Analysis of Surface Plasmons in a Planar Waveguide System with Spectral Detection — Results of Model Investigations

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The paper presents the results of numerical investigations of the phenomenon of plasmon resonance in a planar waveguide structure, applied in the construction of sensor with spectral detection.

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1. Model investigations of planar structures — assumptions

The paper presents the results of model investigations performed on the theory and software dealt with in the paper [1].

The model investigations presented in this paper required some assumptions, in compliance with which a model of a planar waveguide was used, made by means of the ion exchange Na⁺ \leftrightarrow K⁺ performed on glass BK-7 in a bath of melted KNO₃ at a temperature of 673.15 K for one hour. The calculated profile [2, 3] of the refracting index was then approximated by a system of 14 layers with a constant thickness $d = 0.5 \ \mu m$ and a stepwise changing refracting index.

As the material dispersion of the waveguide layers caused by the ion exchange in the glass BK-7 is inconsiderable (at the polarization TM the refractive index changes in the interval from 450 nm to 780 nm only by 0.00013) [4], this dispersion was disregarded, assuming that the profile of the refracting index as a function of the wavelength changes according to the following law:

$$n(x,\lambda) = n(\lambda) + \Delta n(x)$$

where $n(\lambda)$ — dispersive dependence of the refracting index of the substrate (glass BK-7), $\Delta n(x)$ — spatial distribution of the refractive index caused by the ion exchange.

The assumed dispersive dependences have been taken over, respectively, for the substrate glass from the publication [5], water and SiO₂ from [6, 7], the metal layers Ag, Au and the dielectric layer Al₂O₃ from [8].

Model investigations were carried out on a model of a planar plasmon sensor with spectral detection, the aim of which was to record slight changes of the refractive index occurring in a watery medium — the analyte. The dispersion of this medium was assumed to be the same as that of water.

2. The effectivity of surface plasmons exciting

The effectivity of surface plasmons exciting was investigated in the system presented in Fig. 1. On the planar waveguide an adhesive chromium layer was deposited with a thickness of 2 nm, as well as a film of gold, 10 to 100 nm thick. Above this layer there is the analyte (pure water).



Fig. 1. Analysed arrangement of the layers.

The question arises concerning the thickness of the film of gold, at which the maximum coupling of light propagated in the waveguide with the surface plasmon does occur. Expressing this more precisely, we are trying to find such a thickness of the film of gold at which the largest part mode field penetrates the analyte, and thus, is characterized by the highest attenuation. The characteristics shown in Fig. 2 provides an answer to this question. We see a very high maximum of attenuation connected with the excitation of the surface plasmon. Its values are particularly high when the thickness of the film of gold ranges from 20 to 50 nm. Moreover, the maximum of attenuation changes its position in the domain of the wavelength with the change of the thickness of the film of gold, shifting towards the longer waves with the

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increasing thickness of the film of gold within the limits from 10 to 50 nm.



Fig. 2. Spectral characteristics of attenuation of the mode TM_0 as a function of the thickness of the film of gold.

A further increase of the thickness of this film makes it more and more difficult to excite the surface plasmon through this layer. It ought to be kept in mind that the field propagating in the waveguide couples with the surface plasmon through a layer of metal. Putting it more precisely, we do not have to do with a mode field in the waveguide and a field of surface plasmon, connected with a layer of metal, nor their linear combination. We have to do with the field of the entire system of layers which cannot be separated from each other. When the film of gold is too thick (> 70 nm), the distribution of the field in such a system of layers changes its character, and its part penetrating the region in which the investigated analyte is situated is less and less. In the case of a further increase of the thickness of the metal layer, the character of the quoted dependence stops to change. In the range of shorter wavelengths (< 500 nm) and thicker layers of gold (> 70 nm) the attenuation of the mode is still comparatively high, though this is not connected with the excitation of the surface plasmon, but merely with the form of the dispersive character of the gold and the attenuation of light in such a system. In this range of wavelengths gold does not meet the conditions required to excite effectively the surface plasmons.

The performed model investigations indicate that the most intensive attenuation of the mode TM_0 is achieved when the thickness of the film of gold amounts to $d_{Au} = 40$ nm.

