УДК 621.38
DOI 10.36910/10.36910/6775-2313-5352-2023-22-02
Hetmanchuk V., Machulianskyi O.
National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", Kyiv, Ukraine

THE INFLUENCE OF THE STRUCTURAL PARAMETERS OF THE MATERIALS OF THE SENSITIVE ELEMENT OF THE OPTICAL SENSOR ON ITS SENSORY PROPERTIES

The sensor element of an optical sensor based on surface plasmon resonance is investigated in the paper. In particular, the influence of the components of the sensor element on its sensor properties by modeling design options. The Kretschmann configuration was chosen as the model, which is a glass prism with a multilayer nanoscale structure applied to one face. It was established that the material of the prism affects only the resonance angle of the structure. The thickness of nanoscale gold and silver films varied from 1 to 100 nm. The minimum value of the coefficient was obtained when the thickness of the gold and silver nanoscale films was 50 nm and 45 nm, respectively. The thickness of the silicon dioxide film varied from 10 to 150 nm. In the Au – SiO2 structure, the addition of silicon dioxide improved the optical properties of the multilayer structure. The minimum value of the reflection coefficient has decreased, but the thickness of the silicon dioxide is 3 nm. When the thickness of the dielectric layer increases, the optical properties of the structure deteriorate. The structure of the sensitive element, which uses a nanosized silver film, almost does not change its optical properties when adding a layer of SiO2, its thickness can reach 50 nm.
Keywords: *Optical sensors, surface plasmon resonance, gold, silver, silicon dioxide, glass prism.*

Introduction. Real-time measurement of various physical parameters is important for industrial, environmental, medical and chemical industries [1]. To solve these problems, optical sensors are widely used [2]. The main advantages of these detectors are low noise and high speed. This is due to the fact that the principle of operation of optical sensors is based on measuring the characteristics of light radiation or its changes. An optical sensor is an electronic detector that converts light rays into electronic signals. The measuring system consists of a sensitive element and a measuring device [3].

In particular, optical sensors based on surface plasmon resonance (SPR) are promising [4]. The premise design is the most common for such sensitive elements, this is due to the fact that it is cheap to manufacture, simple to implement and practical to use [5]. This type of sensitive element consists of a glass prism on which a multi-layered nano-sized structure is applied [6]. The multilayer structure consists of a metal and dielectric component, which performs the function of an additional protective layer [7]. The following materials are used to construct the sensitive element of the SPR sensor: Au, Ag, Al, SiO2, TiO2 and various polymers [8, 9, 10].

The principle of operation of such sensitive elements is that electromagnetic radiation is directed at the face of the prism at a certain angle, which passes through it and falls on the metal layer of a multilayer nanoscale structure, free electrons of the metal component are excited. The surface electromagnetic wave begins to move parallel to the multilayer structure. Since the wave is at the boundary between the conductor and the external medium (eg air, water or vacuum), these oscillations are very sensitive to any change in this boundary, such as the adsorption of molecules on the conducting surface. The angle of incidence of the light beam, which causes the SPR phenomenon, depends on the optical properties of the sensitive element, a slight change in the refractive index leads to the fact that the SPR effect does not occur. Therefore, the advantage of SPR sensors is the ability to detect specific substances (cells, molecules, analytes) in the experimental environment [11].

The main characteristic is the minimum value of the reflection coefficient of the structure depending on the angle of incidence. Since the conditions for the occurrence of the PPR effect are affected by various factors, such as: the substance under investigation and its concentration, the research environment, the materials of the sensitive element.

Since individual materials have different optical properties, the optical characteristics of such a design depend on the interaction of its individual components with each other. Therefore, the study of the interaction of materials with a multi-layered nanoscale structure with each other in various combinations is an important aspect in the design of such sensors.

This work examines a sensitive element. Since individual materials have different optical properties, the optical characteristics of such a design depend on the interaction of its individual components with each other and their structural parameters. In this regard, the prediction of the optical properties of such metal-dielectric nanoscale structures must be carried out taking into account the thickness of individual layers and the technological modes of their formation. When developing a sensitive element for an optical sensor, it is necessary to take into account the influence of structural elements on optical parameters with various options for combining materials of a multilayer structure. Therefore, the study of the influence of individual components and materials of the structure is an urgent task. Such dependencies can be obtained by modeling the optical parameters of the sensitive sensor element using information about the optical properties of their structural components.

