J. Nano- Electron. Phys.
3 (2011) No1, P. 721-727

PACS numbers: 68.65.Ac, 78.20.Ci

THE OPTIMIZATION OF OPTICAL THIN FILMS DEPOSITION USING IN-SITU REFLECTIVITY MEASUREMENTS AND SIMULATION

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We have optimized and automated the experimental in-situ reflectivity measurement system for the laser diode (LD) facet coating. We have also developed a reflectivity-simulator program that gives the reflectivity data as a function of the thickness of the film (single or multi-layer) for a given wavelength, which aids in optimizing the above parameters while monitoring the coating of the films in-situ. We report the results for the in-situ reflectivity of a single layer MgF_2 *and a quarter-wave optical thick three bi-layer pairs of* MgF_2 *and silicon on GaAs as a substrate for both the cases. We have achieved up to 83 % experimental reflectivity for the latter case.*

Keywords: *THIN FILM, MULTILAYERS, IN-SITU, REFLECTIVITY, SIMULATION.*

(Received 04 February 2011, in final form 13 October 2011)

1. INTRODUCTION

Thin film optical coating is used for modulating the reflectivity in different kinds of optical components viz. beam splitters, optical filters, polarizers, lenses of cameras and telescopes, including anti-reflection (AR) and high-reflection (HR) coating on the laser diode facets [1]. Owing to its importance, it is essential to monitor the thin film deposition parameters like the deposition rate, substrate temperature, and thickness of the thin film during the deposition.

Although various optical in-situ measurement systems are available, most of these systems employ a very sophisticated instrumentation and are quite complex. We have developed an in-situ reflectivity measurement system for optimization of facets-coating process for laser diodes. We have performed in-situ reflectivity measurements on single layer MgF_2 and a quarter-wave optical thick (QWOT) three bi-layer pairs of MgF_2 and silicon on GaAs as a substrate for both the cases. The measurements were optimized using a simulation program that gives the reflectance of non-absorbing dielectric single or multilayer, or QWOT bi-layer optical facet coatings for the Laser Diode (LD) using LabVIEW (laboratory virtual instrument engineering workbench) (version 8.2). Since the set-up is custom-built for our specific application, it is quite simple, cost-effective and efficient tool for quick optimization and automation of the process.

The mathematical equations used in the simulation to calculate reflectivity of the optical thin-films followed by program execution are discussed in the next section. The experimental detail for the in-situ measurement of reflectivity has been described in section 3. Results of the simulated reflectivity spectra for various optical thin-films are presented in section 4.

2. THEORETICAL BACKGROUND

2.1 Mathematical treatment

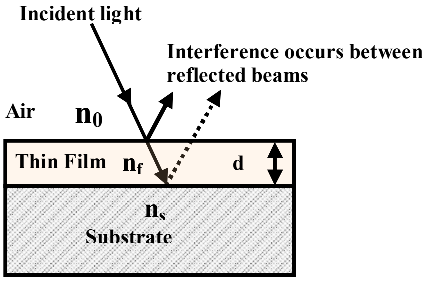


Fig. 1 *– The light reflected from the air-film and the film-substrate boundary produces interference.*

Fig. 1 shows light incident on an air-film interface. The light reflected from the air-film and the film-substrate interface give rise to the interference phenomenon, which results in the change in the reflected beam intensity as the film grows on to the substrate. The reflectance co-efficient, r, of a non-absorbing multilayer dielectric thin-film is given as [2]:

$$r = \frac{Y_0 m_{11} + Y_0 Y_s m_{12} - m_{21} - Y_s m_{22}}{Y_0 m_{11} + Y_0 Y_s m_{12} + m_{21} + Y_s m_{22}} \tag{1}$$

