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GENETIC ALGORITHM APPROACH TO THIN FILM OPTICAL PARAMETERS DETERMINATION *

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Optical parameters of thin films are important for several optical and optoelectronic applications. In this work the genetic algorithm method is proposed to solve optical parameters of thin film values. The experimental reflectance is modelled by the Forouhi – Bloomer dispersion relations. The refractive index, the extinction coefficient and the film thickness are the unknown parameters in this model. Genetic algorithm use probabilistic examination of promissing areas of the parameter space. It creates a population of solutions based on the reflectance model and then operates on the population to evolve the best solution by using selection, crossover and mutation operators on the population individuals. The implementation of genetic algorithm method and the experimental results are described too.

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1 Introduction

Thin films optical data estimation is critical for a variety of applications. Microstructure and composition of thin films are deposition process-dependent and determine values of optical refractive index (n) and extinction coefficient (k). The validity of spectroscopic results is often reported and discussed especially in case of thin films prepared on absorbing or thick substrates when only reflectance measurements are possible. Ellipsometry and reflectometry belong to the most important optical methods appropriated for this analysis. The difference between various optical methods is in the way of the inversion of reflection or transmission data to obtain the optical constants values. The genetic algorithm (GA) implementation in optical parameters solving from the experimental reflectance measurements uses information concerning different regions of parameter space and lends efficiency to the GA approach. The implicit parallel nature of the GA approach makes it an robust method for optimization of functions of many variables [1–5].

2 Optical characterization of thin films

The spectral refractive index, extinction coefficient and the thickness of the film can be found by a reflectance $R(\lambda)$ spectrum of the thin film deposited on transparent substrate. Optical reflection of an ideal paralell-sided thin film on a thick substrate illuminated at normal incidence with

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monochromatic radiation can be described by a classical optics theory. A thin isotropic film with the thickness d is chacterized by the complex refractive index n_1- ik_1 and the substrate is characterized by n_2- ik_2, where n_1,n_2 being the real part and the extinction coefficient k_1, k_2 being the imaginary part of the complex refractive index. The optical reflectance of a parallel–sided thin isotropic homogeneous film on a thick partly absorbing substrate is then given by

$$R = \frac{A + Bx + Cx^2}{D + Ex + Fx^2}. \tag{1}$$

In this equation x= exp(-αd) is the absorbance, α =(4πk_1)/$\lambda$is the absorption coefficient. Let us denote

$$\begin{aligned}
&A' = (1-n_1^2 - k_1^2)(n_1^2 - n_2^2 + k_1^2 - k_2^2) + 4k_1(n_1k_2 - n_2k_1),\\
&B' = 2(1 - n_1^2 - k_1^2)(n_1k_2 - n_2k_1) - 2k_1(n_1^2 - n_2^2 + k_1^2 - k_2^2),\\
&C' = (1-n_1^2 - k_1^2)(n_1^2 - n_2^2 + k_1^2 - k_2^2) - 4k_1(n_ik_2 - n_2k_1),\\
&D' = 2(1-n_1^2 - k_1^2)(n_1k_2 - n_2k_1) + 2k_1(n_1^2 - n_2^2 + k_1^2 - k_2^2),\\
&\varphi = (4\pi \mathrm{n}_1 d)/\lambda,
\end{aligned}$$

then

$$\begin{aligned}
A &= [(1 - n_1)^2 + k_1^2][(n_1 + n_2)^2 + (k_1 + k_2)^2]\\
B &= 2[A' cos\varphi + B' sin\varphi]\\
C &= [(1 + n_1)^2 + k_1^2][(n_1 - n_2)^2 + (k_1 - k_2)^2]\\
D &= [(1 + n_1)^2 + k_1^2][(n_1 + n_2)^2 + (k_1 + k_2)^2]\\
E &= 2[C' cos\varphi + D' sin\varphi]\\
F &= [(1 - n_1)^2 + k_1^2][(n_1 - n_2)^2 + (k_1 - k_2)^2]
\end{aligned} \tag{2}$$

