MODELING OPTICAL RESPONSE OF THIN FILMS: CHOICE OF THE REFRACTIVE INDEX DISPERSION LAW

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***Abstract**: Determination of the so-called optical constants (complex refractive index N, which is usually a function of the wavelength, and physical thickness D) of thin films from experimental data is a typical inverse non-linear problem. It is still a challenge to the scientific community because of the complexity of the problem and its basic and technological significance in optics. Usually, solutions are looked for models with 3-10 parameters. Best estimates of these parameters are obtained by minimization procedures. Herein, we discuss the choice of orthogonal polynomials for the dispersion law of the thin film refractive index. We show the advantage of their use, compared to the Selmeier, Lorentz or Cauchy models.*

***Keywords**: Thin films; Materials and process characterization*

***ACM Classification Keywords**: J.2 Physical Sciences and Engineering (Physics)*

Introduction

The problem of estimation of the optical parameters of thin films: physical thickness (D) and complex refractive index N = n – i*k (real refractive index (n) and extinction coefficient (k)) is challenging from mathematical point of view and has technological and scientific importance. Usually, n and k are unknown functions of the wavelength (λ). The task is to evaluate them by the use of measurable quantities, such as film transmittance (T), front side reflectance (R) and/or backside reflectance (R′). Different methods have been proposed but no one has shown yet absolute advantage over the others. We can say that estimation of thin films optical parameters is more of an art, than scientific analysis. There are several steps that have to be fallowed: a) creation of a model, which describes the optical behavior of the film; b) collecting empirical data; c) fitting the postulated model to the data; d) evaluation of the results. The model of the wavelength dependence of the refractive index is of crucial importance: it defines the number of the unknown parameters and their functional relation. Some of the most popular models are named after the scientists that have proposed them: Cauchy, Drude, Selmeier, Lorentz, etc. Cauchy dispersion law is purely empirical:

$$n(\lambda) = A_0 + \frac{A_1}{\lambda^2} + \frac{A_2}{\lambda^4} + \ldots ,$$

where A_0, A_1, A_2,… are parameters to be determined. The number of terms can reach 10 – 15. Selmeier dispersion is semi-empirical:

$$n(\lambda) = \sqrt{A_0 + \frac{A_1\lambda^2}{\lambda^2 - B_1^2} + \ldots} ,$$

where A_0, A_1, B_1,… are parameters to be determined. More terms can be added for different oscillator positions.

Once the model is assumed, minimization techniques are applied to estimate the unknown parameters to the optical response of the thin film.

Here we shall consider the use of orthogonal polynomials in the dispersion law representation. We shall simulate a measurable quantity (transmittance) with predefined wavelength dependence of the complex refractive index. Then we shall fit the simulated data to different models of refractive index. Parameters in the dispersion law will be estimated, comparing Cauchy, Selmeier and orthogonal polynomials (OP) approaches.

Models and Computational Procedures

We shall consider a thin homogeneous film with wavelength dependence of the complex refractive index and physical thickness of 350 nm. The spectra of n(λ) and k(λ) are shown in Figure 1a and 1b, respectively. The choice of n(λ) and k(λ) is characteristic for many optical materials, such as amorphous semiconductors.

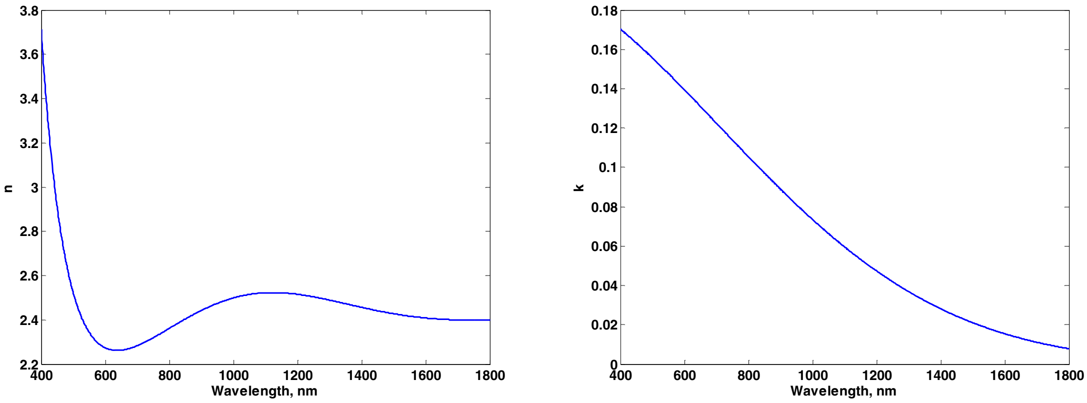

Figure 1. Spectral dependence of the refractive index (a) and extinction coefficient (b)

