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Engineering

THE INFRARED OPTICAL PROPERTIES OF $AL_{0.5}IN_{0.5}SB$ ALLOY WITH NANO COATINGS

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Abstract
In this article, the SiC/Nano GaAs and SiC/Nano InP coatings on $Al_{0.5}In_{0.5}Sb$ alloy are investigated in a theoretical framework. A Special program code written by MATLAB version 10 was performed to describe the reflectivity of coatings as a function of the nano-particles sizes, refractive index, and energy gap. This program is based on the Brus model and the Characteristic Matrix Theory. The results connected with nano-particle size of 3.6 nm in multilayer coatings indicate that our designs achieve high reflectivity. Such as, with six layers, the Air/SiC/Nano GaAs/$Al_{0.5}In_{0.5}Sb$ design gives the reflectivity for S-Polarization Rs=99.9% and for P-Polarization Rp=98.0% for oblique incidence of θ=45° and R=99.9% for the perpendicular incidence. Similarly, the Air/SiC/Nano InP/$Al_{0.5}In_{0.5}Sb$ gives Rs=99.9% and Rp=98.5% for oblique incidence of θ=45° and R=99.8% for the perpendicular incidence. This study set out with the aim of assessing the importance of Air/SiC/Nano GaAs/Al0.5In0.5Sb composition in industrial applications as a highly reflective coating for CO2 laser resonators in the far infrared region.

Keywords: Refractive coating, Nano GaAs particles, Nano InP particles, Brus model, Characteristic Matrix Theory.

摘要：在这项工作中，在理论框架下研究了 Al0.5In0.5Sb 合金上的 SiC /纳米 GaAs 和 SiC /纳米 InP 涂层。由 MATLAB 版本 10 编写的特殊程序代码用于描述涂层的反射率，作为纳米颗粒尺寸，折射率和能隙的函数。该程序基于 Brus 模型和特征矩阵理论。结果与多层涂层中 3.6 纳米的纳米粒度相关，表明我们的设计实现了高反射率。例如，对于六层，Air / SiC / 纳米 GaAs / Al0.5In0.5Sb 设计使得 S 偏振的反射率 Rs = 99.9%，对于倾斜入射 θ = 45°，P 偏振 Rp = 98.0%。垂直入射的 R = 99.9%。类似地，对于垂直入射，θ / 45°和 R = 99.8%的倾斜入射，Air / SiC / Nano InP / Al0.5In0.5Sb 给出 Rs = 99.9%和 Rp = 98.5%。本研究的目的是评估 Air / SiC / Nano GaAs / Al0.5In0.5Sb 组合物在工业应用中作为远红外区域 CO2 激光谐振器的高反射涂层的重要性。

关键词: 折射涂层，纳米 GaAs 颗粒，纳米 InP 颗粒，Brus 模型，特征矩阵理论

I. INTRODUCTION

The study of optical nano-coatings is considered to be interesting topic in various industrial fields. This is owing to their ability to modify the optical properties of the surfaces in order to achieve a high reflectance or a high transmittance depending on the applications employed, such as optical filters or high reflectivity mirrors [1]. The use of semiconductors alloys is very important and interest in the multiple fields industry. This technology has a wide range of semiconductor alloys [2]. The reason why these alloys is an essential materials used in various applications is the possibility of adjusting their properties to a certain wide range by modifying their composition [3]. Besides, nanotechnology has become an important subject of modern science and the focus of attention of various industries. In fact, it has become a key at the forefront of the most important fields in medicine, engineering, chemistry, biology and others. Also, nano-materials play an important role in various industries for opto-electronics devices such as diodes and sensors [4]. Moreover, the nano optical materials have attracted the attention of researchers and scientists working in the field of optics because of the unprecedented properties which are different from traditional materials owing to the effect of quantum confinement [5]. When the crystalline size decreases to be comparable or even smaller than the de Broglie wavelength, the distance between energy levels increases, then, quantum confinement affects the energy gap and the density of states of the materials. Thus, the optical and electronic properties which depend on the nano-particle sizes will be changed. The result of quantum confinement effect leads to what is called quantum dots, in which the electrons and holes are restricted in all three directions, and the system may be described as being zero-dimensional [6,7].

