Determination of the Optical Constants of Thin-Film Coating Material Using Evolutionary Algorithm

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Abstract

Anew mathematical procedure depends on the evolutionary algorithm has been proposed to estimate the optical constants (refractive index, extinction coefficient and thickness) of unknown deposited material on a defined substrate. The transmittance and reflectance experimental data are taken for two materials (Sc_2O_2 and Rh) with two different thicknesses for the wavelengths range (400-850 nm). The resulting optical constants and the theoretical transmittance and reflectance spectra are very close to the experimental data.

Keywords: Optical constants, Thin film coatings

تحديد الثوابت البصرية لمادة غشاء رقيق باستخدام خوارزمية التطور

الخلاصة

تم اقتراح اسلوب رياضي جديد يعتمد على مبادىء نظرية التطور لايجاد الثوابت البصرية المتمثلة بمعامل الانكسار و معامل الخمود وسمك طبقة واحدة مجهولة مرسبة على طبقة أرضية معروفة المواصفات. اخذت القيم العملية لالنعكاسية و النفاذية كدالة للطول الموجي لمادتين هما اوكسيد السكانديوم و الروديوم و لسمكين مختلفين ضمن الطول الموجي 400-850 نانوميتر. لقد بينت النتائج النظرية للثوابت البصرية و منحنيات الانعكاسية و النفاذية مدى المطابقة مع النتائج العملية لهاتين المادتين.

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Introduction

There are numerous applications for optical multilayer interference coatings in science and technology. The coating materials are chosen to be both absorbing and non absorbing materials. The preparation of such a system is based on thermal evaporation in a vacuum which is the most commonly process for economic reasons. It is common knowledge that films produced in different laboratories or different deposition systems have different optical constants. This is because different Deposition geometries and conditions give rise to different film structures and compositions. For the design and manufacture single or multilayer coatings, a good knowledge of the refractive indices and absorption coefficients of the coatings materials is needed. Many papers with different ideas and mathematical equations are proposed to determine the optical constants (refractive index, extinction coefficient, thickness) of one layer deposited on a substrate. The problem of finding the optical constants is an inverse problem via using the spectrum of normal reflectance or/and transmittance to optimize the equation of reflectance or/and transmittance to get minimum error between the theoretical and experimental data by varying the optical constants.

The methods of estimating the optical constants can be divided to two categories; the first one is the methods depending on interference fringes which can also be called (the envelop method). The envelope methods depend on some boundary conditions which divided the transmission spectral curve to many regions upon the values of the absorption coefficient or the numbers of maxima and minima of the spectrum. This method was firstly proposed by Swanepoel (1), and then many authors depend on the same technique but with some improvements taking into account even the reflectance or transmittance spectrum (2-10). The basic disadvantage of this procedure it cannot be applied for the reflectance or transmittance spectrum that have not any minima and maxima points.

The second methods are depend on optimizing merit function by using any appropriate method of optimization, such as least square method or successive regression method or even the relatively new method such as genetic or evolutionary algorithm methods. The optimization methods are used by many authors (11-20) but it is not very convenient due to the fact that the system is satisfied by many solutions and it is difficult to identify the real physical one. Although these methods can obtain the optical constants and thickness of the thin film even its reflectance or transmittance spectrum have no maxima and minima points.

In this paper, a new method has been proposed based on the evolutionary algorithm to determine the optical constants of one layer deposited on known transparent substrate. The only input data are the transmittance and reflectance spectra have been needed to obtain the optical constants.

Many research institutes used an experimental data [23] of reflectance and transmittance as input data to obtain both the optical constants and optical spectra theoretically, by using different optimization methods which is useful to compare our results with those.

Mathematical form of the optical properties

The basic function of the approaches to the evolutionary algorithms for designing multilayer systems is to find the values of the optical constants of the film that bring the theoretical optical performance close to the target specification over the desired wavelength band. The mathematical assumptions used in this study are:

1) The radiation is incident normally on the materials layers.
2) The best solution for designing depends on the basis of minimizing merit function.

