Optical and Acoustical Methods in Science and Technology

Analysis of Surface Plasmons in the Optical Planar Waveguide with Spectral Detection

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The paper deals with investigations concerning the plasmon resonance in an optical planar waveguide structure, applied in the construction of sensors with spectral detection. The surface plasmons in a multi-layer planar structure (with complex refractive indices) have been described, as well as the way of numerical solutions of physical equations describing the propagating electromagnetic field in such structures. The physical interpretation of obtained results has been presented, too.

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1. Introduction

Surface plasmons were observed for the first time by Wood already at the beginning of the 20th century, in the course of investigating the diffraction of light on metallic grids (the so-called Wood anomalies). Later on, the phenomenon of surface plasmons was used for the purpose of measuring the optical properties of thin metallic layers.

Literature all over the world provides references concerning the application of the surface plasmon resonance (SPR) in numerous devices, e.g. light modulators [1] and spatial modulators of light [2], bistable devices [3], facilities for the generation of the second harmonic [4], tunable optical filters [5]. The two latest decades yielded a lot of information concerning the application of SPR in sensors. At first these were devices constructed basing on Kretschmann’s configuration (of the surface type) [6], later also devices with planar optical waveguides [7, 8] and strip waveguides [9]. At the same time, the structure and physical principles of operation of such waveguide polarizers [10] were presented. Lately the microscopy of the near field has been vehemently developing [11].

The phenomena utilized in these devices and the description of the properties of surface plasmons in layered structures are based on the description of the electromagnetic surface wave in layered media containing metallic layers. Therefore, further on the electromagnetic surface wave will be dealt with.

Most of these publications, both theoretical and experimental ones, assume the detection of the measurement signal on one given wavelength. This is an amplitudinal detection, sensitive to changes of attenuation in the path of transmission. The present paper is devoted to the spectral detection of the SPR measurement signal. The detection concerns the position of the minimum spectral transmittance. The publications [12–16] also deal with the problem, but do not profoundly. Therefore, further investigations have been required, leading to the publication of the present paper.

2. Electromagnetic surface wave

The electromagnetic surface wave propagates along the boundary between two media characterized by different values of the dielectric permittivity. The amplitude of this wave fades exponentially in both media. Its existence is predicted by Maxwell’s equations with considered respective boundary conditions. If the vector of the magnetic field of this wave is situated in the incident plane, perpendicularly to the direction of propagation of the wave, the wave displays the polarisation of the $p$-type (type TM). In the case of such a polarized wave we have to do with discontinuity of the normal component of the electric field at the boundary between the media, due to the presence of the surface electrical charges along this boundary. The electromagnetic wave is responsible for the changes in the density of the surface charge and it is strictly connected with them. This is the way this wave is connected with the boundary between the media, and hence its surface nature. When both media are non-lossless such a wave is called surface Fano wave, and if one of the media is lossy, it is called Zenneck’s wave [17–19].

3. Stratified system

3.1. Theoretical description of the arrangement of the layers

In order to describe the phenomena occurring in the planar system, the arrangement of the layers presented in Fig. 1 was considered. The number of layers in the structure is unlimited. The respective layers are homogeneous, generally characterized by a complex refractive index; thus they may be both dielectric or metallic layers [20–22].

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Fig. 1. Geometry of the considered arrangement of layers. Inserts in the figure shows the spatial distribution of the magnetic field $H_y(x)$.

Light propagates perpendicularly to the plane $XOY$ in the direction of $+Z$ (right-handed coordinate system). In the direction $Y$ the layers are arranged from $-\infty$ to $+\infty$, so that in the solutions they should not depend on the coordinate $Y$. We assume that we have to do with monochromatic wave and the dependence on time takes the form $exp(i\omega t)$. The amplitudes of the fields satisfy in each layer the Helmholtz equation:

$$\nabla^2 \psi_k + k^2 \psi_k = 0,$$

(1)

where $\psi_k$ denotes $E_Y$ or $H_Y$, respectively, for the wave TE or TM, $k$ — denotes the number of the given layer, $k_k = \frac{k_0 n_k}{\omega}$ — wave number in the $k$-th layer where $k_0 = \frac{\lambda_0}{2\pi}$ is the wave number of light in vacuum, $\lambda_0$ — wavelength in a vacuum.

