UDK 519.6; 535.345.67

A.V. Mitsa, I.V. Fekeshgazi, F.E. Geche, V.M. Kotsovsky

MATHEMATICAL MODELING OF INFLUENCE OF LAYER NANODEFECTS ON THE LIGHT TRANSMISSION BY OPTICAL ELEMENTS WITH MULTILAYER INTERFERENCE SYSTEMS

The analysis of defects parameters influence on the light spectra transmission by optical elements with interference coating have been carry out. It is established that the maximum and spectral distribution of transmission curve essentially depend on parameters and space position of defect. The obtained results are important in fabrication of optical elements with multilayer coatings as for laser technique, as the spectacles lens.

Keywords: modeling, light transmission, multilayer interference coating, structure defects, interconnection of parameters.

Introduction

Production of qualitative interference optical elements (interference filters, antireflective coatings, light beam and spectra disconnectors and polarizers) demands the matters of the high level of cleanliness and stability of its parameters both for substrate and layers and also of technological regime of their deposition. The presence of non-uniformly distributed in the space nanodimension defects (emptiness or inclusions of foreign alien) give rise to change the transmission spectra of the interference systems. The results obtained for practically used interference coatings (in particular of spectacles optical lenses) are given in this report.

Experimental samples

All measurements were performed on the transparent substrates (spectacles lens) from material with refraction index equal to 1.9 [1]. The multilayer systems (MLS) was deposited on its working surfaces (see Fig. 1). It was formed by layers with unequal geometrical thicknesses. At the absence of defects the MLS consist on four layers (Fig. 1a and Fig. 1b: MLS-0), while at the presence of one (such as emptiness or inclusions of foreign alien) there are six layers (fig.1b: MLS-1, MLS-2 and MLS-3).

Shape forms of all defects may be represented as spherical (MLS-1), rectangular (MLS-2), cylindrical (MLS-3) and on more complicated one

---

(see Fig. 1 b). The cross-section of defect by the plane that include the direction of light propagation are presented in Fig. 1.The layers parameters are given in the Table 1.

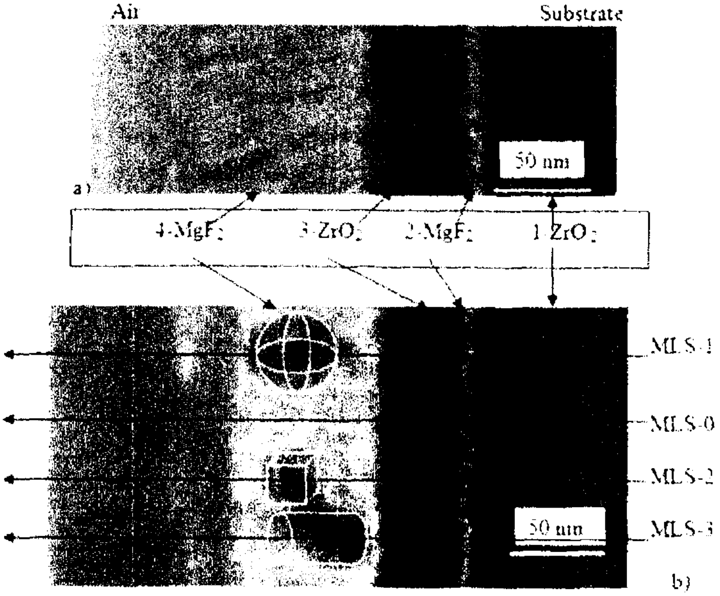

Fig.1. – Cross-section of MLS structures without defects (fig. 1a, 1b system MLS -0) and with defects (fig. 1b: systems MLS -1, MLS -2 and MLS -3).

Table 1.

Types of MLS and thickness of the layers, *nm*

Subst. of the layers	Types of MLS and thickness of the layers, *nm*													
	MLS-0		MLS-1-1		MLS-1-2		MLS-2-1		MLS-2-2		MLS-3-1		MLS-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 or Air	-	-	40	84,4	40	40	25	53	25	25	50	105,5	50	50
MgF_2	-	-	18	24,8	18	24,8	25	37,4	25	37,4	20	27,6	20	27,6

The first and the third layer of ML systems, were made from ZrO_2 (n_H = 2.11), the second, fourth and sixth layers – from MgF_2 (n_L = 1.38). It will be consider the two type of defect material: ZrO_2 or air.