The merit function (*MF*) employed in this study is the basic one that is used to represented the difference between the target and the computed reflectance and transmittance over a range of wavelengths, the chosen merit function

$$MF=\left[\frac{1}{w}\sum_{j=1}^{w}\frac{(R_j-R_j^{'}(\lambda))^2}{\delta R}+\frac{(T_j-T_j^{'}(\lambda))^2}{\delta T}\right]^{\frac{1}{2}} \quad \text{……. (1)}$$

(R_j, T_j) are the theoretical reflectance and transmittance at the wavelength λ, respectively. ($R_j^{'}$, $T_j^{'}$) are the target (or experiment) reflectance and transmittance, respectively. δR and δT is the tolerance at the wavelength λ. In general δR and δT is set to 0.01, *w* is the number of interesting points of the target reflectance that used to compute the merit function.

It is obvious that the goodness of the solution depend on the value of merit function, when its value approaches to zero means that the resulting refractive indices and thicknesses of all layers make the reflectance or transmittance spectrum approaches to the target spectrum.

Minimization Using Evolutionary Algorithm

The evolutionary algorithms (22) are adaptive methods which may be used to solve search and optimization problems. It works with a population of individuals, each representing a possible solution to a given problem. Each individual is assigned a fitness score according to how good a solution to the problem it is. The highly fit individuals are given opportunities to reproduce by cross-over and mutation operation with other individuals in the population. This produces new individuals as offspring, which share some features taken from each parent. The least fit members of the population are less likely to get selected for reproduction, and so excluded.

A whole new population of possible solutions is thus produced by selecting the best individuals from the current generation, and mating them to produce a new set of individuals. This new generation contains a higher proportion of the characteristics possessed by the good members of the previous generation. In this way, over many generations, good characteristics are spread throughout the population. By favoring the mating of the more fit individuals, the most promising areas of the search space are explored. If the evolutionary algorithm has been designed well, the population will converge to an optimal solution of the problem. The basic operations used to reach the final solution are:

1) Create random solutions (by using any random values generators).
2) Cross over operation.
3) Mutation operation.
4) Replacement operation.

The last three operations are repeated until reaching minimum fitness value which represents the good optimum solution. A computer program (**Evotic**) has been designed as illustrated in Appendix (1). This program can vary the optical constant to get minimum merit function value which can be achieved when making the reflectance and transmittance spectrum approaches to the target spectrum.

Target Spectrum

The basic aim of this paper is to use experimental reflectance and transmittance data as the input data (Table (1)) [23] to estimate the optical constants theoretically and then comparing these output optical constants data with the experimental data of Table (1).

The substrate used for the coatings was 38.6 mm diameter by 3 mm thick of fused silica which has a refractive index given by:

$$n_s^2 = 1 + \frac{0.69617\lambda^2}{\lambda^2 - 0.0046792} + \frac{0.40704\lambda^2}{\lambda^2 - 0.013512} + \frac{0.89748\lambda^2}{\lambda^2 - 97.93} \qquad \ldots (2)$$

For wavelength (λ) measured in µm.

The dielectric coating materials selected for this study were Scandium oxide (Sc_2O_3) of 99.99% purity, this material is considered as transparent material over the range of wavelength (400 to 850 nm), which means that the extinction coefficients are zero. Two different thicknesses were made (224.5 and 452.5 nm). The second material is Rhodium (Rh) of 99.9% purity, this material is considered as absorber for the wavelength range (400 to 850 nm).

Also, two thicknesses were made (14.2 and 27.1 nm).

All measurements were taken with the argon-ion laser and NWC transmittance data and OCLI reflectance data taken on spectrophotometer-type instruments.

The Theoretical Results

The basic assumptions of program (**Evotic**) to determine the optical constants are:

1) The refractive index of the coating material has the theoretical formula:

$$n^2 = 1 + \frac{A_1 \lambda^2}{\lambda^2 - A_2} + \frac{A_3 \lambda^2}{\lambda^2 - A_4} + \frac{A_5 \lambda^2}{\lambda^2 - A_6} \quad ..(3)$$

A_1 ,A_2 ,A_3 ,A_4, A_5, A_6 are constants to be determine using the evolutionary programming.

