32^{nd} European Modeling & Simulation Symposium
17^{th} International Multidisciplinary Modeling & Simulation Multiconference

ISSN 2724-0029 ISBN 978-88-85741-44-7 © 2020 The Authors.
DOI: 10.46354/i3m.2020.emss.042

Calculation of refractive index and extinction coefficient of perfluorinated polymer films using new numerical algorithm in prism coupling technique

Viktor I. Sokolov[1,2,*], Ivan O. Goriachuk[1] and Alexander S. Akhmanov[1,2]

[1]Institute on Photonic Technologies, Federal Scientific Research Center «Crystallography and Photonics», Russian Academy of Sciences
[2]Federal Research Center «Scientific Research Institute for System Analysis», Russian Academy of Sciences

[*]Corresponding author. Email address: visokol@rambler.ru

Abstract

Amorphous perfluorinated polymers are of great interest for integrated optics and photonics due to their high optical transparency, low refractive index and index dispersion. Therefore, methods for accurate measuring optical parameters and thickness of light-guiding polymer films are important. We present new approach and numerical algorithm for calculating refractive index, extinction coefficient and thickness of anisotropic polymer films from angular reflection spectra measured by prism coupling technique. The proposed algorithm is valid both in the «low» and «high» coupling limits and takes into consideration the angular divergence of the Gaussian probe beam.

Light-guiding film of proprietary amorphous perfluorinated polymer was fabricated on silicon substrate with thermally grown silica oxide layer. Angular reflectivity spectra of polymer film were measured with TE and TM polarized Gaussian laser beams using the prism coupling technique. Refractive index n, extinction coefficient m and thickness H_f of the film were calculated numerically from reflectivity spectra using the new strategy and fitting algorithm. It was shown that the developed approach is effective and permits to determine n and m of anisotropic polymer films with accuracy $\pm 1 \times 10^{-4}$ and $\pm 1 \times 10^{-5}$ correspondingly.

Keywords: prism-coupling technique, simulation of reflection spectra, thin anisotropic films, light-guiding structures, amorphous perfluorinated polymers, calculation of refractive index and extinction coefficient of thin films, fitting algorithms.

1. Introduction

The prism coupling technique is a powerful tool for measuring refractive index n, extinction coefficient m and thickness H_f of dielectric films (Sotsky et al., 2013; Khomchenko, Sotsky et al., 2002; Pasmooij et al., 1989; Sokolov et al., 2015; Goriachuk et al., 2018; Sokolov et al., 2018). However, the implementation of this technique for determination of optical parameters of thin polymer films often requires sophisticated approaches for the following reasons. First, the polymer films are usually anisotropic with different n and m in the plane of the film and perpendicular to this plane. Second, polymer films can have non-uniform distribution of n and m in the direction perpendicular to the film plane due to the porosity or preferential orientation of the polymer macromolecules on the film/substrate interface. Third, the waveguide modes of low and high orders have different degree of localization in the light-guiding film and therefore different sensitivity to the optical parameters of the films. In this paper, we propose a novel approach, which permits to improve the accuracy of determination of optical parameters and thickness of anisotropic polymer film. The approach can be used for the analysis of single-layer and multilayer thin-film structures. It is valid in the «low» and «high» coupling limits and takes into consideration the angular divergence of the probe Gaussian laser beam.

2. Materials and Methods

2.1. Synthesis of amorphous perfluorinated polymer

We have synthesized new proprietary amorphous perfluorinated polymer by copolymerizing dioxole and ether monomers under high pressure (1200 MPa) without any initiators. The scheme of the synthesis is presented in Figure 1.

