Optimization and prospects of the use of antireflection optical films in biomedicine

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ABSTRACT

The work is devoted to the optimization of the structure of a multilayer anti-reflective film with good integral optical properties in a wide range of angles of incidence and wavelengths of the infrared range, coinciding with the absorption of CO_2, and for both types of polarization of the incident wave. The optimization is performed on the basis of the initial solution of the problem, which is adjusted to a quarter-wave optical thickness of each layer(SiO_2, SiO, $SiO_{1<x<2}$, Si), where the optical thickness is chosen from the condition of maximum sensitivity to the absorption spectrum of carbon dioxide (CO_2). The matrix method is used to determine the integral reflection coefficient. Next, the thickness of the layers of the system is optimized by finding the global minimum of the function that determines the total amount of reflected radiation in a given range of wavelengths and angles of incidence of radiation. It is shown that by means of statistical modelling it is possible to determine the thickness of the film layers, which provides a systematic improvement in the value of the integral reflection coefficient. It is also shown that by means of statistical modelling it is indeed possible to obtain an optimized film structure, despite a small improvement in the integral reflection coefficient (less than 1%). Therefore, the developed analysis method has important practical significance for the analysis and detection of absorption effects of optical radiation of non-interference origin. The results of the research are also compared with studies using the Swanepoel method and published in literary sources. The obtained results are of practical interest in biomedical applications: biocompatible thin films of implanted organs, optical sensors for medical diagnostic systems, since in biological structures non-interference absorption effects of the optical range have a systematic and clearly expressed appearance.

Keywords: anti-reflective coating, statistical optimization, integral reflection coefficient, biomedicine, IoT

1. INTRODUCTION

The use of anti-reflective coatings in various optical devices and technologies is widely known. They are used to reduce the reflectance of incident optical radiation in classical optical devices[1], to increase the absorption coefficients of solar energy in solar photovoltaic cells in a wide range of angles of incidence and for the entire visible part of the spectrum, to increase the efficiency of photodetectors tuned to a certain wavelength, including infrared[2], to shield the unwanted effects of electromagnetic radiation in IoT devices that use absorbed electromagnetic radiation[3], to prevent the formation of standing waves in photolithography production processes[4]. The long history of the use of anti-reflective coatings and research related to their manufacturing technologies have resulted in a number of different ways to obtain them: single-layer films, multilayer films, gradient films. The most complex in terms of their manufacture, and therefore the most expensive, are gradient films. But their importance is becoming increasingly important, because a new task arises: ensuring certain characteristics for metamaterials, and especially metasurfaces. This issue arises in connection with the need to protect against electromagnetic radiation such devices as radars, transmitting and receiving antennas, which use metamaterial technology, and in which reflected radiation significantly degrades the quality of communication and the resolution of detection devices. Between optical and radio wave devices is the terahertz range, which is increasingly

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finding its application in science and technology, which also increases interest in modeling surfaces that have specified reflection characteristics in a certain range of angles and wavelengths.

Another important area of application of multilayer and gradient films with low reflectance coefficient is autonomous devices that are able to accumulate energy in order to receive power supply to maintain their functioning. Devices that are able to accumulate electrical energy from the environment are especially relevant as applied to the Internet of Things technology. Such devices that operate in the optical range are called “self-powered devices”[5]. Among such devices, one can distinguish devices with a phase gradient of the surface[6], which leads to the conversion of incident radiation into a surface wave, the energy of which is accumulated in the center of the device, which has radial symmetry.

Another trend related to the development of autonomous storage devices is the simultaneous combination of solar cells and the ability to absorb and convert electromagnetic radiation energy, especially in the range in which its intensity increases due to the spread of wireless telecommunication technologies[7]. This is achieved through the use of a metasurface that is sensitive to radio frequency radiation in the Wi-Fi range and is simultaneously optically transparent.

An important aspect of the application of thin films for detecting radiation in the optical range is biotechnology and biomedicine. Thus, in works[8,9], integrated devices designed for monitoring enzymatic biochemical analysis, which are manufactured using the “laboratory-on-a-crystal” technology, are considered. The importance of research into the properties of multilayer films is also significantly increasing due to the development of capabilities for their production: additive manufacturing, ultraviolet lithography, etc.[4].

