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MODELLING OF SPECTRAL CHARACTERISTICS OF INHOMOGENEOUS (GRADIENT) ANTI-REFLECTIVE COATINGS BASED ON CHALCOGENIDE GLASSES

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Modelling of optical properties and optimization of the structure of gradient chalcogenide film with different distribution of the refractive index for the anti-reflective coatings of high reflective materials here present.

Keywords: Mathematical modeling, Gradient chalcogenide films, Inhomogeneous films, Multidimensional search, The refractive index distribution

1. Introduction

A wide possibility of variants for spectral characteristics of thin-film coatings allows one to use them in nearly every technical device in the space apparatus, gas-analyzers, optical instrument-making industry, optical system for fundamental research, etc. [1,2] In many emerging areas of technology factors between the costs for the assembled products and the optical coatings may range from 10 to 1000. [2].

The development of new methods of preparing films for optical purposes, improvement of technological facilities has resulted in widening the range of film materials for optical coatings, integrated and power optics and revealed the peculiarities in optical properties according to the profile of films [3-6]. Thus, the analysis data of new chalcogenide and oxide materials films witness that at the interface of a high-refractive non-crystalline film-substrate and film-vacuum the inhomogeneities of composition and refractive index, respectively, occur [3-6]. New experimental data about optical properties of films have essentially stimulated us the development of new methods of designing interference coatings which would include the data about optical characteristics of transition regions at the interfaces of layers and the transition film-substrate region.

Computer calculation methods have some advantages, the main of which is universality [1,2,4]. They do not require search of solution of complex non-linear equations with which the analytical theory of coatings synthesis is concerned. Computer methods allow one to optimize the thickness of interference coating layers, whereas this important scientific-practical problem could not have been solved by analytical methods so far. That is why the use of computer methods allows one to obtain better results while solving the problem of synthesizing the optical layered coatings than by using other approaches. In its turn a great variety of computer methods also leads to not a simple problem of choosing the most effective of them while solving the specifically taken problem [4].

One of the important problems in optical instrument-making industry is the problem of antireflecting Ge and Si high-refractive crystals [1,2,4,7]. There exist possibility in this case the stacks of alternating high and low index films to replace by continuous refractive index profile along an axis that is perpendicular to the film surface [8]. Such system does not contain internal interfaces, and therefore one expects better mechanical properties as well as a better optical performance due a to lower level of scatter losses [2].

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2. Results and discussion

Measuring the dispersion of the refractive index of chalcogenide glasses showed that for the wavelengths larger than 1 μm for low absorbing As_2S_3 - GeS_2 glasses a weak dependence of the refractive index on the wavelength in infrared (IR) is observed. For GeS_2 glass at λ= 0.63 μm the refractive index n=2.05. The maximal value of the refractive index (n=5.0) in IR region is found for the films based on Ge-Te glasses [4]. Therefore, while synthesizing atireflecting coatings the class of chalcogenide glasses as a high-refractive layer allows one to choose refractive indices within wide limits.

We have revealed that at vacuum evaporation of GeS_2 a condensed layer has an inhomogeneous structure. On the concentrational Auger profile of the element at film-substrate interface in the transition region the enrichment of the film in germanium is observed which is of linear character or proportional to ln(x) [9]. The concentrational dependence of the refractive index of Ge-S glasses point to the fact that for $Ge_{40}S_{60}$ composition the refractive index n=2.6 at λ= 0.63 μm. In the simplest approximation the profile of the refractive index of GeS_2 films is layered-inhomogeneous. The near-surface and transition regions of the film have the refractive index of 2.6, and a central part of the film has 2.05 at λ=0.63 μm. By varying the evaporation conditions of GeS_2 glass one may vary the composition of an inhomogeneous film and the refractive index from 2.6 to 2.05, respectively.

By using the modelling of the influence of the refractive index profile of GeS_2-based non-absorbing inhomogeneous films on their spectral characteristics, one can select such profiles of the refractive index distribution over the film depth which would provide for a maximal antireflection of Ge and Si substrates.

To find optimal parameters of an inhomogeneous film different methods of multi-dimensional search of functional F extremuma for non-linear functions without limitations have been used. Among them methods of configurations (Hook-Jives), Rozenbroke, the fastest descent, conjugate gradients (Fletcher-Reeves, Pollack-Riviera), variable metrics (Davidson-Fletcher-Powell, Goldfarbe, Fiakko-McCormick, Greenstadt). Among methods of conjugate gradients the best in respect to this task was that of Fletcher-Reeves, and among methods of variable metrics was the method of Davidson -Fletcher-Powell. But if take into consideration all the methods, the most effective ones are direct search methods – methods of configurations (Hook-Jives) and Rozenbrok.

Table.

Distribution	Refractive index of substrate $n_s = 3.4$		Refractive index of substrate $n_s = 4.0$	
	Depth *d*, nm	Functional *F*	Depth *d*, nm	Functional *F*
Linear	845.1	0.8940305	821.2	0.8917372
Quadratic	871.9	0.9049775	853.0	0.8994528
Exponential	865.9	0.9039553	864.5	0.8930525
Logarithmic	802.6	08768864	781.5	0.8777495

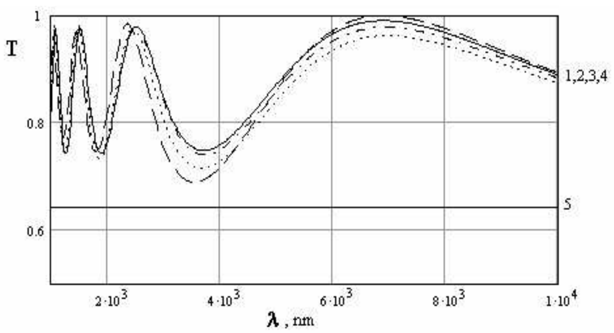

Fig. 1. Spectral characteristics of an inhomogeneous film based on g-GeS_2, whose refractive index n varies from 2.6 to 2.05 for different distributions n on the substrate with n_s=4: 1 – exponential distribution at *d*=864.5 nm; (dotted line); 2 – quadratic distribution at *d*=853.0 nm; (full line); 3 – linear distribution at *d*=821.2 nm; (dashed line); 4 – logarithmic distribution at *d* = 781.5 nm; (broken line); 5 – transmission of Ge substrate without an inhomogeneous film.

The calculated results are given in Table. As we see for Ge and Si substrates by using any considered distribution with the optimal choice of a geometric depth one can obtain good results. But it is better to use inhomogeneous films with quadratic or exponential distribution of the refractive index (Fig.).

3. Conclusions

The mathematical model of an inhomogeneous non-absorbing film with different distributions of the refractive index has been developed. Optimal parameters and the possibility anti-reflecting of high-refractive substrates in infrared spectral range have been studied.

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