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SIMULATION OF SURFACE PLASMON PROPAGATION IN PLANAR WAVEGUIDES

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Surface plasmon propagation in a multilayer planar waveguide structure was studied. We are proposing an algorithm for solving the characteristic equation in order to determine the complex effective refractive index n_{eff}. The absolute minimum of the complex characteristic equation is determined in three steps considering the nodes of an increasingly refined mesh. After each step a new mesh is created around the node of the previous mesh in which the minimum was found. Tests on a 4-layer structure proved that the algorithm is convergent, rapid and accurate.

Keywords: surface plasmons, planar waveguides, plasmonic waveguides.

1. Introduction

Surface plasmons are free electron oscillations that exist at the interface between a metal and a dielectric medium, materials with opposite signs of the real parts of the dielectric constants [1-3]. Their propagation creates a localized electromagnetic wave, which attenuate rapidly during the propagation due to the intrinsic electron oscillation damping loss in the metal. Surface plasmon waves guided by multiple parallel thin metal films placed closely together have been studied [4]. Surface plasmon resonance found applications in various devices, as light modulators [5-6], bistable devices [7], second harmonic generation facilities [8] and tunable optical filters [9]. Sensors were built as SPR applications, using Kretschmann's configuration [10], planar waveguides [11-12] and strip waveguides [13]. These promising applications created a need for modeling with the aim to better design the waveguide. In this paper we changed our approach in

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modeling plasmon propagation in planar waveguides [14-15], finding an absolute minimum by mesh refining.

2. Surface plasmon propagation equations

Equations describing surface plasmon propagation are derived from Helmholtz equation applied for each layer. The layers geometry taken into consideration is presented in Fig. 1. Noting by N the number of layers, each layer (or medium) k (layer ordinal number, varying from 0 to N) has refractive index n_k and thickness d_k. First and last medium is semi-infinite, of refractive indices n_0 and n_N and thicknesses d_0 and d_N.

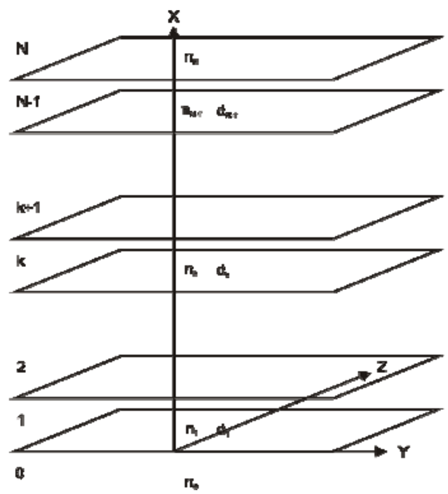

Fig. 1. Schematic representation of the layers geometry. At left layer ordinal number. For k = 0 to N, n_k – complex refractive index of the layer, d_k – the thickness of the same layer.

As derived in [16], the amplitudes of the fields satisfy the next equation:

$$\frac{d^2\psi_k}{dx^2} + \gamma_k^2 \cdot \psi_k = 0\ , \qquad (1)$$

where ψ_k denotes E_Y (for the wave TE) or H_Y (for the wave TM), k denotes the number of the given layer (from 0 to N) and γ_k represents component of the wave vector along the X direction:

$$\gamma_k = k_0 \cdot \sqrt{n_k^2 - n_{eff}^2}\ , \qquad (2)$$

where $k_0 = \frac{2\pi}{\lambda_0}$ represents the wavenumber at wavelength λ_0 in vacuum, n_k is the refractive index of the k^{th} medium and n_{eff} denotes the complex effective refractive index. Equation (1) has as solution for any arbitrary layer that expressed in equation (3), which includes two components of the distribution of amplitudes along the axis +X and -X.

