ON A DIRECT APPROACH TO THE SOLUTION OF INVERSE OPTICAL PROBLEMS

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Abstract: The evaluation from experimental data, of physical quantities, which enter into the electromagnetic Maxwell equations, is described as inverse optical problem. The functional relations between the dependent and independent variables are of transcendental character and numeric procedures for evaluation of the unknowns are largely used. Herein, we discuss a direct approach to the solution, illustrated by a specific example of determination of thin films optical constants from spectrophotometric data. New algorithm is proposed for the parameters evaluation, which does not need an initial guess of the unknowns and does not use iterative procedures. Thus we overcome the intrinsic deficiency of minimization techniques, such as gradient search methods, Simplex methods, etc. The price of it is a need of more computing power, but our algorithm is easily implemented in structures such as grid clusters. We show the advantages of this approach and its potential for generalization to other inverse optical problems.

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Introduction

A 'direct problem' in mathematics and physics is referred as an evaluation of a dependent variable from a set of independent variables, which enter in some functional relations, usually partial differential equations. In optics, this direct problem can be defined as finding the response of an optical object to electromagnetic radiation, forming a solution of the Maxwell equations and their boundary conditions [1]. The so-called 'inverse optical problem' is the evaluation of the object characteristics from experimentally observed data. Herein, we focus on a specific inverse problem of great importance to fundamental and applied science, namely the determination of the complex refractive index (N = n – i*k) and physical thickness (D) of very thin films from spectrophotometric quantities, such as transmittance (T), front side reflectance (R) and backside reflectance (R').

In optics, for many cases of practical interest N is an unknown function of the radiation wavelength (λ). The functional relations between {n(λ), k(λ), D} and {T(λ), R(λ), R'(λ)} are of transcendental character, so inverse optical problems are nonlinear and they are solved by numeric optimization techniques, which have some disadvantages [2]. The derivative methods (Gauss – Seidel, steepest descent, etc.) are not reliable, because of their dependence on the initial guess and they fail when the numeric evaluation of the gradient is not effective. The Simplex or direct search methods are derivative free, but their dependence on the initial guess of the unknowns is very substantial. The principle difficulty for finding a robust and efficient solution to the inverse problem that we shall discuss below comes from the fact that for small D (when $D/\lambda \rightarrow 0$) the optical response becomes less sensitive to {n, k} values. We propose a new algorithm for the direct numeric solution of the above optical problem and explore its potential for generalization and application to other inverse problems.

Algorithm and Computational Procedures

We consider a very thin homogeneous film with wavelength dependence of the complex refractive index in the visible spectral range. Spectrophotometric experiments are simulated numerically at normal incidence of light. That is, measurable quantities {T(λ), R(λ), R'(λ)} are calculated for specific parametric values {n(λ), k(λ), D} by the help of the Abeles characteristic matrix, which gives an exact solution of the Maxwell differential equations [1].

To those 'true' measurable values, experimental noise is added. We assume random experimental uncertainty with zero mean and variance, equivalent to that of high precision equipment, i. e. Cary 5E (Varian corp.).

Once the 'experimental data' is obtained we proceed to the evaluation of the parameters {n(λ), k(λ), D} at each wavelength, meaning that the evaluation is wavelength orientated and independent one from each other. The criteria for successful evaluation are that the three parameters under estimation must result in measurable quantities that satisfy simultaneously the uncertainty conditions on the observables. First, we define the range in the parametric space, where solutions will be searched for. This can be done on the basis of some preliminary information of general character, say whether the film material is a metal, dielectric or semiconductor. The range is increased by 30 – 50 % of the minimum to maximum expected values for each parameter. Second, a mesh grid is defined, where the step for a change of each variable must still have a physical meaning, simulating a quasi continuous change in the measurable quantities. These two inputs to the calculation procedure are not relevant for the numeric approach; they just limit the number of necessary computer evaluations. Third, for each point of the parametric mesh, direct calculations of the measurable quantities are done. Those calculations are rigorous, no approximations are maid, and accuracy is limited by the machine precision. Next, all values of the unknown parameters that give observables, which simultaneously fulfill the uncertainty conditions on the measured quantities, are accepted and stored. In other word, we keep all {n(λ), k(λ), D} from the parametric space that result in residuals that fall in the experimental joint confidence region in the observation space {T(λ), R(λ), R'(λ)}. This procedure is computer time consuming but that is the price for making no linearization, neither on the goal function, nor on the model function of the dependent variable.