The purpose of the work: to study the sensory properties of various structures of the sensitive element by modeling their optical characteristics.

Modeling methodology

Krechman's model was chosen for simulation [12]. It is based on the PPR effect and is a prism on which a multilayer nanoscale structure is applied (Fig. 1). Modeling was carried out for the following structures:

The first design is a prism and a sensitive element made of a nano-sized metal layer;

The second structure is the Prism and the sensitive element of the structure is a nano-sized metal layer with an additional protective nano-sized dielectric layer.

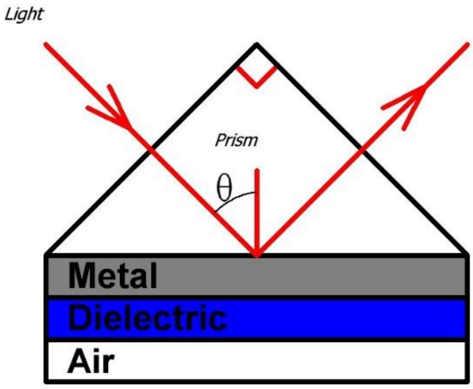

Figure 1 – Kretschman's model

Electromagnetic radiation passes through the prism with a specified length of electromagnetic radiation and its angle of incidence. The light that falls on the boundary of the distribution of the prism - metal, excites the molecules found in the air. An additional dielectric layer serves to protect the metal film from the influence of the molecules of the substance under study and improves the optical properties of the system.

The reflection coefficient for such a structure in accordance with is determined by the ratio [13]:

$$R = \left| \frac{r_{12} + r_{23}\exp(-2k_2 d)}{1 + r_{12}r_{23}\exp(-2k_2 d)} \right|^2 \qquad (1)$$

where k is the wave vector, d is the thickness of the metal layer, r_{ij} is the reflection coefficient at the interface between the two media.

$$r_{ij} = \frac{\frac{k_i}{\varepsilon_i} - \frac{k_j}{\varepsilon_j}}{\frac{k_i}{\varepsilon_i} + \frac{k_j}{\varepsilon_j}} \qquad (2)$$

where, ε is the dielectric constant of the medium, i, j = 1, 2, 3, depending on the medium.

$$k_i = k_0 \left[\varepsilon_i - \varepsilon_1 \sin^2\theta \right]^{\frac{1}{2}} \qquad (3)$$

where $k_0 = \omega/c$, $\sin\theta$ is the sine of the incidence angle, p of polarized light.

Simulation input data. The following materials SiO_2, MgF_2 were used to analyze the influence of the refractive index of the prism during modeling. Gold (Au) and silver (Ag) are used as a thin metal layer. The thickness of the metal varied from 1 to 100 nm. Silicon dioxide (SiO_2) was chosen as an additional dielectric component. This is due to its structural and technological features. The thickness of the additional dielectric layer varied from 1 to 150 nm. The dielectric constants of the materials are listed in Table 1 [14]. Laser radiation with a wavelength of λ = 633nm is used as a source of external electromagnetic (EM) radiation.

Winspall software (Resonant Technologies GmbH) [15] was used for simulation. It was tested and confirmed experimentally in the laboratory of the Max Planck Institute (MPI, Framersheim, Germany.

Table 1 – Optical parameters of the components of the sensitive element

Prism			Metal			Dielectric		
Material	n	k	Material	n	k	Material	n	k
MgF2	1,38	0	Au	0,178	3,07	SiO2	1,51	0
SiO2	1,51	0	Ag	0,151	3,97			

Research results and discussion of results. For the first structure (a prism and a sensitive element made of a nano-sized metal layer), modeling of structures using metal films of gold or silver was carried out. The minimum values of the reflection coefficient were obtained for structures with a gold film thickness of 50 nm. and silver - 45 nm. In fig. 2 shows examples of the dependence of the reflection coefficient on the angle of incidence of electromagnetic radiation with different prism materials for a structure with a nanosized gold film. And in fig. 3 shows examples of the corresponding dependence for a structure based on a metallic layer of silver.