2) The extinction coefficient of the coating material has the mathematical formula:

$$k = B_1 + B_2 \lambda + B_3 \lambda^2 \quad .... (4)$$

B_1 ,B_2 ,B_3 are constants. These mathematical formulas for both refractive index and extinction coefficients can take many different shapes depending on the material and the wavelength range.

The testing of evolutionary algorithm to estimate the optical constants theoretically have two directions depends on the two input experimental data which differ in thicknesses for both Scandium Oxide and Rhodium. The results of the four experiments are:

1) Scandium Oxide

The theoretical results using (Evotic) program are:

a) The refractive index of the coating layer for both thicknesses is:

$$n^2 = 1 + \frac{1.60864\,\lambda^2}{\lambda^2 - 0.032378} + \frac{0.777177\,\lambda^2}{\lambda^2 - 0.013432} + \frac{0.330865\,\lambda^2}{\lambda^2 - 40.88458}$$

b) For the thin Scandium Oxides, the resultant coating layer thickness is (221.9 nm), which is very close to the real experimental value (224.5 nm) with error about (1.1 %). The mean percentage error between experimental and theoretical reflectance is about (0.23 %).

c) For the thick Scandium Oxide, the resultant coating layer thickness is (455.86 nm), which also close to the real experimental value (452.5 nm) with error about (0.7 %). The mean percentage error between experimental and theoretical reflectance is about (0.92 %).

The comparisons of the theoretical with the experimental values are shown in Figure (1), while Figure (2) shows the theoretical and experimental reflectance.

2) Rhodium

The theoretical results for thin Rhodium (Thickness 14.2 nm) are:

a) The refractive index of the coating layer is:

$$n^2 = 1 + \frac{2.17160\,\lambda^2}{\lambda^2 - 0.006873} + \frac{8.82488\,\lambda^2}{\lambda^2 - 0.001506} + \frac{2.72105\,\lambda^2}{\lambda^2 - 46.29752}$$

b) The extinction coefficient of the coating layer is:

$$k = 0.843657 + 3.795618 * \lambda + 0.60007 * \lambda^2$$

c) The coating layer thickness is (14.02 nm), with error 1.3 %. The mean error percentage for reflectance, transmittance and absorptance are (0.25 %, 0.28 %, 0.36 %) respectively.
While the theoretical results for thick Rhodium (Thickness 27.1 nm) are:
a) The refractive index of the coating layer is:

$$n^2 = 1 + \frac{6.07087\,\lambda^2}{\lambda^2 - 0.00288} + \frac{5.49754\,\lambda^2}{\lambda^2 - 0.00066} + \frac{0.22919\,\lambda^2}{\lambda^2 - 47.48964}$$

b) The extinction coefficient of the coating layer is:

$$k = 1.30274 + 3.72406 * \lambda + 0.26631 * \lambda^2$$

c) The coating layer thickness is (24.35 nm), with error 10 %. The mean percentage error of reflectance, transmittance and absorptance are (0.13 %, 0.02%, 0.12 %) respectively.
The experimental and theoretical refractive indices are shown in Figure (1), while Figure (3) shows the extinction coefficients and Figure (4) illustrates the experimental and theoretical reflectance and transmittance.

Discussion

Figures (1-4) shows the theoretical results of the optical constants, the transmittance and reflectance spectra which are very close to the experimental results [23]. The error in transmittance and reflectance spectra is less than 1 % for all the four experiments, while the error in thicknesses less than 1.3%. The mean error in refractive indices for Sc_2O_3 is (1.2%), while the mean errors in refractive indices for Rh are (17%, 32%), and in extinction coefficients (7.5%, 2.3%) for the thicknesses (14.2 and 27.1 nm) respectively.
Obviously, the coincidences between the input (experiment) results and the theoretical results are very good for Sc_2O_3, while the results for reflectance, transmittance and thicknesses for Rh are very good in spite of relatively large error in refractive indices and extinction coefficients. This error is due to the possibility of non-unique solutions which is the major problem for any optimization method.
To illustrate the ability of evolutionary technique comparing with other mathematical techniques, we put the result of thickness of the unknown coating layer for all these techniques (Table 2) as a comparison with the evolutionary technique.
Thus, the evolutionary algorithm can be considered as promising technique to solve the optimization problems without needing to any additional constraints conditions.

