International Journal of Electrical, Electronic and Communication Sciences
ISSN: 2517-9438
Vol:6, No:8, 2012

Modeling of Sensitivity for SPR Biosensors-New Aspects

Volodymyr Chegel

***Abstract*—**The computer modeling is carried out for parameter of sensitivity of optoelectronic chemical and biosensors, using phenomena of surface plasmon resonance (SPR). The physical model of SPR-sensor's is described with (or without) of modifications of sensitive gold film surface by a dielectric layer. The variants of increasing of sensitivity for SPR-biosensors, constructed on the principle gold – dielectric – biomolecular layer are considered. Two methods of mathematical treatment of SPR-curve are compared – traditional, with estimation of sensor's response as shift of the SPR-curve minimum and proposed, for system with dielectric layer, using calculating of the derivative in the point of SPR-curve half-width.

***Keywords*—**Surface Plasmon Resonance, modeling, sensitivity, biosensor

I. Introduction

A number of works related to modeling of SPR-sensors sensitivity is published [1,2,4]. Usually the modeling of sensitivity performs for such multilayers structure: glass prism - metal layer - biomolecular layer. However, the presence of additional dielectric layer on the top of metal can be considered as advantage due to possibility of multiple using of expensive SPR - chips and as possibility to avoid the negative influence of the applied metal (gold, silver) on a biomolecule. Unfortunately, only few works present modeling of sensitivity for SPR sensors with additional layer on the surface of metal. In the work [1] the sensitivity of gas sensor with presence of dielectric above the gold layer was simulated with dependence of sensitivity on the form of SPR – curve and height position of its minimum. In works [2] sensitivity of SPR-sensor simulated without a dielectric layer, but using gel matrix as the layer - sorbent of biomolecules.

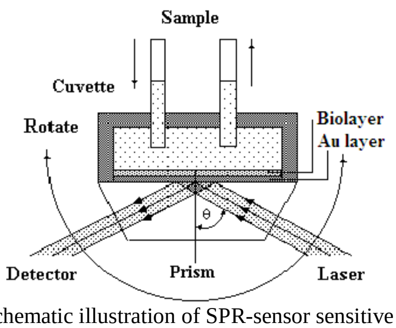

Fig. 1 Schematic illustration of SPR-sensor sensitive element

V. I. Chegel is with the Functional Optoelectronic Transducers Department, V.E.Lashkarjov Institute of Semiconductor Physic National Academy of Science of Ukraine, 41, pr. Nauki, 03028 Kiev, Ukraine, (e-mail: vche111@yahoo.com).

The modeling of sensitivity of SPR-sensor, made on «particle linkage» technology was carried out in work [4]. Such type of technology based on the effect of increase of SPR-response, when little particles of optically active materials, for example, colloidal gold or titan dioxide were linked with biomolecules, adsorbed on the surface of metal-carrier of plasmon oscillations. Every of mentioned work have proposed the particular variant of multilayer system, where influence of optical and geometrical parameters for each of layer on sensitivity of whole system don't considered in details.

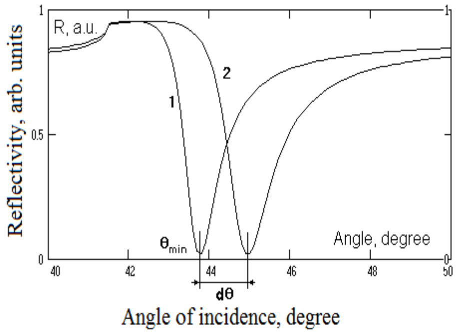

Fig. 2 Dependence of reflectance on angle of incidence for SPR – sensor (SPR-curves). 1-bare gold surface, 2 - with some layer of adsorbed biomolecules

More generalized is offered here variants of modeling of multilayer system with simple gold layer, gold with dielectric layer and gold with dielectric layer and with layer of biomolecules, adsorbed on the gold or dielectric. Such approach covers any possible variants of estimation of sensitivity for system gold – dielectric - biomolecular layer. In present work we discuss the possibility to theoretically significant increasing of SPR response using metal layers and dielectric covers with different optic parameters. The offered model theoretically allows considering system with n-layers, though in practice it is no necessary.

II. Theory

For sensors based on phenomena of Surface Plasmon Resonance ATR (Attenuated Total Reflection) - technology mostly is used. As informative parameter the reflective characteristic of intensity of p-polarized laser irradiation on output of the optical block is utilized (Fig. 1, Kretschmann configuration).