The field of the mode has been assumed to take the following form:

$$\psi_k(x, z) = \psi_k(x) exp(-j k_z z),$$

(2)

where $k_z = \beta + j \alpha$ is the $z$-th component (in the direction of propagation) of the complex constant of propagation, $\beta$ — propagation constant ($\beta > 0$ — for propagation in the direction of $+Z$), $\alpha$ — constant of attenuation ($\alpha < 0$ — attenuation), $k_z = k_0 n_{eff}, n_{eff}$ — effective refracting index of the mode, $j$ — imaginary unit.

Substituting (2) into (1) we get

$$\frac{d^2 \psi_k}{dx^2} + \gamma_k^2 \psi_k = 0,$$

(3)

where

$$\gamma_k = k_0 \sqrt{n_k^2 - n_{eff}^2},$$

(4)

$\gamma_k$ — component of the wave vector along the $X$ direction.

Expression (4) determines the quantity $\gamma_k$ with accuracy to the sign. Further on, one of the two values will be chosen for which $\text{Im}\{\gamma_k\} < 0$.

The solution of Eq. (3) for any arbitrary layer is expressed by the formula (5) and includes two components of the distribution of amplitudes along the axis $+X$ and $-X$.

$$\psi_k(x) = A_k e^{-j \gamma_k (x-x_{k-1})} + B_k e^{j \gamma_k (x-x_{k-1})}$$

for $\gamma_k \neq 0$,\n
$$\psi_k(x) = A_k + B_k x$$ for $\gamma_k = 0$, \n
(5)

where $A_k, B_k$ — constant values, $d_k = x_k - x_{k-1}, d_0 = 0$.

As $n_k$ generally is a complex quantity, the values $A_k, B_k, \gamma_k, n_{eff}$ are also complex values. The function $\psi_k(x)$ for the case $\gamma_k = 0$ has been applied here because of the formal reasons, but it will not be taken into account in further considerations being rather improbable in numerical solutions. Wishing the field to disappear outside the system of layers, we assume that

$$A_0 = 0, \ B_0 = 1, \ B_N = 0.$$ \n
(6)

Moreover, at each boundary between the layers, the conditions of continuity must be satisfied, which in the case of the boundary $k$ may be expressed as follows:

$$\psi_k(x) = \psi_{k+1}(x)|_{x=x_k}$$ for the modes TE and TM,

(7)

$$\frac{d\psi_k(x)}{dx} = \begin{cases} \frac{d\psi_{k+1}(x)}{dx}\bigg|_{x=x_k} & \text{for the modes TE,} \\ \frac{n_k^2}{n_{k+1}^2} \frac{d\psi_{k+1}(x)}{dx}\bigg|_{x=x_k} & \text{for the modes TM.} \end{cases}$$

(8)

Taking into account the conditions of continuity at the boundaries of the layers (7) and (8) in the set of Eqs. (5), we get the relation of recurrence which permits to determine $A_{k+1}$ and $B_{k+1}$, when the values $A_k$ and $B_k$ are known

$$A_{k+1} = \frac{1}{2} (1 + \Gamma_k) A_k e^{-j \gamma_k d_k} + \frac{1}{2} (1 - \Gamma_k) B_k e^{j \gamma_k d_k},$$

$$B_{k+1} = \frac{1}{2} (1 - \Gamma_k) A_k e^{-j \gamma_k d_k} + \frac{1}{2} (1 + \Gamma_k) B_k e^{j \gamma_k d_k}$$

(9)

where

$$\Gamma_k = \frac{n_k}{n_{k+1}} \kappa_k,$$

$$\kappa_k = \begin{cases} 1 & \text{for TE,} \\ \frac{n_k^2}{n_{k+1}^2} & \text{for TM.} \end{cases}$$

Equation (9) can be more conveniently expressed by the matrix

$$\begin{pmatrix} A_{k+1} \\ B_{k+1} \end{pmatrix} = W_k \begin{pmatrix} A_k \\ B_k \end{pmatrix},$$

(10)

where

$$W_k = \begin{pmatrix} \frac{1}{2} (1 + \Gamma_k) e^{-j \gamma_k d_k} & \frac{1}{2} (1 - \Gamma_k) e^{j \gamma_k d_k} \\ \frac{1}{2} (1 - \Gamma_k) e^{-j \gamma_k d_k} & \frac{1}{2} (1 + \Gamma_k) e^{j \gamma_k d_k} \end{pmatrix}.$$