Last step in the algorithm is to remove the 'outliers' from the sample parametric data and make a robust estimate of the unknowns. Here the main difficulty is that these outliers cannot be rejected as due to random errors. Besides they do not have some pre-determined statistical distribution, i.e. they are not just extreme values of random variables that occur naturally but infrequently [2]. To deal with that problem we have incorporated two independent and parallel decision making subroutines, referred bellow as Fit1 and Fit2. The first one is related to the distribution-free tests. The median of the parametric sample vector is evaluated as an estimate of the ensemble mean. Then, by the help of interquartile range of values of the sample realization, the upper and the lower 25% of the data are eliminated. Keeping the difference of 75% to 25% percentiles, we obtain an estimate of the spread of the body of the parametric values. The second subroutine makes use of the mode function for the estimation of each of the parametric realizations. The mode function for a continuous probability distribution evaluates its density function. The two subroutines are different mathematical implementations of the intuitive picture that when we get closer to the 'true value' of an unknown parameter, the relative frequency of the parameter realization is asymptotically increased.

Model, Results and Discussion

We define a model of a thin homogeneous film with physical thickness of 15 nm. The wavelength dependence of the film complex refractive index is that of bulk gold in the range 400 – 800 nm. This is expensively studied case, because very thin gold films are largely used in nanotechnologies, and, on the other hand, the evaluation of the complex refractive index is difficult in the red part of the spectrum due to strong correlation of front and backside reflectance. 'True values' for {T(λ), R(λ), R'(λ)} are generated and 'experimental noise' is added. We defined a relative uncertainty in T(λ) as derived from random values with zero mean and standard deviation of 0.0025. Reflection measurements are less accurate, so we used a standard deviation for R(λ) and R'(λ) of 0.0050. Then, a mesh grid is defined in the parametric space. The range of n(λ) is between 0.1 and 1.7, the range of values for k(λ) is between1.5 and 5.5 and that of D is from 8 to 25 nm. The step in the D parameter is chosen to be 1 nm, the step in n(λ) is $5*10^{-4}$ and that for k(λ) is $1*10^{-4}$. The film is supported by a substrate of refractive index 1.5.

In Figure 1 we show results of the fit for D = 12 nm. The length of realization by Fit1 (see text above) is 14 estimations, and for Fit2 – 15 estimations of the parameters n and k out of needed realizations of 21 (that is the number of wavelength estimations). It is obvious that for certain λ the fit results in no acceptable solution. The

values of the refractive index are overestimated, in order to catch up with the underestimated physical thickness. The normalized norm of the fit for n(λ) is 0.0144 (Fit1) and 0.0145 (Fit2). The results for k(λ) is 0.115 (Fit1) and 0.117 (Fit2). We remind that evaluated observables {T(λ), R(λ), R'(λ)} with these parameters satisfy the uncertainty conditions.