The simulated measurement is the spectrum of transmission in VIS at normal incidence of light calculated by the help of Abelès characteristic matrix [1], Figure 2. The measurable quantity is T ~ tt* (* stands for complex conjugate). The amplitude transmittance t is a complex quantity, related to N and D by transcendental equations [1]. During the fitting calculations, we have assumed that the physical thickness D and the extinction coefficient k(λ) are known, so that there is no fitting on these quantities. In this way we have strongly reduced parameter interactions. We have used associated Legendre functions $P(m,p;\lambda)$ of degree p and order $m = 0,1,...,p$, as orthogonal polynomials. Thus, the dispersion law for n(λ) stands as:

$$n(\lambda) = A_0 P(0, p; \lambda) + A_1 P(1, p; \lambda) + A_2 P(2, p; \lambda) + ...$$

For Cauchy, Selmeier or OP dispersion laws, 8-9 coefficients are need for relevant representation of the refractive index n(λ), shown in Figure1a. The nonlinear data-fitting problem is solved by the Levenberg-Marquardt method (unconstrained minimization) [2].

Results and Discussion

Calculations of the film optical response and preliminary fits showed that Selmeier model of the refractive index has to be disregarded: it cannot describe properly the 'experimental' data, shown in Figure 2. In order to compare the Cauchy and OP models, we have used 8 coefficients in their corresponding presentations, so that the degrees of freedom in the two cases are the same. Levenberg-Marquardt procedures demand initial guess of the unknown parameters. For each fit, we have put 7 of the coefficients equal to zero, while the first one is 20% up of its initial 'true' value. After the termination of the minimization, one step refinement of the estimations is undertaken as well. The results obtained with the two models differ significantly. The residual error of the fit with the Cauchy model is an order of magnitude greater. The residual error of the fit with OP reaches 0.1%, which is equal to the experimental uncertainty of high precision spectral instruments. This means that further improvement of the fit is meaningless. The minimization procedure is much faster in latter case – the consumed CPU time is ~20 times greater for the Cauchy case. In Figure 3 the relative errors of the estimated wavelength dependence of the refractive index are shown. This is an illustration of the performance of the Cauchy and OP models.

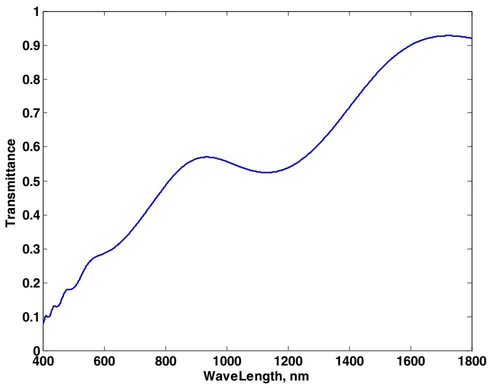

Figure 2. Calculated transmittance of the thin film as 'experimental' data for the fit

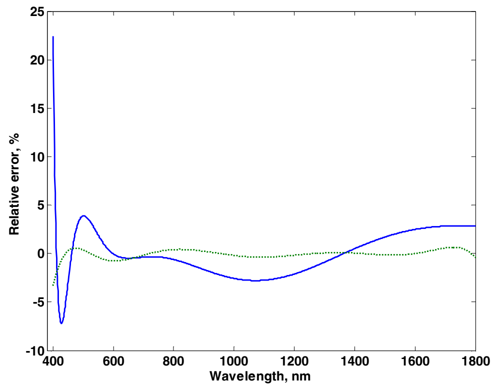

Figure 3. Relative error of refractive index fit: (dots) orthogonal polynomials; (line) Cauchy law

The advantages of fitting orthogonal polynomials to experimental data are well-known [2]. In our case, the situation is more complicated because of the nonlinear functional dependence of the target on the fitting parameters. However, the main advantage of this approach is sustained: due to the orthogonal property, each coefficient in the dispersion law representation can be determined independently from the others. If one has already obtained an evaluation of m^{-th} degree polynomial, an additional term in the dispersion law ((m+1) degree polynomial) requires only one new coefficient to be determined. The other coefficients remain the same, unlike in the Cauchy or Selmeier case. In the Cauchy case, high order polynomials may result in ill conditioned matrices. Besides, the joint confidence region in the parameter space, estimated by the covariance matrix, has minimum volume.

Conclusion

We have shown that the use of orthogonal polynomials in refractive index modeling is effective and highly productive. Although the involved coefficients have no physical meaning, this is also true for the Cauchy and Selmeier models. The OP principal feature is that the number of parameters to be fitted can be kept low at initial steps and then it can be increased, retaining the intermediate results. The orthogonal polynomials approach can be of use in many branches of material science, including photonic crystal design, optimization of elements for effective conversion of solar radiation, etc.

Acknowledgments

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