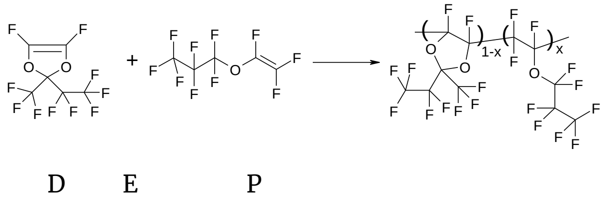

Figure 1. Scheme of synthesis of amorphous perfluorinated polymer P by copolymerizing dioxole D and ether E under high pressure. *x* is molar concentration of ether in the polymer macromolecule.

2.2. Fabrication of light-guiding polymer film

The film was spin-coated from the pertinent polymer solution on the silicon wafer with thermally grown «thick» SiO_2 oxide layer (estimated thickness ≈ 3.7 μm) using SPIN-1200T spinner (Midas System Co., Ltd.). The thickness of the polymer film was estimated to be ≈ 2.5 μm. The photograph of the structure is presented in Figure 2.

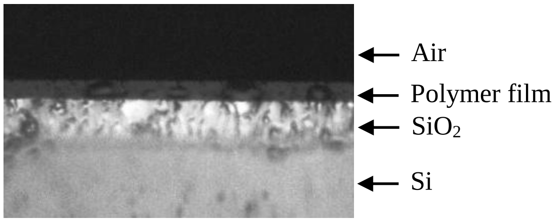

Figure 2. Perfluorinated polymer film on silicon substrate with thermally grown SiO_2 oxide layer (butt view).

2.3. Measuring reflection spectra of polymer film using prism coupling technique

Angular reflection spectra $R_{TE}(\theta)$, $R_{TM}(\theta)$ for TE and TM polarized probe laser beams correspondingly were measured using a prism coupler Metricon2010/M (Metricon Inc.). The device was equipped with a He-Ne laser (λ = 632.8 nm), having the diameter of the beam at the waist 0.65 mm and the angular divergence Δθ = 0.07 deg. Since there are variations of laser beam intensity (typically at the level of ±1%) during the scan, the prism coupler was modified by directing a small part of the probe beam to the reference photodetector. By normalizing the reflected beam intensity to the intensity of the reference beam we could improve the accuracy of $R_{TE}(\theta)$, $R_{TM}(\theta)$ measurement, which was estimated to be ±0.2%. The measured normalized reflection spectra are given in Figure 3.