Optical constants can be solved from a nonlinear equation

$$R_{exp}(\lambda) - R_{theor}(\lambda, n_1, k_1, d) = 0 \tag{3}$$

The reflectance R_{theor} is calculated according to equation (1) and fitted to the measured reflectance R_{exp} by GA method. The Forouhi and Bloomer dispersion equations are used for n_1 and k_1 description [6]:

$$\begin{aligned}
n_1 &= n(\infty) + \frac{B_0 E_\nu + C_0}{E_\nu^2 - BE_\nu + C} \quad k_1 = \frac{A(E_\nu - E_g)^2}{E_\nu^2 - BE_\nu + C}\\
B_0 &= \frac{A}{Q}\left(-\frac{B^2}{2} + E_g B - E_g^2 + C\right) \quad C_0 = \frac{A}{Q}\left((E_g^2 + C)\frac{B}{2} - 2E_g C\right)\\
Q &= \frac{1}{2}\left(4C - B^2\right)^{1/2}
\end{aligned} \tag{4}$$

where E_ν denotes the photon energy and $E_g$denotes the energy gap.

3 The GA method for optical parameters solution

GA-based optimization is a stochastic search method that involves the random generation of potential design solutions and then systematically evaluates and refines the solutions until a stopping criterion is met. The GA is based on the principles of evolution - calculation is carried out for a sequence of populations. The population is represented by the block of binary numbers in our implementation. Each row in the block is an individual that represents one solution to the design problem. One individual is made up of all of the design variables concatenated. Initially, the population is generated randomly, and then the solutions are ranked from best to worst and a specified number of the lowest ranked individuals are replaced with combinations of the highest ranked individuals. The process of determining which of the highest ranked individuals are to be used is called selection. There are several differing methods of selection that can be used. Once selected, two individuals go through a process called crossover. During the crossover operation the two individuals (or parents) exchange a segment of the binary digits creating two new individuals (offspring). Another basic GA operation is mutation. The mutation operation randomly mutates the bits within the individual based on the mutation probability set by the user. Finding optimal values for the parameters used in the GA operations can be problematic. Parameter values that result in a relatively fast convergence for one problem may be slow for another. The algorithm can generate inferior points if the design variables are not represented accurately enough, or if the feasible domain of the problem is irregular. So, there is no absolute guarantee that the GA will converge to the best solution, but in most cases, it will converge to a very good approximation of the best solution. The GA may also require a large amount of computational time to generate solutions when compared to a conventional gradient-based optimization method. Therefore, the main advantage is that it solves problems that include discrete-type variables and problems where global rather than local solutions are sought. In order to extend the GA to a multiobjective problem, some steps have to be taken. The methods considered in this paper are briefly explained in the following sections.

a) Problem formulation and coding of variables. The reflectance model is developed according to Eq.(1). Each variable in the reflectance function is represented by a binary string. The length of the string is determined by the desired precision. Strings, representing all variables, are then concatenated to form an individual.

b) Generation of initial population An initial population of individuals is randomly generated. Each individual consists of a sequence of binary values with a length of 64 bits. Each model parameter X_i is represented by the 16 bit sequence as a constituent part of the individual.

<table>
<tr><td colspan="16">X1</td><td colspan="16">X2</td><td>...</td><td colspan="6">X4</td></tr>
<tr><td>1</td><td>1</td><td>1</td><td>1</td><td>1</td><td>1</td><td>1</td><td>1</td><td>1</td><td>1</td><td>1</td><td>1</td><td>1</td><td>1</td><td>1</td><td>1</td><td>1</td><td>1</td><td>1</td><td>1</td><td>1</td><td>1</td><td>1</td><td>1</td><td>1</td><td>1</td><td>1</td><td>1</td><td>1</td><td>1</td><td>1</td><td>1</td><td>...</td><td>...</td><td>1</td><td>1</td><td>1</td><td>1</td><td>1</td></tr>
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Fig. 1. Construction of the individual of the population.

c) Fitness assignment. The fitness value F is a measure of a string quality with respect to the consistency of theoretical reflectance R_{theor} with experimental one R_{exp} and fitness can therefore be defined as appropriate function of reflectance function parameters. The reflectancies giving rise to good agreement between experimental and calculated data have low fitness. The evolution of the GA is such that the strings of lowest fitness have the best chance of passing on their characteristics to the next population. The fitness function

$$F = \sum_{\lambda} \left(R_{\exp}(\lambda) - R_{theor}(\lambda) \right)^2 \tag{5}$$

provides good discrimination between good and bad synthetized reflectancies within the population at all stages of the evolution of the population.

d) Selection. In the evolution process pairs of strings are selected from the population on the basis of their fitness. The selection probability is higher for strings with lower fitness value. Only the strings of lowest fitness are chosen to form the next population. This step ensures that the overall quality of the population increases during evolution process.

e) Crossover and Mutation. The selected individuals are crossed-over and mutated to produce the next generation. That is, each individual exchanges a segment of its binary string. Double point crossover is used in this work with random selection of cutting points within the string length.