Analysis of the curves shown in fig. 2 and fig. 3 shows that for a structure based on a SiO2 prism, the value of the plasmon resonance formation angle is smaller than for a MgF2 prism. Silver-based structures are characterized by lower values of the reflection coefficient than gold-based structures. The numerical values of these parameters are presented in Table 2. The values of the reflection coefficient on the straight sections of the curves for the silver-based structure are greater by 0.2 than for the gold-based structure.

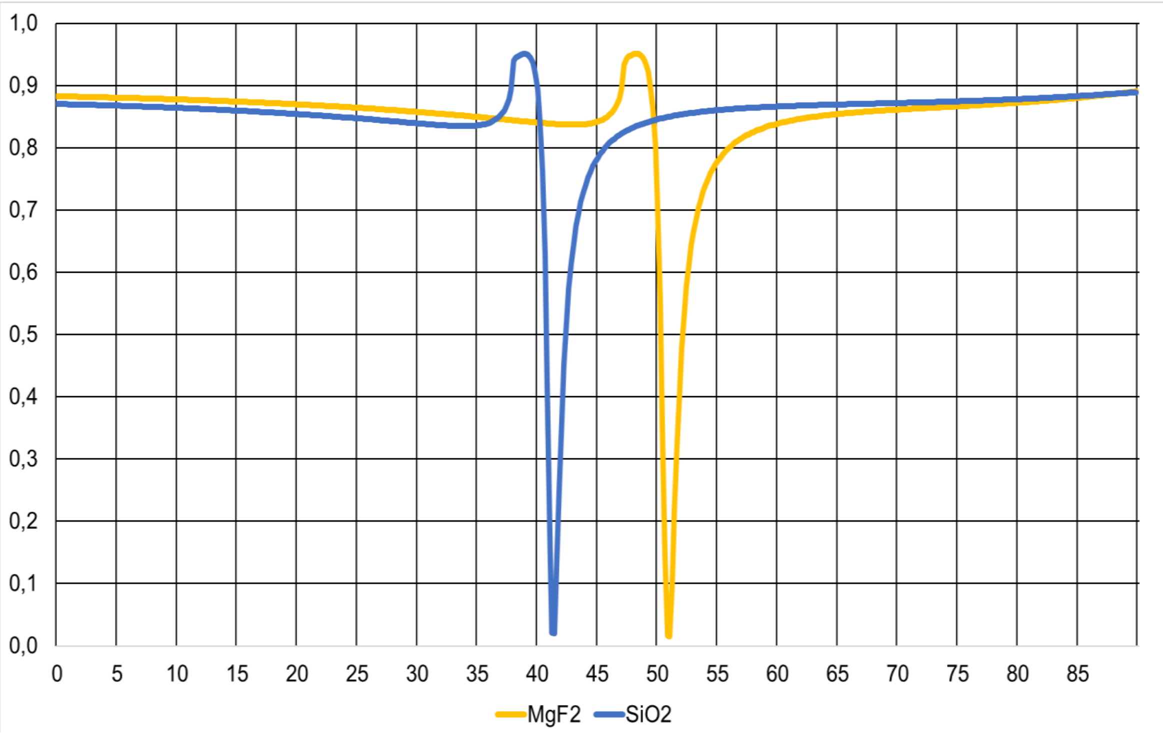

Figure 2 – Dependence of the reflection coefficient on the angle of incidence of electromagnetic radiation for the first design based on a 50 nm thick gold film with different prism materials

For the second design (prism and sensitive element of the structure, a nano-sized metal layer with an additional protective nano-sized dielectric layer), the structures were modeled using metal films of gold or silver, on which an additional dielectric layer of silicon dioxide was applied. The minimum values of the reflection coefficient were obtained for the structures of a nanoscale gold film 50 nm thick, with a silicon dioxide layer 3 nm thick, or a silver nanoscale film 45 nm thick, with a silicon dioxide layer 50 nm thick.

In fig. 4 shows the dependence of the change in the reflection coefficient on the angle of incidence of laser radiation, for a metal-dielectric structure based on Au-SiO2, with different prism materials.

