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Study of the Variation of the Optical Properties of Nano-GaAs Coating with Particle Size

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In this work, the optical properties of nano-GaAs coating are studied as a function of its particle size. Bulk Si is used as a basis for multi-layer optical reflection of nano-GaAs coating. This study is done by using a program performed in Matlab software, aiming to calculate the variation in reflectivity of the perpendicular and oblique incident light at wavelength of 1064 nm with particle size, refractive index and energy gap of the coated multi-layer. This program is based on the Brus model and characteristic matrix theory. The results show that the reflectivity of Air/Si/Nano-GaAs/Si design, with particle size P_s which equal is to 3.6 nm is ($Rs = 100\%$, $Rp = 99.8\%$), approximately for oblique incidence at 45° and $R = 99.98\%$ for a perpendicular incidence. Given such a high reflectivity gained by this design, this study makes a major contribution to the field of fabricating Nd-YAG laser resonators.

Keywords: High-reflected coatings; nano-GaAs particles; Brus model; characteristic matrix theory.

1. Introduction

Dielectric materials can be used to design a high-reflectance coating by taking the advantage of their different refractive indices.[1] It is well known that many opticals, such as refractive index and energy gap, depend on the particle size in nanomaterials.[2] Semiconductor materials are considered as suitable materials for nanoscale devices. The nanomaterials have properties that are quite different from their bulk counterparts.[3] The quantum confinement effects on the physical properties of nanomaterials arise from the confinement of the electronic particles, such as electrons, by potential barrier within a particular small region of space.[4] Quantum dots are such cases in which the electrons are bound in all the three directions. When the dimensions of the nanostructured particles are very small and approach the de Broglie wavelength, the quantization effects take place. The optical and electronic properties of the materials are affected by quantum confinement because the distance between the energy levels increases by decreasing nanoparticle sizes.[4,5] Abed and Al Rashid[1] designed a high-reflection coating that depends on the variation of refractive indices in the NIR spectral region (700–2500 nm). Ramizy and Al Rashid[2] designed and optimized a silicon quantum-dot antireflection coating with high performances for UV light.

Mohammed and Al-Rashid[6] designed a high reflectance nanocoating for ruby laser resonators. Also, Abed and Al-Rashid[7] studied the effects of nanoparticle sizes on the transition of CdTe thin films at visible wavelengths. This work offers some important insights into examining the effect of changing the size of nano-GaAs on its optical properties when it is being used as a coating material. These findings provide significant insights for future research due to the possibility of fabricating solid-state laser resonator working at 1064 nm wavelength based on using multi-layer quarter wavelength on an Si substrate. Our novelty and motivation use nanomaterials coating for Nd-YAG laser resonators, which have not been theoretically studied. This study presents an optimization of nanocoating for laser applications.

2. Theory

2.1. *The Brus model*

The Brus model is one of the most widely used optical models. It shows that the energy gap of the semiconductor in quantum dots depends on the particle size.[8] The values of the effective masses of electrons and holes play an important role in this model. The variation of the energy gap leads to the well-known equation of Brus[8]

$$\Delta E_g = \frac{\hbar^2\pi^2}{2r_{\text{ps}}^2}\left[\frac{1}{m_e^*}+\frac{1}{m_h^*}\right] - \frac{1.786\,e^2}{\varepsilon r_{\text{ps}}} - \frac{0.124e^4}{h^2\varepsilon^2} \times \left[\frac{1}{m_e^*}+\frac{1}{m_h^*}\right]^{-1}, \tag{1}$$

where r_{ps} is the particle radius, m_e^* is the effective mass of the electron, m_h^* is the effective mass of the hole and ε is the relative permittivity.

With E_g^{bulk} being the bulk energy gap and $E_g^{\text{nano}}(r_{\text{ps}})$ being the quantum dot energy gap, then Eq. (1) gives[9]

$$E_g^{\text{nano}}(r_{\text{ps}}) = E_g^{\text{bulk}} + \Delta E_g. \tag{2}$$

The energy gap increases when particle size decreases as shown in the second term of Eq. (2). If the second and third terms of Eq. (1) can be ignored compared to the first term, then Eq. (2), becomes

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

The Bohr radius of the Acetone ($\alpha_\circ$) can be defined as[10]

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

where $\varepsilon_\circ$ and ε_r are the vacuum permittivity and permittivity of the semiconductor, respectively. When r_{ps} is close to the Bohr radius given by Eq. (4), then one can expect variations of the energy gap with particle sizes.

