Optimization of parameters of integrated optical waveguides based on thin-film Sol-gel structures by using mathematical modelling

S.A. Aliev, K.D. Pakhlavonova, A.R. Ravin, N.S. Trofimov, T.K. Chekhlova

Peoples' Friendship University of Russia (RUDN University), 6 Miklukho-Maklaya Street, Moscow, 117198, Russian Federation
E-mail: alievsamiralievich@gmail.com

Abstract. An algorithm for calculating optical waveguide film parameters was proposed, the use of which makes it possible to reduce the time for processing experimental data. The developed algorithm was tested using experimental data of waveguides samples with a wave-guiding layer of zirconium dioxide sol-gel films. A comparison of the developed algorithm and the Wolfram Mathematica program showed a good agreement of the results, as well as the developed method advantage in terms of using ease and timesaving spent on processing the results.
Keywords: mathematical modelling, integrated optics, optical waveguide, sol-gel technology, temperature optical coefficient.

1. Introduction.

Nowadays, progress in the photonics and integrated optics is associated with the development of new technologies and materials for the formation of optical waveguides, which can provide improved characteristics and expand the functionality of devices based on them. In recent years, titanium dioxide films formed by the sol-gel method and its analogs [1–4] have been successfully used in optical waveguides creation. Films made by this technology have a number of specific properties, the most important of which are the possibility of varying the refractive index of films by changing the parameters of the technological mode, a large negative thermo-optical coefficient (TOC), which determines the prospects of their use in devices of integrated optics and FOCL. Negative TOC finds application in temperature adjustment of integrated-optics interference devices, such as narrow-band filters, resonators, Mach-Zander interferometers, multiplexers/demultiplexers, etc. A large thermo-optical coefficient is especially important for creating thermo-optical selectors, switches, and other thermo-controlled devices. Noticing that, the temperature coefficient of the effective refractive index of the waveguide is important for the waveguide devices of photonics, because of its dependence on the waveguide layer thickness and the refractive indices of the substrate and the upper framing medium.

The parameters of optical sol-gel waveguides, such as thickness and refractive index of waveguide layer, depend on the parameters of the technological mode, which include the composition of the film-forming mixture, the method of film deposition and subsequent temperature processing.

The development of the technology for creating such waveguides and the optimization of their parameters for a particular device assumes experimental studies of a large series of samples made with different parameters of the technological mode and the calculation of their parameters. Decision, based on the research results, is made on the appropriate adjustment of the parameters of the technological order to obtain samples with the specified parameters. In this case, processing of a large experimental database is required and an express analysis of the parameters of optical waveguides is necessary.

The work is dedicated to the creation of an algorithms for calculating optical waveguide film parameters, the use of which makes it possible to reduce the time for processing experimental data. The developed algorithm applied for research of waveguide samples based on previously little-studied zirconium dioxide films. In particular, there are no data on studies of the thermo-optical coefficient and the temperature coefficient of the effective refractive index of zirconium dioxide waveguide. The study of manufactured samples was carried out by fixing the excitation angle of the waveguide by laser radiation.

The program with algorithms processes the input data in the form of an array of angles, and checking 240 values takes about 2 minutes, which in the usual calculation method would take a lot of time. The development of a mobile version for Android OS is also underway.

2. Mathematical modelling of the calculation of the optical waveguide parameters.

In the simplest case, an optical waveguide is a substrate with a film deposited on its surface with a refractive index greater than the refractive index of the substrate. The effective refractive index (ERI) of an optical waveguide is determined by the thickness of the waveguide film and the refractive indices of the materials from which the waveguide is formed. As is known, the refractive indices of materials and the thickness of the waveguide film depend on the temperature in accordance with their TOC and the coefficient of expansion of the film material, respectively. The arrangement diagram for determining the temperature dependence of ERI using the Peltier element is shown in Fig.1.
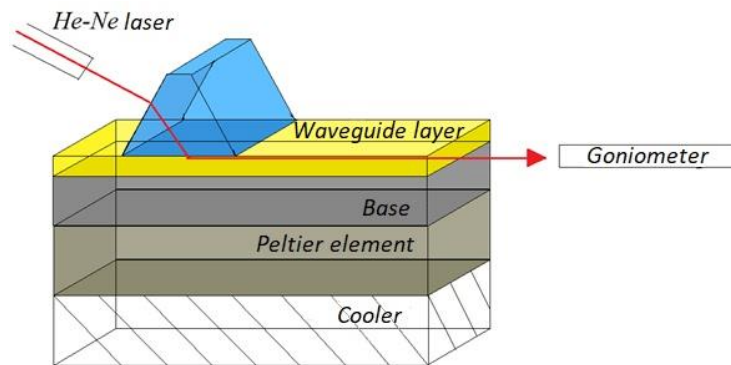