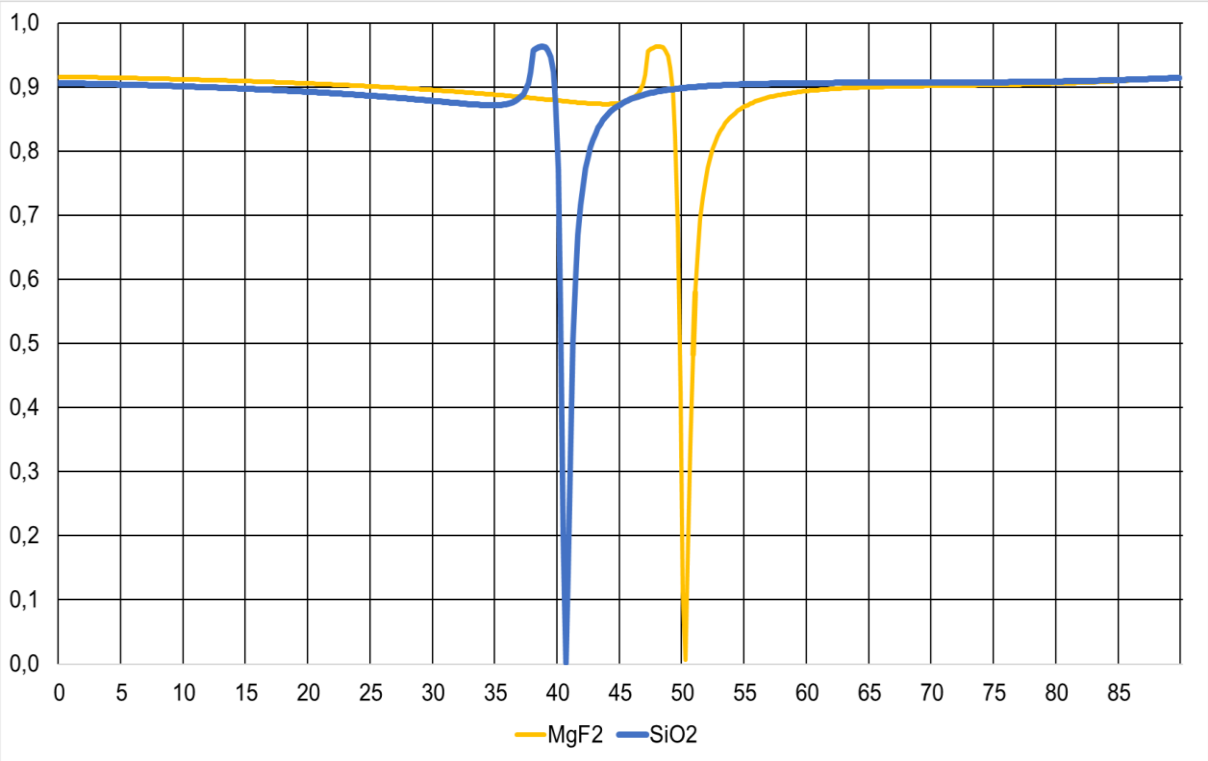

Figure 3 – Dependence of the reflection coefficient on the angle of incidence of electromagnetic radiation for the first design based on a 45 nm thick silver film with different prism materials

