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Determination of Thickness and Optical Parameters of Thin Films from Reflectivity Spectra Using Teaching-Learning Based Optimization Algorithm

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In this paper, we report a simple method to extract thickness and refractive index of thin-film from experimentally measured reflectivity spectra using teaching-learning based optimization (TLBO) algorithm. The algorithm finds thickness and refractive index by fitting an experimentally measured reflectivity spectra with theoretically ones generated by transfer matrix approach. The value of refractive index as a function of wavelength is determined by considering sellmeier dispersion relation. The algorithm is implemented by means of an interactive numerical simulation using LabVIEW as a programming tool. To check the effectiveness of the self-developed program, it is tested on different thin-film samples prepared from some commonly used optical materials such as MgF_2, Al_2O_3 and SiO_2 using electron beam evaporation technique. The values of thicknesses and refractive index spectra for different thin-film samples obtained by TLBO algorithm are verified using standard spectroscopic ellipsometry measurements. It is found that there is an excellent agreement between the results obtained by the TLBO algorithm and those by ellipsometry. It is also demonstrated that a simple reflectivity measurements give the valuable information about the thickness and dispersive refractive index over a range of wavelengths, which are obtained by our self-developed simulation program based on TLBO algorithm.

Keywords: Thin film, TLBO Algorithm, Optical Constant, Reflectivity, LabVIEW.

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1. INTRODUCTION

Thin-films are widely used as an anti-reflection (AR) coating to avoid undesirable surface reflection in many optoelectronics devices like solar cell [1], laser diode (LD) [2] and superluminescent light emitting diode (SLED) [3]. Usually, semiconductor materials used for fabrication of optoelectronic devices exhibit high surface reflectivity of about 30-40 % due to mismatch in refractive index at the interface between ambient medium, usually air, and the semiconductor active layer materials. The photon collection in solar cell and photon emission in SLED and LD can be improved by applying the AR films at the interface between ambient medium and the semiconductor active layer materials. The desired spectral characteristics viz. reflectivity and transmissivity spectra of such AR films can be obtained by tuning the thickness (t) and refractive index (n) of the thin- film materials. Therefore, an accurate knowledge of the t and n of thin-films are always crucial in order to design the optical coatings, consequently, the performance of the optoelectronic devices can be improved. Moreover, for the optimization of deposition condition for optical coatings, frequent measurements of t and n are inevitable. Thus, a simple and readily available technique to evaluate the t and n for optical thin-films is of great importance.

Several methods such as wavelength scanning [4-6], spectroscopic ellipsometry [7-9] and waveguide coupling [10-12] have been used to determine t and n of optical thin-films. The wavelength scanning method uses either reflectivity or transmissivity spectra for the extraction of t and n of the film. One of the most important classes of wavelength scanning method is spectrum fitting, in which the experimental reflectivity or transmissivity spectra are fitted with the theoretical ones using some optimization algorithms. Several global optimization algorithms such as particle swarm optimization [13] genetic algorithm [14, 15], pattern search [16] and artificial neural network [17] have been employed for the estimation of t and n of thin-films in the literature. These methods are robust, stochastic and generally do not rely on the initial conditions. However, they require their own algorithm-specific input parameters for searching the optimum solution. For example, GA utilizes the mutation rate and crossover rate. Similarly, PSO uses the inertia weight, social and cognitive parameters. The improper selection of such parameters can either increase computation time or lead the solution to the local optimum rather than global one. Moreover, these parameters are problem specific and to find the optimum values of these parameters are quite difficult. Thus, they may affect on the performance of the algorithm.

A novel global optimization algorithm namely the teaching-learning based optimization (TLBO) algorithm, introduced by Rao et al. [18], considerably overcomes these limitations. The algorithm has been extensively applied to a wide range of optimization problems [19-20]. There are some attractive features of the TLBO, which make it a very effective and efficient. For example, it does not require any knowledge about the algo-

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rithm specific parameters. Further, the convergence of the solution to the global optimum is almost independent on the initial conditions. It works with only a few control parameters such as population size and number of iterations which are common for all nature-inspired algorithms. So far, to the best of our knowledge, the TLBO has not yet been applied for the determination of t and n of thin-film in the literature.

In this paper, a spectroscopic reflectometry method is used to measure the reflectance of optical thin-films. This method is relatively a very simple, non-destructive and generally easy to setup in the laboratory. The measured reflectivity spectra are then fitted with theoretical ones with the help of TLBO algorithm. The algorithm is implemented using LabVIEW (laboratory virtual instrument engineering workbench, version-10) as a programming tool.