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Table (1) Experimental data of optical Parameters and optical constants.

Material	Thickness (nm)	λ (nm)	T Transmittance	R Reflectance	A Absorptance	n	k
Sc_2O_3	224.5	450.0	91.57	08.43	00.00	1.700	0.00
		488.0	87.04	12.96	00.00	1.820	0.00
		500.0	85.76	14.24	00.00	1.860	0.00
		514.5	85.10	14.90	00.00	1.864	0.00
		550.0	84.06	15.94	00.00	1.844	0.00
		600.0	85.61	14.39	00.00	1.842	0.00
		650.0	89.30	10.70	00.00	1.836	0.00
		700.0	93.03	06.97	00.00	1.828	0.00
		750.0	95.60	04.40	00.00	1.817	0.00
		800.0	96.63	03.37	00.00	1.780	0.00
Sc_2O_3	452.5	450.0	89.22	10.78	00.00	1.860	0.00
		488.0	85.64	14.36	00.00	1.832	0.00
		500.0	86.45	13.55	00.00	1.848	0.00
		514.5	89.23	10.77	00.00	1.854	0.00
		550.0	95.75	04.25	00.00	1.866	0.00
		600.0	91.93	08.07	00.00	1.863	0.00
		650.0	85.07	14.93	00.00	1.816	0.00
		700.0	85.86	14.14	00.00	1.836	0.00
		750.0	91.07	08.93	00.00	1.840	0.00
		800.0	95.35	04.65	00.00	1.851	0.00
Rh	14.2	450.0	16.43	43.67	39.90	2.40	3.28
		500.0	16.71	43.22	40.07	2.60	3.40
		550.0	16.84	43.11	40.05	2.78	3.53

		600.0	16.94	42.94	40.12	2.95	3.65
		650.0	17.05	42.84	40.11	3.11	3.77
		700.0	17.15	42.82	39.92	3.23	3.91
		750.0	17.26	42.72	40.02	3.35	4.03
		800.0	17.41	42.65	39.94	3.42	4.17
Rh	27.1	450.0	05.57	55.97	38.46	2.27	3.25
		500.0	05.94	56.49	37.57	2.39	3.41
		550.0	06.18	56.98	36.84	2.51	3.58
		600.0	06.36	57.45	36.19	2.62	3.74
		650.0	06.52	57.70	35.78	2.75	3.88
		700.0	06.65	57.97	35.38	2.87	4.03
		750.0	06.77	58.08	35.15	3.01	4.15
		800.0	06.88	58.20	34.92	3.14	4.28

Table (2) Thickness results comparison

Institution	Method	Sc_2O_2 Thickness nm		Rh Thickness nm	
		Thin	Thick	Thin	Thick
Real Experiments Values Michelson laboratory		224.5	452.5	14.2	27.1
University of New Orleans	Reflection Ellipsometry	228.2	462.6	15.5	31.6
Centre d'Etudes des Couches Minces	Wide-Band Spectrophotometric	217.6	447.8	----------	----------
Optical Coating Laboratory Inc.	Modified Valeev Turning point	219.0	447.4	17.2	30.1
Vought Corporation	Algebraic Inversion	225.0	450.0	12.0	27.5
National Research Council of Canada	Inverse Synthesis	221.2	450.3	16.9	31.7
Optical Science Center	Envelope	219.4	449.6	17.0	----------
Present Work	Evolutionary Algorithm	221.9	455.9	14.0	24.4