3. Spectral sensitivity of a sensor as a function of the thickness of the metal layer

This section deals with the answer to the question how to choose the proper thickness of the layer of metal so that the sensor would in a watery medium display the maximum spectral sensitivity. It ought to be stressed that this need not be the case when the surface plasmon is excited with the maximum effectiveness, because in the course of changes of the refractive index of the analyte also the field of the excited mode is reconstructed. The considered arrangement of layers has been presented in Fig. 1.

In order to assess the spectral sensitivity of the sensor, two groups of curves of spectral attenuation of the mode TM_0 were plotted. One of them, presented in Fig. 3 is based on the assumption that the medium above the film of gold is water.



Fig. 3. Changes of the spectral characteristics of the sensor in the course of changes of the thickness of the film of gold. All the curves were determined basing on the assumption that water was applied as the analyte.

The other group (Fig. 4) was plotted, assuming that above the gold there is a substance, the dispersive characteristics of which are the same as those of water, but its refractive index had increased by $\Delta n = 0.04$ over the entire considered range of the spectrum.



Fig. 4. Changes of the spectral characteristics of the sensor in the course of changes of the thickness of the film of gold. The respective curves were determined basing on the assumption that the analyte is water with a refracting index increased by $\Delta n = 0.04$.

Comparing these two diagrams, we see that due to the increase of the refracting index of the analyte the curves of attenuation are shifted towards the longer waves. An increase of attenuation is also to be seen in the second case.



Fig. 5. Shift of the plasmon minimum (sensitivity) caused by the increase of the refracting index of the analyte as a function of the thickness of the film of gold. Solid circles — position of plasmon's minimum for $n(H_2O)$ analyte, circles — for $n(H_2O)+0.04$, triangles — plasmon's minimum displacement.

In order to assess the spectral sensitivity of the sensor to changes of the refractive index, the position of the maximum values of the respective curves were determined, as well as their differences concerning the identical thicknesses of the films of gold. The results have been presented in Fig. 5. The obtained result indicates that the sensitivity of this system initially increases with the growing thickness of the film of gold. As soon, however, as the value $d_{Au} = 50$ nm has been reached the value of sensitivity became constant. Therefore, there is no reason to apply films of gold thicker than 50 nm. A further increase of the thickness of gold may even reduce considerably the sharpness of the maximum, so that in the course of measurements it may become difficult to identify it, as can be seen in Figs. 3 and 4. The sensitivity estimated basing on the data quoted in Fig. 5:

$$S = rac{\partial \lambda_{\min}}{\partial n} \,,$$

where λ_{\min} — wavelength corresponding to the minimum transmission in the system, n — refractive index of the analyte at a layer thickness of 50 nm, amounts to about 2350 nm/RIU (RIU — refractive index unit). Assuming that the maximum of attenuation can be localized with an accuracy of about 1 nm, the changes of the refracting index of the analyte can be recorded with an accuracy of about 4.2×10^{-4} .

4. Linearity of the sensor response

Let us try to find the answer to the question whether the response of the sensor depends linearly on the refractive index of the analyte. This is an important problem connected with the practical application of the sensor.

In order to answer this question, the layer arrangement presented in Fig. 1 was investigated within the range of wavelengths from 350 nm to 850 nm. The refractive index of the analyte, was changed in the range

 $\Delta n = 0 \div 0.14$ (such a change corresponds to changes of the refracting index which can be achieved by mixing water and glycerol in adequate proportions). Figure 6 illustrates the attenuation of the mode TM_0 as a function of the wavelength (the parameter is the refractive index of the analyte). This diagram displays the different character of attenuation in the left-hand part of the diagram ($\lambda < 650$ nm) and in its right-hand part $(\lambda > 650 \text{ nm})$, i.e. in the case of smaller refracting indices of the analyte $(n_{\text{anal}} < n(H_2O) + 0.04)$ and the higher ones $(n_{\text{anal}} > n(\text{H}_2\text{O}) + 0.04)$. In the case of wavelengths below 650 nm gold does not completely satisfy the conditions required for the formation of surface plasmons: hence the irregular character of the curves of attenuation. Above this value the curves are quite regular, characterized by a considerable attenuation, exceeding 700 dB/cm.