2. IMPLEMENTATION OF TLBO ALGORITHM FOR EXTRACTION OF THICKNESS AND REFRACTIVE INDEX OF THIN FILM

TLBO is inspired by the traditional classroom teaching-learning process between the teacher and learners (students). It utilizes the basic principle of the effect of teacher's knowledge on results of learners in the classroom. It is a simple population based algorithm that relies on the solutions of population to proceed towards the global optimum like other optimization algorithms. In TLBO, a group of learners in the classroom indicate the population. Different design variables (i.e. unknown parameters) are similar to different subjects offered to learners during their course work. The performance of the learners is determined based on their obtained results or grades by defining problem specific suitable objective function called "fitness function" $F(X)$. The most knowledgeable learner in the entire classroom is considered as the teacher who shares his or her knowledge with other learners. In this algorithm, the performance of a learner is improved by the propagation of knowledge though two phases, i.e. the "teacher phase" and the "learner phase". These both phases are explained in details elsewhere [21]. The extraction of the t and n are carried out by utilizing the set of experimentally measured reflectivity data of thin-film over the wavelength range. In the present study, the two term sellmeier dispersion relation [22, 23] is considered to find the dispersive n over the wavelength range using the following Eq. (1).

$$n^2(\lambda) = 1 + \frac{B_1\lambda^2}{\lambda_2 - C_1^2} + \frac{B_2\lambda^2}{\lambda^2 - C_2^2} \quad (1)$$

Therefore, the t and each sellmeier coefficients B_1, C_1, B_2, and C_2 are considered as a set of unknown parameters denoted as $X_i = (B_{1i}, C_{1i}, B_{2i}, C_{2i}, t_i)$, which is identified as a learner. Thus, a learner X_i learns five subjects viz. B_{1i}, C_{1i}, B_{2i}, C_{2i}, and t_i. Here, $i = 1, 2, 3…N$, where N indicates the total number of learners in the class (classroom strength). The quality of learner (X_i) can be judged based on the value of fitness function. In our program, the fitness function is defined as,

$$F(X) = \frac{\left\{\sum_{k=1}^{p}\left[R^{\exp}(\lambda_k) - R^{cal}(\lambda_k, B_{1i}, C_{1i}, B_{2i}, C_{2i}, t_i)\right]^2\right\}}{p} \quad (2)$$

Where, $R^{\exp}(\lambda_k)$ is the experimental value of reflectivity at wavelength λ_k, and $R^{\text{cal}}(\lambda_k, B_{1i}, C_{1i}, B_{2i}, C_{2i}, t_i)$ is the calculated value of reflectivity at wavelength λ_k based on the five subjects such as B_{1i}, C_{1i}, B_{2i}, C_{2i} and t_i offered to a learner using transfer matrix method [24]. The p is the total number of wavelength steps in the reflectivity spectrum. The values of offered subjects are tuned during the teacher and the learner phase in such a way that the fitness value of learner according to Eq. (2) is minimized during every TLBO iterative process. This iterative process is continued until the best fit between the experimental and calculated values of reflectivity is achieved over the defined wavelength range. At the end of the program, the obtained optimum values of sellmeier coefficient are used to calculate the n over the wavelength range by considering the optical dispersion model as shown in Eq. (1). In the present study, we have considered thin-film structure which is non-absorbing over the wavelength of interest. For the execution of the TLBO, the three control parameters viz. learner size, number of iterations and search space (range of upper and lower limits for unknown variables) are mainly required and fed as input parameters in the program. These parameters are optimized systematically for the present problem. TLBO algorithm is implemented using the flow chart given in the literature [18, 21, 25] for the extraction of t and n. The terminology of TLBO in the context of present problem is shown in Table-1. The classroom strength (i.e. number of sets of layer thickness (t) and sellmeirer coefficients) and the numbers of iterations were fixed to 1000 throughout the exercise. The process of determining an optimum set of t and sellmeier coefficients was repeated for 100 times for each sample.

