Theoretical study of the optical properties of HgS/Na_3AlF_6, HgS/MgF_2 and CdS/Na_3AlF_6 thin films

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Abstract

The optical properties of multi-layers thin films, to be used as resonator for
Nd:YAG, is studied in this work via computer simulation. The output coupler
was designed to be fabricated by successive thin layers to achieve very high
transmittance at optical wavelengths around 1064 nm for Nd:YAG laser. In
addition, different optical filters were examined to control the transmittance
and reflectance for the same laser wavelength. Three samples of dielectric
materials composed of HgS/Na_3AlF_6, HgS/MgF_2, and CdS/Na_3AlF_6 were used
and compared with each other in transmittance, reflectance, physical
thickness, optical thickness and full width at half maximum. The results
showed that the best transmittance was achieved with HgS+Na3AlF6 where
the transmittance for 1064 nm increased to 95.74 %.

Keywords

Optical filters; Nd-YAG laser resonator; Multi-layers thin films

Introduction

A dielectric film stack consists of layers of two different materials alternately deposited on a substrate. Each layer has a thickness of one quarter of the reference wavelength. These thin films are used as mirrors, reflectors, filters, beam splitter. All lasers resonators made use of one or more of these components. A designed sequence of the thin film filters was the following schemes: Air/(HL)^nHH(LH)^n/substrate, where H means material with High refractive index, L means material with Low refractive index and n is a real number [1]. The large difference between the refractive indices of the materials can improve the optical characteristics of the filters. Therefore, CdS and HgS were chosen as the high refractive index (H) (2.5 and 2.9) while Na$_3$AlF$_6$ and MgF$_2$ were chosen as the low refractive index (L) (1.35 and 1.38) [2]. One of the most important lasers using different types of optical components is the Nd–YAG with the famous wavelength of 1064 nm. Nd:YAG crystal is the most widely used solid-state laser medium due to its excellent optical and mechanical properties. The Nd:YAG has the advantages of excellent thermal properties, ease of fabrication, low manufacturing costs, high neodymium concentration without any decrease in the optical quality, no growth limitation of shape and size and ease of power scaling [3,4].

Generally, most of the researches on Nd:YAG lasers focused on ^{4}F$_{3/2}$-^{4}I$_{11/2}$ transition at the 1064 nm wavelength and also focused on how to develop the Nd:YAG resonator in this wavelength [5]. Usually these resonators are composed of thin films, with specific optical characteristics, deposited on substrate.

Concerning the optical properties of graphene, the so-called thin-film limit (TFL) or thin-film approximation, obtained by taking the zero-thickness limit in classical formulae for the optical absorptance A, reflectance Rand transmittance T, is frequently discussed. Apart from graphene, the TFL has found applications in a variety of characterization methods, including differential reflectance spectrometry and infrared spectroscopy, as well as in polarimetry of very thin layers and low absorptance spectroscopy [6].

For the optical properties of the thin films, many characterization techniques, such as x-ray diffraction and band gap calculation from transmission and reflectance, cannot provide reliable information due to the small thickness, whereas simulation is a powerful tool owning to its high sensitivity to the film thickness and optical properties [7], both of which are important for understanding the materials properties and optimizing the performance of the optical component [8].

Film thickness and refractive index were measured by spectroscopic ellipsometry. Atomic Force Microscopy (AFM) was used to confirm the thickness evaluation and to control the surface roughness. The influence of temperature, annealing time and argon pressure were studied for the passivation improvement [9].

Material and method

In order to examine the performance of the different filters composed of HgS/Na_3AlF_6, HgS/MgF_2 and CdS/Na_3AlF_6, a number of titrations for them was done in transmittance, physical thickness, optical thickness, geometric thickness and full width at half maximum (FWHM).

The physical thickness (d) is given by:

$$d = \frac{0.25 \times \lambda_0}{n} \tag{1}$$

where (d) in nm, λ_0 is the reference wavelength also in nm and η is the refractive index [10].

The geometric thickness (QWOT) is

$$QWOT = \frac{d}{\lambda_0} \tag{2}$$

From equation (2) it can be seen that the geometric thickness is dimensionless quantity [11]. Optical thickness (Optical depth) is a measure of transparency. If I_0 is the intensity of radiation of the source and I is the observed intensity after a given path, then optical depth τ is defined by the following equation [12]:

$$\frac{I}{I_0} = e^{-\tau} \tag{3}$$

From Eq.(3) it can be seen that the optical thickness is dimensionless quantity.

Full width at half maximum (FWHM) is an expression of the extent of a function, given by the difference between the two extreme values of the independent variable, at which the dependent variable is equal to half of its maximum value [13].

Results and discussion

Table 1 lists the details of the transmittance spectrum and the results of the designed thin films, with varying thickness and glass substrate of 1.50664 refractive index, which were designed by alternating dielectric multilayer films to meet the requirements of high transmittance to 1064 nm. Figures 1 to 3 show the transmission spectra of these materials with maximum transmittance at 1064 nm. A computer program, using optical admittance loci analysis was run for thin film calculations, at the reference wavelength (λ_0) 1064 nm, getting the best results of different transmittance percentage with different thicknesses [10]. We need to titrate these different materials to choose the best one.

