EFFECTS OF LAYER NANODEFECTS ON THE LIGHT TRANSMISSION BY OPTICAL ELEMENTS WITH MULTILAYER INTERFERENCE COATINGS

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The light transmission properties of optical elements with multilayer interference coatings (MLS) have been studied. The decreasing of transmittance maxima for optical elements with coating containing the defects is found to be stronger for larger refractive indices of the defect material. The shape of transmission curves substantially depends on the defect dimensions along the direction of light propagation and its arrangement in the layer bulk. The results obtained are necessary for the developing of a technology in fabrication of the optical elements with MLS as for the laser technique, as for the optical lenses.

1. Introduction

It is well-known that high-quality and optically uniform films are widely used in the functional elements of optoelectronic and laser technique such as filters, antireflection coatings, light beam- and spectra disconnectors, polarizers, et al. [1]. At present, the electrical and optical properties of insulated films, their dependence on the fabrication technologies, the influence of nanodefects in the film bulk on the film properties, and the capabilities of their practical applications have been studied rather well. The results of these researches have been discussed at many conferences [2, 3]. Modern technologies of thin-film deposition demand that defects were absent in the film bulk, because the presence of emptiness or foreign substance inclusions leads to significant decrease in the film's parameters and even up to their destruction. However, it cannot always be avoided. Therefore, the influence of nano-sized defects on the properties of thin films has been widely studied in many works. In this work the theoretical and experimental results of the nanodefects influence on the optical transmission spectra of a 4-layers interference system of the antireflection type, which is widely used in practice (especially for manufacturing of the optical lenses) are investigated.

2. Experiment

The multilayer interference coatings are widely used in the modern fabrication of the optical lenses. They are created by periodically depositing of zirconium oxide (ZrO_2, it has a high refractive index $n_A = 2.11$) and magnesium fluoride (MgF_2, it has a low refractive index $n_B = 1.38$) layers. The layers are deposited one after another on a transparent substrate (the corresponding refractive index is $n = 1.9$). It was found that the depo-

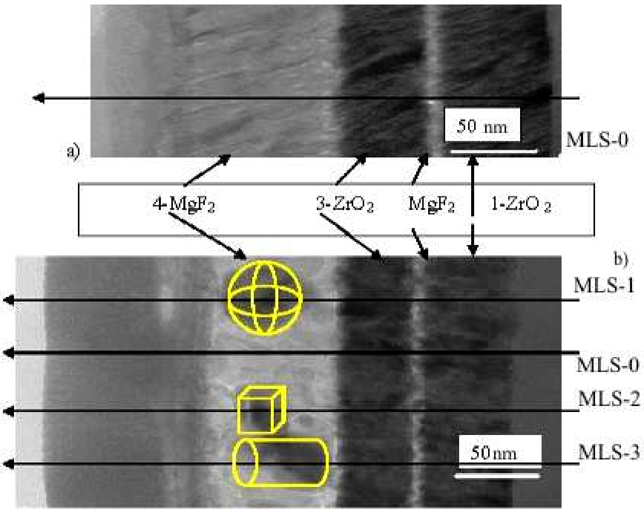


Fig. 1. Transverse cross-section of MLSs: free of defects (*a*, system MLS-0) and with defects (*b*, systems MLS-1, MLS-2, and MLS-3)

sition of only four layers with different geometrical thicknesses is enough to increase the light transmittance of optical lenses (see the multilayer structure (MLS) MSL-0 in Fig. 1,*a*). However, it happens in practice that defects can occur in a certain layer (as a rule, in the external, thick layer of MgF_2 contacting with air). In this case, the 4-layers structure transforms into a 6-layers one (see the MLS-1, MLS-2, and MLS-3 in Fig. 1,*b*), because the defect itself forms two boundaries. By their spatial configuration, all defects can be classified as spheres (MLS-1), parallelepipeds (MLS-2), or cylinders (MLS-3). The transverse cross-section of a MLS by a plane, which coincide with the direction of light propagation are showen in Fig. 1,*b*. The geometrical and optical thicknesses of layers for all obtained MLSs are presented in Table 1.