For conditions of total internal reflection practically 100 % of reflected laser beam energy is fixed by photodetector, except for vicinity of angle of incidence $\theta = \theta_o$,

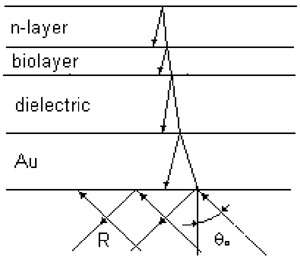

Fig. 3 The scheme of considered multilayer system

where value of wave vector of photon is compared with (or begins to exceed) the value of the wave vector of surface plasmon.

$$k_{sp}^{0} = k_{ph}^{0} = n_0 \left(\omega/c\right) \sin\theta_0 \quad , \qquad (1)$$

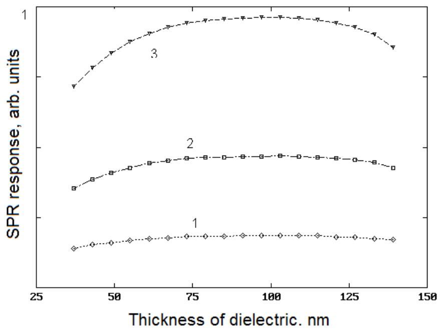

Fig. 4 Dependence of SPR - response on the thickness of layer Au (N_{Au} = 0.15 + 3.6i) .1-for layer of biomolecules (N_{mol} = 1.46) with thickness d_{mol} = 2 nm, 2 - 5 nm, 3 -10 nm

where k_{sp} is the wave vector for surface plasmon propagating along the interface gold - environment, c - speed and ω - frequency of light, k_{ph} - the wave vector for photon, n_o - coefficient of refraction of the prism. The sharp dipping of the reflection curve (Fig. 2), fixes the absorption of light energy and occurrence of the collective oscillation of free electrons at the surface layer of metal. Similar effect can be observed only for metals, having high concentration of free electrons, such as copper, gold and silver. The conditions of occurrence of resonance oscillations directly depend on the condition at the interface: metal – ambient. SPR angle (θ_{min}) is displaced (SPR-response) with change of the dielectric characteristics of an ambient (Fig. 2). The value of SPR-response ($d\theta_{min}$) in relation to change of the complex index of refraction or thickness of biomolecular layer above metal is the parameter of SPR biosensor sensitivity. In this study the program, allowing step by step varying the dielectric constant (n_i, k_i) and thickness (d_i) of each layers of multilayer system (Fig. 3) in the wide range of technologically possible values was developed. For all variants the SPR-response ($d\theta_{min}$) is calculated under detection of the tested layer with thickness d_{mol} and optical parameters close to biomolecules layer (N_{mol} = 1.46, d_{mol} = 2, 5 or 10nm). Accordingly, the sensor sensitivity:

$$S = \frac{d\theta_{\min}}{d_{mol}(n,k)} \qquad (2)$$

As initial, the following effective values, describing above multilayer structure, were taken: Au layer - complex coefficient of refraction N_{Au} = 0.15 + 3.6i, d_{Au} = 45nm; dielectric layer - N_d = 1.5 + 0i; glass prism - N_g = 1.51; ambient (phosphate buffer solution) - N_a = 1.334. Further, some of this parameters will be varied to optimize the sensor's sensitivity.

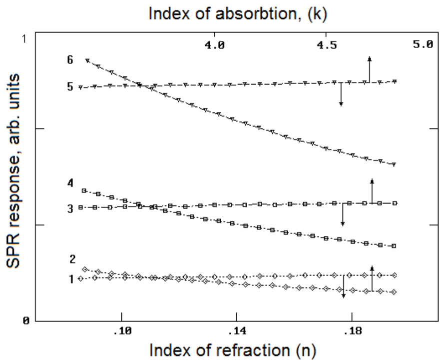

Fig. 5 Dependence of SPR-response on value of n and k of a gold layer (d_{Au} = 45nm). 1, 2 - for biomolecules layer (N_{mol} = 1.46) with thickness d_{mol} : 1, 2 = 2nm, 3, 4 - 5nm, 5, 6 - 10nm

The values of SPR-response at the beginning ($d\theta_{min\ b}$) and end ($d\theta_{min\ e}$) of variation diapason, where parameter of sensitivity rises, was taken as average (because of probable nonlinearity) parameter of efficiency Q, showing, as varied parameter of multilayer system influences on sensors sensitivity.