As the values of the coefficients $A_0$ and $B_0$ have been assumed (cf. Eq. (6)), basing recurrently on Eq. (10), all the unknown indices $A_k$ and $B_k$ can be determined. This is, however, reduced to the following expression:

$$\begin{pmatrix} A_N \\ B_N \end{pmatrix} = W_{N-1} \cdots W_{N-2} \cdots W_1 W_0 \begin{pmatrix} A_0 \\ B_0 \end{pmatrix}.$$ \n
(11)

The values in matrices $W_k$ depend on the physical parameters of the $k$-th and $k+1$-th layers, and not on the coefficients $A_k$ and $B_k$. Thus, the matrices $W_k$ may be
multiplied independently of the knowledge of the coefficients $A_0$, $B_0$, $A_N$, $B_N$. The product of the matrices $W_k$ describes the physical properties of the successive layers as a function of the effective refractive index $n_{\text{eff}}$. The dependence on $n_{\text{eff}}$ is concealed in the component of the wave vector along the axis $X$, i.e. in the quantity $\gamma_k$.

The formal reason, i.e. in order to multiply the matrices successively according to the number of the layer, Eq. (11) has been transformed as follows:

$$
\begin{pmatrix}
A_0 \\
B_0
\end{pmatrix} = G(n_{\text{eff}}) \begin{pmatrix}
A_N \\
B_N
\end{pmatrix},
$$

(12)

where

$$
G(n_{\text{eff}}) = C \cdots G_0 \cdots G_k \cdots G_{N-1},
$$

$$
C = \frac{1}{\det(W_0) \cdots \det(W_k) \cdots \det(W_{N-1})},
$$

$$
G_k = \begin{pmatrix}
\frac{1}{2} \left( 1 + \Gamma_k \right) e^{j \gamma_k d_k} & -\frac{1}{2} \left( 1 - \Gamma_k \right) e^{j \gamma_k d_k} \\
-\frac{1}{2} \left( 1 - \Gamma_k \right) e^{-j \gamma_k d_k} & \frac{1}{2} \left( 1 + \Gamma_k \right) e^{-j \gamma_k d_k}
\end{pmatrix}.
$$

The last Eq. (12) may also be expressed as

$$
\begin{pmatrix}
A_0 \\
B_0
\end{pmatrix} = \begin{pmatrix}
g_{11}(n_{\text{eff}}) & g_{12}(n_{\text{eff}}) \\
g_{21}(n_{\text{eff}}) & g_{22}(n_{\text{eff}})
\end{pmatrix} \begin{pmatrix}
A_N \\
B_N
\end{pmatrix},
$$

(13)

where

$$
G(n_{\text{eff}}) = \begin{pmatrix}
g_{11}(n_{\text{eff}}) & g_{12}(n_{\text{eff}}) \\
g_{21}(n_{\text{eff}}) & g_{22}(n_{\text{eff}})
\end{pmatrix}.
$$

Substituting into Eqs. (15) the conditions which should ensure the disappearance of the field outside the arrangement of the layers (6), the last equation is reduced to the following set of equations:

$$
\begin{cases}
g_{11}(n_{\text{eff}}) A_N = 0, \\
g_{21}(n_{\text{eff}}) A_N = 1.
\end{cases}
$$

(14)

The first of these two Eqs. (14) is the so-called characteristic one for the system of layers and permits to determine $n_{\text{eff}}$ — the refractive indices of the respective modes. In order to determine the distribution of the fields of modes, however, further coefficients $A_k$, $B_k$ are required, calculated by means of Eq. (10), after a previous substitution of the determined $n_{\text{eff}}$. The distribution of the fields can now be determined making use of Eq. (5). The distribution of the field is: $H_Y$ at the polarization TM (or $E_Y$ at the polarization TE). The other components at the polarization TM can be determined applying Maxwell’s equations

$$
E_z = \frac{j}{\omega \varepsilon} \frac{\partial H_y}{\partial x}, \quad E_x = \frac{-k}{\omega \varepsilon} H_y.
$$

(15)

Coming back to the first equation in the set (14), it must satisfy the formula (when $A_N \neq 0$):

$$
g_{11}(n_{\text{eff}}) = 0.
$$

(16)

As the solution of this equation is to be looked for in the domain of complex number, it disintegrates into a set with two true (real) equations of the complex variable $n_{\text{eff}}$:

$$
\begin{cases}
\Re\{g_{11}(n_{\text{eff}})\} = 0, \\
\Im\{g_{11}(n_{\text{eff}})\} = 0.
\end{cases}
$$

(17)

It is to be kept in mind that the coefficients in this set of equations, viz. the parameters of the layers, the wave numbers, are generally complex values, and that the equations are nonlinear equations, because of searching $n_{\text{eff}}$. This is why the solutions had to be found by means of numerical methods.