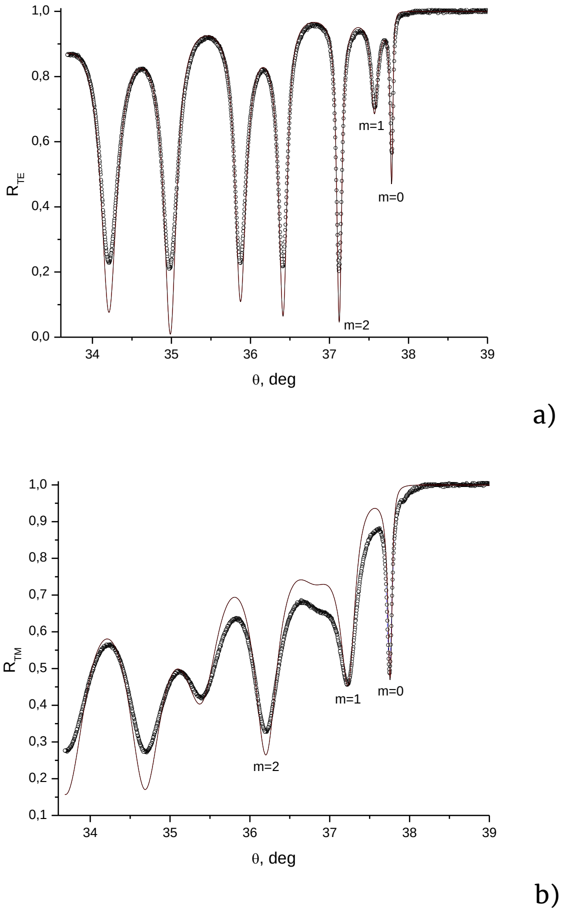

Figure 3. Reflection coefficients $R_{TE}(\theta)$ (a) and $R_{TM}(\theta)$ (b) measured with Metricon2010/M prism coupler for TE and TM polarized probe Gaussian beams (open circles). Calculated reflection spectra $R_{TE}(\theta)$, $R_{TM}(\theta)$ are shown by solid lines. Sharp dips with *m* = 0, 1, 2 etc. (*m* – lines) correspond to the excitation of TE and TM waveguide modes of zero, first etc. orders in the polymer light-guiding film. Optical parameters of silicon substrate are n_{Si} = 3.883, m_{Si} = 0.01963.

In Figure 3 the simulated reflection spectra, which were calculated using the model of uniform anisotropic polymer film and that of two-dimensional probe Gaussian beam, are also presented. The new mathematical algorithm we used to calculate $R_{TE}(\theta)$, $R_{TM}(\theta)$ is based on the fitting approach and equations presented earlier (Sokolov et al., 2018). According to this approach the mean-square difference D_{abs} between the measured and calculated reflection spectra is minimized by varying following parameters of the structure:

a) ordinary refractive index n_o of the polymer film in the film plane and non-ordinary n_{eo} in the direction perpendicular to the film plane, which correspond to

TE and TM polarization of the probe laser beam,

b) thickness H_f of polymer film,

c) thickness H_{SiO2} of thermal oxide layer,

d) thickness H_i of the air gap between the measuring prism and the sample in the prism coupling technique.

The abovementioned parameters, which provide the smallest D_{abs} value, are believed to be the real parameters of the film.

2.4. Calculation of refractive index and extinction coefficient of polymer film

One can see from Figure 3 that calculated positions of *m* – lines fit very well those of measured ones. Therefore one can conclude that calculated refractive indices n_o = 1.32004 and n_{eo} = 1.32036 of the polymer film are close to the real ones. However, there is essential difference in the depth of *m* – lines in Figure 3. To our opinion, this is due to the following reasons. First, in the simulation we have supposed that extinction coefficients m_o and m_{eo} of the polymer film are negligible ($m_o = m_{eo} = 0$). Second, we have not taken into account the non-uniformity of optical constants of thermal oxide layer in the direction perpendicular to the film plane as well as some transition layers on the silica-silicon interface. Thus, to improve the quality of fitting one should optimize the extinction coefficients m_o, m_{eo} of polymer film. The pertinent simulation should be done, however, in the reduced angular range, which includes the excitation of fundamental TE and TM waveguide modes only. These modes are highly localized in the polymer light-guiding film and therefore are less sensitive to *n* and *m* of thermal oxide layer and transition layers. On the other hand, one should use fitting in the broad angular range to calculate the thickness H_f of the polymer film with high accuracy.

To realize this strategy we have calculated H_f as a function of N_{max} parameter, where N_{max} is the number of measured points in the angular reflection spectra (increasing N_{max} corresponds to increasing angular range of $R_{TE}(\theta)$ and $R_{TM}(\theta)$ spectra). The calculated H_f vs N_{max} is presented in Figure 4. One can see that the deviation of polymer film thickness from the optimal value H_f = 2510.81 nm does not exceed ±6 nm (±0.24%).

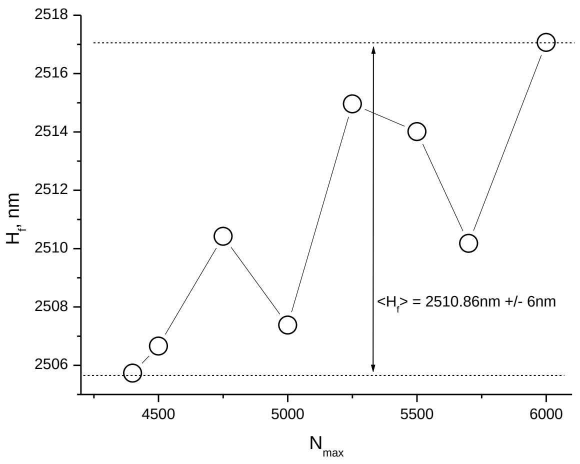

Figure 4. Calculated thickness H_f of the polymer light-guiding film as a function of N_{max} parameter, where N_{max} is the number of points in the measured angular reflection spectra $R_{TE}(\theta)$ and $R_{TM}(\theta)$.