II. THEORY

A. Brus model

The first theoretical calculation of semiconductor nano-particles based on effective mass approximation (EMA) was reported by Brus. In this approximation, an exciton is considered to be confined to a spherical volume of the crystallite and the masses of electrons and holes are replaced with effective masses (m^*_e and m^*_h) to define the energy gap [8]:

$$\Delta E_g = \frac{\hbar^2 \pi^2}{2 r_{ps}^2}\left[\frac{1}{m_e^*}+\frac{1}{m_h^*}\right] - \frac{1.786\, e^2}{\varepsilon\, r_{ps}} - \frac{0.124 e^4}{\hbar^2 \varepsilon^2}\left[\frac{1}{m_e^*}+\frac{1}{m_h^*}\right]^{-1} \quad \dots (1)$$

where $r_{ps}$is the particle radius, m^*_h is the effective mass of the hole, m^*_e is the effective mass of the electronand ε is the relative permittivity, also known as the effective energy gap. The energy gap then is [9]:

$$E_g^{nano}(r_{ps}) = E_g^{bulk} + \Delta E_g \quad \dots (2)$$

Where: $E_g{}^{bulk}$ is the bulk energy gap and (r_{ps}) is the energy gap in the quantum dots. In the first term of equation (1) we can observe that the energy gap is inversely proportional to r^2_{ps}. The energy gap increases when the particle size decreases. In the second term we can notice the energy gap decreases with decreasing r_{ps} as a consequence of the increased strength of the coulombic interaction. The second and third terms are very small compared to the first, so they can be neglected. Then, equation 2 becomes:

$$E_g^{nano}(r_{ps}) = E_g^{bulk} + \frac{\hbar^2 \pi^2}{2 r_{ps}^2}\left[\frac{1}{m_e^*}+\frac{1}{m_h^*}\right] \quad \dots (3)$$

Based on equation 2, we expect the energy gap will increase as the size of the particle decreases due to the effect of the quantum confinement, which has a significant effect when the radius of the particles r_{ps} is equal to or smaller than the Exciton Bohr radius $\alpha_\circ$ [10]:

$$\alpha_\circ = \frac{4\pi\varepsilon_\circ \varepsilon_r \hbar^2}{e^2}\left[\frac{1}{m_e^*}+\frac{1}{m_h^*}\right] \quad \dots (4)$$

where ε_r and $\varepsilon_\circ$ are the permittivity of the semiconductor and vacuum respectively.

B.The relation between energy gap and refractive index

There is a strong correlation between the energy gap Eg and the refractive index n. Several studieshave been made to find mathematical relationships between refractive index and the energy gap. The following relationship is found to be the most accurate [11]:

$$n = \alpha + \beta E_g \quad \dots (5)$$

$\beta = -0.62\ \mathrm{eV}^{-1}$ and $\alpha = 4.048$with

Considering the simple physics of light refraction and dispersion, an empirical relationship is proposed as $n = 1 + \sqrt{(\frac{A}{E_g + B})^2}$, where A = 13.6

eV and B = 3.4 eV. Equation 5 is independent of the temperature. And in this equation, since $\beta < 0$, we see that the refractive index decreases with the increase of the energy gap. From equation (3), we can say that the refractive index of the quantum dots decreases with decreasing particle size.

C. The characteristic matrix of multilayer coating

The characteristic matrix which connects tangential components to the electric and magnetic fields can be expressed as [12]:

$$\begin{bmatrix} E_a \\ H_a \end{bmatrix} = \begin{bmatrix} 1 \\ Y \end{bmatrix} = \begin{bmatrix} \cos\delta & i\sin\delta/\eta_1 \\ i\eta_1 \sin\delta & \cos\delta \end{bmatrix} \begin{bmatrix} 1 \\ \eta_{sub} \end{bmatrix} \dots (6)$$

The input optical admittance [13]:

$$Y = \frac{H_a}{E_a} \qquad \dots (7)$$

Also:

$$Y = \frac{\eta_{sub}\cos\delta + i\eta_1 \sin\delta}{\cos\delta + i(\eta_{sub}/\eta_1)\sin\delta} \qquad \dots (8)$$

Y is usually referred to as the characteristic optical admittance.