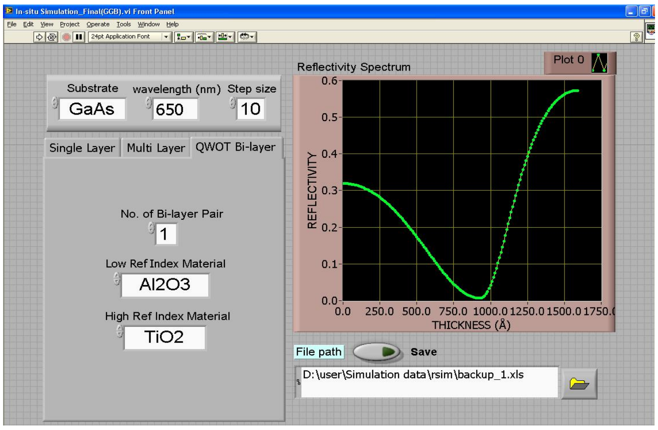
where, $Y_0 = \sqrt{\varepsilon_0/\mu_0 n_0^{'}}$ and $Y_S = \sqrt{\varepsilon_0/\mu_0 n_S^{'}}$ with n_0' and n_s' being the effective refractive indices of the incident medium and the substrate, respectively, and are given as $n'_0 = n_0 \cos\theta_0$ and $n'_s = n_s \cos\theta_s$ for s or perpendicular polarization. In case of p or parallel polarized light, n'_0 and n'_s are given as $n'_0 = n_0/\cos\theta_0$ and $n'_s = n_s/\cos\theta_s$. Here, n_0 and n_s are the refractive indices of the incident medium and the substrate whereas θ_0 and θ_s are the angles of incidence in the incident medium and the substrate, respectively. In equation **(1)**, m_{11}, m_{12}, m_{21}, and m_{22} are the elements of characteristic matrix, **M**, of the entire system with p layers in a multilayer stack, which is the resultant of the product (in proper sequence) of the individual 2×2 matrices for each layer in the multilayer stack, that is:

$$\mathrm{M} = \mathrm{M}_1 \, \mathrm{M}_2 \, \mathrm{M}_3 \ldots \ldots \mathrm{M}_p = \begin{bmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{bmatrix} \tag{2}$$

However, the layer matrix is a complex matrix [2]. Hence, elements m_{12} and m_{21} in above equations are purely complex whereas the other two elements, i.e. m_{11} and m_{22}, are real. Thus, the reflectance coefficient r is an imaginary quantity. So, the reflectance, $R = r{\cdot}r^*$ gives,

$$R = \frac{\left(n_0^{'} m_{11} - n_s^{'} m_{22}\right)^2 + \left(n_0^{'} n_s^{'} m_{12} - m_{21}\right)^2}{\left(n_0^{'} m_{11} + n_s^{'} m_{22}\right)^2 + \left(n_0^{'} n_s^{'} m_{12} + m_{21}\right)^2} \tag{3}$$

Equation **(3)** determines the reflectance of the non-absorbing multilayer dielectric thin-film. This equation is used in the computer simulation program.


In-situ Simulation_Final(GGB).vi Front Panel

Substrate: GaAs
wavelength (nm): 650
Step size: 10

No. of Bi-layer Pair: 1
Low Ref Index Material: Al2O3
High Ref Index Material: TiO2

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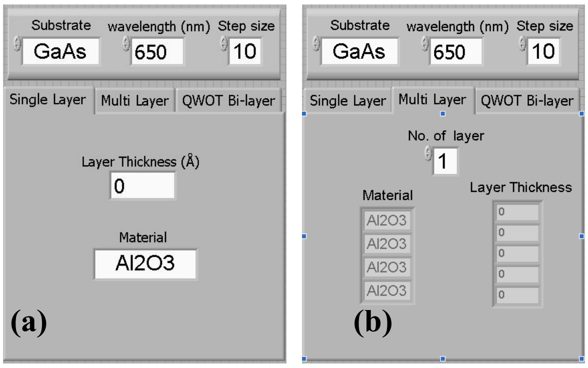
Fig. 2 *– The front-panel of the LabVIEW program for reflectivity simulation of the optical thin film*