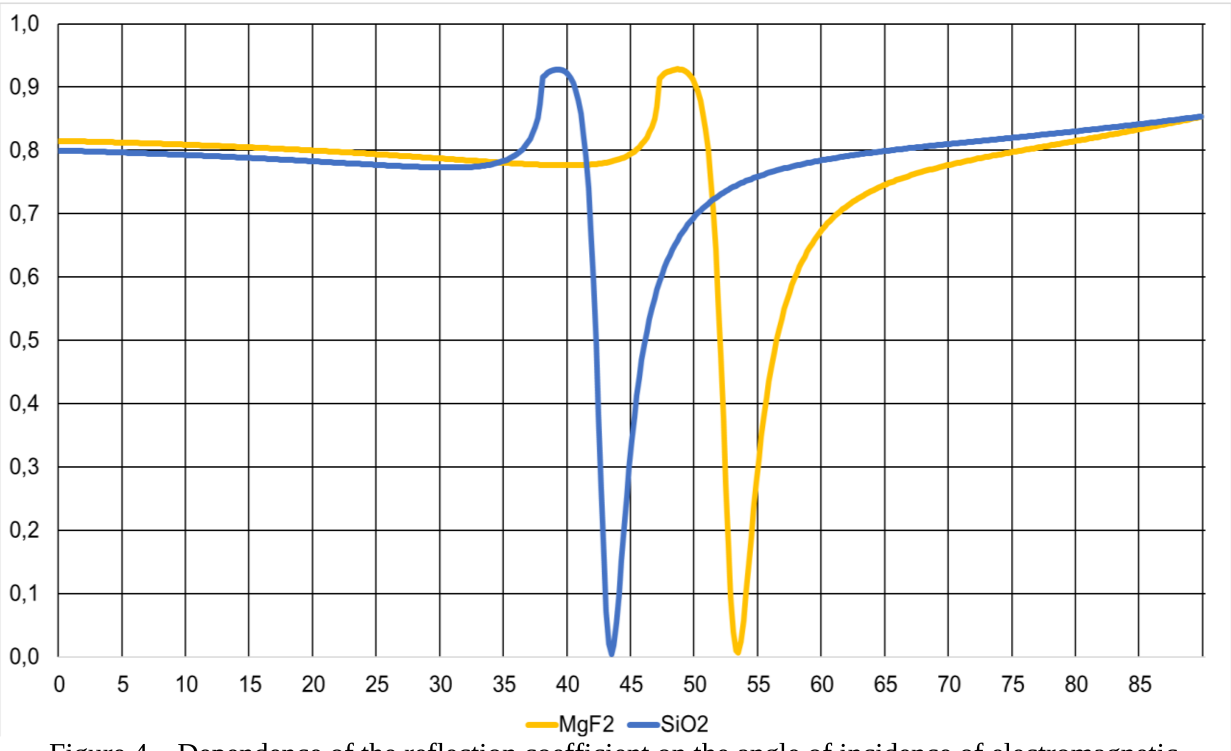

Figure 4 – Dependence of the reflection coefficient on the angle of incidence of electromagnetic radiation for the second design based on a 50 nm thick gold film, with an additional 3 nm thick silicon dioxide dielectric layer, with different prism materials

Analysis of the curve shown in fig. 4 shows that for a structure based on a thin film of gold, an additional dielectric layer of silicon dioxide reduces the minimum value of the reflection coefficient, and its value in the sections of the curves before and after the PPR effect, the resonance angle increased.

