflection of a selective electromagnetic wave in a multilayer optical system, allows to analyse the spectra of reflections given by the studied thin films, and the influence of some parameters on the reflection rate.

To know the spectral responses of a layer stack, it is enough to know the optical indices of the materials used, the phase and the thicknesses of the layers deposited.

A quarter-wave delay layer provides good reflection than a half-wave layer.

The increase in thickness has an influence on the spectral bandwidth of the reflected wave.

A quarter-wave delay must be chosen for a pair of materials, and for a stack of layers, in order to achieve maximum reflection.

Increasing the number of patterns to increase light reflection is limited.

References

[1] G. Fragneto, « Réflectivité de neutrons : exemples d'études des systèmes en matière molle », vol.11, p 89, 2010.

[2] L.R.Brovelli, U.Keller, « Simple analytical expressions for thr reflectivity and the penetration depth of Bragg mirror between arbitary media »Optics Communications, 1995, Pages 343-350.

[3] E. Yablonovitch. Photonic crystals : what's in a name ? Optics and Photonics news, 18, 12-13, mars 2007.

[4] Willey, R. R. (2011). Practical Design of Optical Thin Films, Willey Optical.

[5] [5] P. Louda, «Applications of thin coatings in automotive industry, » Journal of achievemens in materials and manufacturing engineering, vol. 24, pp. 51-56, 2007.

[6] Ritter, E. (1981). "Properties of optical film materials." Applied Optics 20(1) : 21-25.

[7] Traylor Kruschwitz, J. D. and W. T. Pawlewicz (1997). "Optical and durability properties of infrared transmitting thin films." Applied Optics 36(10) : 2157-2159.

[8] Thielsch, R., A. Gatto, et al. (2002). "A comparative study of the UV optical and structural properties of SiO2, Al2O3, and HfO2 single layers deposited by reactive evaporation, ion-assisted deposition and plasma ion-assisted deposition." Thin Solid Films 410(1): 86-93.

[9] Field, E., J. Bellum, et al. (2016). Laser Damage Comparisons of Broad-Bandwidth, High-Reflection Optical Coatings Containing TiO2, Nb2O5, or Ta2O5 High Index Layers.

[10] Zukic, M., D. G. Torr, et al. (1990). "Vacuum ultraviolet thin films. 1: Optical constants of BaF2, CaF2, LaF3, MgF2, Al2O3, HfO2, and SiO2 thin films." Applied Optics 29(28) : 4284-4292.

[11] D. I. Babic et S. W. Corzine, « Analytic expressions for the reflection delay, penetration depth, and absorptance of quarter-wave dielectric mirrors », IEEE Journal of Quantum Electronics, vol.28, no 2, pp. 514 - 524, 1992.

[12] M. Idir, A. Mirone, G. Cauchon, et P. Dhez, « Optiques de Bragg-Fresnel. Principes et applications », *Ann. Phys. Fr.*, vol. 22, p 2. C1-139-C1-146, févr. 1997, doi: 10.1051/anphys/1997030.

[13] H. Macleod, Thin-film optical filters, Third ed., CRC Press, 2001.

[14] Hoang Le-Huy « Introduction à MATLAB et Simulink », Département de génie électrique et de génie informatique Université Laval Université Laval Québec, CANADA, sept 1998, p3.

[15] Imemoriam, « Special thanks to joe Macke for providing this PDF of the military handbook (MIL-HDBK-141)», 5 Oct 1962.