Table 1 – The terminology of TLBO algorithm equivalent to the set of thickness of layer and Sellmeier Coefficient

TLBO terms	Equivalent to thickness of layer and sellmeier coefficients
Learner (i.e. individual)	A set of layer thickness and sellmeier coefficients
Classroom strength (i.e. population)	Number of sets of thickness and sellmeier coefficients
Subjects	Thickness of the layer and each sellmeier coefficient
Teacher (X_{teacher})	Best set of thickness and sellmeier coefficient in the population with minimum value of fitness function
Mean value of a particular subject for all learners (X_{mean})	Mean value of a particular set of layer thickness and sellmeier coefficients
Search space	Range of minimum and maximum values for each sellmeier coefficient and layer thickness

3. SAMPLE PREPARATION AND SPECTROSCOPIC REFLECTOMETRY MEASUREMENT

A thin-film of commonly used optical coating materials such as magnesium fluoride (MgF_2), aluminum oxide (Al_2O_3) and silicon dioxide (SiO_2) are deposited individually on Indium Phosphide (InP) substrate at temperature 100 °C under high vacuum (10^{-6} mbar). The deposition is accomplished using a 3 kW e-beam evaporation system equipped with 180° bend e-beam gun facility (Hind High Vacuum Co. (P) Ltd.). During the growth of the film, the thickness and deposition rate are monitored by a quartz crystal oscillator inbuilt inside the chamber. The uniformity of the coating is achieved by rotating the substrate with constant rpm during the deposition. The substrate temperature is attained by employing the radiant heater arranged inside the chamber.

The optical reflectivity spectra of coated samples are measured using self-assembled reflectometry measurement set up developed at our laboratory. The set up consists of light source (Ocean Optics – Model No. HL-2000), Monochromator (oriel cornerstone – 260 ¼ m), lock-in amplifier (SR-830), optical chopper (SR-540) and silicon detector (Edmond optics – NT53-373). All InP coated samples are characterized for reflectance measurement in the wavelength range 450-950 nm in step of 5 nm wavelength resolution at near normal incidence.

4. RESULTS AND DISCUSSION

In the present paper, the use of TLBO algorithm is demonstrated first time for extraction of refractive index and thickness of thin-film. However, it is very crucial to check the effectiveness of TLBO algorithm before its implementation for practical use. Thus, we use standard ellipsometric measurement as an experimental verification tool. To varify our appraoch, thin-film samples of different materials are prepared on InP susbtrate using electron beam evaporation technique. The reflectivity spectra of these samples are measured using developed spectroscopic reflectivity measurment setup and finally fitted with the help of developed program based on TLBO algorithm to extract the refractive index and thickness of thin-films. The values of refractive index spectra and thickness of samples obtained TLBO algorithm are verfied by using ellipsometric measurements on same samples. The spectral dependencies of measured ellipsometric parameters ψ and Δ are fitted using suitable models to extract film thickness and the refractive index (n) in order to obtained the best fit between experimental and simulated spectra. The obtained results of different thin-films samples are analyzed and discussed in in this section.

4.1 A Single Layer MgF_2 Coated on InP Substrate

The experimentally measured (black dotted line) and its best-fit reflectivity spectrum (red curve) obtained by TLBO algorithm for single layer MgF_2 coated on InP substrate is shown in Fig. 1a. It is clearly observed that the experimental curve exactly overrides on the fitted curve. Fig. 1b shows the experimentally measured ellipsometric parameters (ψ, Δ) values versus wavelength and their corresponding fitted curves obtained using model generated parameters (ψ, Δ) for same single layer MgF_2 film coated on InP substrate.

The thickness of the single layer MgF_2 film obtained by the TLBO algorithm and those by ellipsometry were found to be 1326 Å and 1327 Å, respectively (shown in Table 1). Fig. 1c shows the wavelength dependent