$$Q = \frac{d\theta_{\min b}}{d\theta_{\min e}} \qquad (3)$$

The program is based on the calculating of integrated Fresnel coefficient R for p-polarization of light [3]. In case of i layers is convenient to calculate R, using a formalism of the scattering matrix [3],

$$S = I_{10}L_1 I_{12} L_2 ... I_{(J-1)J} L_J ... I_m L_{m(m+1)} , \qquad (4)$$

where matrix of interface between layers

a and b: $$I_{ab} = \begin{bmatrix} 1 & r_{ab} \\ r_{ab} & 1 \end{bmatrix},$$

where r_{ab} - Fresnel coefficient of reflection for the appropriate interfaces,

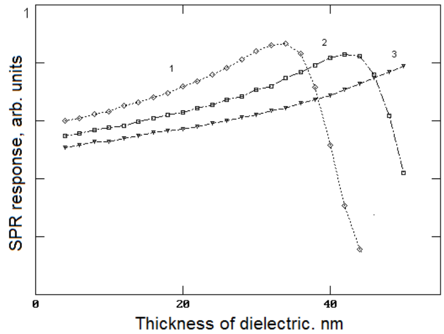

Fig. 6 Dependence of SPR-response on k of Au layer (k_{Au}) and thickness of the dielectric layer (d_d) with registration of the layer of biomolecules with N_{mol} = 1.46 and d_{mol} = 2nm. (1) - 0.15 + 3.4i, (2) - 0.15 + 3.6i, (3) - 0.15 + 3.8i

and matrix of the layer: $L = \begin{bmatrix} e^{\beta_i} & 0 \\ 0 & e^{-\beta_i} \end{bmatrix}$,

where β - phase thickness of appropriate layer:

$$\beta = 2\pi\left(\frac{d}{\lambda}\right)N\cos\varphi\,, \qquad (5)$$

where d - thickness of the appropriate layer, φ - angle of refraction for the appropriate layer (Fig.3), λ - length of a wave (in our case 632,8 nm), N-complex coefficient of the refraction for appropriate layer. The reflection coefficient of multilayer structure is determined by elements of first column of a scattering matrix:

$$R = \frac{S_{10}}{S_{00}} \qquad (6)$$

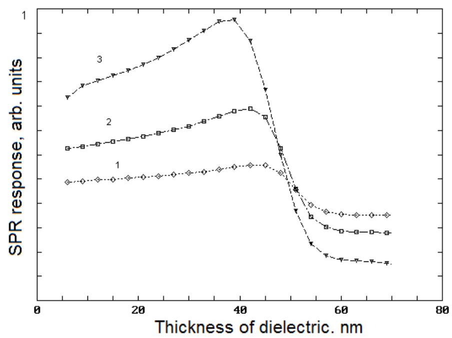

Fig. 7 Dependence of SPR-response on the thickness of a dielectric layer (N_d = 1.5). 1-for registration of biomolecules layer (N_{mol} = 1.46) with thickness d_{mol} = (1) -2 nm, (2) - 5nm, (3) - 10nm

III. Analysis of Results of Modeling

A. Model without dielectric layer

The results of modeling show, that sensitivity of considered

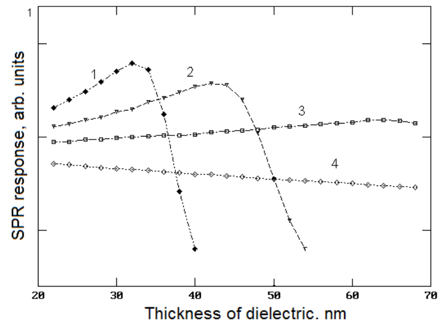

Fig. 8 Dependence of SPR-response on coefficient of refraction and thickness of dielectric layer for registration of biomolecular layer with N_{mol} = 1.46 and d_{mol} = 2nm. 1 - (N_d = 1.35), 2 - (N_d = 1.5), 3 - (N_d = 1.55), 4 - (N_d = 1.6)

SPR-biosensor changes depending on the parameters of multilayer structure in the wide range of values, especially for biomolecular layers with large size of biomolecules (Fig. 4). Actually, if for the biomolecular layer with thickness d_{mol} = 2nm the change of sensitivity for variation of gold film thickness is almost not observed, for the detection of molecules with size d_{mol} = 10nm the SPR-response $d\theta_{min}$ has expressed spherical form with a maximum in area of gold film thickness d_{Au} = 100nm (Fig.5) However, parameter of the efficiency Q is about identical for all considered cases (1.333 for d_{mol} = 2nm and 1.332 for d_{mol} = 10nm). The bigger efficiency is observed with modeling of influence on sensors sensitivity from the side of complex refraction coefficient of gold film (Fig.4). The value of Q varies from Q = 1.9 for biolayer with d_{mol} = 2nm up to Q = 1.63 (d_{mol} = 10nm). Parameter Q more depends on the coefficient of absorption k_{Au} whereas on n_{Au} a little. Maximal sensitivity of SPR - sensor without dielectric layer was observed with thickness of a gold layer approximately 80 nm with minimal value of k_{Au}.