The comparison of radiation transmission spectra shown that the spectra in the zone of MLS-0 (Fig.1a and Fig. 1b) without defects are identical to the transmission spectra of the MLS free on defects (fig.1b).

The analysis of results

The multilayer structures shown on Fig. 1a and Fig. 1b can be schematically represent as transparent substrate S with a refraction index n_S, on which one after another in consecutive order deposited the layers A with high refraction index n_A and layers B with low refraction index n_B (Fig.2), namely:

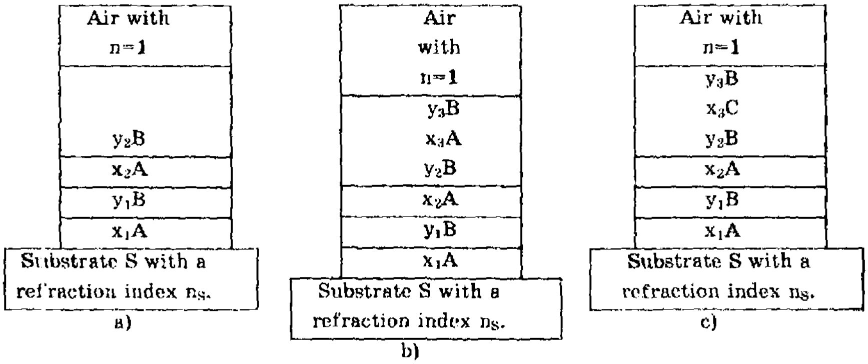

Fig. 2. Model of MLS structure without defects (a) and with the ZrO_2 (b) or air (c) defects.

The geometric and optical thicknesses of layers are determine by the factors x_i and y_i at the corresponding quarter-wave layers A and B for which the following ratio is correct $n_A d_A = n_B d_B = \lambda_0/4$. The geometrical view of defect structures MLS layer are present on Fig. 3. The MLS structure will be as in Fig 2b when the defects substance is from the same as B layer or as the Fig. 2c, when the defect is from the air.

To estimate the influence of changing interference systems parameters on the resulting transmission the matrix method was used. It based on the determination of a characteristic matrix [2]. If the geometrical thickness of a layer is equal to d, and refraction coefficient is equal to n, the characteristic matrix of the homogeneous dielectric film has the appearance:

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

where $\delta(n,d,\lambda)=2\pi nd\cos\theta/\lambda$ - is the phase thickness of a layer, $p=\sqrt{\varepsilon/\mu}\cos\delta$. In the case when the direction of propagation of radiation coincides with a perpendicular to the interface, $\delta=0$ and correspondingly $p=n$.

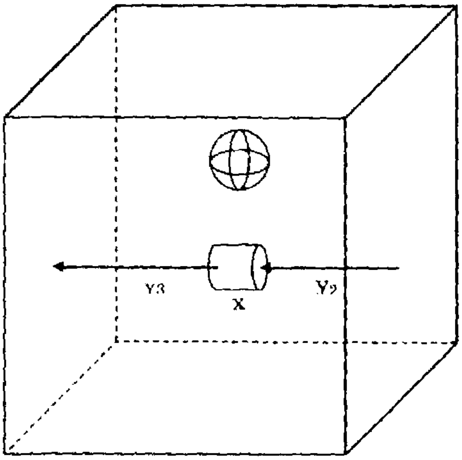

Fig.3. Geometrical view of the structures the MLS defect layer.

Knowing a characteristic matrix of one layer (1), we can determine a characteristic matrix of k-th layer of MLS, as a product of matrixes of each layer:

$$M(\bar{n},\bar{d},\lambda)=M_k(n_k,d_k,\lambda)\cdot M_{k-1}(n_{k-1},d_{k-1},\lambda)\cdot\ \cdot M_2(n_2,d_2,\lambda)\cdot M_1(n_1,d_1,\lambda), \qquad (2)$$

where Mj – is a characteristic matrix of j-th layer; $n=(n_1,n_2,\dots,n_{k-1},n_k)$ - is a vector of the values of refraction indices of layers; $\bar{d}=(d_1,d_2,\dots,d_{k-1},d_k)$ - is a vector of geometrical thicknesses of layers.