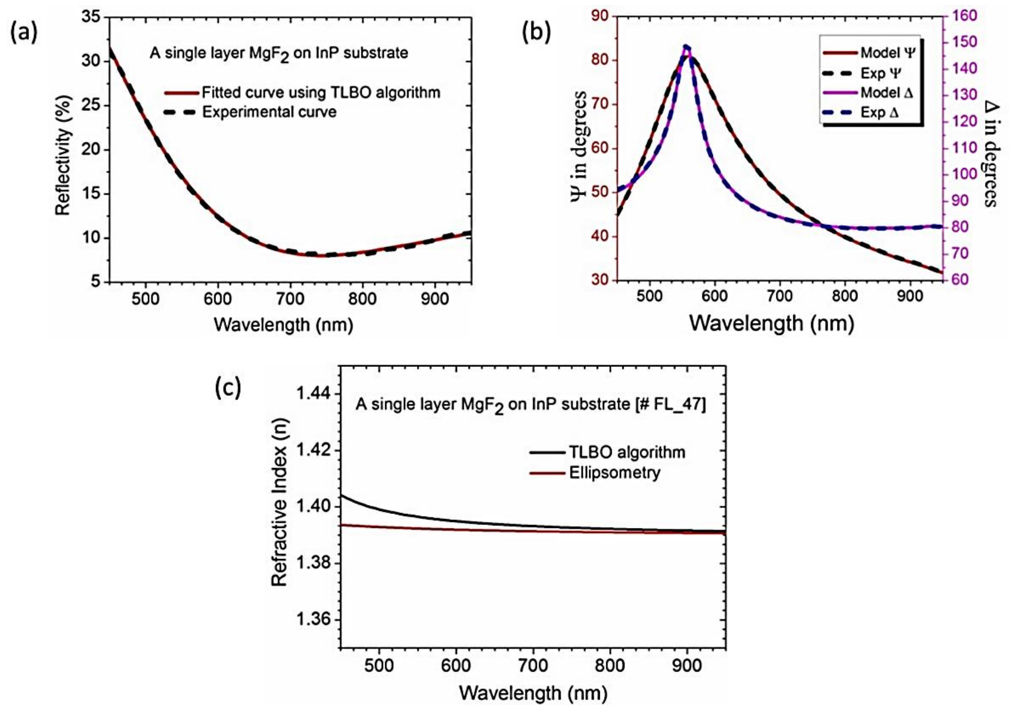

Fig. 1 – Reflectivity spectrum of a single layer MgF_2 (a). Ellipsometric parameters variation versus wavelengths for a single layer MgF_2 (b). Refractive index variation versus wavelengths for a single layer MgF_2 (c)

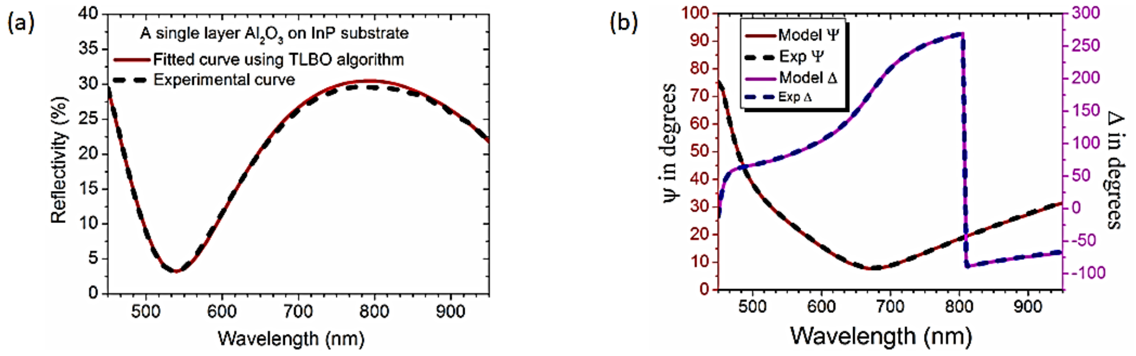

Fig. 2 – Reflectivity spectrum of a single layer Al_2O_3 (a). Ellipsometric parameters variation versus wavelengths for a single layer Al_2O_3 (b)

refractive index for MgF_2 film as obtained by the TLBO approach (black curve). For the same sample, the corresponding values obtained by the ellipsometry are also shown in Fig. 1c (red curve). From the Figure, it is evident that the obtained values of refractive index over entire wavelength range for a single layer MgF_2 film are in very good agreement with the results obtained from ellipsometry measurement as well as those reported in the literature [26].

4.2 A Single Layer Al_2O_3 Coated on InP Substrate

In order to further verify the reliability of the program, we have tested it on a single layer Al_2O_3 film deposited on InP susbtrate. The experimentally measured (black dotted line) and fitted reflectivity spectrum (red line) over the wavelength range 450-950 nm obtained by the approach is shown in Fig. 2a.

As seen from the Figure, the derived reflectivity spectra from the obtained values of thickness and refractive index are exactly overides on the experimental spectra which reveal the effectiveness of the algorithm. Fig. 2b depicts the experimentally measured ellipsometric parameters variation with respect to wavelengths and their corresponding fitted curves obtained using model generated parameters for a single layer Al_2O_3 film. The extracted thickness values by our method and those obtained by ellipsometry are shown in Table 2. Even, for the case of single layer Al_2O_3 film, we have found extremely good agreement in thickness values between the TLBO approach and ellipsometry method.