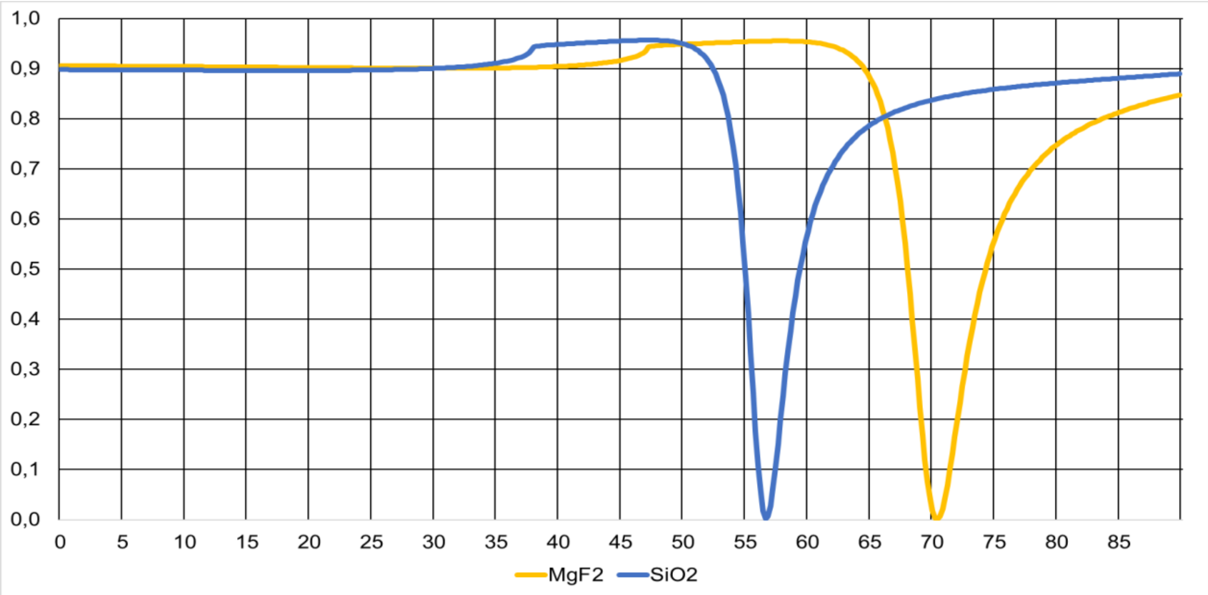

Figure 5 – Dependence of the reflection coefficient on the angle of incidence of electromagnetic radiation for the second design based on a silver film 45 nm thick, with an additional dielectric layer of silicon dioxide 50 nm thick, with different prism materials

For structures based on silver, the dependence of which the image in fig. 5, an additional silicon dielectric layer with a thickness of 50 nm has a minimal effect on the optical properties. Thus, the value of the reflection coefficient during the formation of the PPR is of the order of one ten-thousandth of a unit, and in the segments before and after the effect of the PPR, the change is insignificant. However, the resonance angle has increased significantly. The numerical values of these parameters are presented in Table 2.

Table 2 – Values of resonance angle and reflection coefficient for structures

	Gold		Gold - silicon dioxide	
Prism material	Reflection coefficient	Excitation angle	Reflection coefficient	Excitation angle
MgF_2	0,015	51	0,006	53
SiO_2	0,019	41	0,004	43
	Silver		Silver - Silicon dioxide	
Prism material	Reflection coefficient	Excitation angle	Reflection coefficient	Excitation angle
MgF_2	0,007	50	0,002	70
SiO_2	0,002	40,5	0,0001	57

Conclusions. The influence of the material of the prism and the additional dielectric layer on the optical properties of the sensitive element of the optical sensor has been established. The material of the prism affects only the resonance angle of the structure. For the SiO_2-based structure, it decreases by about 10 degrees relative to the values for the MgF_2-based structure.

An additional dielectric layer based on silicon dioxide improves the optical properties of the system. Thus, the minimum reflection coefficient decreased by approximately 3 times compared to structures with metal films. The lowest value of the reflection coefficient is observed for a structure based on silver with a thickness of 45 nm, with a prism based on SiO_2, and a dielectric component of the same material with a thickness of 50 nm, it is 0.0001.

The thickness of the additional dielectric layer of silicon dioxide for structures based on gold nanoscale films is 3 nm, and for such structures based on silver 50 nm, respectively. But gold has a high affinity for human cells and does not undergo oxidation, so it can be used in the medical field. Silver-based structures allow you to apply a large protective layer of silicon dioxide, but are vulnerable to oxidation, so such structures can be used in aggressive environments, for example, in the chemical, environmental and industrial sectors.

The research used macroscopic values of the parameters of the nanoscale components of the structure, but it is known that their real parameters differ significantly from the macroscopic ones.

To increase the accuracy of the simulation of the metal-dielectric structure in further studies, it will be necessary to take into account dimensional changes in the optical parameters of the nanoscale metal component [16].

References

1. Truong Thi Vu Nu, Tran Thi Nhu Hoa, Eunjoo Nam and Tai Tan Nguyen, Blood-based immunoassay of tau proteins for early diagnosis of Alzheimer's disease using surface plasmon resonance fiber sensors, RSC Advances, 2018.

2. E. D. Paul Regtien, Sensors for Mechatronics, Elsevier, 2018.

3. Yoshinori Kagawa, Masahiro Satoh, Takayuki Numata, Hiroshi Ishida and Norihiro Umeda, "Compact SPR Gas Sensor for Mobile Robot Olfaction Using Metal Nanostructure and LED Light Source," in *SENSORS*, Tokyo, Japan, 2007.

4. F. Vollmer and D. Yu, Surface Plasmon Resonance, 2022.

5. Celina M. Miyazaki, Flávio M. Shimizu and Marystela Ferreira, "Surface Plasmon Resonance (SPR) for Sensors and Biosensors," *Micro and Nano Technologies, Nanocharacterization Techniques,* pp. 183 - 200, 2017.