The optimal value Hf = 2510.81 nm was taken into account for determination of m_o and m_{eo} of polymer film in the reduced angular range $\theta \in 37.65$ - 38.35 deg., in which only the fundamental TE and TM waveguide modes with $m = 0$ are excited by the probe laser beams. The results of the fitting procedure are shown in Figure 5 and are summarized in Table 1. It should be noted, that the fitting procedure was performed for TE and TM polarizations simultaneously, since the calculated thickness of the film does not depend upon beam polarization, and takes into account the angular divergence of the probe Gaussian laser beam.

Table 1. Refractive index *n* and extinction coefficient *m* of perfluorinated polymer film calculated using fitting algorithm in the angular range 37.65 - 38.35 deg.

Polarization	*n*	*m*
TE (n_o, m_o)	1.32011	2.00×10^{-4}
TM (n_{eo}, m_o)	1.32023	2.77×10^{-4}

One can see from Figure 5 and Table 1 that the developed approach is effective and permits to determine *n* and *m* of anisotropic polymer films with accuracy $\pm 1 \times 10^{-4}$ and $\pm 1 \times 10^{-5}$ correspondingly.

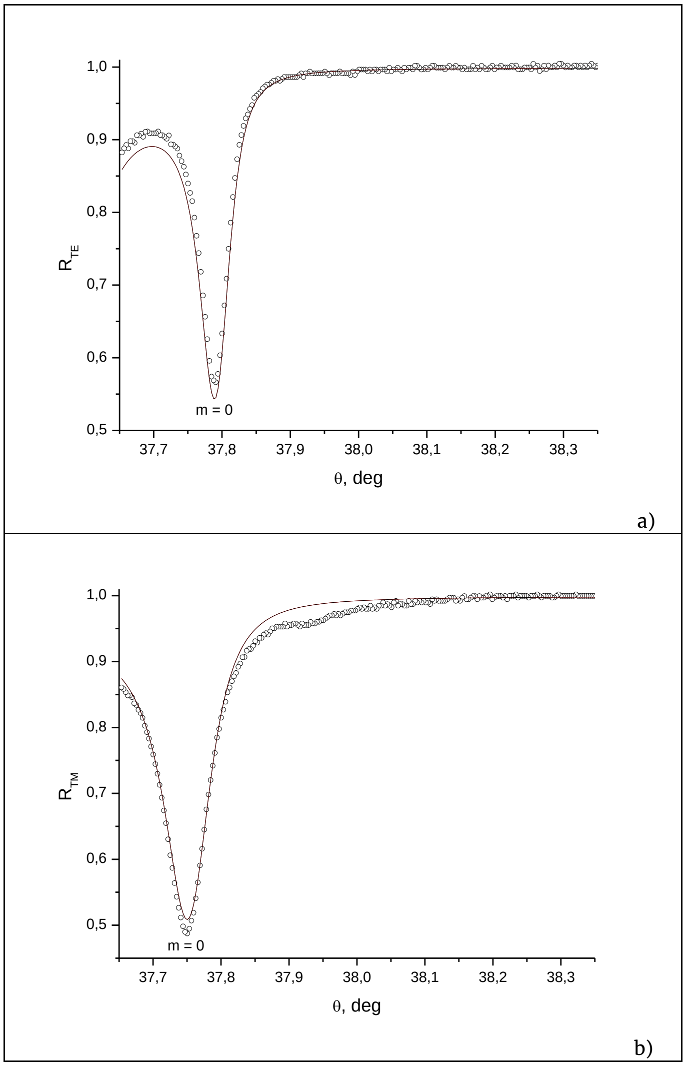

Figure 5. Reflection spectra $R_{TE}(\theta)$ (a) and $R_{TM}(\theta)$ (b) measured with Metricon2010/M prism coupler in the angular range 37.65 - 38.35 deg. (open circles). Calculated spectra $R_{TE}(\theta)$, $R_{TM}(\theta)$ are shown by solid lines. Optical parameters of Si substrate are n_{Si} = 3.883, m_{Si} = 0.01963.

3. Results and Discussions

Amorphous perfluorinated polymers are of great interest for integrated optics and photonics due to their high optical transparency, low refractive index and index dispersion. Therefore, methods for synthesis and accurate measurement of optical parameters and thickness of polymer films are important. It is known, that thin light-guiding polymer films are usually anisotropic with different ordinary n_o and extraordinary n_{eo} refractive index in the film plane and in the direction perpendicular to the film plane. By using proprietary synthesized amorphous perfluorinated polymer we have shown that extinction coefficient in light-guiding polymer films also can be anisotropic, see Table 1. Thus, the prism coupling technique in combination with advanced simulation tools permits to determine not only refractive index and thickness of anisotropic polymer films but also the extinction coefficient of the films with high accuracy.