3. Results and Discussion

The multilayer structures shown in Fig. 1 can be schematically presented as transparent substrate S characterized by the refractive index n_S, on which layers A with a high refractive index n_A and layers B with a low refractive index n_B have been periodically deposited (see Fig. 2). The optical thicknesses of the layers are determined by the factors x_iA and y_iB for the corresponding quarter-wavelength layers A and B, which satisfy the relations $n_A d_A = n_B d_B = \lambda_0/4$, where d_A and d_B are the geometrical thicknesses of layers A and B, respectively, and λ_0 is the working wavelength (it can be determined by the color of lense glass). The geometrical scheme of defect-including layers in the MLS is shown in Fig. 3. The corresponding structures in such layers presented in Fig. 2,*b*, if the defect substance is the same as substance of layer A, or in Fig. 2,*c*, if the defect is formed by air (emptiness).

To estimate the influence of the MLS parameters on the changing of the resulting transmittance, the matrix method was used. It based on the determination of a characteristic matrix. If the geometrical thickness of the layer is equal to d, and its refractive index is n, the characteristic matrix of a homogeneous dielectric film can be presented in the form

$$M(n,d,\lambda) = \begin{Vmatrix} \cos\delta(n,d,\lambda) & -(i/p)\sin\delta(n,d,\lambda) \\ ip\sin\delta(n,d,\lambda) & \cos\delta(n,d,\lambda) \end{Vmatrix}, \quad (1)$$

where $\delta(n,d,\lambda) = 2\pi nd\cos\theta/\lambda$ is the phase incursion on the layer, $p = \sqrt{\varepsilon/\mu}\cos\delta$, and θ is the angle between the direction of radiation propagation and the normal to the layer interfaces [4–6]. In the case when the direction of radiation propagation coincides with the normal to the interfaces, $\theta = 0$, and, therefore $p = n$.

If the characteristic matrix is known for each layer, the characteristic matrix for a structure involving k layers can be determined as a product of all these matrices,

$$M\left(\bar{n},\bar{d},\lambda\right) = M_k\left(n_k,d_k,\lambda\right) M_{k-1}\left(n_{k-1},d_{k-1},\lambda\right) \times$$

$$\times \cdots \times M_2\left(n_2,d_2,\lambda\right) M_1\left(n_1,d_1,\lambda\right), \quad (2)$$

where M_j is the characteristic matrix for the j-th layer, $\bar{n} = (n_1, n_2, \ldots, n_{k-1}, n_k)$ is the vector of the refractive indeces values for all layers, and $\bar{d} = (d_1, d_2, \ldots, d_{k-1}, d_k)$ is the vector of geometrical thicknesses of the MLS.

Taking Eq. (2) into account, it can be find the transmittance for a MLS consisting of 4 layers with given parameters $\bar{n}$, $\bar{d}$, and λ,

$$T(\bar{n},\bar{d},\lambda) = 1 - \left[\left|\frac{n_0(M_{11}(\bar{n},\bar{d},\lambda) + n_S M_{12}(\bar{n},\bar{d},\lambda)) - (n_S M_{22}(\bar{n},\bar{d},\lambda) + M_{21}(\bar{n},\bar{d},\lambda))}{n_0(M_{11}(\bar{n},\bar{d},\lambda) + n_S M_{12}(\bar{n},\bar{d},\lambda)) + (n_S M_{22}(\bar{n},\bar{d},\lambda) + M_{21}(\bar{n},\bar{d},\lambda))}\right|\right]^2, \quad (3)$$

T a b l e 1. MLSs types and layer thickness, nm

Layer substance	MLS types and layer thickness, nm													
	MSL-0		MSL-1-1		MSL-1-2		MSL-2-1		MSL-2-2		-3-1		MSL-3-2	
	geom.	opt.	geom.	opt.	geom.	opt.	geom.	opt.	geom.	opt.	geom.	opt.	geom.	opt.
ZrO_2	60	126.6	60	126.6	60	126.6	60	126.6	60	126.6	60	126.6	60	126.6
MgF_2	10	13.8	10	13.8	10	13.8	10	13.8	10	13.8	10	13.8	10	13.8
ZrO_2	50	105.5	50	105.5	50	105.5	50	105.5	50	105.5	50	105.5	50	105.5
MgF_2	80	110.4	22	30.4	22	30.4	30	41.48	30	41.48	10	13.8	10	13.8
ZrO_2	–	–	40	84.4			25	53			50	105.5		
Air					40	40			25	25			50	50
MgF_2	–	–	18	24.8	18	24.8	25	37.4	25	37.4	20	27.6	20	27.6