Fig. 6. Spectral characteristics of the attenuation of the mode TM_0 in the layer system presented in Fig. 1.



Fig. 7. Dependence of the position of the plasmon minimum (mode TM_0) as a function of the refractive index of the analyte.

In spite of that, unfortunately, the successive curves are the result of equally distant changes of the refractive index of the analyte, denoting not the same distances between the positions of the maximum values of attenuation. This is confirmed by the characteristics presented in Fig. 7.

5. The influence of an additional dielectric layer on the characteristics of the layer system

Let us analyze the influence of additional dielectric layers on the parameters of the propagation of the layer system. On a gradient waveguide two layers of metal were deposited: an adhesive layer of chromium, 2 nm thick, and an active film of gold with a thickness of 50 nm. On both these layers a dielectric SiO_2 buffer layer was deposited, and above the buffering layer there is the analyte, i.e. a substance with a similar dispersion as that of water. But for the purpose of analyzing its refractive index may be increased without changing the shape of the dispersive characteristics. This arrangement of layers is to be seen in Fig. 8.



Fig. 8. The analysed arrangement of layers.

Model investigations were carried out in order to find the position of the maximum of spectral attenuation of the mode TM₀ as a function of the thickness of the buffering layer. A parameter in these investigations was the refractive index of the analyte, changing within the range from the refracting index of water $n(H_2O)$ to the refractive index $n(H_2O)+0.12$. The form of these characteristics was also checked in the situation when the buffering layer is not above but below the film of gold without any contact with the analyte. This situation was denoted in the diagram by a negative thickness of the SiO₂ layer.

Figure 9 proves that placing the buffering layer under the active film of gold does not affect essentially the attenuation of the layer system, whereas placing it on the active layer in direct contact with the analyte affects the shape of the attenuation characteristics, including the position of the maximum of attenuation. The maximum of attenuation shifts towards the longer waves with the increasing thickness of this layer.

The regularity consisting in the fact that the shift caused by the buffering layer decreases with the increasing refracting index of the analyte, is also evident. Due to the application of the buffering layer the spectral characteristics of attenuation are shifted considerably towards longer waves only in the case of analytes with a refractive index not deviating from that of water, but the shift decreases with the increase of this index.

The question also arises how the arrangement of the layers should be designed in the case of the determined wavelength of the monochromatic source of light, so that it may be adjusted to the preset refractive index of the analyte. The parameter which will be chosen is the thickness of the buffering layer situated in the layer system



Fig. 9. Position of the plasmon minimum as a function of the thickness of the buffering SiO₂ layer. The parameter of the respective curves is the refractive index of the analyte, $n_{\rm analyte} = n({\rm H}_2{\rm O}) + \Delta n$. The meaning of negative values of the thickness of the SiO₂ layer is dealt with in the text.

between the active film of gold and the analyte. Let us assume for the purpose of further consideration that this wavelength amounts to $\lambda = 680$ nm.

Figure 10 provides an answer to this question, presenting the calculated characteristics of attenuation of the mode TM_0 depending on the thickness of the buffering SiO₂ layer. The parameter is the change of the refracting index of the analyte $(n_{analyte} = n(H_2O) + \Delta n)$.



Fig. 10. Attenuation of the mode TM_0 as a function of the thickness of the buffering layer. A parameter is the refractive index of the analyte $n_{\text{analyte}} = n(\text{H}_2\text{O})$. The wavelength was assumed to be equal to $\lambda = 680$ nm.

Following the selection of the thickness of the buffering layer, another question arises, viz. what will be the characteristics of such a system as a function of changes of the refractive index of the analyte.

Figure 11 presents this characteristic. It is evidently nonlinear, even not unequivocal in a large range of changes of the refractive index. If, however, this range were narrowed, the system of measurements might prove to be very sensitive to even slight changes of the refractive index of the analyte.



Fig. 11. Attenuation of the mode TM_0 as a function of the refractive index of the analyte. A parameter is the thickness of the buffering layer. The wavelength was assumed to be $\lambda = 680$ nm.