Figure 1. Arrangement for determining the temperature dependence of ERI using the Peltier element.

The effective refractive index of an optical waveguide was calculated using dispersion equations that determine the relationship between the effective refractive index for the corresponding mode, the thickness of the waveguide layer, the refractive indices of the environment forming the waveguide, and the wavelength taking into account *n(T)* and *h(T)* [5]. For the TE and TM modes, the dispersion equations have the form:

$$h = \frac{\lambda}{2\pi\sqrt{n^2-\gamma_{TE}}} \cdot \left(Arctg\sqrt{\frac{\gamma_{TE}^2-n_1^2}{n^2-\gamma_{TE}^2}} + Acrtg\sqrt{\frac{\gamma_{TE}^2-n_2^2}{n^2-\gamma_{TE}^2}} + \pi(m-1) \right) \qquad (1)$$

– for TE waves and

$$h = \frac{\lambda}{2\pi\sqrt{n^2-\gamma_{TM}}} \cdot \left(Arctg\left(\frac{n}{n_1}\right)^2\sqrt{\frac{\gamma_{TM}^2-n_1^2}{n^2-\gamma_{TM}^2}} + Arctg\left(\frac{n}{n_2}\right)^2\sqrt{\frac{\gamma_{TM}^2-n_2^2}{n^2-\gamma_{TM}^2}} + \pi(m-1) \right) \qquad (2)$$

- for TM waves.

where n_1, n, n_2 are the refractive indices of air, the film and the substrate, respectively, *m* is the number of the waveguide mode, *γ* is the phase retardation factor, which can be interpreted as the effective refractive index for the waveguide mode, which takes a certain value for a given thickness of the

waveguide layer. It is convenient to solve transcendental equations for h/λ, setting different values of the ERI for known n_1, $n_2(T)$, $n_3(T)$. The radiation is introduced into the optical waveguide by optical tunneling through a medium with a refractive index of $n_3 > \gamma$ at certain angles of incidence depending on the ERI and n_3 or by the diffraction method.

The parameters of optical waveguides based on sol-gel materials, such as the refractive index $n(T)$ and layer thickness h, depend on the parameters of the technological mode, which include the composition of the film-forming mixture, the annealing temperature, etc. Therefore, the task is to determine the parameters of the waveguide for specific parameters technological mode. The thickness of the waveguide layer h is calculated by measuring the angles of excitation of the experimental waveguide and determining γ using the dispersion equations. If the refractive index n is unknown, then by measuring the angles of excitation on two modes and determining γ for these modes using the dispersion equations, we can determine the unknowns n and h.

3. Calculation methods.

Dispersion equations (1) and (2) are transcendental. One of the examples of thickness dependences on the refractive index of the waveguide layer, constructed with known phase delay coefficients of the TE and TM modes, is shown in Figure 2.
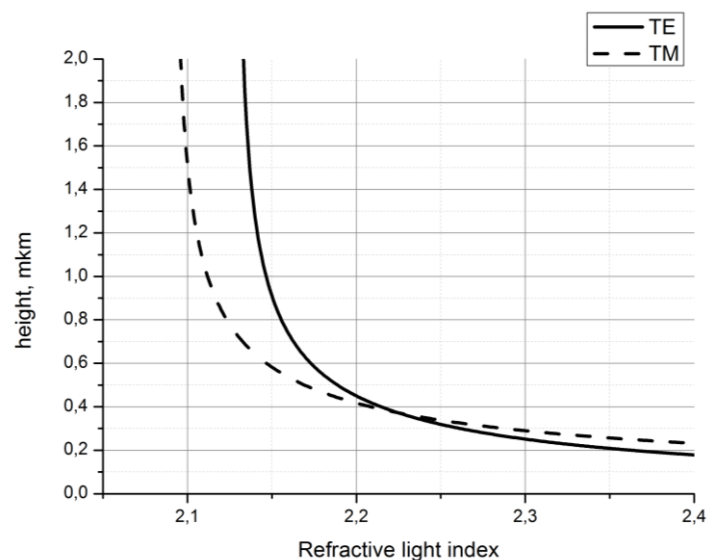