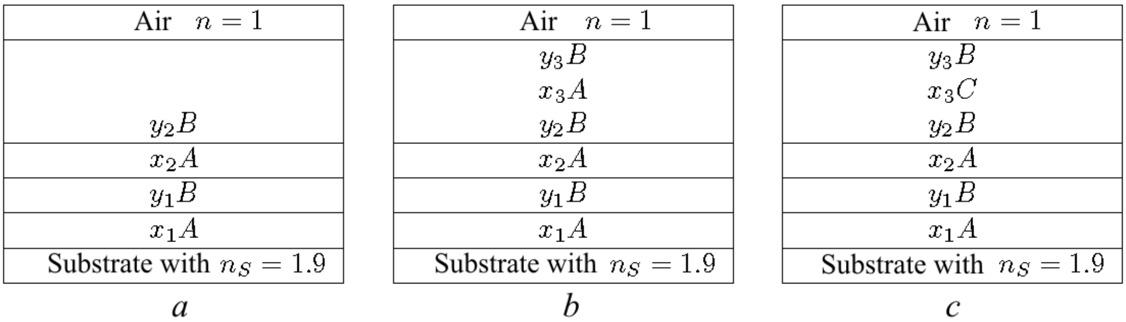


Fig. 2. Models of MLSs free of defects (*a*), with defects formed by ZrO_2 (*b*) and by air (*c*)

where n_0 and n are the refractive indices of the external environment and the substrate, respectively; and M_{11}, M_{12}, M_{21}, and M_{22} are the elements of the characteristic matrix M [5–7].

In the numerical calculations of MLS transmission spectra, the objective functional was taken in the form

$$\max_{\bar{n},\,\bar{d}} F(\bar{n}, \bar{d}) = \left(\frac{1}{L} \sum_{i=1}^{L} T^2 \left(\bar{n}, \bar{d}, \lambda_i \right) \right)^{1/2}, \qquad (4)$$

where L is the number of a grid points within the spectral interval from λ_1 to λ_2. For a uniform grid with the step $\Delta\lambda$,

$$L = \frac{\lambda_2 - \lambda_1}{\Delta\lambda} + 1\,, \qquad (5)$$

where λ_1 and λ_2 are the short- and the long-wave boundaries of the research spectral region [6, 7].

The spectral dependences of the MLS transmittance were calculated by formula (3) with the using of the layer parameters presented in Table 1. The results of calculations are presented in Fig. 4. It was found that the existence of defects in a MgF_2 layer gives rise to a considerable decrease of the transmittance maxima and their shift toward the long-wave spectral region. A more essential decrease of the transmission coefficient was observed in the case of a higher refractive index of the defect, e.g., ZrO_2 (curves *3-1* and *3-2* in Fig. 4), or defect has larger geometrical size [9, 10].

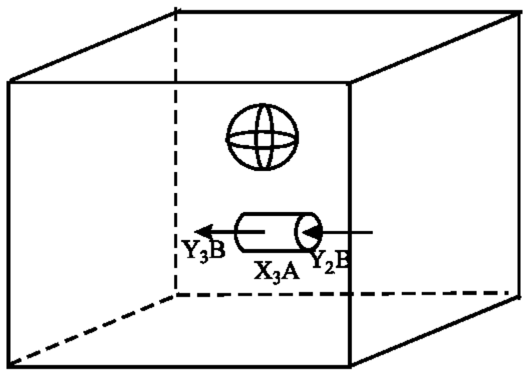


Fig. 3. Geometrical view of a defect layer in the MLS

The existence of the layer defects formed by ZrO_2 changes the character of the transmission spectra (see Fig. 4,*a*). In particular, there appears a minimum in a region of 525 nm, the maximum of the curve shifts towards the long-wave region and its amplitude decreases by approximately 10%. If the layer defects are formed by the air (Fig. 4,*b*), the