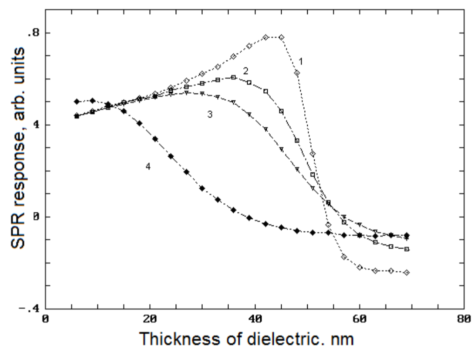

Fig. 9 Dependence of SPR-response on the coefficient of absorption and thickness of dielectric layer (N_d = 1.5). 1-for registration of biomolecules layer (N_{mol} = 1.46, d_{mol} = 2nm). 1-(k_d = 0.0i), 2-(k_d = 0.02i), 3-(k_d = 0.04i), 4-(k_d = 0.2i)

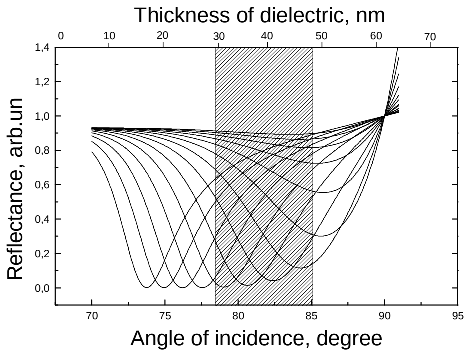

Fig. 10 Calculated SPR-curves for structure Au-dielectric (N_d=1.5+0i) for step by step increasing of thickness of dielectric (step 5 nm). Selected angle region – zone of strong increasing of SPR response $\Delta\theta_{min}$

B. Model with dielectric layer

In the case of model with dielectric layer the more complex dependence on SPR-response from thickness and complex coefficient of refraction of a dielectric layer is observed. Sensor's sensitivity smoothly grows with presence of the dielectric layer (N_d = 1.45) for all thickness of biomolecular layers up to some crucial values, and then sharply falls (Fig. 6-9). Exception is the case, when coefficient of absorption k_d of dielectric grows up to 0.2, where sensitivity falls with presence of the dielectric layer with any thickness (curve 4, Fig. 9). The maximal value of parameter of efficiency (Q = 1.4) is observed with full absence of light absorption in dielectric layer (k_d = 0) (curve 1, Fig.9) and with it's minimal value for gold (curve 1, Fig. 6). The crucial value of dielectric layer thickness, where sensitivity of SPR-sensors starts to decrease, depends on the dielectric parameters of gold (Fig. 5) and dielectric layer (Fig. 6-9) as well as on the size of biomolecules (Fig. 7) and changes from 32 nm (curve 1, Fig. 8) up to 65 nm (curve 3, Fig. 8), for k_d = 0. For value of k_d = 0.02 properties of a dielectric layer as amplifier of SPR - response are reduce to minimum, and with k_d = 0.2 sensitivity decreases for all cases.

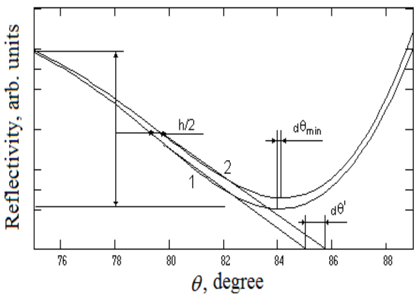

Fig. 11 Comparison of SPR-response for traditional method ($d\theta_{min}$) and for derivatives method (dθ'). Modeling of presence of biomolecules layer with d_{mol} = 10nm on the dielectric layer d_d = 50nm (N_d = 1.5 + 0.02i). 1 – SPR - curve without biomolecular layer, 2 - with biomolecular layer