From (2) it is easy to find a value of a MLS transmission at the fixed values of $\bar{n}$, $\bar{d}$ and λ:

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

where n_0, n_S – are the refraction indices of external environment and substrate accordingly, M_{11}, M_{12}, M_{21}, M_{22} - are the elements of a characteristic matrix Mj.

For the numerical calculation of the transmittance spectra of MLS the objective function is represented as [3-5]:

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

where L – is a number of a grid points for a spectral interval from λ_1 to λ_2. At the its uniform distribution with a step $\Delta\lambda$

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

where λ_1 and λ_2 – are the short-wave and the long-wave boundary accordingly of researched wave spectral region.

The spectral dependences of the MLS transmission was calculated by using the formula (3) and represented in Tables 1 and in the Fig. 3 layers parameters are presented in Fig. 4. It was shown, that the existence of the defects in the volume of MgF_2-layer give rise to essential change of MLS transmittance, decreasing of a spectra maximum and to its displacement in the short wave range. The more considerable effects observed when the defect is from the substance with higher refractive indices (curves 3.0, 3-1 and 3-2 in Fig. 4).

The more detailed examination of transmittance dependences were made by changing the defect parameters. The data for layers structure at the different type of defect with the constant longitudinal geometric value equal to 20 nm, but different optical thicknesses determined by the refractive indices of defect substances are presented in Table 2. The correspondence spectra of MLS-n are presented in fig. 5.

Table 2

Types of MLS-n systems with 20 *nm* geometric value of defect from substance with different refractive indices

Substance of the layers	Types of MLS-n and thickness of the layers, *nm*									
	MLS-0		MLS-n=1		MLS-n=2		MLS-n=3		MLS-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
Mater with n-	-	-	20	20	20	40	20	60	20	80
MgF_2	-	-	30	41.4	30	41.4	30	41,4	30	41,4

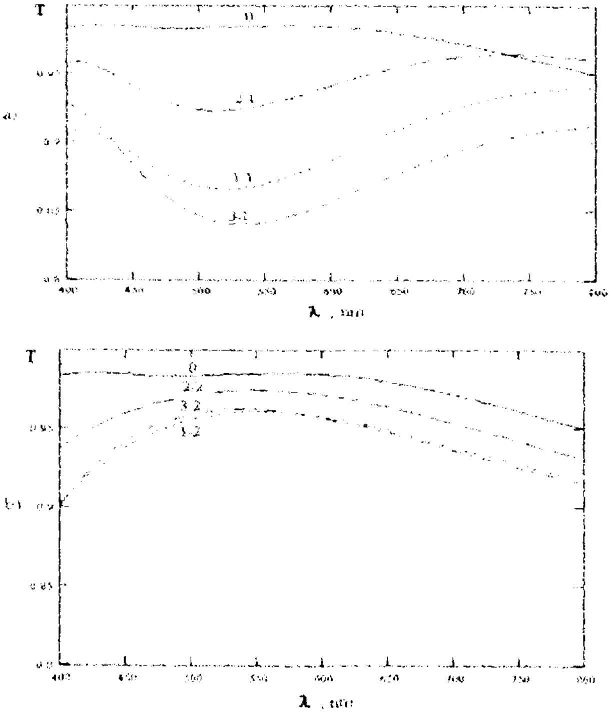

Fig. 4. The transmission spectra of MLS without defects (curve 0) and with defects from ZrO_2 (curves 1-1, 2-1, 3-1 on fig. 4a) or defects from air (curves 1-2, 2-2, 3-2 on fig 4b).

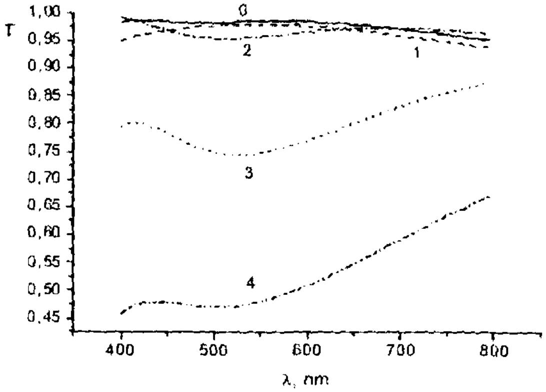

Fig. 5. The transmittance spectra of MLS-n without defects (curve 0) and with the defects from substances with refractive indexes $n = 1$ (curve 1), $n = 2$ (curve 2), $n = 3$ (curve 3), $n = 4$ (curves 4).