The comparison of dispersive values of refractive index obtained by TLBO and ellipsometry for Al_2O_3 film is shown in Fig. 3. As seen from the Figure, although the deviation in the values of refractive index obtained by TLBO from those obtained by ellipsometry is slightly higher in case of Al_2O_3 film than that for the MgF_2, it is still very much within the acceptable range for most optical coating applications.

4.3 A Single Layer SiO_2 Coated on InP Substrate

Again to prove the versatility of developed program for its use in different kind of coating materials, we use the program on a single layer SiO_2 evaporated on InP substrate. Fig. 4a shows the measured and fitted reflectivity spectrum over the wavelength range 450-950 nm for a single layer SiO_2.

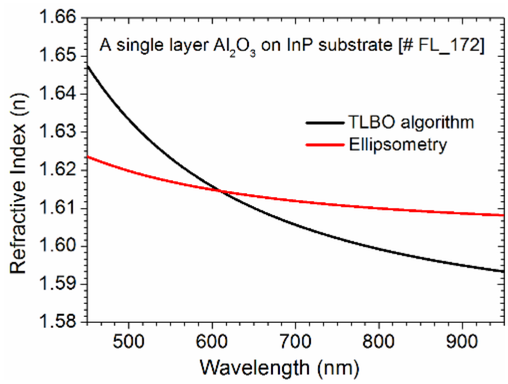

Fig. 3 – Refractive index variation versus wavelengths for a single layer Al_2O_3

From the Figure, it is clearly seen that the computed reflectivity spectrum (red solid line) from the obtained values of thickness and refractive index by our method largely coincides with the experimental curve (dotted black line) which reveal the strength of the algorithm. Fig. 4b indicates experimentally measured ellipsometric parameters (ψ, Δ) values versus wavelength and their corresponding fitted curves obtained using model generated parameters (ψ, Δ) for single layer SiO_2. The fitted curves are completely matched to the measured curved over the entire wavelength range. However, the thickness obtained by TLBO algorithm in this case is a bit deviated than those obtained by ellipsometry.

The variation in the refractive index values obtained by TLBO algorithm and ellipsometry measurement with wavelength for a single layer SiO_2 is displayed in Fig. 4c. Table 2 summarizes the comparison between the thickness values obtained by TLBO algorithm with those measured by ellipsometry for all three coating materials considered in the present work. As evident from the Table, the values of thicknesses obtained by TLBO algorithm, in general, are in excellent agreement with the corresponding values obtained by the ellipsometry for different types of materials. These results prove the potentiality of the present approach.

To further analyse the results, we have calculated the relative errors in thickness value and average relative error of the refractive index data for each sample. The error values for thickness and refractive index are also summarized in Table 2. The values of errors in thickness for a single layer MgF_2 and Al_2O_3 films were found 0.07 % and 0.03 %, respectively. However, this error was slightly higher in case of a single layer SiO_2, which is around 3 %. This higher error may be attributed to the non-uniformity of film during growth process.

In case of refractive index data, we calculate the relative error over the entire dispersive spectra for each sample. The average relative error was found to be almost less than 1 % in each sample. However, we observed marginally higher deviation in refractive index values obtained by TLBO approach from those obtained by ellipsometry, as evident from the average relative errors. We believe that these deviations in the values of refractive index are partly due to limitation in the measurement of reflectivity spectrum. In the present work, the reflectivity spectrum is measured at near normal incidence in our case (about 5° from the normal). However, transfer matrix approach used to calculate the reflectivity spectrum assumes perfectly normal incidence. It is quite difficult to arrange the angle of incidence at perfect normal due to the mechanical limitations of the setup in practical case. This introduces a marginal error in the fitting, especially in case of calculation of refractive index as a function of wavelength. This error can be reduced by further improving the reflectivity measurement setup for future application. In addition to these measurement issues, the simulation program also assumes a perfectly homogeneous films and sharp interfaces. However, in practice, it is not possible to achieve sharp interfaces during experiment, which can add the deviation in measured values of reflectivity. Ultimately, this fact may affect on the values of refractive index more dominantly than they can affect the thickness value due to inherent nonlinearity and the higher power terms involved in the sellmeier dispersion equation.