Figure 2. Mathematical model of dependences h(γTE, γTM), where the intersection point contains the solution of the dispersion equations.

The intersection point of the functions corresponds to the solution of the dispersion equations in the form of thickness (OY axis) and the waveguide refractive index (OX axis). To find it, the method of simple iterations, the method of chords and tangents (the combined method) and the method of half division (dichotomy) were considered. For each method, a processing algorithm is written in the C ++ programming language.

The point of the method of simple iterations [6] is the gradual refinement of the root value. The model from Figure 2 calculates the values at the points ni and ni+1, and compares the difference between them. The iteration goes from left to right as the functions narrow to their point of intersection. Each next "step" approximates the root value, while solving the functions a = |funcTE (step) -funcTM (step)| will not be less than the value of the error eps. If the "step" is greater than necessary and the variable value is missed and the functions begin to diverge, then step variable will return to the previous successful point and change the step by several orders of magnitude in accordance with the specified error parameter eps. The basic block diagram of the algorithm is shown in the diagram (Fig. 3).
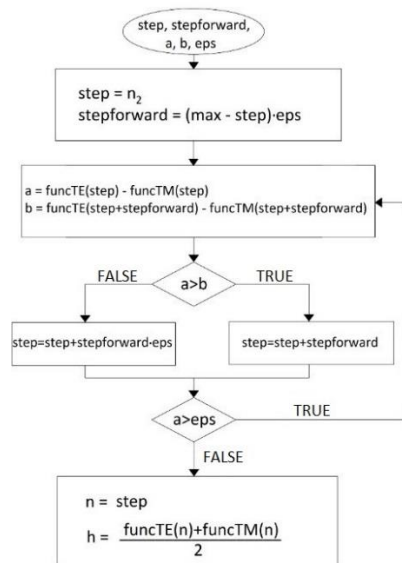
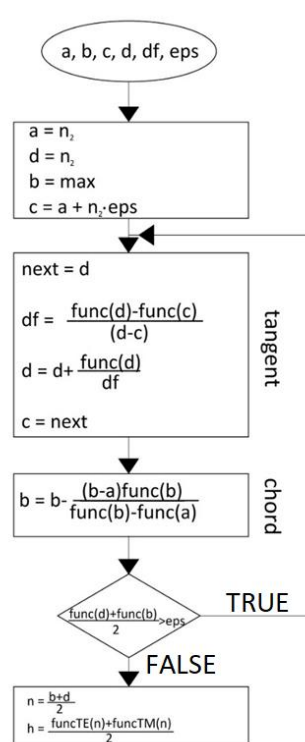**Figure 3.** Algorithm of the method of simple iterations.

Figure 4. Algorithm of the combined method (method of chords and tangents).
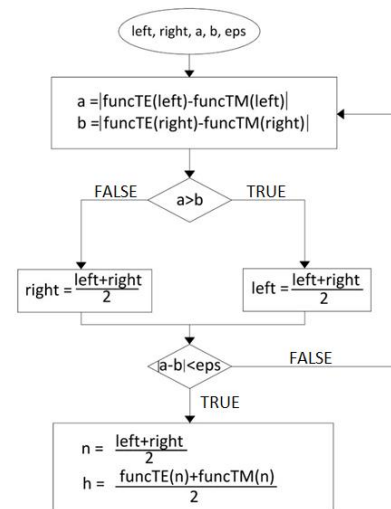
Figure 5. Algorithm of the half division method (dichotomy method).

Almost all iterative methods, including the method of simple iterations, have an important merit: they do not accumulate calculation errors. This error is equivalent to some degradation of the next approximation.