6. The influence of the kind of metal layer on the characteristics of the layer system

In order to find out, to which extent the kind of the applied metal layer affects the properties of the layer system, two most essential metals have been taken into consideration, viz. gold and silver. So far numerous results have been quoted concerning layer system containing a layer of gold. Similar model investigation have been performed concerning system including a layer of silver.

In both these cases it has been assumed that we have to do with an identical gradient waveguide as described above. Upon this waveguide an adhesive layer of chromium was deposited, 2 nm thick, and then a film of gold with an optimal thickness (keeping in mind the spectral sensitivity to changes of the refractive index of the analyte). In the case of gold this thickness amounts to 50 nm and in the case of silver to 40 nm. Above these layers there is the analyte. Up till now it has been assumed to be a substance with the same dispersion as that of water and that its refractive coefficient can be changed by $\Delta n \ (\Delta n = 0.00 \div 0.12)$ within the entire range of the spectrum.

The further part of the paper presents the results of model investigations concerning the spectral characteristics of attenuation of the mode TM_0 , determined for various refractive indices of the analyte. In Fig. 12 the results concerning a system with a film of gold have been gathered, and in Fig. 13 those of layer with a layer of silver. For the sake of facilitating comparisons in both these diagrams the same scale has been applied.

The comparison of the characteristics of both these systems speaks for the layer of silver, due to several reasons. Firstly, its characteristics are more homogeneous in a wider range of wavelengths, displaying a higher attenuation of about 1000 dB/cm (in the case of gold it amounts only to 600 dB/cm). The presented diagrams also indicate a higher sensitivity of the spectral characteristics of attenuation to changes of the refracting index of the analyte in the case of the system with a layer of



Fig. 12. Spectral characteristics of the attenuation of a layer system including a film of gold.



Fig. 13. Spectral characteristics of the attenuation of a layer system including a film of silver.

silver. As a matter of fact, the only factor speaking in favour for gold is its chemical stability, which is, however, essential because it is very often used, in the layers of gold. But in systems in which the metal layer does not contact directly the analyte, the application of silver layers ought to be considered as being of much importance.

7. The effect of a spatial distribution of the refractive index of the waveguide upon the characteristics of the layer system

In order to investigate the effect of the spatial distribution of the refractive index of a planar waveguide contained in the layer structure upon the characteristics of such system model investigations had been carried out. Assuming that identical layer structures deposited on multimode planar waveguide would have to be compared, i.e. on a gradient and on step-index one. The thickness of the latter waveguide was chosen so as to contain the same number of modes as the considered gradient waveguide. The gradient waveguide was assumed to have been formed in result of the ion exchange Na⁺ \leftrightarrow K⁺ in glass BK-7 for 4 h at a temperature of 673 K. The waveguide of the step-index type, on the other hand, results from depositing on the substrate (glass BK-7) a homogeneous waveguide layer with a thickness of 5 μ m and a refractive



Fig. 14. Results of calculations concerning the gradient waveguide (as described in the text).



Fig. 15. Results of calculations concerning the step-index waveguide (described in the text).

index of the same value as that of the refractive index of the gradient waveguide on the surface ($\Delta n = 0.00882$). Applying these parameters of the step-index waveguide, both waveguides contain the same number of modes. On both of them first a layer of chromium, 2 nm thick, was deposited, followed by a film of gold with a thickness of 50 nm. Above the last layer there is the analyte (pure water), which does not undergo any changes while its properties are being investigated. As both these layer systems are composed of the same materials, their dispersive properties are in these investigations the same.

The results of investigations concerning the system of layers with a gradient waveguide have been presented in Fig. 14, and those concerning the step-index waveguide in Fig. 15. The maximum values of the attenuation of all modes in both cases are positioned, at the same spot $(\lambda = 550 \text{ nm})$ which indicates that the position of the plasmon resonance is in the domain of wavelengths conditioned first of all by the dispersive characteristics of the materials composing the layer system. No influence is, however, exerted on them by the spatial distribution of the refractive index, although it affects essentially the attenuation of the respective modes. While in the case of the gradient waveguide the mostly attenuated mode is the mode of zero order, and the mode of higher orders are less and less attenuated, in the case of the step-index waveguide it is just the opposite. The reason for this must be accounted for by the distribution of the fields in both types of waveguides.

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