Parameter of efficiency Q decrease with increasing of k_d for dielectric, (Figure 9, Q = 1.11 for k_d = 0.04 and Q = 1.24 for k_d=0), whereas without dielectric layer Q decrease, if value of k_{Au} for gold raises (Fig. 5). The calculated optimal parameters for dielectric layer with fixed thickness of a gold layer (45 nm) and coefficient of refraction of dielectric layer N_d = 1.5 is: thickness of the dielectric layer 30-50 nm with full absence of light absorption in dielectric layer (k_d=0) (curve 1, Fig. 9) and with it's minimal value for gold (curve 1 Fig. 5). Taking into account the optimized characteristics of a layer of gold (N_{Au} = 0.15 + 3.4i, d_{Au} = 80 nm), theoretically, best rough characteristics for layers gold - dielectric in limits of described model are, for Au: 0.15 + 3.4i, d_{Au} = 80nm, for dielectric: d_d = 20nm, N_d = 1.5. It is necessary to note, that with other base values for a gold film the dependence of sensitivity on parameters of dielectric layer can be changed.

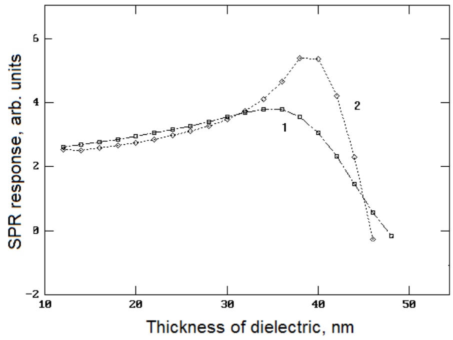

Fig. 12 Dependence of SPR-response for traditional method (1) and derivatives method (2) with variation of dielectric thickness d_d from 10 nm up to 60 nm (biomolecular layer thickness d_{mol} = 10 nm).

C. Method of derivatives

The observable peak character of dependence of sensitivity for SPR-sensor on parameters of multilayer structure is easily explained by change of the form of SPR - curve during variation of parameters of model (Fig. 10). Actually, if for small thicknesses of a dielectric layer the form of SPR-curve differs from a classical form a little, with further increasing of dielectric thickness the minimum of curve is displaced to the right upwards, curve extends and with some threshold value of dielectric thickness great changes of the SPR-curve's form occurs, which explain decreasing of sensor's sensitivity. In this case is attractive, especially for significant values of dielectric thickness, the presentation of the function of sensor's sensitivity as derivative $S = dR/d\theta$ in some certain point, for example, at half-width of SPR-curve (Fig. 11). Here as parameter of sensitivity the shift of crossing point for tangent to SPR- curve and ordinate axis before and after of adsorption of biomolecules can be considered. As obvious from comparison of the diagrams of sensitivity (Fig. 12) for proposed method of derivatives and traditional method of shift for SPR-curve, the first one expresses greater parameter of efficiency, especially with dielectric thickness, close to crucial (Q = 2.12 for a method of derivatives and Q = 1.49 for traditional. With thickness, far from crucial, both methods have similar sensitivity.

IV. CONCLUSION

Parameter of sensitivity for SPR - biosensors is one of important in monitoring of biomolecules, especially for molecules with small mass (<100 Dalton) or for small concentration of analyte (< 1µg/ml). The presented work expands opportunities of a SPR-method, because the obtained results of modeling allow not only to choose the optimal parameters with designing of SPR-sensors, but also to specify researched parameters of bioobjects, provided by direct dependence of SPR-response on values of dielectric constants and thickness of multilayers structure. Actually, it is necessary to have a number of specific nomograms for calculating of the SPR-response which take into account a real values of materials that applied.

REFERENCES

[1] J. Homola, “Model of a chemo-optical sensor based on plasmon excitation in thin silver films”, *Sensors and actuators B*, vol. 11, pp. 481-485, 1993.
[2] B. Liedberg, I. Lundstrom, E. Stenberg, “Principles of biosensing with an extended coupling matrix and surface plasmon resonance, ”*Sensors and Actuators B*, vol. 11, pp. 63-72, 1993.
[3] R. M. A. Azzam and N. M. Bashara, “*Ellipsometry and Polarized Light*”, North-Holland, Amsterdam, 1977.
[4] P. T. Leung, D. Pollard-Knight, G. P. Molan, M. F. Finlan, “Modelling of particle-enhanced sentitivity of the surface-plasmon resonance biosensor, ”*Sensors and actuators B*, vol. 22, pp. 175-180, 1994.