The point of the combined method [7] consists in splitting the segment [n; max] into three segments with the help of the chord and the tangent. A new segment selects from the intersection point of the chord with the x-axis to the intersection of the tangent with the x-axis, on which the function changes sign and contains the solution. The construction of chords and tangents continues until the required accuracy of the solution eps is achieved. Next, the solution algorithm is applied (Fig. 4).

The considered method is one of the fastest methods for solving a nonlinear equation (it has a high rate of convergence). However, one of the main requirements for the convergence of this method (and its main disadvantage) is the localization of the initial approximation in a sufficiently small localization of the root of the equation.

The point of the half division method [7] (dichotomy) is to construct segments ([left; right]), but at each step the next segment is divided in half, and the next segment is the half in which the function values at the ends of the segment (a, b) have different signs. The process continues until the length of the next segment becomes less than the value of eps. Then the midpoint of the segment will be an approximate root value with an accuracy of eps/2. The algorithm of this method is shown in the diagram (Fig. 5).

The dichotomy method is easily implemented and is the most universal among iterative methods of root refinement. The method always converges, but the rate of convergence is small, since the accuracy increases only twice during one iteration. Its application guarantees obtaining a solution for any continuous function f(n) if an interval is found in which it changes sign. One of the drawbacks of the

half division method is the convergence of an arbitrary root from the search area — almost all iterative methods have it. In this case, only the removal of previously found roots can help.

4. Making samples. Materials and methods.

Photo plates with a refractive index of $n_2 = 1,512$ were used as substrates. Substrates were cleaned by sequential washing in a 30% KOH solution, chromium mixture, and distilled water with drying in a stream of purified air.

The main reagents that were used during the experiment:

Zirconium N-Propoxide (TPOZ)

Acetylacetone $CH_3CH(OH)CH_5$

Isopropyl alcohol C_2H_5OH

The sol is obtained by mixing zirconium n-propoxide (TPOZ) with an equivalent molar amount of acetylacetone. Then isopropyl alcohol is added to adjust the viscosity of the sol. Acetylacetone is used as a stabilizer. By solving the chemical task, the ratio of the mixed components was calculated [8]:

$$TPOZ:CH_3CH(OH)CH_5 = 3:1.$$

The resulting solute had a yellow color and crystals formed in it. The solute was continuously stirred in a vessel for about 30 minutes at room temperature, the crystals decayed and dissolved in the solute while stirring.

The substrate was placed vertically down into the solute three times, and between this was dried in an oven for 10-15 minutes at a temperature of 100℃. After the third drawdown, the waveguides were placed in quartz tubes and were annealed in a furnace for 3 hours at a temperature of 450℃.

5. Results and its discussion

Samples of waveguides based on zirconium h-propoxide films that had 2 TE and TM- waveguide modes were investigated. The measurements were carried out using a technique developed in [9] using the Peltier module; the temperature of the samples was changed from 25°C to 100°C with a step of 5 ± 1°C. Using the measured excitation angle, the effective refractive index versus temperature was calculated and plotted (Fig.6). Dotted lines indicate areas of error.
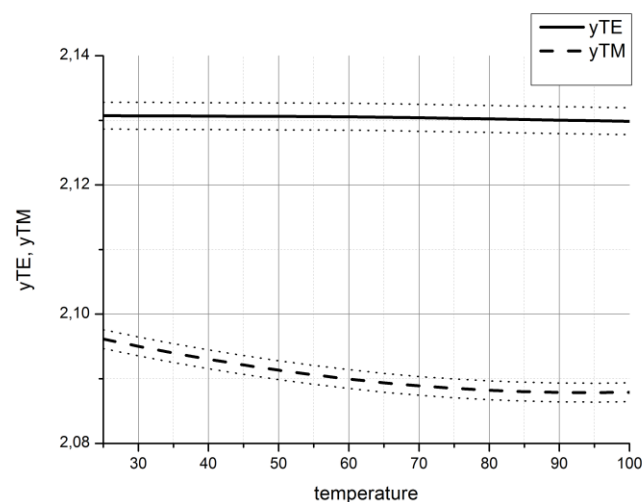

Figure 6. The dependence of the effective refractive index on temperature.