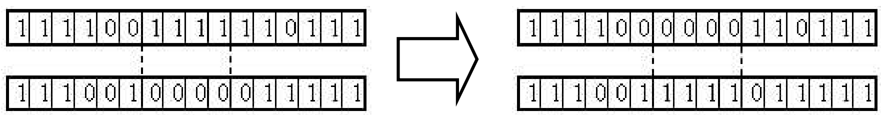

Fig. 2. Two point crossing procedure.

After crossing procedure the two new offsprings from the two parents are produced mixing their genetic information.

The mutation operation occur independent of crossover. In the mutation procedure strings are selected randomly from the population and random changes are made to part of their symbols to generate new mutant strings. The introduction of mutant strings within the population is necessary to maintain the diversity and prevent the GA converge to a false optimum. It allows the new regions of parameter space to be explored. For a given population, certain regions of parameter space might not be accessible through the crossing procedure alone, because crossing procedure does not introduce new information into population, it only mixes the existing information. After crossover and mutation occur the next generation is formed.

Steps a) through e) are repeated until the decision maker pauses the algorithm in order to impose/review constraints on the objectives or until the stopping criterion has been satisfied. Advantages of the GA method for optical parameters solution include the fact, that the GA calculation does not stop when a local optimum of the hypersurface is reached. Before running the GA we fix some parameters for optimization process – the number of populations, the number of individuals in each population, the crossing probability and the probability of mutation. It is necessary to make an appropriate choice of the reflectance model parameters d,$n(\infty)$ and E_g

too. An instant set of model parameters is represented by a binary string and inserted into population as its individual. The values of these parameters are real numbers. Our application use strings of 16 binary numbers to construct a constituent part of individual for each parameter of the reflectance model.

The number of individuals in the population remains constant for all generations as well as the number of crossing and mutation operations. The selection process is based on the so-called 'roulette-wheel' selection procedure, in which strings in a given population are selected with probability proportional to their fitness and copied into a temporary population. Crossing and mutation operations are then performed by selecting strings from this temporary population. The parent chromosomes used to create the mutants are not replaced by the mutants but remain within the intermediate population. The next population is produced by taking the best members of the intermediate population (individuals with the lowest fitness). It is guaranteed, that the fitness value for the best solution R in the population P_{j+1} is less or equal to the value of fitness for the best reflectance R in population P_j. In summary the best model reflectance survive onto successive populations.

In our work the GA calculation involved a population size of 1000 individuals (optional). In each generation, *CP* crossing and *MP* mutation operations were carried out, where *CP* is optional value of crossing probability (usually 20% of population size) and *MP* is optional value of mutation probability (40%). The progress of the GA reflectance solution calculation can be monitored by plotting the evolution of the best fitness values as a function of the generation number. The best reflectance solution are searched in several independent GA evolution processes. The first GA evolution searches optimal reflectance function parameters in wide interval of the parameter space while the next refinement steps are performed in the regions defined by formula $< X - 0.1X, X + 0.1X >$. The X value is the value of the individual variable of the hypothetical reflectance function, reached in the previous step of GA evolution process.

4 Experimental results

At the effectiveness of the GA method of the equation 1 inversion study we simulated a set of the experimental reflectance functions by a computer. We systematically modified the model parameters of the thin films. In independent successive steps we changed all values of the reflectance function variables $\{d$, n(∞), E_g, A, B, $C\}$. The optical parameters n_2, k_2 in this experiments were taken for the Si substrate from [8]. Various probabilities of the mutation and crossover operators as well as the influence of various individual and generation counts were studied. The values of the theoretical reflectance model reached by the GA method converge very closely to the simulated experimental reflectance model in all studied cases. The fitness function values F decrease rapidly in the early stages of the GA calculation, where the most significant improvements in the quality of the best reflectance solution occur. Computer simulation results are summarized in table 1. Presented differences between simulated values and GA output values for the refractive index Δn and the extinction coefficient Δk are typical values reached for thin films of the thickness d and various values of other simulated reflectance function variables. Genetic algorithm solution in this table uses one iteration cycle in wide search parameter space and one iteration cycle when using refinement method. The iteration cycle length is given by generation count. We use 500 GA generations, 1000 individuals, the probability of the crossing operator