T a b l e 2. Types of MLS-n system with 20 nm defect from substances with different refractive indices

Layer substance	MLS types and layer thickness, nm									
	MSL-0		MSL-n=1		MSL-n=2		MSL-n=3		MSL-n=4	
	geom.	opt.	geom.	opt.	geom.	opt.	geom.	opt.	geom.	opt.
ZrO_2	60	126.6	60	126.6	60	126.6	60	126.6	60	126.6
MgF_2	10	13.8	10	13.8	10	13.8	10	13.8	10	13.8
ZrO_2	50	105.5	50	105.5	50	105.5	50	105.5	50	105.5
MgF_2	80	110.4	30	41.4	30	41.4	30	41.4	30	41.4
defect	–	–	20	20	20	40	20	60	20	80
MgF_2	–	–	30	41.4	30	41.4	30	41.4	30	41.4

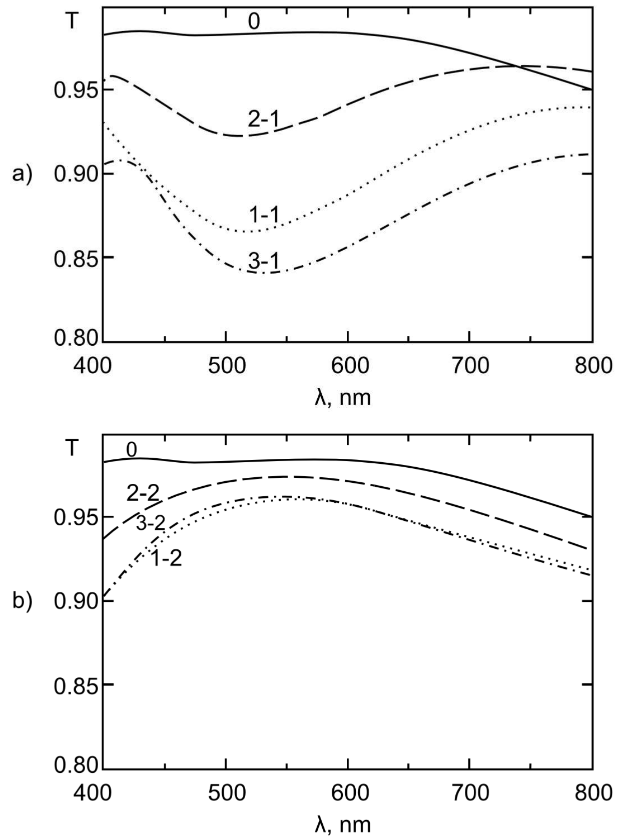


Fig. 4. Transmission spectra of MLS free of defects (curve *0*) and with defects formed by ZrO_2 (*a*, curves *1-1*, *2-1*, *3-1*) and by air (*b*, curves *1-2*, *2-2*, *3-2*)

character of the spectral dependence remains preserved, but its maximum shifts towards the short-wave range.

It was found that the transmission spectrum for MLS-0 (free of defects, Fig. 1) is identical to those in a MLS-0 region free from defects in Fig. 1,*b*, i.e. the defects are electrically neutral and do not influence on the optical characteristics of the nearest regions.

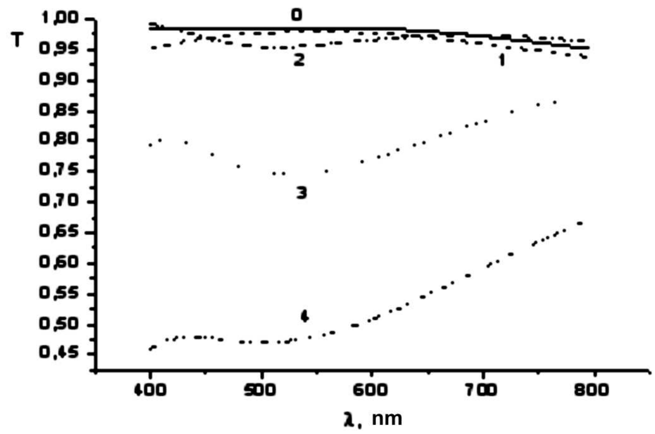


Fig. 5. Transmission spectra for MLS-n free of defects (*0*) and with defects formed by a substance with the refractive index $n = 1$ (*1*), 2 (*2*), 3 (*3*), and 4 (*4*)