For a system consisting of q thin films on a substrate, then:

$$\begin{bmatrix} E_a \\ H_a \end{bmatrix} = \left\{ \prod_{r=1}^{q} \begin{bmatrix} \cos\delta_r & i\sin\delta_r/\eta_r \\ i\eta_r \sin\delta_r & \cos\delta_r \end{bmatrix} \right\} \begin{bmatrix} 1 \\ \eta_{sub} \end{bmatrix} \qquad \dots (9)$$

The phase thickness is given by: $\delta_r = 2\pi n_r d_r \cos\theta_r / \lambda$.

Equation (9) provides all the necessary information for the calculation of the reflectivity (R) in the case of structures with several layers [14]. Figure 1 represents a system consisting of two thin films on a substrate. However, there are three terms a, b and c.

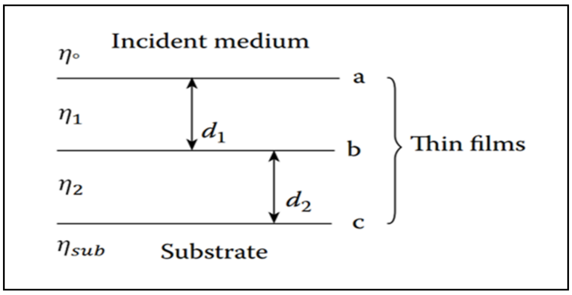


Figure 1. A system composed of two thin films (q=2) on a substrate [15].

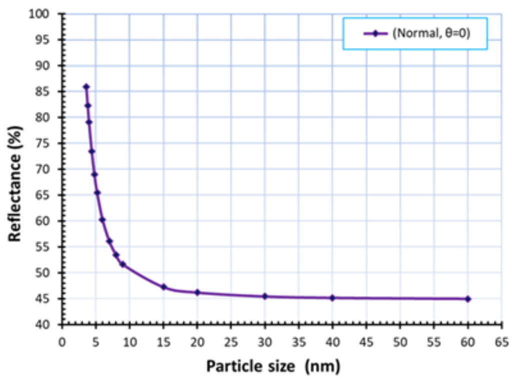
Thus, we found the reflectance from Fresnel's equations:

$$R = \left(\frac{\eta_\circ - \eta_1}{\eta_\circ + \eta_1}\right)^2 \dots (10),$$

where $\eta_\circ$ and η_1 are the optical admittance for median incidence and the transmittance respectively [16].

III. Suggested Design of an Air/SiC/Nano GaAs coating on Bulk $Al_{0.5}In_{0.5}Sb$

The alloy $Al_{0.5}In_{0.5}Sb$ has a refractive index n =3.13 and reflectivity (26.23%) is very low. When the substrate is coated with a single layer of (Nano GaAs) with the particle size Ps=3.6 nm, we notice a very low reflectivity is achieved in the case of vertical incidence (R=12.5%) and (Rs=16.9%, Rp=11.6%) in the case of oblique incidence of (θ=45°) for the design (Air/Nano GaAs/$Al_{0.5}In_{0.5}Sb$). This design can be used as an anti-reflective coating. However, it is also desirable to obtain a high reflection for some applications. The design (Air/SiC/Nano GaAs/$Al_{0.5}In_{0.5}Sb$) is proven to give the best reflectance at the design wavelength λ_o =10600 nm. The design of (Air/SiC/Nano GaAs/$Al_{0.5}In_{0.5}Sb$) shows a constant reflectance for the coating material of (20-60 nm). There is no effect of quantum confinement on the vertical component. The particle size of the coating in the range (10-20 nm) leads to increase the design reflectance. The increasing in the reflectance is due to the slightly decrease of coating refractive index. The refractive index with the particle size of $Ps > 10\, nm$, which approach to the Bohr radius of GaAs decrease to minimum values, due to the quantum confinement effect. The decrease of the refractive index is related to the increasing of the reflectivity to the maximum value of (Rs=92.2%, Rp=70.2%) for oblique incidence of (θ=45°) and (R=85.9%) for a perpendicular incidence when the particle size of the coating material is Ps = 3.6 and by using two layers of coating as shown in figures 2 and 3.