3. The Characteristic Matrix Theory of Multi-Layer Coatings

This theory has the following mathematical form for q thin films[11]:

$$\begin{bmatrix} B \\ C \end{bmatrix} = \left\{\prod_{r=1}^{q}\begin{bmatrix} \cos\delta_r & i\sin\delta_r/\eta_r \\ i\eta_r\sin\delta_r & \cos\delta_r \end{bmatrix}\right\}\begin{bmatrix} 1 \\ \eta_m \end{bmatrix}, \tag{5}$$

where $\delta_r = 2\pi n_r d_r \cos\theta_r/\lambda$ is the phase thickness, η_m is the refractive index of the substrate, B and C, respectively stand for the electric and magnetic fields, and η_r is the optical permittivity. Equation (5) is well known as the modified characteristic matrix equation.[12] Also, it has all the necessary information to describe the optical parameters like reflectivity R and transmittance T for multi-layer structures.[13] One can see from Fig. 1 that with two layers of thin films on a substrate, there are three interfaces, and hence, three terms a, b and c.

The electromagnetic field can be separated into electric and magnetic fields, then can be connected to these fields as[15]:

$$\eta = \frac{H}{E}, \tag{6}$$

in case of vertical incidence, ($\eta = y = n\gamma$), where y, n and γ are the medium permittivity (at the vertical incidence), the real refractive index and the per-

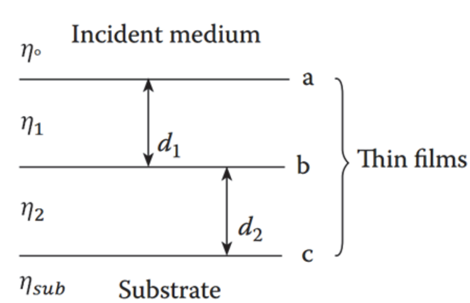


Fig. 1. Two layers of thin films on a substrate.[14]

mittivity of free space, respectively. Numerically, $y = n$ in free space units, then[14]

$$\eta_0 = y_0 = n_0\gamma = n_0, \quad (7)$$

in the first medium, then, whereas in the second medium is it

$$\eta_1 = y_1 = n_1\gamma = n_1. \quad (8)$$

For P-Polarization and S-Polarization, in oblique incidence, one can use the following equations[16]:

$$\eta_p = n/\cos\theta, \quad (9)$$

$$\eta_s = n\cos\theta, \quad (10)$$

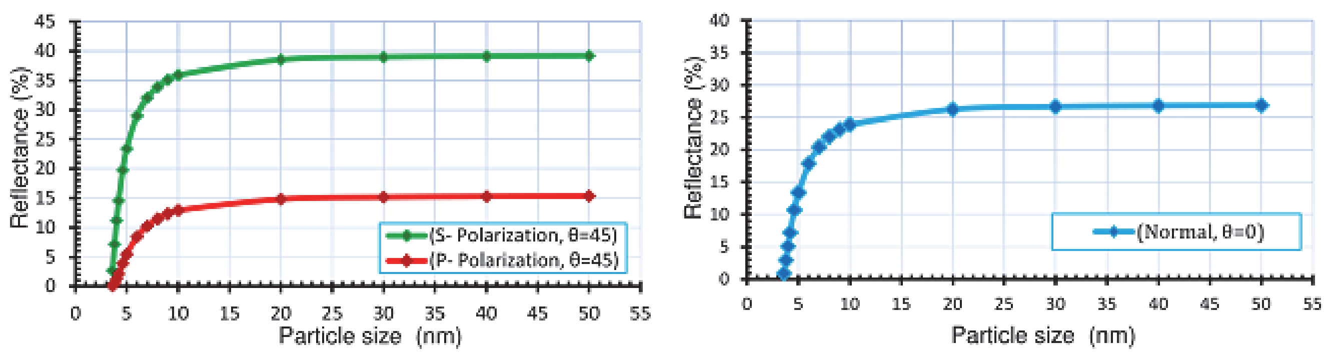
where θ is the incidence angle in the first medium which is connected with the refraction angle through Snell's law.[16]

4. Results and Discussion

The MATLAB program is developed to calculate the variation of optical properties like reflectivity, refractive index and energy gap, with the nanosize of GaAs particles. This program is suitable to the goal of optimizing reflective optical coatings by tuning the particles size for the 1064 nm wavelength region of the electromagnetic spectrum.