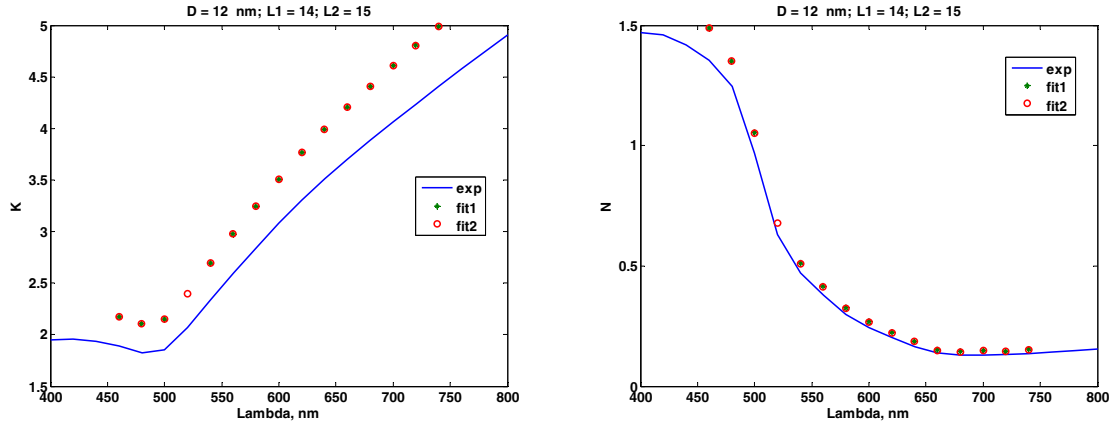

Figure 1. Spectral dependence of the extinction coefficient (a) and refractive index (b), D = 12 nm

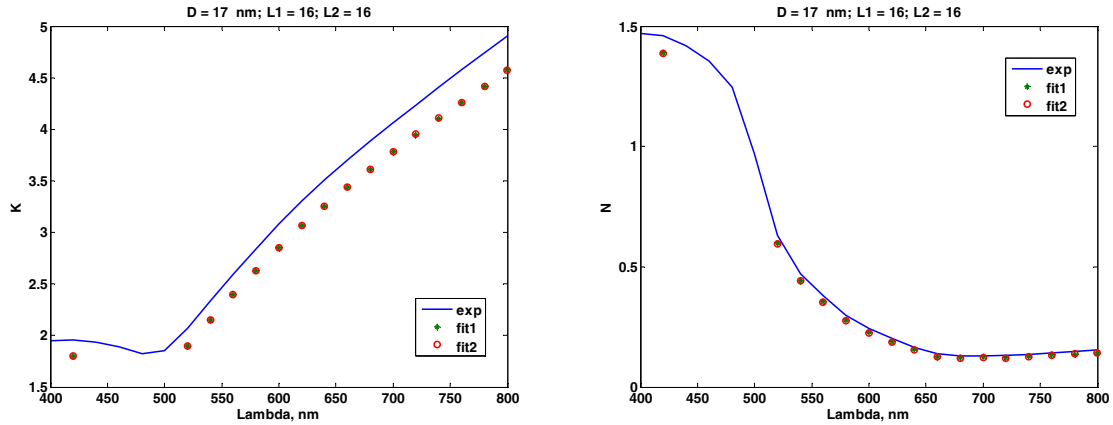

Figure 2. Spectral dependence of the extinction coefficient (a) and refractive index (b), D = 17 nm