Tab. 1. Experimental results. $\sum_{\mathrm{i}} \mathrm{SQR}\,(\Delta \mathrm{x}) = \sum_{i} (x_{theor} - x_{\exp})_i^2$

d	ΣSQR(Δn)	ΣSQR(Δk)
nm	1.00E-08	1.00E-08
100	1.25	2.34
200	1.46	1.88
300	1.38	1.83
400	1.82	1.96
500	1.77	2.11
600	1.63	1.65
700	1.12	1.54
800	0.92	1.57
900	1.03	1.28
1000	0.89	1.33

CP = 0.2 and the probability of the mutating operator *MP* = 0.4 in these simulations. The values of *CP* and *MP* operators are set after empirical search concerning the speed of GA convergence.

Very good agreement of the refractive index and extinction coefficient spectral dependencies with the envelope method results was obtained for several reflectance function simulations [7]. The differences when comparing GA and envelope method results are of 10^{-1} order of magnitude in the $\sum_{i} (n_{theor} - n_{\exp})_i^2$ value.

Similar results were obtained in the real sample studies. Reflectance measurements were carried out by a double-beam Carl Zeiss Jena spectrophotometer Specord M40 at room temperature. The possibilities of the GA method illustrates the ZnO thin film sample case. The ZnO sample was deposited on the polished Si substrate by rf. diode sputtering. The thickness of the film estimated from deposition conditions was 1000 nm. The absolute errors of the reflectance measurements were ~ 0.01. The experimental reflectance of the sample is in Fig.3. The values of spectral dependencies of the refractive index and extinction coefficient reconstructed by the GA method are summarized in in Fig.4.

The spectral dependencies of the optical constants of the ZnO sample determined by the GA method are smaller than values reported for bulk material. The values of the refractive index decrease uniformly in the whole wavelength range while the values of the extinction coefficient slightly increase. This result is in agreement with the Kramers – Krönig relations.

5 Conclusion

The GA method is used for the optical parameters of thin film determination from experimental reflectance measurements. Using the GA inversion of the reflectance function enables relatively arbitrary constraints and objectives to be incorporated painlessly into a single optimization method. There are many different settings associated with predictions in optical parameters solutions. Most of these settings are maintained automatically using rules of the GA that create

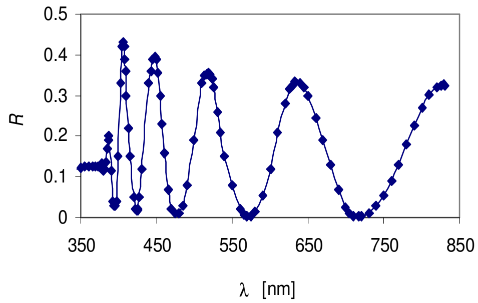

Fig. 3. ZnO/Si reflectance.

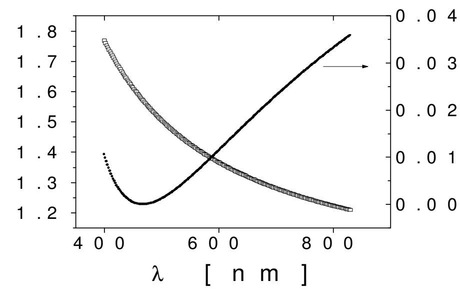

Fig. 4. The refractive index and extinction coefficient of the ZnO sample.

the best results in the general case. However, by fine-tuning these settings, it can be possible to get significantly better results from previous predictions. It can take a significant amount of time to determine what settings give better results. To speed this process in the direction of the best solution, GA approach can be made to experiment and supplemented with the direct search methods, especially when the extended set of independent model variables is refined. In this work the values of $n\left(\infty\right),\ n_2,\ k_2$ and E_g were fixed during the GA optimization. We search unknown model parameters in two independent steps – in the wide region of the parameter space and then we refine obtained results near their values obtained in the previous step. This treatment can speed up the GA solution and enables comfortable estimation of unknown optical constants values of the real sample. The results of the computer simulation of the hypothetical thin film reflectance show good convergence of the GA solution to the simulated parameter values. Reconstructed spectral dependencies of the optical constants of the real ZnO sample are in agreement with the envelpe method results.

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