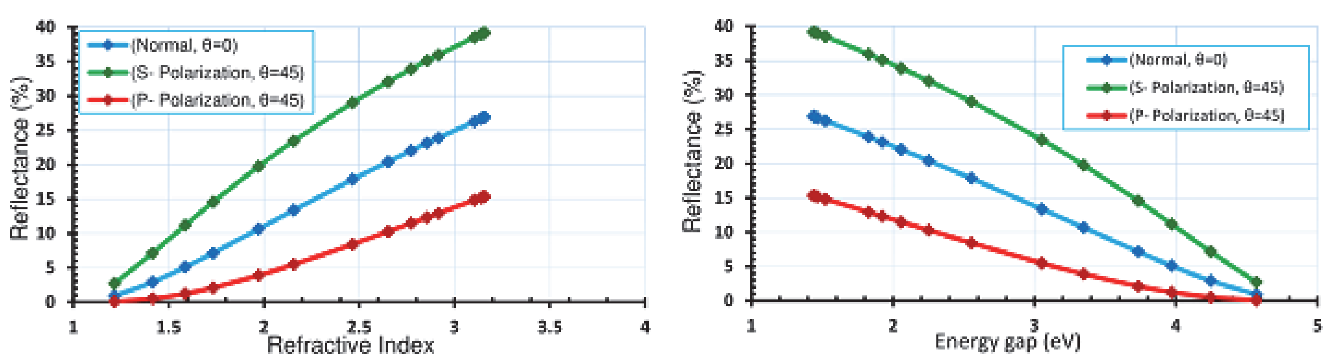
4.1. *Reflectivity of nano-GaAs coating as a function of the particle size*

The reflectivity of nano-GaAs coatings has been computed while varying the particle size ($\text{ps} = 2r_{\text{ps}}$).[17] The angles that are used to compute the reflectivity values are 0° and 45°. Figures 2 and 3 show that the reflectivity is varying with particle size, reflective index and energy gap of single-layer GaAs coating. Figure 4 shows the variation of the reflective index and energy gap with the particle size. The energy gap and reflective index change with particle size when the size is less than 20–50 nm. One can see from these figures that there is a direct proportion between refractive index and particle size, while there is an inverse proportion between the energy gap and the particle size. All these cause the reflectivity value to increase. These changes are very small until the particle size becomes smaller or equal to the Bohr radius of the



(a) (b)

Fig. 2. Variation of GaAS reflectance with particle size when (a) $\theta = 45°$, (b) $\theta = 0°$.



(a) (b)

Fig. 3. Variation of GaAs reflectance with (a) refractive index, (b) energy gap.

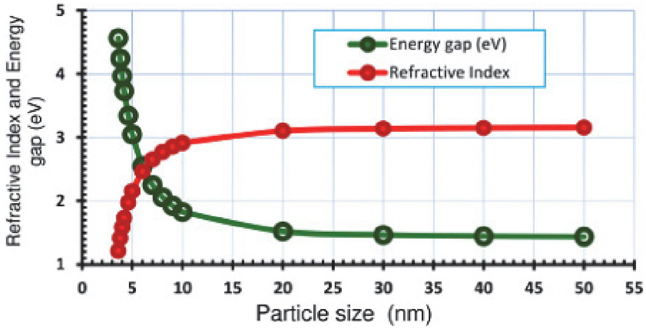


Fig. 4. Variation of refractive index and energy gap of GaAs with the particle size.

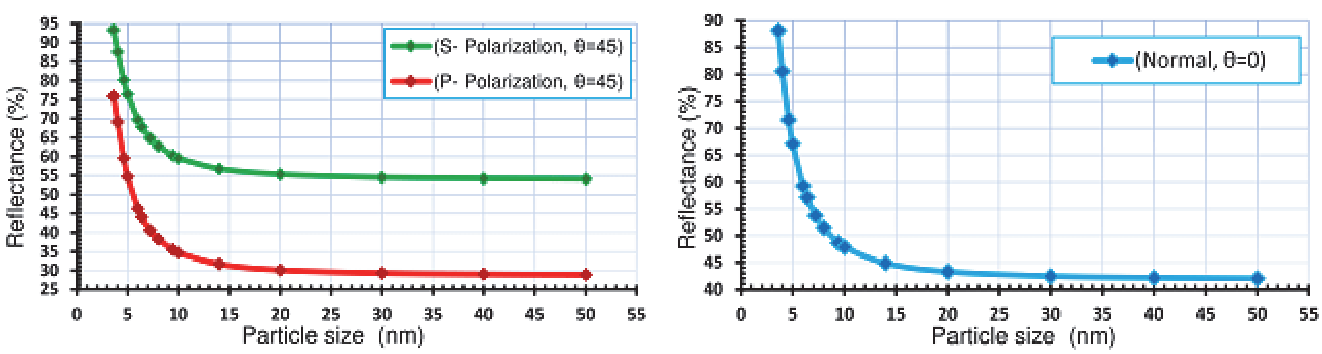
excitation. The results show that the minimal reflectivity is $R = 0.9299\%$ when $\theta = 0°$, and Rs = 2.7155%, Rp = 0.0737% when θ is 45°.