2.2 Program execution

In the case of optical films, two parameters are necessary to determine the reflectivity of the thin film viz. the physical thickness and the refractive index of the material [3]. The other input parameters are the refractive index of the substrate material, wavelength of interest, and thickness (step size). All these parameters are provided on the front panel of the program, shown in Fig. 2. Fig. 3 shows the other control parameters to be fed in the input in program. The program executes as per the data flow arranged using the graphical programming code in the back panel of the program viz. block diagram.


(a)

Substrate: GaAs
wavelength (nm): 650
Step size: 10
Layer Thickness (Å): 0
Material: Al2O3

(b)

Substrate: GaAs
wavelength (nm): 650
Step size: 10
No. of layer: 1

Material	Layer Thickness
Al2O3	0
Al2O3	0
Al2O3	0
Al2O3	0
	0

Fig. 3 *– The input parameters for single layer (a) and multilayer (b) in-situ reflectivity simulation*

3. EXPERIMENTAL

3.1 Sample preparation

The deposition of single layer MgF_2 and a QWOT three bi-layer pairs of MgF_2 and silicon on GaAs as a substrate for both the cases was carried out under the high vacuum (10^{-5} mbar) using e-beam evaporation system (EBG-6K, HINDHIVAC).

The GaAs test substrate was used to optimize the deposition conditions as well as the reflectivity of the coated material. The quartz crystal monitor was used for measuring the thickness of the sample. For the better control of the deposition parameters viz. thickness and deposition rate, e-beam evaporation system is interfaced with the thin film deposition controller (SQC-112C, Sigma Instruments). The substrate was rotated with 120 rpm inside the vacuum chamber during the deposition with the help of a dc motor in order to get uniform coating. The substrate was maintained at 100 °C substrate temperature using radiant heater during the deposition. The deposition rate was 4 Å/s.

3.2 In-situ reflectivity measurement

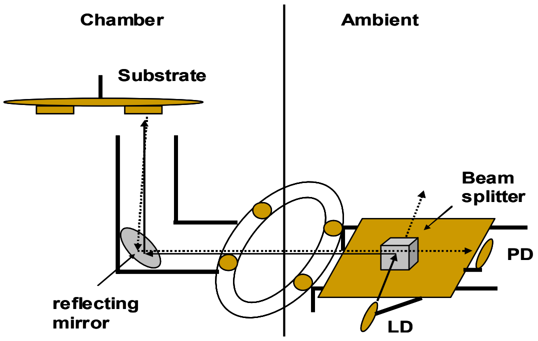


Fig. 4 *– A schematic diagram of the experimental in-situ reflectivity measurement setup*

Fig. 4 shows a schematic diagram of the experimental setup for measuring in-situ reflectivity. The laser beam enters in to the vacuum chamber through a glass view port of the chamber and reflects back on the photo-detector (BPW-34) from the sample at normal incident angle. We have used a