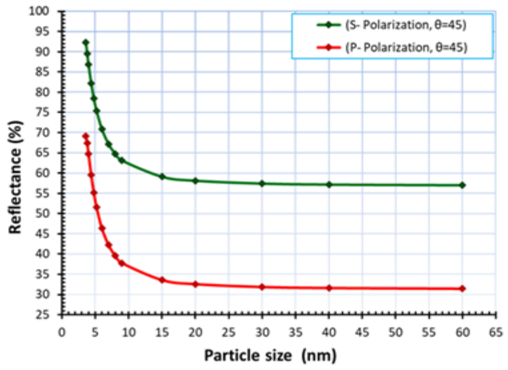


Figure 2. Design reflectance for Air/SiC/Nano GaAs/$Al_{0.5}In_{0.5}Sb$ as a function of the particle size with designing wavelength λo=10600 nm at (a) the vertical incidence and (b) for Incidence angle of 45^o.

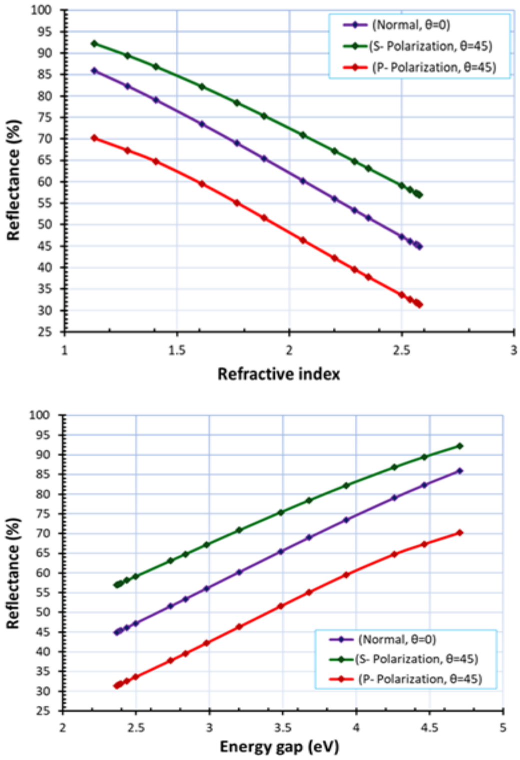


Figure 3. Reflectance of Air/SiC/Nano GaAs /$Al_{0.5}In_{0.5}Sb$ (a) as a Function of the Refractive Index and (b) as a function of the energy gap.

By adding six layers of (Air/SiC/Nano GaAs) coating, the reflectivity increases to 99.9% when a particle size of Nano GaAsis Ps=3.6 nm, as shown in figures 4 and 5.