### 3.2. The method of solving characteristic equations

In order to find solutions of the set of Eqs. (17), consisting in the determination of $n_{\text{eff}}$ (effective refractive indices) and the distribution of the fields, a numerical program has been developed. As far as the solution of non-linear equations by means of numerical methods in the domain of real numbers does not prove to be a problem, solutions in the domain of complex numbers (on the complex plane) have not rendered up to now any general algorithms of procedures.

The first problem which had to be solved was the separation of the solutions (the number of which had been earlier unknown). For this purpose on a rectangular complex region a network of adequately densely distributed points was constructed, in which — in order to separate the minimum values — the surface, defined in the following way, could be sampled:

$$
F(n_{\text{eff}}) = |\Re\{g_{11}(n_{\text{eff}})\}| + |\Im\{g_{11}(n_{\text{eff}})\}|.
$$

(18)

This surface is rather complex, and the derivative is not everywhere continuous. Evidently, the places in which the value of this surface is nought, are the solutions which have to be found, but not all the minimum values in this surface are the required solutions. What is more, this method is rather slowly convergent. Therefore, it was applied to separate the places indicating that nearby there may be the solution that is being looked for. Then, around these places equations of two planes (constructed at three points of the surrounding) were determined, defined by both these Eqs. (17). These planes approximated the surfaces resulting from (17) in their immediate neighbourhood. Having got these two planes, their common point with the third plane $Z = 0$ was determined. Such a procedure is quickly convergent if we approach a solution while starting this procedure (provided the surfaces defined by Eqs. (17) can be approximated by the planes).

As in this consideration no assumptions have been made concerning the number of layers, this method may be also applied to find one’s own solutions and field modes in planar gradient waveguides. What is merely required is to approximate the gradient distribution of the refracting index basing on the arrangement of many layers with a homogeneous refractive index within each of them. Therefore, this method is adequate for the solution of planar waveguides real parameters. The obtained numerical programme has been organized in such a way that it can be used to determine solutions, taking into account the dispersive properties of all the layers in this model. This feature is extremely important in the case of modelling the phenomena occurring in waveguides in which the excited surface plasmons are to be investigated, and
their excitation is detected spectrally. The solution of the layer arrangement is a set of the effective complex refractive indices of the respective waveguide modes. Their real part $\text{Re}(n_{\text{eff}})$ is responsible for the phase velocity of the mode, whereas the imaginary part is responsible for its attenuation.

4. Interpretation of the numerical results

As the own solutions of the layer arrangements with complex parameters are complex quantities, there arise some problems in their interpretation. In the case of real parameters of the arrangement of the layers we merely need to mark the solutions with numbers in the order of the decreasing refractive indices and thus decide which mode is the mode of the zero order and which is a mode of the higher order. Such a procedure is, however, unjustified in the case of the solution of a layer system with complex parameters. The program developed and applied by the author of the presented paper classifies the solutions in the order of the decreasing real part of the solutions. This does not suffice, however, to interpret the solutions. Further on, the shapes of the fields of the respective modes must be considered. As an example of the procedure to be followed in every case after numerical results have been obtained, let us quote the example of the arrangement of the layers defined in Fig. 2.

Fig. 2. The considered arrangement of layers.

Besides the gradient waveguide resulting from the exchange of ions $\text{Na}^+ \leftrightarrow \text{K}^+$, taking place in glass BK-7 at a temperature of 673 K in the time $t = 1$ h, this system includes a dielectric buffering layer of $\text{Al}_2\text{O}_3$ with a thickness of 200 nm. This layer is coating with a layer of chromium, 2 nm thick, and an active layer of silver, 40 nm thick. Above this system of layers there is an analyte. In the considerations it has been assumed that water is used as the analyte, the refractive index of which had been increased by $\Delta n = 0.12$. The behaviour of modes with the polarization TM of the arrangement of layers as function of the wavelength was investigated within the range from 350 nm to 850 nm. The obtained results have been gathered in Fig. 3.