The diagram of interdependences between the of the MLS layer parameters at longitudinal values of defects from ZrO_2 are presented in Table 3 and Fig. 6a and on its space dislocation - in Table 4 and Fig. 6b for the longitudinal X_3A=20 nm value of defect .

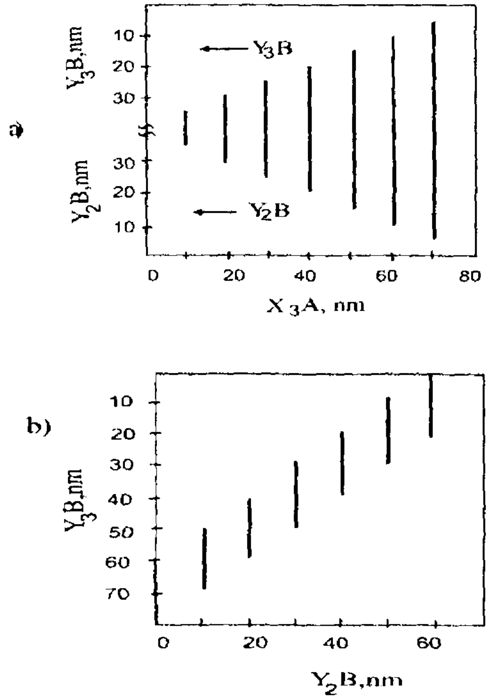

Fig.6. Diagram of interdependences between the MLS-D layer parameters at lon-gitudinal scale of defects (Fig. 6 a) and on its space dislocation MLS-P (Fig. 6 b).

Table 3.

Interdependency of MLS-D layers dimensions Y_2B and Y_3B at different longitudinal values of X_3A for defects from ZrO_2

Substance and designation of layers	Types of MLS D and thickness of the layers, *nm*																	
	MLS-D0		MLS-D1		MLS-D2		MLS-D3		MLS-D4		MLS-D5		MLS-D6		MLS-D7		MLS-D8	
	geom	opt.	geom	opt.	geom.	opt.	geom	opt.	geom	opt.	geom.	opt.	geom.	opt.	geom.	opt.	geom	opt.
ZrO_2X_1A	60	126,6	60	126,6	60	126,6	60	26,6	60	126,6	60	126,6	60	126,6	60	126,6	60	126,6
MgF_2Y_1B	10	13.8	10	13.8	10	13,8	10	13,8	10	13,8	10	13.8	10	13,8	10	13,8	10	13.8
ZrO_2X_2A	50	105.5	50	105.5	50	105,5	50	105,5	50	105.5	50	105,5	50	105,5	50	105,5	50	105,5
MgF_2Y_2B	40	55,	35	48,3	30	41,4	25	4,5	20	27,6	15	20,7	10	13,8	5	6,9	0	0
ZrO_2X_3A	0	0	10	13,8	20	42,24	30	63,3	40	84,4	50	105,5	60	126,6	70	147,7	80	168,8
MgF_2Y_3B	40	55,2	35	48,3	30	41,4	25	4,5	20	27,6	15	20,7	10	13,8	5	6,9	0	0

Table 4.

Interdependency of MLS-P layers dimensions Y_2B and Y_3B at different space position of the defects from ZrO_2 with the longitudinal geometric value of X_3A= 20 nm

Substance and design- nation of layers	Types of MLS P and thickness of the layers, *nm*															
	MLS-P0		MLS-P1		MLS-P2		MLS-P3		MLS-P4		MLS-P5		MLS-P6		MLS-P7	
	geom.	opt.	geom.	opt.	geom.	opt.	geom.	opt.	geom.	opt.	geom.	opt.	geom.	opt.	geom.	opt..
ZrO_2X_1A	60	126,6	60	126,6	60	126,6	60	126,6	60	126,6	60	126,6	60	126,6	60	126,6
MgF_2Y_1B	10	13,8	10	13,8	10	13,8	10	13,8	10	13,8	10	13,8	10	13,8	10	13,8
ZrO_2X_2A	50	105,5	50	105,5	50	105,5	50	105,5	50	105,5	50	105,5	50	105,5	50	105,5
MgF_2Y_2B	40	55,2	0	0	10	13,8	20	27,6	30	41,4	40	55,2	50	69,4	60	82,8
ZrO_2X_3A	0	0	20	42,2	20	42,2	20	42,2	20	42,2	20	42,2	20	42,2	20	42,2
MgF_2Y_3B	40	55.2	60	82,8	50	69,4	40	55,2	30	41.4	20	27,6	10	13,8	0	0