The development of methods for modeling the properties of multilayer films provides an opportunity not only to improve their properties, but also to significantly increase the reliability of experimental results of the study of such properties. Thus, in work[10], the combination of experimental studies of the transmission spectra of thin films and the method of modeling the transmittance coefficient improved by the authors (Swanepoel method) made it possible to detect the displacement of local minima of the transmittance coefficient from the real minima, which is only 0.4%-1.2%. Thus, the authors of the work managed to detect the influence of the absorption properties of the semiconductor, which is due to non-interference mechanisms. The accuracy of the algorithm described by the authors is at the level of 0.06-0.1% for the lower and upper envelope of the oscillating transmission spectra of thin films[11,12,13].

2. METHOD FOR CALCULATING THE REFLECTANCE OF A MULTILAYER FILM

The matrix method is well known for its efficiency in calculating complex multilayer coatings, and it has been used for quite some time. Let us consider the essence of this method for calculating the reflection coefficients of electromagnetic waves (Figure 1).

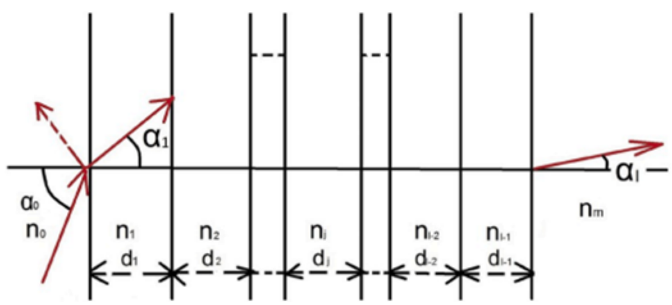

Figure 1. Discretized structure of a multilayer film.

According to the matrix method, the complex film is replaced by a discrete structure, each of which is characterized by a thickness and a macroscopic refractive index of the wave. The matrix of each layer connects the electromagnetic field vectors of the incident and refracted waves[14–18]:

$$\begin{cases} \begin{bmatrix} E_i \\ H_i \end{bmatrix} = \|M_{i-1}\| \times \begin{bmatrix} E_{i-1} \\ H_{i-1} \end{bmatrix} \\ \|M_i\| = \begin{bmatrix} m^i_{11(s,p)} & \sqrt{-1} \cdot m^i_{12(s,p)} \\ \sqrt{-1} \cdot m^i_{21(s,p)} & m^i_{22(s,p)} \end{bmatrix} \\ m^i_{11(s,p)} = cos\varphi_i, m^i_{12(s,p)} = sin\varphi_i / n_{i(s,p)}, m^i_{21(s,p)} = n_{i(s,p)} \cdot sin\varphi_i, m^i_{22(s,p)} = cos\varphi_i \\ \varphi_i = \frac{2\pi n_i d_i}{\lambda}, n_{i(s)} = cos\alpha_i, n_{i(p)} = \frac{n_i}{cos\alpha_i} \end{cases}, \quad (1)$$

where α_i is the angle of the Pointing vector in each layer,"s" and "p" denote s- and p- polarization of the wave.

The final relationship between the fields of the incident wave and the wave behind the film has the form:

$$\begin{cases} \begin{bmatrix} E_0 \\ H_0 \end{bmatrix} = \|M\| \times \begin{bmatrix} E_{l-1} \\ H_{l-1} \end{bmatrix} \\ \|M\| = \prod_{i=1}^{l-1} \|M_i\| = \|M_1\| \times \|M_2\| \times \cdots \times \|M_{l-1}\| \end{cases}, \quad (2)$$

where l is a number of layers, $\|M\|$ is a resulting matrix.

The resulting expression for the reflection coefficient of an overall film is the following formula:

$$r = \frac{n_0 \cdot M_{11} - n_s \cdot M_{22} + n_0 n_s \cdot M_{12} - M_{21}}{n_0 \cdot M_{11} + n_s \cdot M_{22} + n_0 n_s \cdot M_{12} + M_{21}}, \quad (3)$$

where M_{ij}, $i, j \in \{1,2\}$ are coefficients of the resulting matrix, n_0 is the is the refractive index of the environment, n_s is the refractive index of the substrate.