Data for structure layers with different types of defects, which have the same longitudinal size of 20 nm – i.e. the layers have different optical thicknesses, which is governed by the refractive index of the defect substance, are presented in Table 2. The corresponding transmission spectra are shown in Fig. 5. Their analysis give us that higher is the refractive index of the defect substance, the more strong change in the character of these curves are observed, such as the formation of the curve minimum, the decrease of the absolute value of transmittance almost in 2 times at $n = 4$, and the shift of the curve maximum toward the long-wave interval.

It were also analyzed the dependences of the MLS transmittance on the defect parameters in more details, in particular, on their geometrical dimensions and their arrangements relative to the boundaries of MgF_2 layer, in which they are located. The diagrams of interrelations between the parameters of MLS and the geometrical dimensions of the ZrO_2 defects are shown in Table 3 and in Fig. 6,*a*. The corresponding dependences on the spatial arrangement of defects, provided that the longitudinal

T a b l e 3. Interrelations between MLS-D layers parameters Y_2B and Y_3B at various longitudinal dimensions X_3A of ZrO_2 defects

Substance and layer notation	MLS-D types and layer thickness, nm								
	MSL-D0	MSL-D1	MSL-D2	MSL-D3	MSL-D4	MSL-D5	MSL-D6	MSL-D7	MSL-D8
ZrO_2X_1A	60	60	60	60	60	60	60	60	60
MgF_2Y_1B	10	10	10	10	10	10	10	10	10
ZrO_2X_2A	50	50	50	50	50	50	50	50	50
MgF_2Y_2B	40	35	30	25	20	15	10	5	0
ZrO_2X_3A	0	10	20	30	40	50	60	70	80
MgF_2Y_3B	40	35	30	25	20	15	10	5	0

T a b l e 4. Interrelations between MLS-P layers Y_2B and Y_3B at various spatial positions of ZrO_2 defects and with a constant longitudinal size $X_3A = 20$ nm

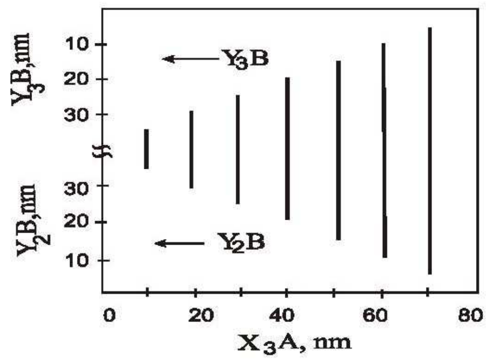
Substance and layer notation	MLS-P types and layer thickness, nm							
	MSL-P0	MSL-P1	MSL-P2	MSL-P3	MSL-P4	MSL-P5	MSL-P6	MSL-P7
ZrO_2X_1A	60	60	60	60	60	60	60	60
MgF_2Y_1B	10	10	10	10	10	10	10	10
ZrO_2X_2A	50	50	50	50	50	50	50	50
MgF_2Y_2B	40	0	10	20	30	40	50	60
ZrO_2X_3A	0	20	20	20	20	20	20	20
MgF_2Y_3B	40	60	50	40	30	20	10	0

size of the defect, $X_3A = 20$ nm, is constant, are presented in Table 4 and in Fig. 6,*b*.

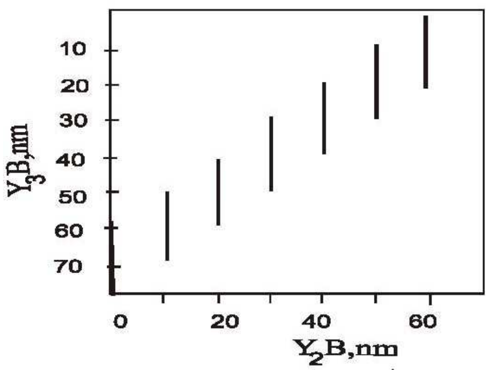
The transmission spectra, corresponding to the diagram 6,*a* and parameters from Table 3, are presented in Fig. 7,*a*. One can see that, if the longitudinal dimension of the defect grows, there appears a minimum in the region of 500–550 nm, which shifts to the long-wave region of the spectrum. A similar dependence is also observed, if the position of a defect relatively to the boundaries is varied (Table 4 and diagram 6,*b*). However, Fig. 7,*b* demonstrates that the approach of the defect to the interface between media lead to a shift of the formed minimum to the short-wave spectral region.