4.2. *Design of an Air/Si/Nano-GaAs coating on Bulk Si*

Figures 5 and 6 show the reflectance of Air/Si/Nano-GaAs design, this (Air/HL/Sub) achieves the highest reflectance for a wavelength if $\lambda = 1064$ nm. A constant reflectance is obtained for Air/Si/Nano-GaAs/Si design when the particle size is in 20–50 nm range, where the effect of the quantum confinement at the size is virtually nonexistent, at the particle size from 7–20 nm, can be observed increasing in the value of design Reflectance. The refractive index of coating decreases fast, when the particle size is smaller than 7 nm, this results from quantum confinement getting increasingly important, when the particle size approaches the Bohr radius of GaAs. This results in high reflectivity, while approaching maximum value of Rs = 93.3%, Rp = 75.9% at $\theta = 45°$ and $R = 88.0911\%$, when $\theta = 0°$ for a particle size of 3.6 nm and one layer of coating.

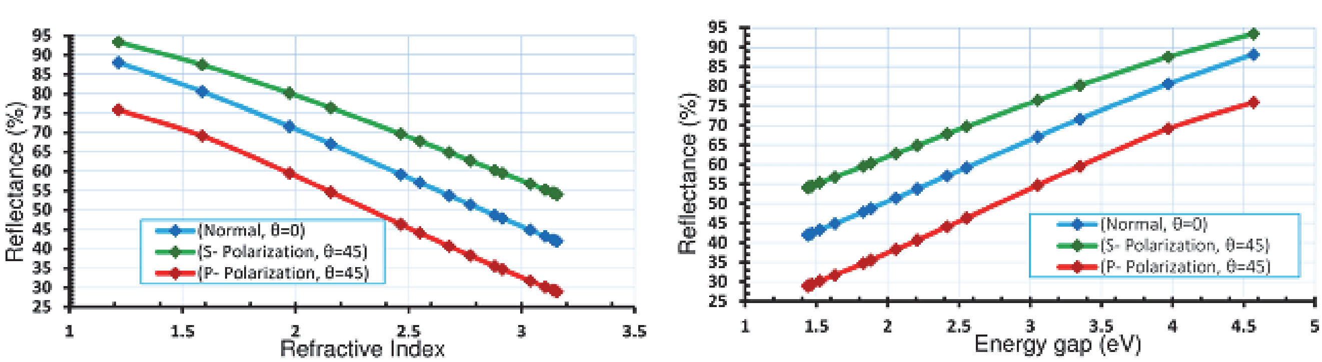
The reflectivity approaches 100% approximately, if one can add four layers from (Air/Si/Nano-GaAs) coating with particle size of 3.6 nm, as shown in Figs. 7 and 8.

The effect of the number of layers on reflectivity to layer Air/Si/Nano-GaAs design is shown in Table 1. One can see that the four-layered coating



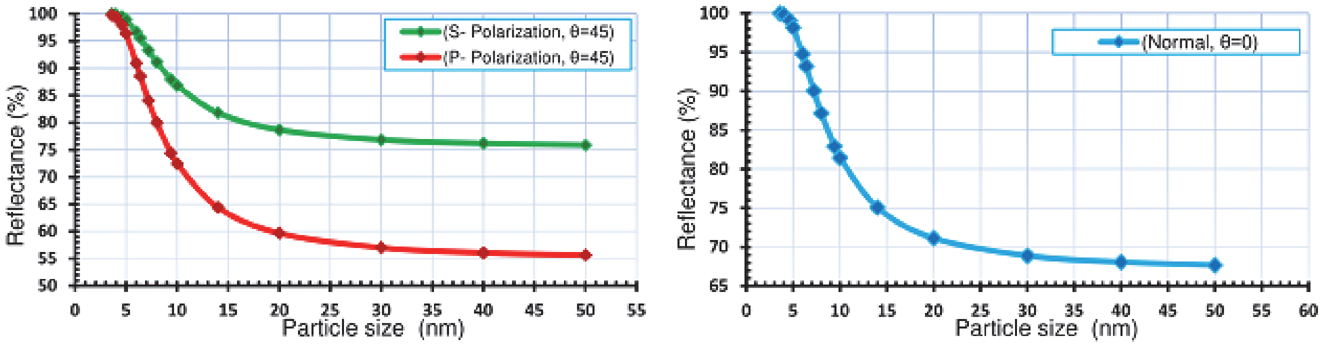
(a) (b)