3. RESULTS OF THE RESEARCH

Previously we investigated[2] the properties of a complex multilayer film designed to improve the efficiency of an infrared diode operating in the infrared spectral region specified by the frequency range [3.5-5] microns. The film, which is deposited on the surface of the active material - indium antimonide (InSb), consisted of four layers: silicon dioxide (SiO_2), monoxide (SiO), silicon suboxide ($SiO_{1<x<2}$) and silicon (Si). The thickness of each layer is chosen from the condition of equality of a quarter of the reference wavelength ($\lambda_0/4$, $\lambda_0 = 450$ nm). It is shown that a low value of the reflection coefficient could be achieved for such film. At the same time, the value of the studied angles is limited to a rather narrow range from -6° to +6°, which occurs in optoelectronic converters of the AK9710ADF01 type, developed by Asahi Kasei. In this study, we determine the integral part of the reflected light generated by the LED used in the AK9710ADF01 optocoupler, taking into account the possible expansion of the range of angles of incidence of radiation on the surface of the photodetector. Fig. 2 shows the reflection coefficients (a) and the spectrum of reflected radiation (c and d), calculated for the normal angle of incidence.

From the figures, we can conclude that the spectrum of reflected radiation remains quite high for the wavelength that is the maximum for incident radiation. Let us also consider the possibility of the device operating in the case of multiple radiation sources, and for this purpose we will increase the range of incidence angles (Fig. 3).

From Fig. 3 we can conclude that the reflection coefficient increases significantly for large angles of incidence, especially for the p-polarized wave (Fig. 3b), which can increase to almost 80%, while for the p-polarized wave it does not exceed 15%. This is due to the significant integral value of the reflection coefficient for the entire range of angles and wavelengths from 2.6 to 5.5 microns, which is emitted by LEDs used for carbon dioxide detection (Fig. 2b).

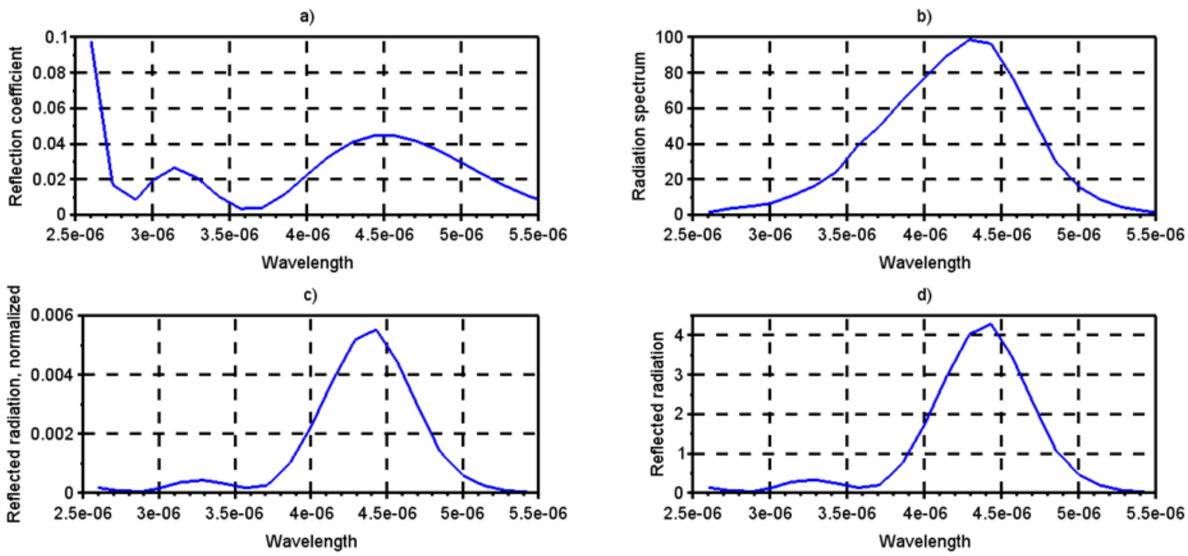

Figure 2. Reflectance coefficient (a), reflected radiation spectrum (c and d) and incident radiation spectrum (b) for a four-layer film deposited on indium antimonide (InSb), calculated for normal incidence on the photodetector surface.