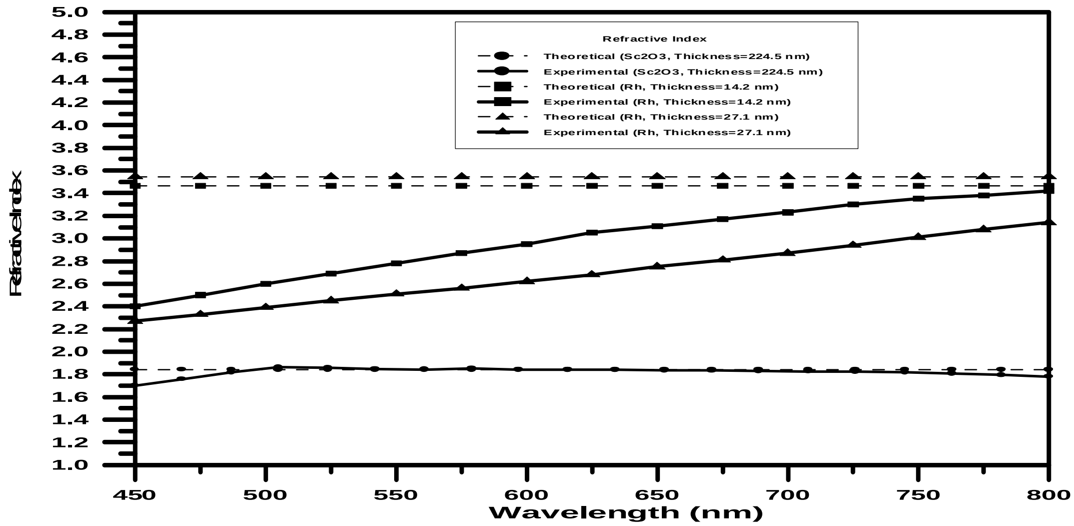

Figure (1) Experimental and theoretical refractive index versus wavelengths for Scandium Oxide and Rhodium.

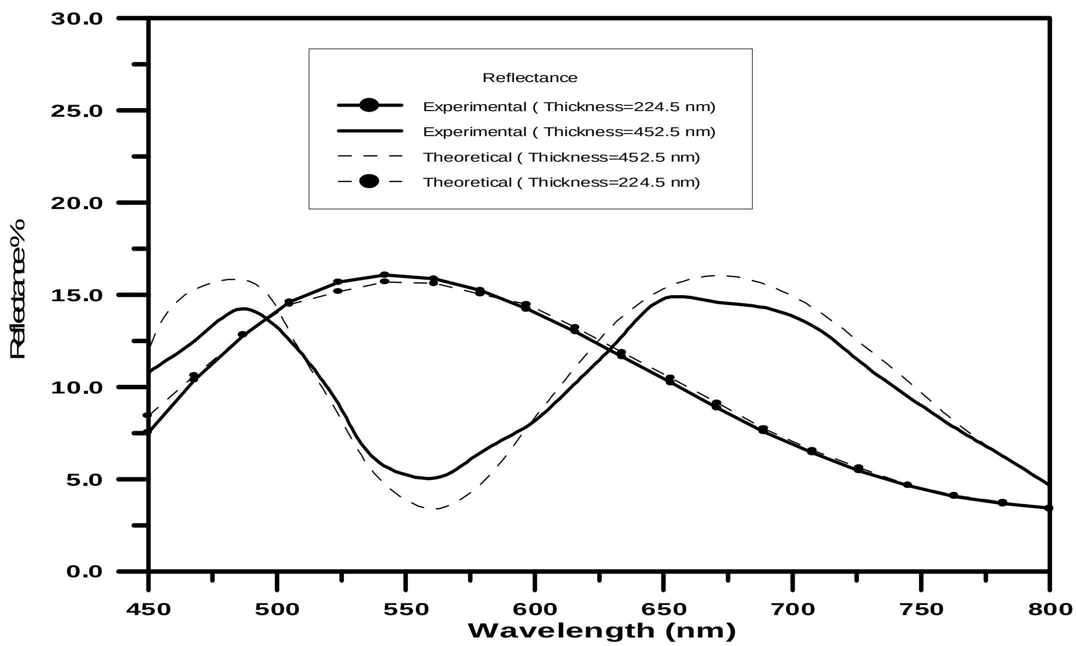

Figure (2): Experimental and Theoretical reflectance versus wavelength for Scandium Oxide.