Fig. 5. Variation of the reflectance of (Air/Si/Nano-GaAs/Si) design when $n_{sub} = 3.6$, $L = 0.25\lambda_o$ and $\lambda_o = 1064$ nm with the particle size at (a) $\theta = 45°$ and (b) $\theta = 0°$.



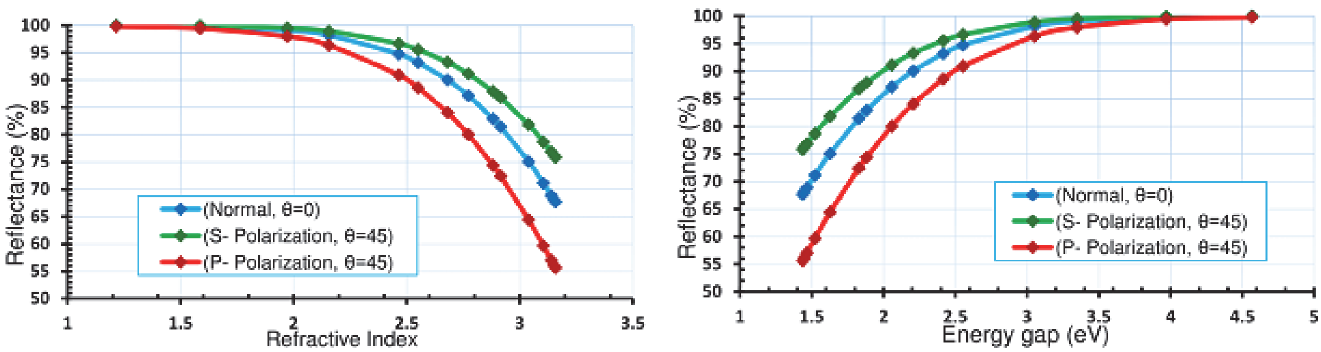
(a) (b)

Fig. 6. Variation of the reflectance of (Air/Si/Nano-GaAs/Si) with (a) refractive index, (b) energy gap.



(a) (b)

Fig. 7. Variation of the reflectance of Air/Si/Nano-GaAs/Si with particle size, when $n_{\rm sub} = 3.6$, $L = 0.25\lambda_o$ and $\lambda_o = 1064$ nm for (a) $\theta = 45°$ and (b) $\theta = 0°$.



(a) (b)

Fig. 8. Variation of the reflectance Air/Si/Nano-GaAs/Si with the (a) refractive index, (b) energy gap.

Table 1. Effects of the number of layers on reflectivity of (Air/Si/Nano-GaAs) design with particle size 3.6 nm and $\theta = 0°$ and $\theta = 45°$.

N = number of coating layer	Refractive index	$R\%$	$Rs\%$	$Rp\%$
1	1.2159	88.0911	93.3772	75.8726
2	1.2159	98.5644	99.4001	94.9458
3	1.2159	99.8352	99.947	99.0152
4	1.2159	99.9812	100	99.8108

gives a reflectivity of virtually 100% approximately. Then, the Air/Si/Nano-GaAs coating can be used in many industrial applications in different spectrum regions that need high reflectivity, such as Nd-YAG laser resonator, instead of gold.

5. Conclusions

The nanoparticle size is proportional directly and inversely to the refractive index and energy gap, respectively, this leads to increase in reflectivity of the coatings when the particle size approaches the Bohr radius of the excitation because the quantum confinement is not existent in the particle size less than 7 nm. The reflectivity depends on the number of layers and it increases with the number of layers increasing. The results show that four layers from Air/Si/Nano-GaAs design with bulk Si substrate containing particle size of 3.6 nm, θ at 0° and 45° and wavelength of 1064 nm, give high reflectivity approaching 100% approximately. These coatings can be suggested for use in industrial application instruments that need high reflectivity such as with Nd-YAG laser resonators.

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