The numeration of the modes presented in the diagram results merely from the values of the actual part of the effective refractive index, i.e. the mode with the highest value in the real part is zero mode, whereas that with a lower value is a mode of the first order. In order to prove that such an interpretation is inadequate, let us consider the same solutions, taking, however, also into account the distribution of the modes of the fields. The evolution of the fields as a function of the wavelength has been presented in Fig. 4, showing in which way the spatial distributions of the mode fields are changing in the function of the wavelength concerning each mode. The upper curves of the distribution of the fields correspond to modes of the lower order, the bottom curves to modes of the higher order. Scanning these distributions, we can classify them into four groups which are the leading groups. They have been denoted by the symbols A, B, C, and D. The axis of coordinates ($Y$-axis) indicates in the diagram the position of the boundary between the analyte and the silver layer.

Group A. The shape of the field indicates that this is the mode $\text{TM}_1$. The plasmon field connected with it is excited along the boundary between the buffering layer ($\text{Al}_2\text{O}_3$) and the layer of chromium. Thus, the excitation occurs inside the arrangement of layers and “sees” the analyte only to a slight extent. This mode exists in the system merely in a small range of wavelengths, because already at a wavelength of 470 nm it is cut off.

Group B. This is the mode $\text{TM}_0$. The plasmon field connected with this mode is excited similarly as before along the boundary between the buffering layer ($\text{Al}_2\text{O}_3$) and the layer of chromium. Thus, the excitation occurs inside the arrangement of layers and “sees” the analyte only to a slight extent. This mode exists in the system merely in a small range of wavelengths, because already at a wavelength of 470 nm it is cut off.

Group C. The shape of the field module inside the dielectric waveguide indicates that it is also the $\text{TM}_0$ mode, although in this case the plasmon field is excited along the boundary between the analyte and the silver layer. This mode occurs only at the wavelength of about 490 nm, and is from the very beginning characterized by an extremely large attenuation of the order 1700 dB/cm. The attenuation decreases with the increasing wavelength, and at 810 nm, more or less, the attenuation again rises to about 300 dB/cm.

Fig. 3. Results of the numerical simulation of the arrangement of layers presented in Fig. 2.
Group D. The field of this mode differs considerably from those described so far. First of all, it is connected with the boundary between the analyte and the silver layer. Most of the energy of this field is localized in the analyte, and the field in the waveguide occurs “so to say by chance”. The field of this mode reminds one remarkably the distribution of the surface plasmon field, with which we have to do in Kretschmann’s volumetric systems. Because of the strong interaction with the analyte, the attenuation of this mode is considerable, amounts to more than 1800 dB/cm. The characteristic feature of this solution is the extremely large variation of both the real and imaginary parts of the effective refractive index as a function of the wavelength. This is why this mode is a leading mode only in a narrow range of wavelengths (760 nm to 800 nm). It occurs also beyond this region, but because of the narrow range of variation of the wave vector which can be excited in the waveguide, this mode cannot be excited by the waveguide mode. Referring to the accepted nomenclature, it is short-range plasmon mode (SRSP) excited by a planar waveguide.

Figure 5 presents the corrected interpretation of the results obtained in the course of numerical calculations. Such an analysis cannot be performed automatically making use a numerical programme. It must be carried out each time after having got the numerical results.

One more feature ought to be mentioned here, not encountered in layered system with real parameters. The number of modes in systems with real parameter decreases with the increase of the wavelengths. In the case presented in Fig. 5 the number of modes varies with the increasing wavelengths in the following way:

- 350–470 nm ⇒ 2 modes (A,B),
- 480–600 nm ⇒ 2 modes (B,C),
- 610–750 nm ⇒ 1 mode (C),
- 760–800 nm ⇒ 2 modes (C,D),
- above 800 nm ⇒ 1 mode (C).

This indicates that while developing the software for the purpose of solving a characteristic equation, it is impossible to find solutions by releasing stepwise the complex parts of the parameters of the arrangement of layers, because this might cause omission of some solutions. In our case solution D would be omitted.
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