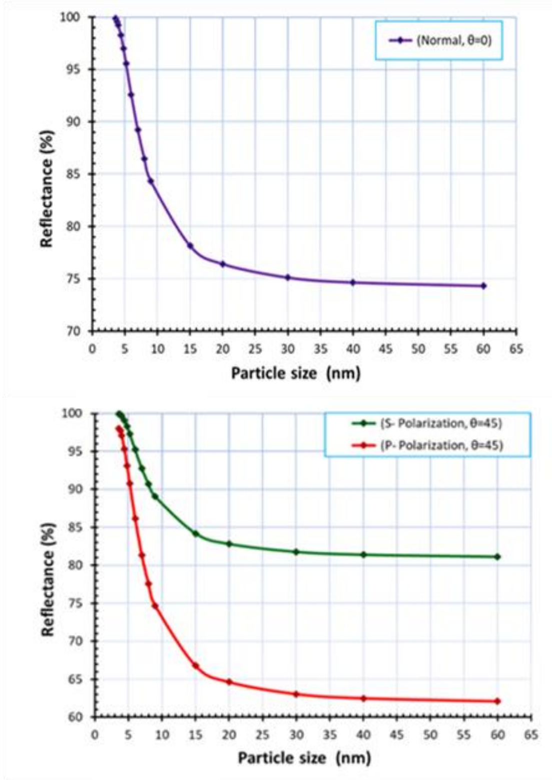


Figure 4. Design reflectance for Air/SiC/Nano GaAs/$Al_{0.5}In_{0.5}Sb$ as a function of the particle size with designing wavelength λ_o=10600 nm at (a) the vertical incidence (b) for incidence angle of 45^o.

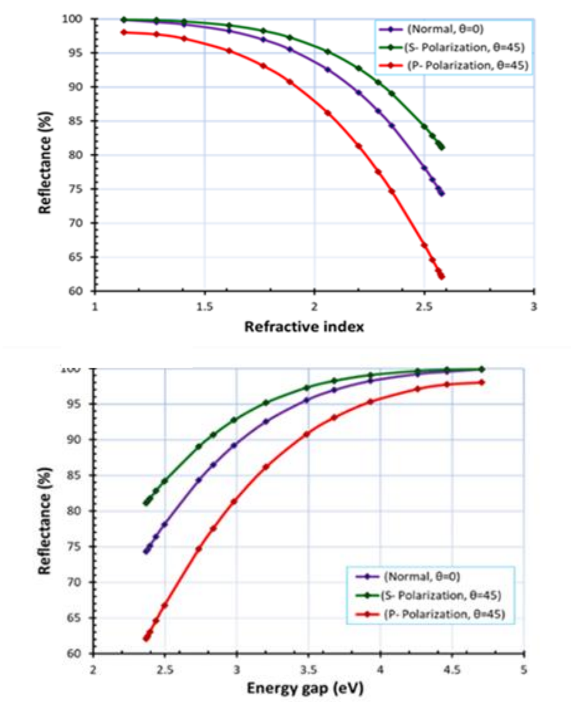


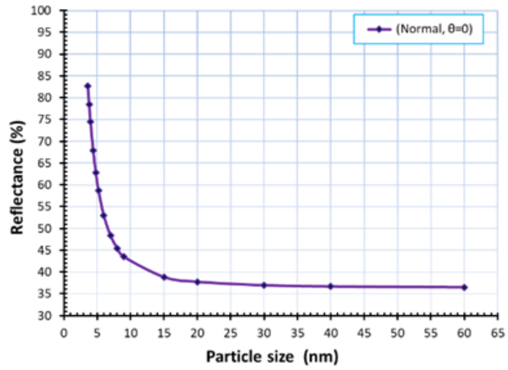
Figure 5. Reflectance of Air/SiC/Nano GaAs/$Al_{0.5}In_{0.5}Sb$ (a) as a function of the refractive index (b) as a function of the energy gap.

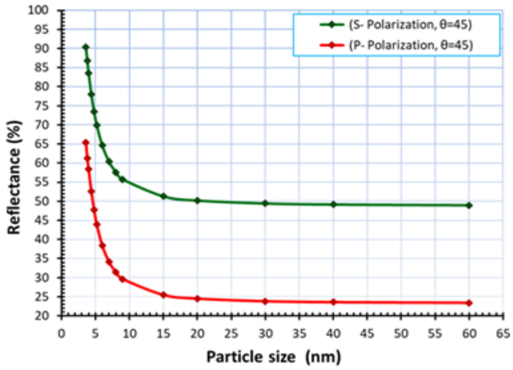
Table 1.
The change in the reflectivity of Air/SiC/Nano GaAs/$Al_{0.5}In_{0.5}Sb$ for the vertical and oblique incidence with particle size Ps = 3.6 nm and refractive index 1.21, as the number of layers is increased.

Here N is the number of a coating layer.