4. Conclusions

We have presented a new approach and numerical algorithm for calculating refractive index, extinction coefficient and thickness of anisotropic polymer films from angular reflection spectra measured by prism coupling technique. The fitting algorithm takes into consideration the angular divergence of Gaussian probe beams. It was shown that the developed approach is effective and permits to determine *n* and *m* of anisotropic films with accuracy $\pm 1 \times 10^{-4}$ and $\pm 1 \times 10^{-5}$ correspondingly. The algorithm was successfully applied to the light-guiding film fabricated with proprietary amorphous perfluorinated polymer.

Funding

This work was supported by the Ministry of Science and Higher Education of the Russian Federation within the State assignment FSRC «Crystallography and Photonics», Russian Academy of Sciences, in part of developing polymer light-guiding structures, Russian Foundation for Basic Research (projects No. 20-07-01038 A and No. 18-29-20102 MK) in part of synthesis of amorphous perfluorinated polymers.

References

Goriachuk, I.O., Glebov, V.N., Maliutin, A.M., Sokolov V.I. (2018). Analysis of multilayer metal-dielectric thin-film structures using prism coupling technique. I3M EMSS 2018, September 17-19, 2018, Budapest, Hungary.

Khomchenko, A.V., Sotsky, A.B., Romanenko A.A., Glazunov E.V., Kostyuchenko, D.N. (2002). Determining thin film parameters by prism coupling technique. Technical Physics Letters 28:467-470.

Pasmooij, W.A., Mandersloot, P.A., Smit, M.K. (1989). Prism coupling of light into narrow planar optical waveguides. Journal of Lightwave technology 7:175-180.

Sokolov, V.I., Akhmanov, A.S., Goriachuk I.O. (2018). Modeling of waveguide modes excitation in thin-film multilayer structures by TM-polarized Gaussian light beam. I3M EMSS 2018, September 17-19, 2018, Budapest, Hungary.

Sokolov, V.I., Glebov, V.N., Malyutin, A.M., Molchanova, S.I., Khaydukov, E.V., Panchenko, V.Ya. (2015). Investigation of optical properties of multilayer dielectric structures using prism-coupling technique. Quantum Electronics, 45:868–872.

Sotsky A.B., Chudakovskii P.Y., Steingart L.M., Jackson J.H., Sotskaya L.I. (2013). Prism excitation of leaky modes of thin films. Technical Physics. The Russian Journal of Applied Physics 58:1651-1660.