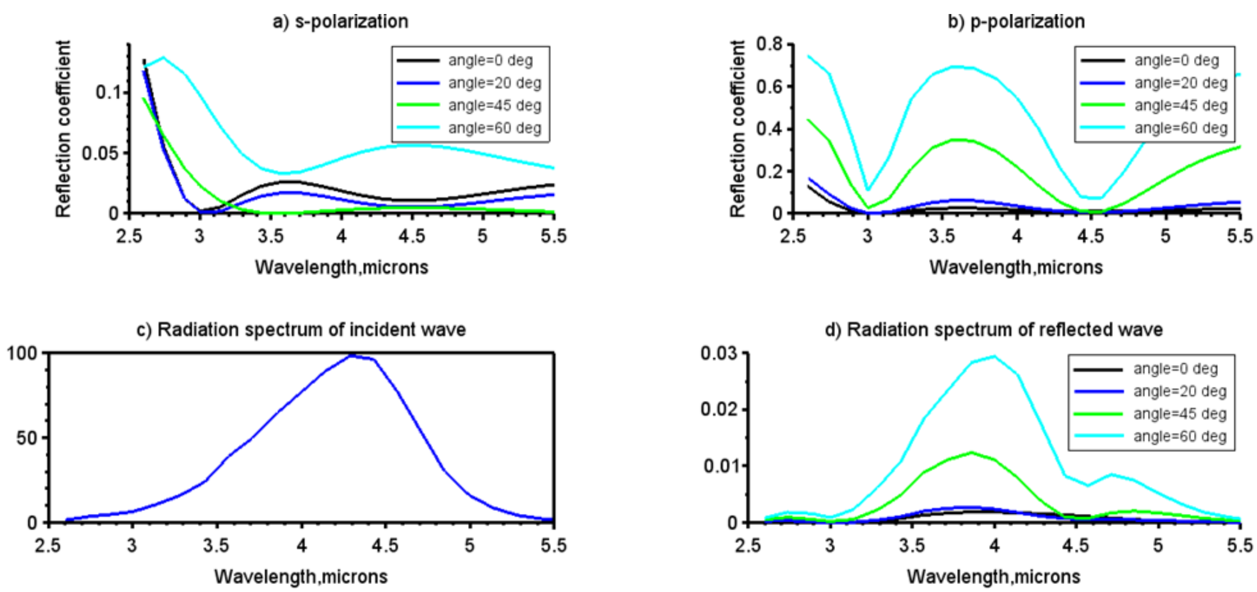

Figure 3. Reflectance coefficient (a), reflected radiation spectrum (c and d) and emitted radiation spectrum (b) for a four-layer film deposited on indium antimonide (InSb), calculated for the range of incidence angles from 0° to 60° on the photodetector surface.