$$\psi_k(x) = A_k \cdot \exp\left[-i \cdot \gamma_k \cdot \left(x - x_{k-1}\right)\right] + B_k \cdot \exp\left[i \cdot \gamma_k \cdot \left(x - x_{k-1}\right)\right], \quad (3)$$

where A_k and B_k are complex constants, $d_k = x_k - x_{k-1}$, $d_0 = 0$. Each of them is attached to a layer k (from 0 to N). Initial and final values are $A_0 = 0$, $B_0 = 1$ and $B_N = 0$, because we want the field to disappear outside the system of layers. In this situation d_0 and d_N are zero. Constants A_k and B_k can be determined iteratively as:

$$\begin{aligned} A_{k+1} &= A_k \cdot \frac{1+\Gamma_k}{2} \cdot \exp\left(-i \cdot \gamma_k \cdot d_k\right) + B_k \cdot \frac{1-\Gamma_k}{2} \cdot \exp\left(i \cdot \gamma_k \cdot d_k\right) \\ B_{k+1} &= A_k \cdot \frac{1-\Gamma_k}{2} \cdot \exp\left(-i \cdot \gamma_k \cdot d_k\right) + B_k \cdot \frac{1+\Gamma_k}{2} \cdot \exp\left(i \cdot \gamma_k \cdot d_k\right) \end{aligned}, \quad (4)$$

Here Γ_k is determined as:

$$\Gamma_k = \begin{cases} \dfrac{\gamma_{k+1}}{\gamma_k} & \text{for TE mode} \\ \dfrac{\gamma_{k+1}}{\gamma_k} \cdot \left(\dfrac{n_k}{n_{k+1}}\right)^2 & \text{for TM mode} \end{cases}, \quad (5)$$

It can be demonstrated that:

$$\begin{bmatrix} A_0 \\ B_0 \end{bmatrix} = g\left(n_{eff}\right) \times \begin{bmatrix} A_N \\ B_N \end{bmatrix}, \quad (6)$$

where $g\ (n_{eff})$ is defined as:

$$g\left(n_{eff}\right) = \begin{bmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{bmatrix} = \prod_{k=1}^{N} \begin{bmatrix} \frac{1+\Gamma_k}{2} \cdot \exp\left(i \cdot \gamma_k \cdot d_k\right) & \frac{1-\Gamma_k}{2} \cdot \exp\left(i \cdot \gamma_k \cdot d_k\right) \\ \frac{1-\Gamma_k}{2} \cdot \exp\left(-i \cdot \gamma_k \cdot d_k\right) & \frac{1+\Gamma_k}{2} \cdot \exp\left(-i \cdot \gamma_k \cdot d_k\right) \end{bmatrix}, \quad (7)$$

Putting the boundary conditions ($A_0 = 0$, $B_0 = 1$ and $B_N = 0$) in equation (6) we get:

$$\begin{aligned} g_{11} \cdot A_N &= 0 \\ g_{21} \cdot A_N &= 1 \end{aligned}, \quad (8)$$

For $A_N \neq 0$ the first condition of equation (8), which is the so-called characteristic equation for the system of layers and permits to determine n_{eff}, becomes (g_{11} is complex):

$$\begin{aligned} \mathrm{Re}\left\{g_{11}\left(n_{eff}\right)\right\} &= 0 \\ \mathrm{Im}\left\{g_{11}\left(n_{eff}\right)\right\} &= 0 \end{aligned}, \quad (9)$$

The solution (complex) of the above equations is the complex effective refractive index, n_{eff}.

3. Simulation algorithm

The idea that substantiates this algorithm is to replace the seeking of zero (the solution) of the complex function g_{11} with finding first of all a minimum of this function over a given domain. In order to do this the function is calculated in the nodes of a mesh that cover the domain of the possible existence of the solution of the form (Re$\{n_{eff}\}$, Im$\{n_{eff}\}$) and an absolute minimum is calculated. The number of mesh nodes should be large enough to avoid missing the true solution but small enough to keep the execution time within reasonable limits. Tests on a three-layer structure indicated a number of nodes satisfying both criteria as being 250. Further there are two more steps in which a minimum is searched again around the minimum found in the previous step.