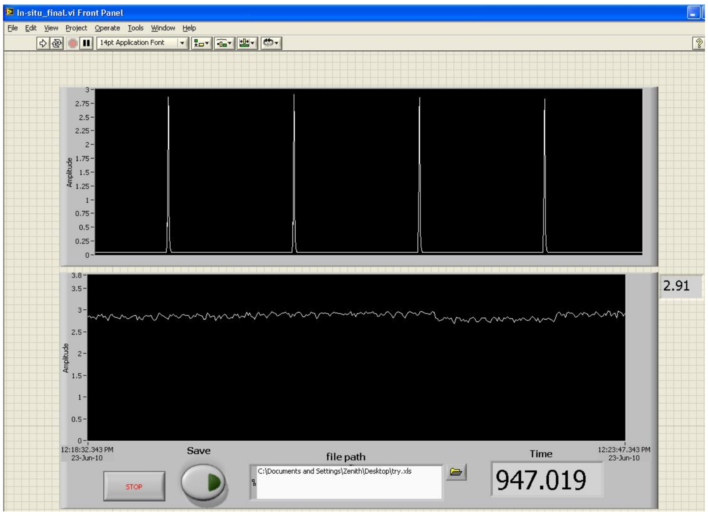


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Fig. 5 *– The LabVIEW front panel showing real time data acquisition as the light reflects from the sample and is detected by the photodetector* commercially purchased red laser diode (λ = 650 nm) as a probe light source for the experiment. To check the stability of the optical power of the laser diode, we operated the laser diode in CW mode continuously for a few minutes before starting the deposition and monitored its optical power as a function of time. We observed negligible variation in optical power. Thus, we can consider the optical power output of the laser diode to be stable during the in-situ reflectivity measurements.

We did not check for the variation of wavelength of the laser diode with time, but as we operate the laser diode at a very low power with controlled operating temperature, we assume that the wavelength of the laser diode is stable over the duration of the experiment. The signal from the photo-detector is fed to a computer through data acquisition card (NI-USB-6251). Fig. 5 shows the acquired data in the front panel of the program built in LabVIEW.

During the deposition, the film grows vertically on the rotating substrate and the light undergoes interference. The change in the intensity of the reflected laser light will produce a sinusoidal curve as the film grows. Fig. 6 shows the real time intensity data acquisition of the reflected laser beam from the sample during the deposition as a function of time.

4. RESULTS AND DISCUSSIONS

The single layer MgF_2 film was deposited at room temperature on the GaAs substrate at the deposition rate of 4 Å/s. Fig. 6 shows the acquired data of the reflected laser light intensity versus time. It is well known that there is direct relation between the film thickness and the film deposition rate. So, one can easily estimate the thickness of the deposited film.

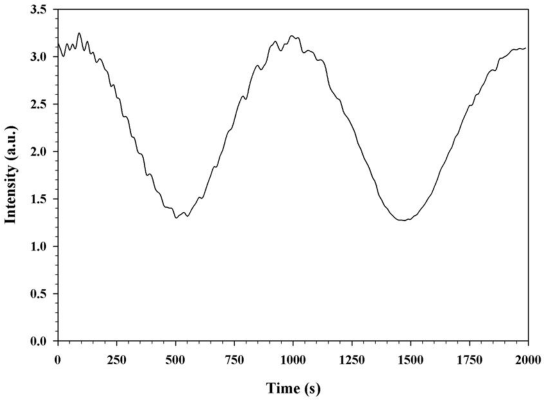

Fig. 6 *– Intensity measurement curve as a function of time for the* MgF_2 *thin film deposited on GaAs substrate.*

Moreover, the natural reflectivity of the substrate GaAs is ~ 32 % and will be modified as the film grows on it. Hence, we can directly get the film reflectivity from the reflected intensity. Fig. 7 shows the experimental as well as the simulated data of the reflectivity of single layer MgF_2. Likewise Fig. 8 shows the reflectivity plot for multilayer stack of material. The three QWOT bi-layer pair of MgF_2 and Si where the former has a low refractive index and the latter has a high refractive index. Starting with the low refractive index material coating on the GaAs substrate, the stack of the layers were deposited in alternation. We have achieved up to 83 % experimental reflectivity. The simulated data, which we have fitted, was fed refractive indices 1.38 and 3.5 for MgF_2 and Si, respectively.

In order to confirm the obtained results, we measured the reflectivity spectrum of the coated samples ex-situ with the standard setup using a broad-band light source, a monochromator, photo-detectors and a lock-in amplifier. Figure 9 shows the reflectivity spectrum for a three QWOT bi-layer pairs of MgF_2-Si measured ex-situ. As shown in the figure, the reflectivity value obtained ex-situ at 650 nm is in good agreement with the value obtained in-situ at the end of the deposition.