Table 1. Transmittance of three filters at wavelength 1064 nm with glass substrate of 1.50664 refractive index

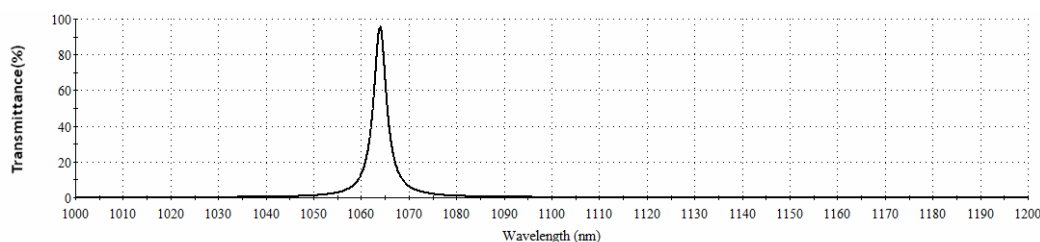| Materials	Refractive index	Physical thickness(nm)	No. of layers	Filter design	Trans. (%)
HgS/Na₃AlF₆	2.9/1.35	1916.02	11	(HL)^3HH(LH)^3	95.74
HgS/MgF₂	2.9/1.3803	1890.06	13	(HL)^3HH(LH)^3	95.74
CdS/ Na₃AlF₆	2.5/1.35	3247.17	21	(HL)^5HH(LH)^5	95.74

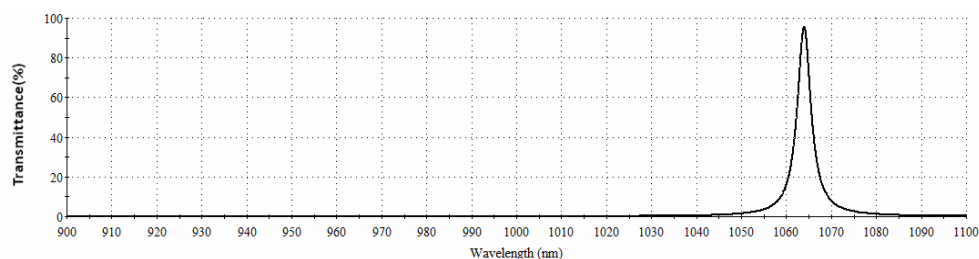**Figure 1.** *Transmission spectrum of HgS/Na₃AlF₆ between 1000 and 1200nm*

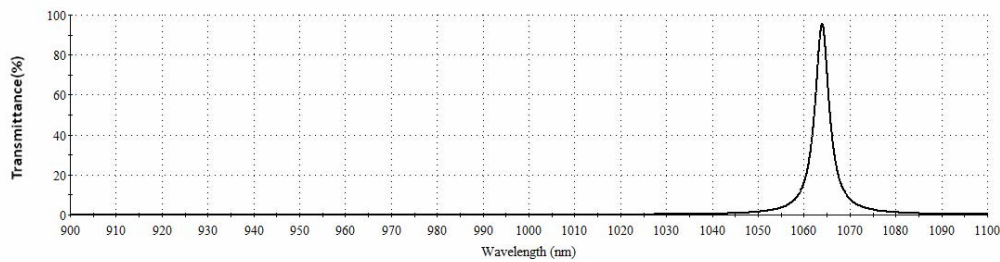**Figure 2.** *Transmission spectrum of HgS/MgF₂ between 900 and 1100nm*

Figure 3. Transmission spectrum of CdS/ Na_3AlF_6 between 900 and 1100nm

Figure 4 shows the values of transmittance (%) of the dielectric materials at 1064 nm. We can notice that the value of the transmittance (%) is almost the same for all the dielectric materials. Therefore, one may look for other titrated material among these dielectric materials to choose the material that has better characteristics than others.
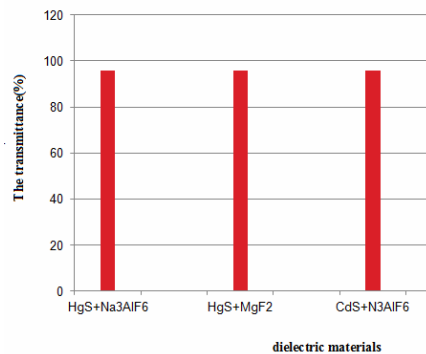

Figure 4. The transmittance (%) of 1064 nm for the dielectric materials

Figure (5) shows the physical thickness for the different dielectric materials. HgS/Na_3AlF_6, and HgS/MgF_2 are thinner than CdS/ Na_3AlF_6. The dielectric material with the lowest physical thickness has the best characteristics. Therefore, HgS/Na_3AlF_6 and HgS/MgF_2 filters are the best between these materials to be chosen for Nd:YAG Laser.
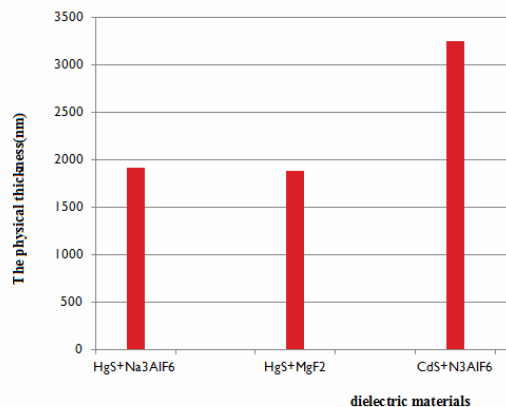