4. Conclusions

In this work were considered the influence of nanodefects in the optical elements with multilayer interference coatings on the transmission spectra. It was found that such defects give rise to a deviation of the optical parameters of real structures from those required by technology. For numerical estimations a model of defect layer structure was proposed. In the frame of this model, the interrelations between the geometrical and optical thicknesses of nearest layers were proposed depending on the defect parameters, such as the defect nature, dimensions, and positions relatively to the boundaries of the defect-including layer. It was found that the



a



b

Fig. 6. Diagrams of interrelations of MSL parameters with the longitudinal size of defects (*d*) and their spatial arrangement (*b*)

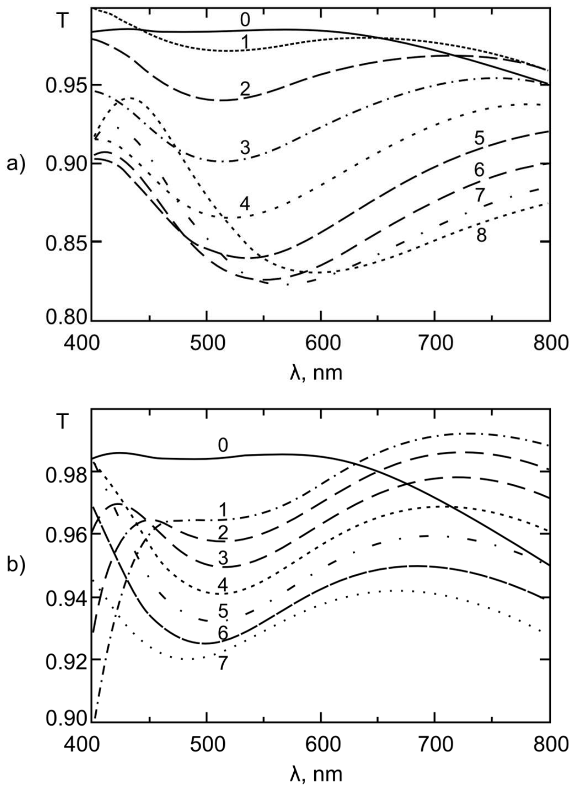


Fig. 7. Dependences of MLS transmission spectra on the longitudinal size of defects (*a*, curves *0* to *7*, the parameters from Table 3, diagram 6,*a*) and their spatial arrangement (*b*, curves *0* to *7*, the parameters from Table 4, diagram 6,*b*)

maxima in the transmission spectra of the optical elements with real defect-including coatings decrease with the growth of the refractive indices of defect substances. The spectral position of the maxima and the shape of transmission curves substantially depends on the defect size along the direction of light propagation, as well as on the defect position in the layer bulk. The obtained results may be used for fabrication of the optical elements (especially, the lenses for glasses) with antireflective coatings.

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ВПЛИВ НАНОДЕФЕКТІВ ШАРІВ НА ПРОПУСКАННЯ СВІТЛА ОПТИЧНИМИ ЕЛЕМЕНТАМИ З БАГАТОШАРОВИМИ ІНТЕРФЕРЕНЦІЙНИМИ ПОКРИТТЯМИ

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Р е з ю м е

Досліджено залежність пропускання світла оптичними елементами з багатошаровими інтерференційними покриттями. Встановлено, що максимуми пропускання оптичних елементів з реальними покриттями, які мають дефекти, знижуються тим сильніше, чим вищі показники заломлення речовини дефектів, а форма кривих пропускання суттєво залежить від розмірів дефектів уздовж напрямку поширення світла та їх положення в об'ємі дефектного шару. Дані результати необхідно враховувати при відпрацьованні технології виготовлення оптичних елементів з багатошаровими інтерференційними покриттями як для лазерної техніки, так і для виробництва оптичних лінз.