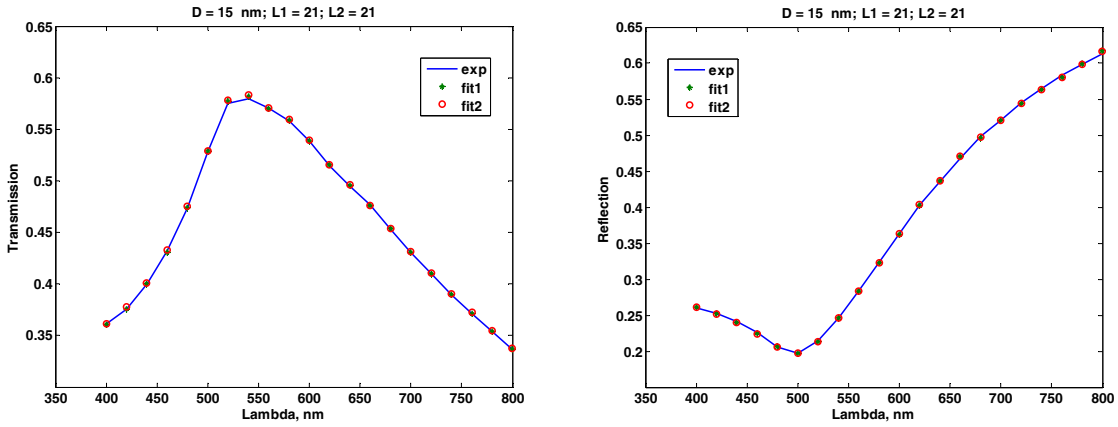

Figure 3. Spectral dependence of the transmission (a) and reflection (b), D = 15 nm

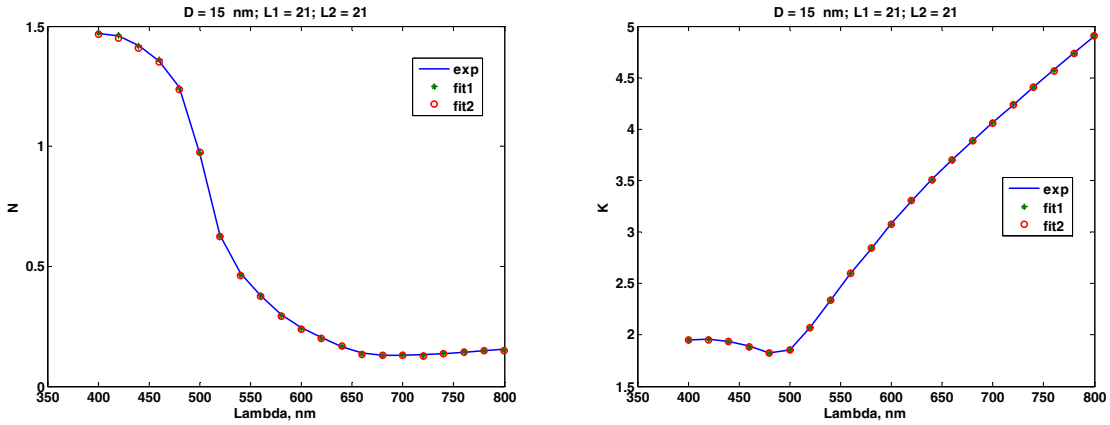

Figure 4. Spectral dependence of the extinction coefficient (a) and refractive index (b), D = 15 nm

In Figure 2 we show the results of a fit for D = 17 nm. The length of realization by Fit1 and Fit2 is 16 estimations, for n and k out of 21 needed realizations on λ. The values of the refractive index are underestimated, in order to catch up with the overestimated physical thickness. The normalized norm of the fit for n(λ) is 0.0059 (Fit1) and 0.0065 (Fit2). The results for k(λ) is 0.06632 (Fit1) and 0.06637 (Fit2).

Figure 3 presents the results for the fit at D = 15 nm. There the length of realization is at maximum and the norms of the estimations are much less than the ones described above. More, the choice of the best physical thickness estimate can be done on considerations on the length of parameter vectors. The normalized norm of the fit for n(λ) is 0.0007 (Fit1) and 0.001 (Fit2). The results for k(λ) is 0.0005 (Fit1) and 0.0007 (Fit2). The norms of the fit on {T(λ), R(λ), R'(λ)} are below 0.03%.

Conclusion

New algorithm is proposed for the solution of inverse optical problems. The unknown parameters evaluation does not need an initial guess and it does not use iterative procedures. Besides, it is derivative free. Thus we overcome the intrinsic deficiency of minimization techniques, such as gradient search methods, Simplex methods, etc. The price of it is a need of more computing power, but our algorithm is easily implemented in structures such as grid clusters. In fact, the simplest form of parallel computing - fractional computing, is neccessary. We have shown with numeric simulations that this approach can be successfully applied to processing of spectrophotometric data. Another advantage is that it has a potential for generalization for other inverse optical problems, related to ellipsometric measurements, FTIR measurements, etc.

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