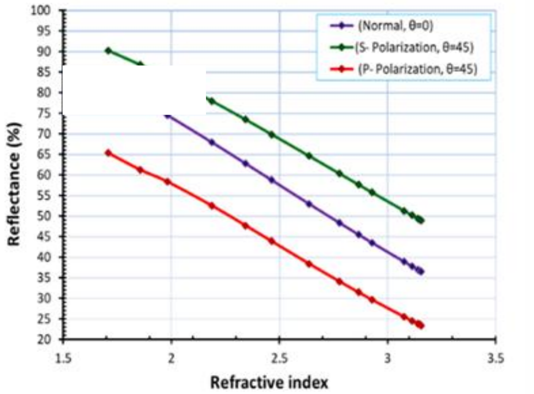
IV. Suggested Design of an Air/SiC/Nano InP coating on Bulk $Al_{0.5}In_{0.5}Sb$

In this design the ($Al_{0.5}In_{0.5}Sb$) substrates were coated with a (Nano InP) layer, i.e (Air/Nano InP/$Al_{0.5}In_{0.5}Sb$) which gave rise to a lower reflectivity for the vertical incidence with (R=0.11%), while in case of oblique incidence (θ=45°) the reflectivity is (Rs=1.94%, Rp=0.56%). This new design, therefore, gives antireflection characteristics, which may be used in optoelectronic applications. To find a design with high reflectivity for the industrial applications a second layer of SiC is added (Air/SiC/Nano InP/$Al_{0.5}In_{0.5}Sb$). This design gives a high reflectivity (Rs=90.3%) for oblique incidence (θ=45°) and (R=82.7%) for perpendicular incidence at λ_o =10600 nm with the particle size of 3.6 nm and by using two layers as shown in figures 6 and 7 .





N	R	Rs	Rp
1	12.557	16.9021	11.6711
2	85.9154	92.2703	70.1825
3	87.4618	93.1567	72.8932
4	98.2302	99.2786	91.9719
5	98.4364	99.3636	92.7454
6	99.8901	99.9888	98.0466



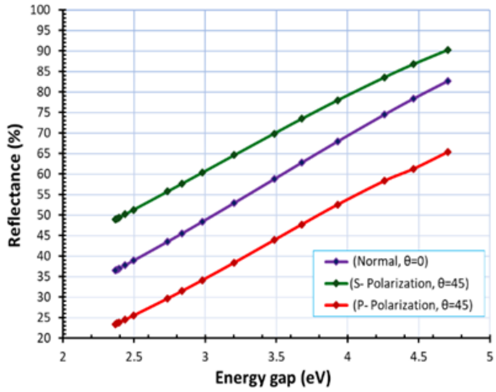
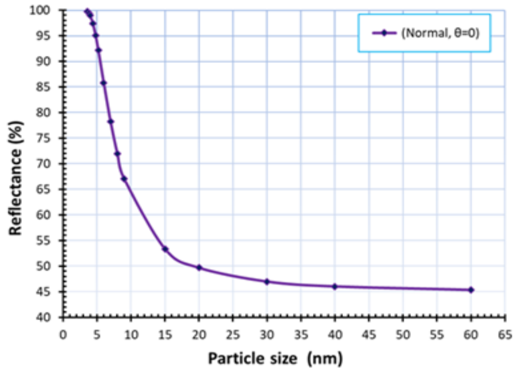
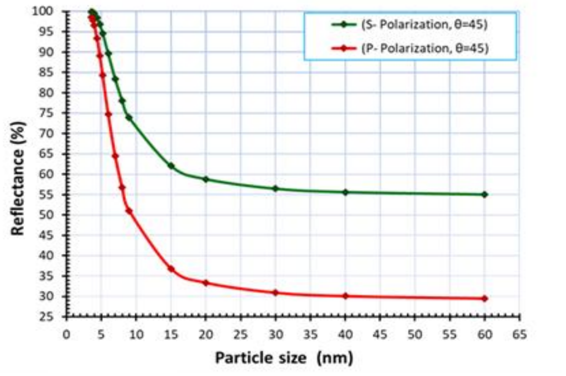


Figure 7. Reflectance of Air/SiC/NanoInP/$Al_{0.5}In_{0.5}Sb$ (a) as a function of the refractive index and (b) as a function of the energy gap.