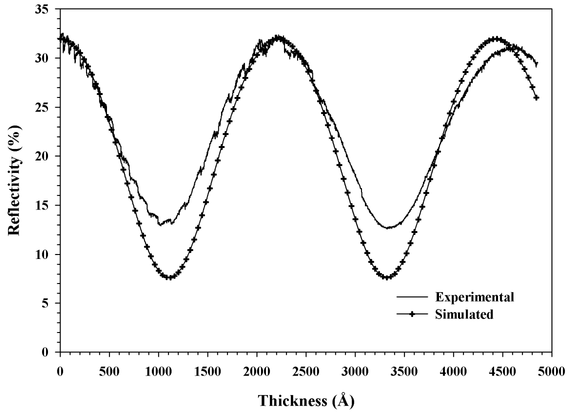

Fig. 7 *– In-situ reflectivity and simulated reflectivity plots for a single layer* MgF_2 *(*$n = 1.43$*) deposited on* GaAs *substrate*

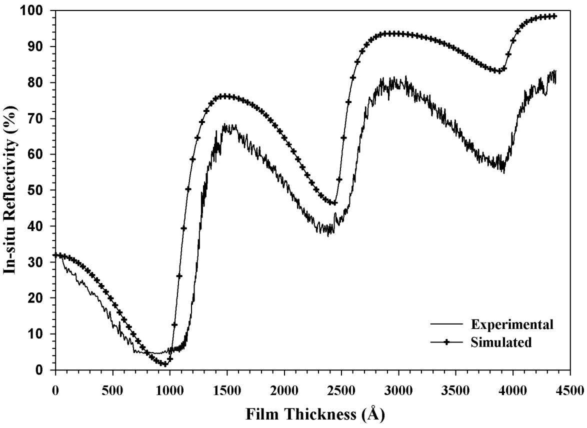

Fig. 8 *– In-situ reflectivity plot for three QWOT bi-layer pairs of* MgF_2-Si

There is a noticeable difference between experimental and simulated value of the reflectivity, especially at the higher thickness as shown in fig. 8. The measured value is lower as compared to the simulated value of the reflectivity. This is mainly due to the usage of bulk values of the material refractive indices during reflectivity simulations. However, it is known that oxides film grown using e-beam evaporation exhibit a variation in refractive index with film thickness [4]. We can easily modify the refractive index for a particular layer and estimate the value of its refractive index by matching the best-fit curve.

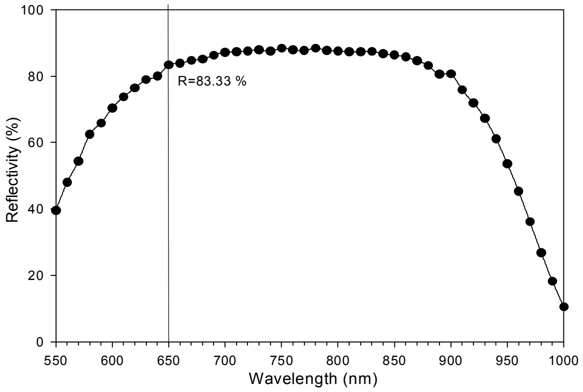

Fig. 9 *– Reflectivity spectrum for three QWOT bi-layer pairs of* MgF_2-Si *measured ex-situ*

5. CONCLUSION

The in-situ reflectivity measurement of the single and multilayer optical thin films has been demonstrated. The change in intensity of the laser light after reflection has been measured to obtain the reflectivity as a function of thickness. Also, we have developed an in-situ reflectivity simulation for the optimization of the in-situ film deposition. The reflectivity simulator provides a very good tool for designing the optical thin films with desired reflectivity response. Also, one can use the simulator for determining the material and the deposition conditions viz., film thickness, and deposition rate for single or multilayer films.

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