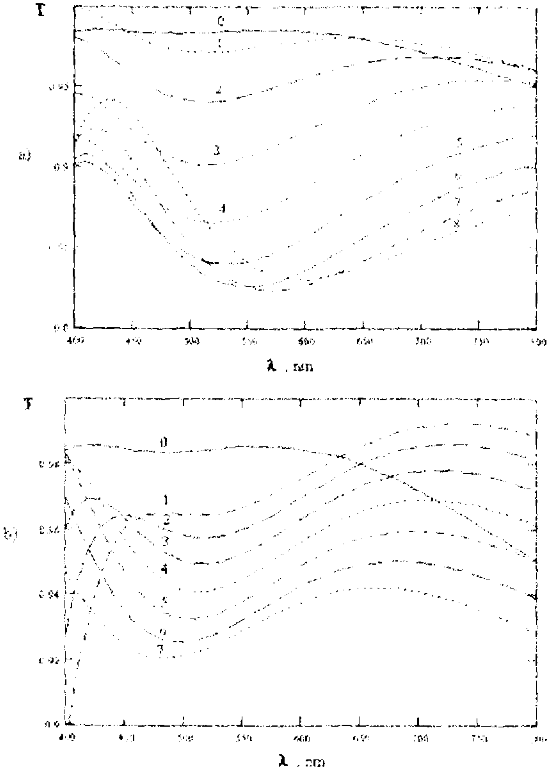

Fig. 7. The dependence of MLS spectra on longitudinal value of defects (fig.7a curves 0-8, data from table 3, diagram of Fig 6a) and on its space dislocation (fig.7b curves 0-7, data from table 4 , diagram on Fig 6b).

The transmittance spectra of corresponding to fig. 5 a diagrams and layer parameters from table 3 and table 4 are presented in Fig. 7a. At the increasing of longitudinal scale of defects (from high refractive substances) the minima of transmittance appear in the wavelength region of 500-550 nm while its position are shifted lo long wave. The similar dependence are observed at the changing of defect space position from the central points (table 4 and diagram of Fig. 5a) but the observed minima are shifted lo short spectra region.

Conclusion

The appearance of nanodefects in the MLS layer of antireflective coatings that give rise to declination the optical parameters of real optical elements from experimentally necessary are observed.

The model of defect layer structure is proposed for establish the interdependences between the MLS layer parameters at the different type of defects, their longitudinal scale and space dislocation. The numerical evaluation of the layers parameters influence of layers parameters on the transmission of MLS with defect are performed.

The decreasing of maximum transmission of the optical element with defect coating is established. At the increasing of longitudinal scale of defects from high refractive substances the minima of transmittance appear in the wavelength region of 500-550 nm while its position are shifted to the long wave. The similar dependences are observed at the changing of defect space position from the central points of defect layer but the observed minima are shifted to short spectra region.

REFERENCES

1. Fekeshgazi I.V., Barna P., Kikineshi O.E., Mitsa O.V., Sidenko T.S. Influence of nanodefects on the light transmission by multilayer interference systems. // Proc. Intern. Scient. Conf. "Physical and chemical principles of formation and modificanion of micro- and nanostructures". 21-23 October 2009. Kharkov. PP. 190-192.
2. Jakovlev P.P., Meshkov B.B. Designing of interference coatings. Moskva. Mechanical engeneering. 1987. – 192 c. (In Russian)
3. Born M., Wolf E. Priciples of optics. 4 ed. Pergamon Press. Oxford 1970.
4. Abeles F. Ann.de Physique. – 1950. V.5. P. 596-640.
5. Pervak Y., Mitsa O., Holovach J., Fekeshgazi I. Influence of transition film-substrate layers on optical properties of multilayer structure // The International Society for Optical Engineering. Vynnytsa. 2000. – Vol. 4425. – P. 321-325.