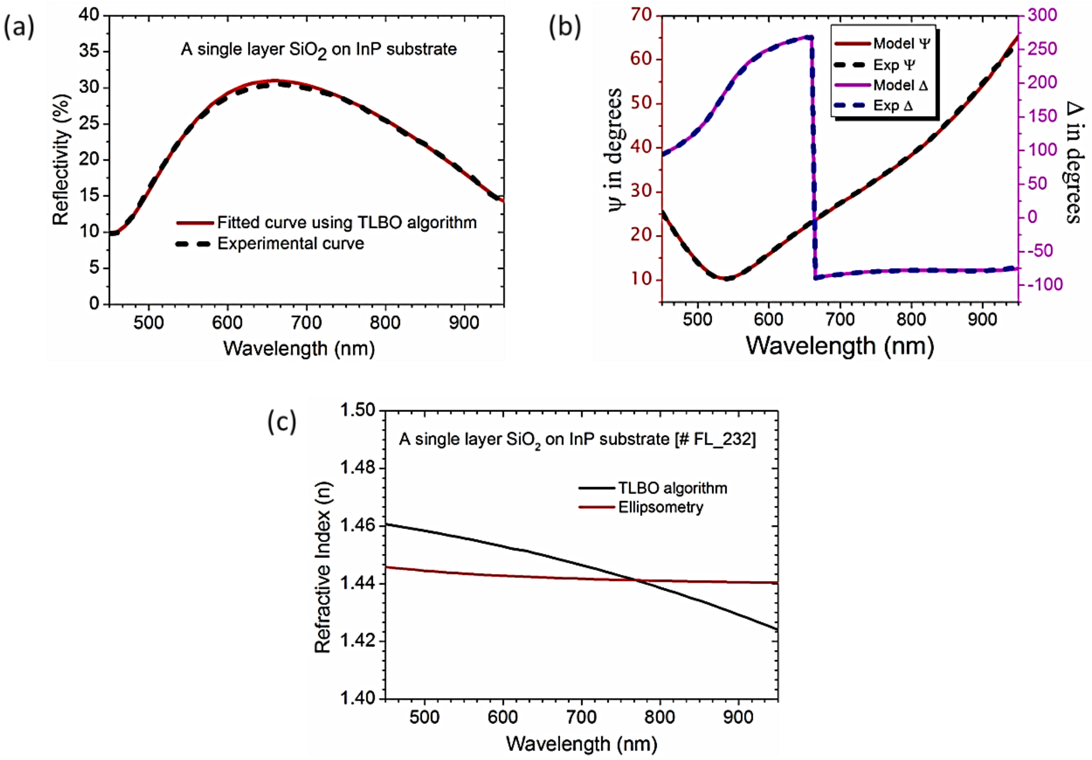

Fig. 4 – Reflectivity spectrum of a single layer SiO_2 (a). Ellipsometric parameters variation versus wavelengths for a single layer SiO_2 (b). Refractive index variation versus wavelengths for a single layer SiO_2 (c)

Table 2 – Calculated thickness from ellipsometry and TLBO algorithm

Sample Code	Types of coating	Thickness (Å) obtained using ellipsometry	Thickness (Å) obtained using TLBO algorithm	Relative errors in thickness (%)	Average relative errors in refractive index (%)
FL_47	A single layer MgF_2 on InP	1327	1326	0.075358	0.199119
FL_172	A single layer Al_2O_3 on InP	2520	2519	0.0396825	0.586557
FL_232	A single layer SiO_2 on InP	2384	2317	2.8104	0.601356

5. CONCLUSION

We have successfully demonstrated a simple technique to estimate thickness and wavelength dependent refractive index from experimentally reflectivity spectra of different thin-films samples using a novel TLBO algorithm. The measured reflectivity spectra of films were fitted with help of TLBO algorithm in order to extract thickness and refractive index of thin-films. To verify the suitability of novel TLBO approach, the same films were subjected to ellipsometry measurements. The obtained values of thickness and refractive index of prepared samples were compared with the corresponding results obtained using standard ellipsometry measurements on the same samples. It was found that the values of thicknesses are in strong agreement with those obtained by ellipsometry measurement in all cases considered here. The dispersive refractive index profiles over the wavelength range 450-950 nm as obtained by TLBO approach are also in good agreement with the ellipsometry results. Thus, it is shown that the thickness and refractive index values could be estimated very consistently for most optical coating applications from a simple reflectivity measurement, which is easily available in small laboratory environment. Finally, it is concluded that a simple reflectivity measurements can yield valuable information about the thickness and dispersive refractive index over the wavelength range by using our program based on TLBO algorithm. In conclusion, we have demonstrated the suitability of a novel TLBO approach for a routine determination of the refractive index and the thickness with good precision for various materials used in optical and optoelectronics devices fabrication.

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