6. A. Heesang, S. Hyerin, C. Jong-Ryul and K. Kyujung, "A Localized Surface Plasmon Resonance Sensor Using Double-Metal-Complex Nanostructures and a Review of Recent Approaches," *Sensors,* no. 18, p. 98, 2017.

7. B. B. Babych, Machulianskyi V. O and Machulianskyi, O. V, "Modeling of metal-dielectric nanocomposite coatings with ferromagnetic inclusions for electromagnetic protection of electronic devices," *Visnyk of Kherson National Technical University,* pp. 104-108, 2018.

8. V. O. Machulianskyi, O. V. Machulianskyi and B. B. Babych, "Determination of the efficiency factors of the absorption and scattering of nickel nanoparticles," *Informatyka, Automatyka, Pomiary w Gospodarce i Ochronie Środowiska,* 2018.

9. O. V. Machulianskyi, "Optical characteristics of nanodimensional particles of chrome," *HERALD OF KHMELNYTSKYI NATIONAL UNIVERSITY,* no. 257, pp. 203-207, 2018.

10. В. В. Гетманчук and О. В. Мачулянський, "Вплив товщини нанорозмірних шарів метало-діелектричної структури на її оптичні характеристики," *Мікросист., Електрон. та Акуст.,* vol. 27, no. 2, 2022.

11. Narjes Amoosoltani, Abbas Zarifkar and Ali Farmani, "Particle swarm optimization and fnite-diference time-domain (PSO/FDTD) algorithms for a surface plasmon resonance-based gas sensor," *Journal of Computational Electronics,* 2019.

12. Shijie Deng, Peng Wang and Xinglong Yu, "Phase-Sensitive Surface Plasmon Resonance Sensors: Recent Progress and Future Prospects," *Sensors,* vol. 17, no. 12, 2017.

13. Md. Moznuzzaman, Md. Rafiqul Islam, Md. Biplob Hossain and Ibrahim Mustafa Mehedi, "Modeling of highly improved SPR sensor for formalin detection," *Results in Physics,* vol. 16, 2020.

14. Palik D. Edward, Handbook of Optical Constants of Solids: Volume 1, Academic Press, 2016.

15. "RES-TEC," RES-TEC, Framersheim, Germany, 2018.

16. O. V. Machulianskyi, "Optical properties of nickel nanoparticles in systems with a statistically inhomogeneous structure," *Microsystems Electronics and Acoustics,* no. 23, 2018.

Гетманчук Віктор, Мачулянський Олександр
Національний технічний університет України "Київський політехнічний інститут імені Ігоря Сікорського"

ВПЛИВ СТРУКТУРНИХ ПАРАМЕТРІВ ПРИЗМОВОГО ОПТИЧНОГО ДАТЧИКА НА ЙОГО СЕНСОРНІ ВЛАСТИВОСТІ

У роботі досліджено сенсорний елемент оптичного датчика на основі поверхневого плазмонного резонансу. Зокрема, вплив компонентів сенсорного елемента на його сенсорні властивості шляхом моделювання конструктивних варіантів. За модель була обрана конфігурація Кречмана, яка являє собою скляну призму з нанесеною на одну граней багатошарову нанорозмірну структуру. Встановлено, що матеріал призми впливає лише на резонансний кут конструкції. Товщина нанорозмірних плівок золота та срібла змінювалася від 1 до 100 нм. Мінімальне значення коефіцієнта було отримано при товщині золотої та срібної нанорозмірних плівок 50 нм і 45 нм відповідно. Товщина плівки діоксиду кремнію змінювалася від 10 до 150 нм. У структурі Au – SiO_2 додавання діоксиду кремнію покращило оптичні властивості багатошарової структури. Мінімальне значення коефіцієнта відбиття зменшилось, проте товщина діоксиду кремнію становить 3 нм. При збільшенні товщини шару діелектрика, оптичні властивості структури погіршуються. Структура чутливого елемента, в якій використовується нанорозмірна плівка срібла, майже не змінює оптичних властивостей при додаванні шару SiO2, його товщина може досягати 50 нм.

Ключові слова: *Оптичні сенсори, поверхневий плазмонний резонанс, золото, срібло, діоксид кремнію, скляна призма.*

Hetmanchuk V., Machulianskyi O.