The simulation of surface plasmon propagation is aimed to be a tool in planar waveguides design. Therefore is important to find out the thickness of a certain layer which ensures the best results. The algorithm allows the user to vary the thickness of a selected layer in order to create a data base of results that will help him designing the waveguide. In our tests, the selected layer was number 2 (gold) in 20 steps of 50 nm. The number of steps, the step size and the layer number to be varied are all settable by user.

The algorithm is described in Fig. 2. After reading structure data from a .csv file (complex refractive index and thickness of each layer), the selected layer (denoted by j) gets a number i_{max} values multiple of Δ_d in a loop (i = 1 to i_{max}). Inside this loop d_j (initialized to 0 outside the loop) is incremented each time by Δ_d and three steps are performed:

- Step 1: initial mesh is set, g_{11} is calculated over this mesh and a minimum is found. The step is performed separately for TE mode and for TM mode.
- Step 2: a zoomed mesh is set, g_{11} is calculated over this mesh and a minimum is found. The step is also performed separately for TE mode and for TM mode.

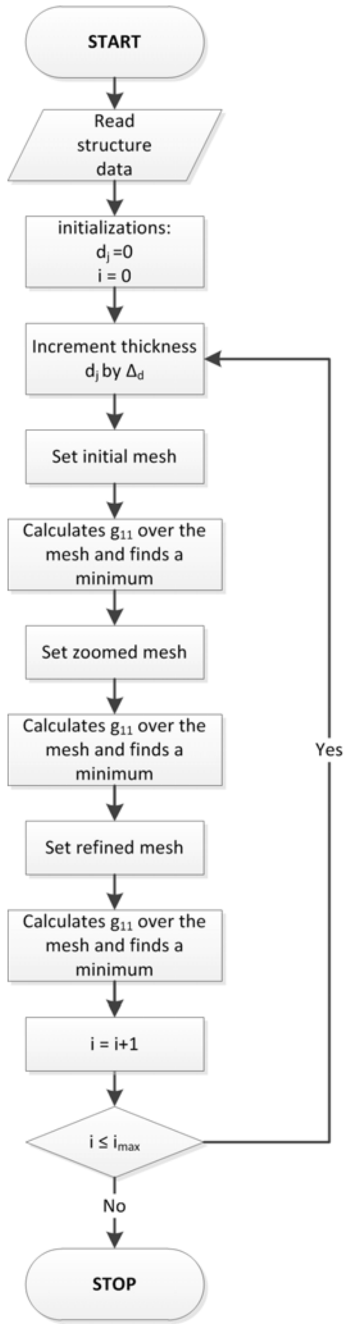

Fig. 2. The algorithm used to simulate the surface plasmon propagation.

- Step 3: a refined mesh is set, g_{11} is calculated over this mesh and a minimum is found. The step is also performed separately for TE mode and for TM mode.

4. Results

The algorithm was tested on the structure presented in Table 1. The structure was a 4-layer one: air – As_2S_3 – gold – BK7 optical glass, studied at the wavelength 632.8 nm.

The meshes (initial, zoomed and refined) had 250 x 250 nodes each.

Table 1. Structure data for algorithm testing.

Layer	Re (n)	Im (n)	d [nm]
0	1.00000	0	0
1	2.47200	0	500
2	0.18377	3.4313	50 to 1000 step 50
3	1.51509	0	0

The results are summarized as plots in Fig. 3. Solution finding process is illustrated separately for TE mode (Fig. 3 (a) to (c)) and for TM mode (Fig. 3 (d) to (f)).