By adding six layers of (Air/SiC/Nano InP) coating, the reflectivity increases to up to 99.88% for a particle size of Ps=3.6 nm, as shown in figures 8 and 9.





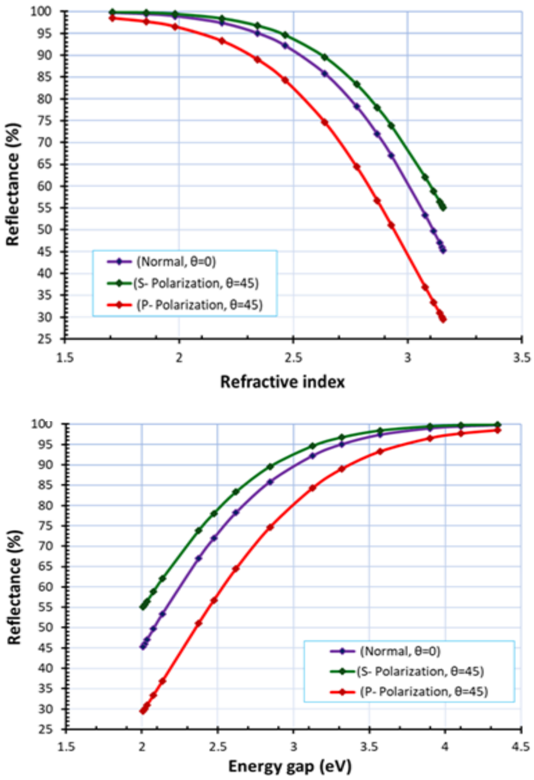


Figure 9. Reflectance of Air/SiC/Nano InP/$Al_{0.5}In_{0.5}Sb$ (a) as a function of the refractive index and (b) as a function of the energy gap.

Table 2.
The change in the reflectivity of Air/SiC/Nano InP/$Al_{0.5}In_{0.5}Sb$ for the vertical and oblique incidence with particle size Ps = 3.6 nm and refractive index 1.70, as the number of layers is increased.

N	R	Rs	Rp
1	0.111	1.9468	0.5656
2	82.7074	90.3001	65.4009
3	88.4718	94.4595	73.7736
4	94.5969	97.1791	85.7438
5	98.8718	99.4927	95.3596
6	99.7685	99.8895	98.5258

Based on the above, the best design is (Air/SiC/NanoGaAs/$Al_{0.5}In_{0.5}Sb$), where high reflectivity was obtained (Rs=99.9%) approximately at incidence angle (45^o) and Ps=3.6 and wavelength λ_o=10600 nm, which can be used in CO_2 lasers.

V. CONCLUSIONS

The reflectance of optical coatings depends on the refractive indexes of the materials and the incidence angle. The refractive index coefficients can be tuned through controlling the particle size of coating material in the design of optical coating for the wavelength 10600 nm by using SiC layer and Nano GaAs layer on alloy substrate of $Al_{0.5}In_{0.5}Sb$ alloy, to obtain a high reflectivity compared to $Al_{0.5}In_{0.5}Sb$ alloy. A high reflective is obtained by adding a six-layer coating of (Air/SiC/Nano GaAs) to reach Rs=99.9% for the design (Air/SiC/NanoGaAs/$Al_{0.5}In_{0.5}Sb$), and adding six-layer coatings of (Air/SiC/Nano InP) to reach Rs=99.8% for the design (Air/SiC/NanoInP/$Al_{0.5}In_{0.5}Sb$) with quarter wavelength thickness. So the design consisting of **(Air/SiC/NanoGaAs /$Al_{0.5}In_{0.5}Sb$)** is the best. A 99.9% reflectivity is achieved at the wavelength of the design when the particle size of the coating is Ps=3.6 nm. The prosperities of this design can be used in optical instruments applications such as lasers, telescopes and microscope.

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