Figure 5. The physical thickness (nm) of the materials

Figure (6) shows the geometric thickness of the used materials. The smallest value of geometric thickness is for HgS/MgF$_2$ which equals 1.77 then for HgS/Na$_3$AlF$_6$ which is equal 1.80 and finally is for CdS/Na$_3$AlF$_6$ which equals 3.05. In thin film coating the smallest geometric thickness provides better coating. Therefore HgS/MgF$_2$ material is the best to act as front Nd:YAG Laser mirror.
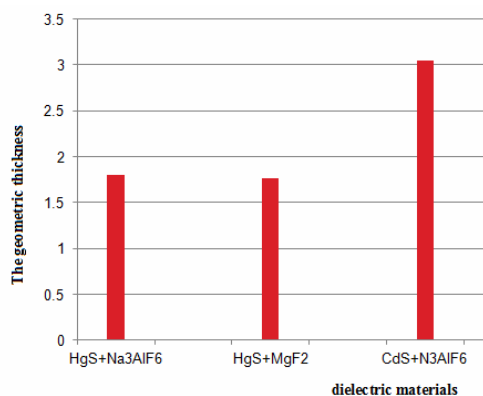

Figure 6. The geometric thickness for different coating materials

Figure (7) shows the optical thickness of the different coating materials. The smallest value of optical thickness is for HgS/MgF$_2$ which equals 14 then for HgS/Na$_3$AlF$_6$ which is equal 14 and finally is for CdS/ Na$_3$AlF$_6$ which equals 22. In thin film coating the smallest optical thickness provide better coating [13]. Therefore, HgS/MgF$_2$, and HgS/Na$_3$AlF$_6$ materials are the best to act as front Nd:YAG laser mirror.

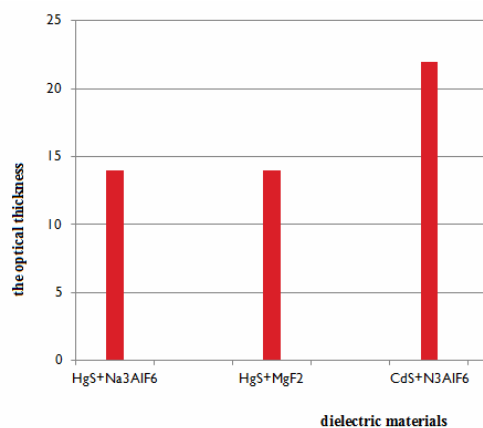*Figure 7. The optical thickness for the used materials*

Figure 8 shows a comparison between FWHM for the three coating materials, HgS+Na$_3$AlF$_6$, HgS+MgF$_2$ and CdS/ Na$_3$AlF$_6$. The dielectric material HgS+Na$_3$AlF$_6$ shows

smaller (FWHM) compared with $HgS+MgF_2$ and CdS/Na_3AlF_6. Therefore, the first material is better in this titration.
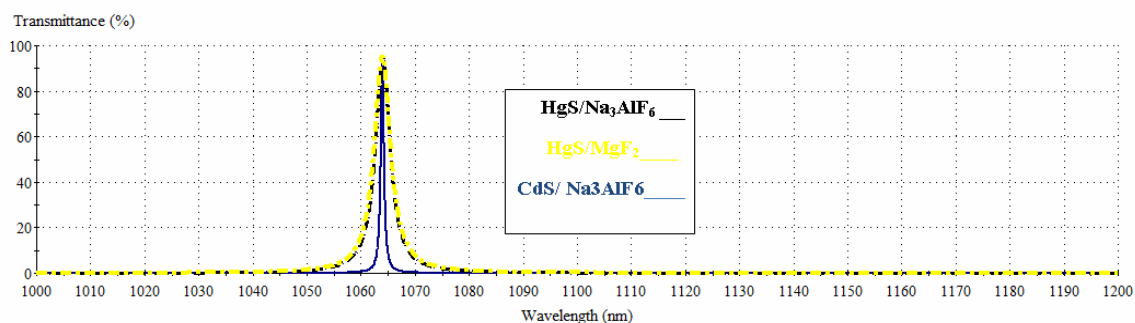

Figure 8. *Comparison between the FWHM for the three dielectric materials ($HgS+Na_3AlF_6$,*

Conclusion

From the obtained results, one can conclude that the best transmittance was achieved with $HgS+Na_3AlF_6$ where the transmittance for 1064 nm reaches to 95.74 %. Among the chosen materials one can built Nd:YAG resonator composed of $HgS+Na_3AlF_6$ With 11 layers as an output coupler. By applying one quarter of the reference wavelength (1064nm) in the calculations for thin film, the best results for Nd:YAG mirrors resonator were achieved.

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