Figure 7 and Figure 8 show the temperature dependences of the thickness and refractive index of the zirconium dioxide film on temperature, respectively. The film thickness decreases with increasing temperature, which is apparently due to the compaction of its structure when the solvent evaporates

(Fig.7). This process ends at a temperature of 85°C, and then the thickness begins to increase in accordance with the coefficient of volumetric expansion of the material.
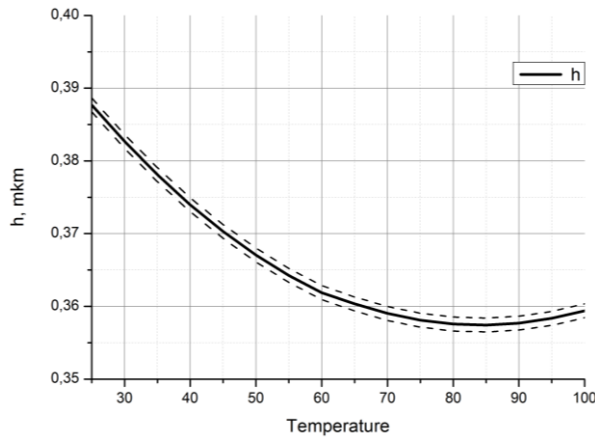

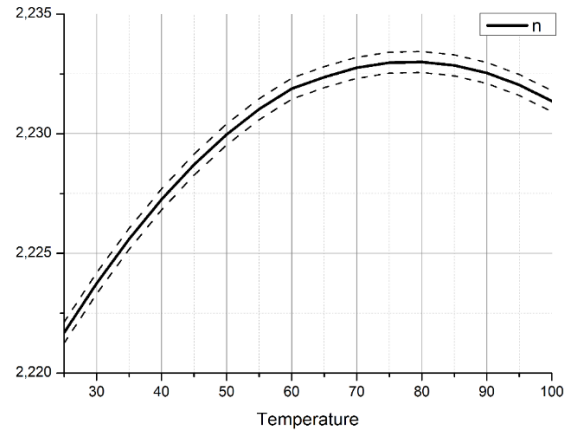**Figure 7.** The dependence of film thickness on temperature.

Figure 8. The dependence of the refractive index on temperature.

In accordance with the film structure change, the refractive index also increases (Fig.8). At a temperature of about 80°C with a further increase in temperature, a decrease in the refractive index is observed, i.e. TOC material becomes negative equal to - $-8,2 \times 10^{-5} \frac{\Delta n}{\Delta T}$. These factors explain the unusual behavior of ERI for the TE and TM modes (Fig. 6), which is associated with the competition of two factors — an increase in the film thickness in accordance with the volumetric coefficient of expansion of the material and a change in its refractive index in accordance with the thermo-optical coefficient, which can be either positive or negative. The influence of these factors depends on the distribution of the wave field in the environments, forming the waveguide [10]. In this case, it appears, that two factors were compensated for the TE wave.

The graphs presented in Figures 7 and 8 were obtained by combining all the methods of calculation with finding the arithmetic mean. For each method, the errors were calculated according to the standard deviation. Also, Wolfram Mathematica 10 software was taken as a well-known and affordable method of calculation. There was used function FindRoot[h(n),{n3,max}] in Wolfram, which searches for a numerical root of h(n), starting from the point n=n3. The faults of each method are listed in Table 1.

Table 1. Faults of each method.

	Wolfram Mathematica 10	The method of simple iterations	The half division method	The combined method (chords and tangents)
n	0,00691	0,006911	0,007803	0,006911
h	0,011886	0,013235	0,013235	0,011891

Calculation errors for deceleration coefficients were about 0,002084 for γTE, and 0,001455 for γTM. From table 1 it is clear, that the most optimal is the combined method (method of chords and tangents), which has the lowest error value.

The temperature properties of zirconia films made by the sol-gel method were investigated with the help of the developed program. It is determined that zirconium dioxide films have a negative thermo-optical coefficient equal to - $-8,2 \times 10^{-5} \frac{\Delta n}{\Delta T}$ in the range of temperatures from 25°C to 100°C.

Acknowledgments

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