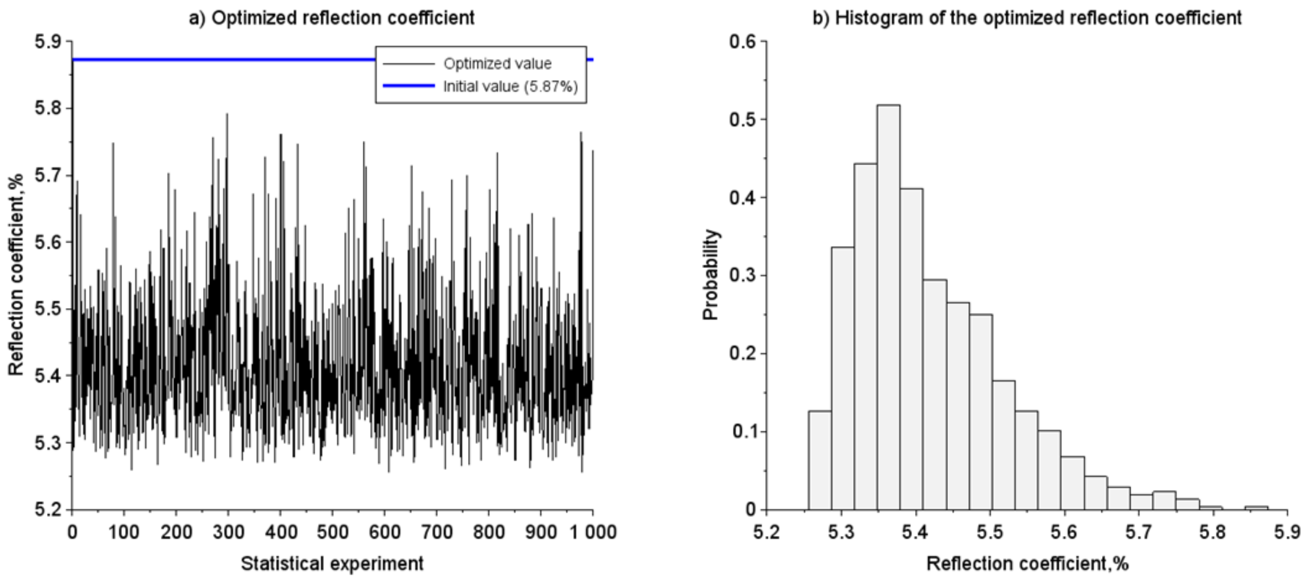

Figure 4. Results of optimization of the integral reflectance index (1000 iterations): optimized reflectance coefficient (a), reflectance coefficient histogram (b).

The next step in the research is to optimize the thickness of the film layers. Optimization problems related to determining the optical thickness a priori may have several local minima, and therefore, for optimization, algorithms for finding the global minimum should be used[13]. To optimize the integral index, we chose a statistical method. Two statistical experiments were conducted: first, the layer thickness was randomly increased in the range from 0 to 15 percent. But this only led to an increase in the integral reflection index. Reducing the layer thickness in the range from 0 to 15 percent led to a systematic improvement in the integral reflection index in each statistical implementation. The calculation results for 1000 iterations are shown in Fig. 4, where the straight line depicts the reflection coefficient for the non-optimized film, the value of which is 5.87%. The statistical values of the optimized reflection coefficient, calculated on a set of 1000 values, are as follows: average value 5.41%; standard deviation 0.1%.

The statistical values of the thickness of layers are as follows: the average thickness and standard deviation of silicon dioxide (SiO_2) - 747÷17 nm; silicon monoxide (SiO) - 570÷13 nm; silicon suboxide ($SiO_{1<x<2}$) - 416÷9 nm and silicon (Si) - 339÷8 nm. Aggregated data of the research results are given in Table 1.

Table 1. Aggregated indicators of the results of optimization of the thickness of film layers.

Film number and composition	**Initial film thickness ($n_i \cdot \frac{\lambda_0}{4}$), nm**	**Statistical optimization of film thickness, nm**	**Statistical average value of the integral reflectance index, %**	**Best integral reflectance index /improvement, %**	**Best film thickness/difference from initial value, nm**
1 (SiO_2)	776	747±17	5.42±0.1%	5.25(-0.64)%	742(-34)
2 (SiO)	592	570±13			589(-12)
3 ($SiO_{0<x<1}$)	433	416±9			400(-33)
4 (Si)	352	339±8			333(-29)

According to the results given in Table 1, optimization of the layer thickness makes it possible to reduce the integral reflection index by 0.64%. This value is very important and significant for further research, since it allows to reveal the action of finer absorption mechanisms caused by the internal quantum photoeffect, which takes place in the volume of each layer of the film. The reduction in the layer thicknesses in this case is from 12 to 34 nanometres. The non-random nature of the obtained results is evidenced by the fact that: 1) an increase in the layer thickness leads to a deterioration in the integral reflection index; 2) the integral reflection index improves for each test, where the layer thickness is reduced by 15% compared to the initial thickness of each layer, which coincides with the classical quarter-wave thickness.

4. CONCLUSIONS

Thus, a review of current trends in modelling and application of complex multilayer surfaces has been conducted. In connection with the improvement of semiconductor technologies, which provide the possibility of manufacturing nanometres-sized structures, the importance of theoretical studies of the properties of such surfaces, in particular gradient surfaces, is increasing, and opportunities arise to effectively solve inverse problems - the problem of synthesizing multilayer or gradient films with specified optical properties.

The combination of the traditional matrix method and the random search optimization algorithm makes it possible to improve the modelling result for the frequency range by almost 0.7%. Such an improvement is important, since it makes it possible to analyse data from experimental studies of multilayer films, in which absorption effects may appear, which have a non-interference origin, but are due to the band structure of the semiconductors used. Comparison with experimental data obtained from literature sources allows us to conclude that the improvement in the accuracy of the matrix method due to additional statistical optimization is commensurate with, or even exceeds the efficiency of other algorithms for modelling multilayer films. The control of the layer thickness, which provides the optimization obtained as a result of the modelling, is quite achievable for modern layer deposition methods that provide accuracy of the thickness value about nanometres.

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