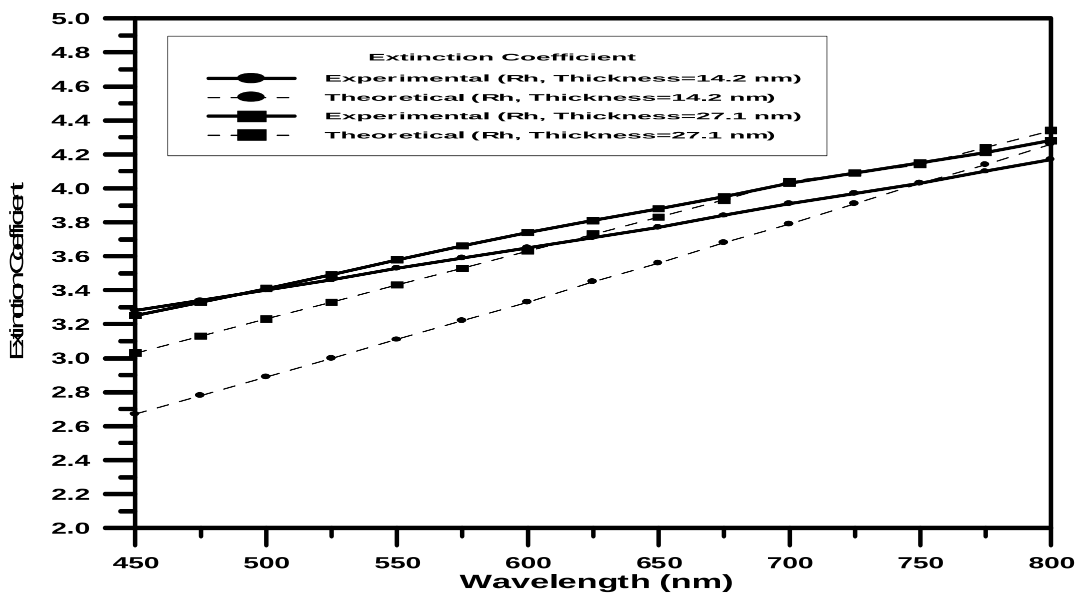

Figure (3) Experimental and theoretical extinction coefficients versus wavelengths for Rhodium.

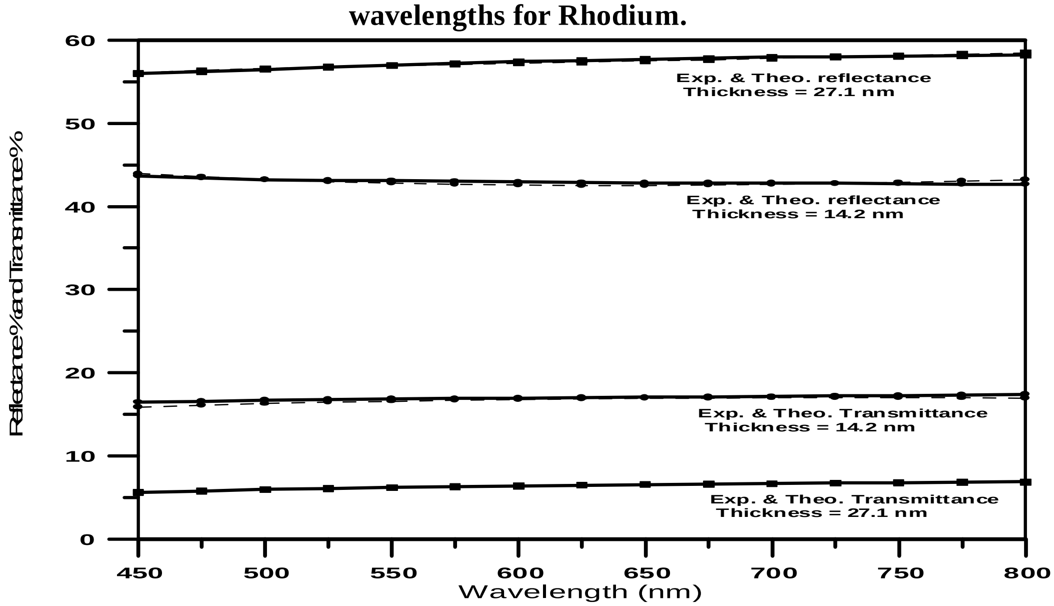

Figure (4) Experimental and Theoretical reflectance and transmittance versus wavelength for Rhodium.

Appendix (1) The Block Diagram of the Computer Program