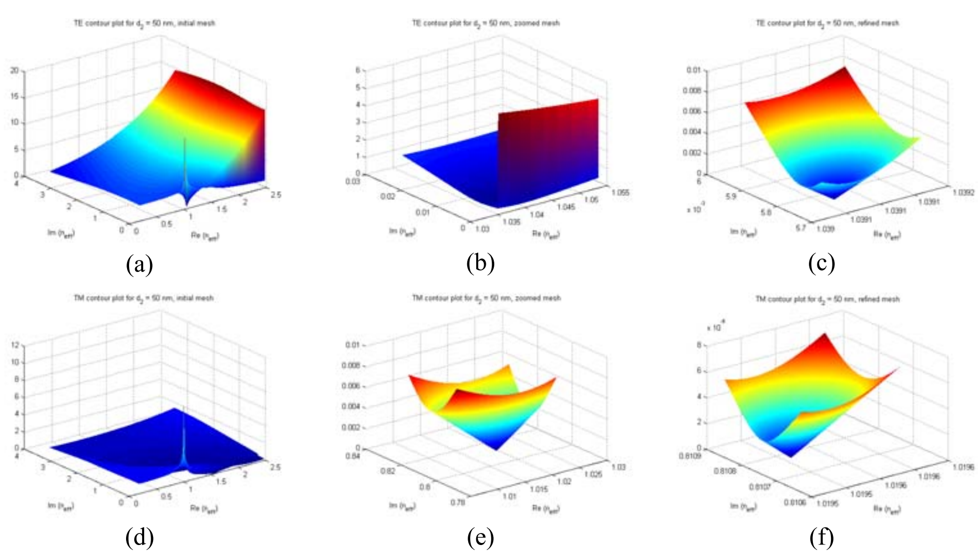

Fig. 3. Plot of Re (g_{11}) illustrating solution finding process for TE and TM modes at d_2 = 50 nm:
(a) TE mode, initial mesh, (b) TE mode, zoomed mesh, (c) TE mode, refined mesh,
(d) TM mode, initial mesh, (e) TM mode, zoomed mesh, (f) TM mode, refined mesh.

Numerical results of this tests are summarized in Table 2. The evolution of the found solution is then visible for each mesh refinement both as graphics and numerical.

Table 2. Results of algorithm tests.

Mode	Result item		Initial mesh	Zoomed mesh	Refined mesh
TE	Re {n_{eff}}	From	0.18377	1.03500	1.03900
		To	2.47200	1.05330	1.03920
		Step	0.0091529	7.3223e-05	5.8579e-07
	Im {n_{eff}}	From	0	0	0.0057097
		To	3.43130	0.02745	0.0059293
		Step	0.013725	0.0001098	8.7841e-07
	min (Re {n_{eff}})	Position	95	57	82
		Value	1.0441	1.0391	1.0391
	min (Im {n_{eff}})	Position	2	54	66
		Value	0.0137	0.0058	0.0058
	$\|g_{11}$ min$\|$		0.3855	0.0027	0
	g_{11} min		0.2248 + 0.3132i	0.0010 + 0.0025i	0
TM	Re {n_{eff}}	From	0.18377	1.00750	1.01950
		To	2.47200	1.02580	1.01960
		Step	0.0091529	7.3223e-05	5.8579e-07
	Im {n_{eff}}	From	0	0.79606	0.81067
		To	3.43130	0.82351	0.81088
		Step	0.013725	0.0001098	8.7841e-07
	min (Re {n_{eff}})	Position	92	165	73
		Value	1.0167	1.0195	1.01954
	min (Im {n_{eff}})	Position	60	135	129
		Value	0.8098	0.81077	0.81078
	$\|g_{11}$ min$\|$		0.0014	0	0
	g_{11} min		-0.0011 - 0.0009i	0	0

5. Conclusions

The algorithm proposed to simulate the surface plasmon propagation proved to be effective and accurate. For each mesh (of 250 nodes) the algorithm finds the local minimum of $|g_{11}|$ at a node placed at position specified in Table 2 as min (Re {neff}) Position and min (Im {neff}) Position, which means the values specified as min (Re {neff}) Value and min (Im {neff}) Value.

Sometimes (as for TM mode case in our example) the solution seems to be found (at a certain tolerance) after the first mesh refinement (zoomed mesh). However, even in this case the second mesh refinement (refined mesh) improves dramatically the accuracy: the refined mesh finds a minimum about ten times lower than the zoomed mesh.

The algorithm provides a useful, accurate and effective tool to design waveguides for surface plasmons.

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