Mode Analysis of Hybrid Plasmonic Waveguide Using Multilayer Spectral Green's Function and Rational Function Fitting Method

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Keywords: Hybrid Plasmonic Waveguide, Spectral Green's Function, Rational Function Fitting, Surface Plasmon, Effective Refractive Index, Propagation Length.

Abstract: A fast and accurate approach to find hybrid plasmonic waveguide mode and its properties is presented in this paper. The method is based on rational function fitting of spectral Green's function of layered hybrid plasmonic waveguide with the use of modified VECTFIT algorithm. Complex modes including surface plasmonic modes of structures with insulator/metal loss can be obtained. The main advantage of this method lies in its simple implementation, speed as well as controllable accuracy. Effective index and propagation length versus thickness of layers are evaluated and excellent agreements with rigorous COMSOL solution (finite element method) are shown.

1 INTRODUCTION

Surface plasmons (SPs) are the interaction of surface electrons of metals with the electromagnetic fields. Unlike surface wave (SW) modes of dielectric waveguide, SPs modes are localized and propagate along interface between dielectric and metal which several optical modules can be developed on the scale of nanometre based on this concept and make these modules widely utilized in information technology, energy and biology (Zia, *et all*. 2004, Brongersma and Kik 2007, Chang and Tai 2011, Kalavrouziotis, *et all.* 2012).

Plasmonic waveguides have advantages of mode size and diffraction limit over the dielectric waveguides while they suffer from large losses due to metal presence. Hybrid plasmonic waveguide (HPW) does not suffer from large losses and diffraction limit due to confinement of mode power in low refractive index region. Various configurations of metal and insulator are reported as HPW structures and for applications like communication (fundamental mode propagation) and biology (multimode propagation) (Sharma and Kumar 2017).

Dispersion equations can be obtained by solving Maxwell's equations for the given geometry and applying proper boundary conditions at the interfaces. In general, dispersion equations have no analytic closed-form solutions and therefore using numerical approach is inevitable. Bisection method (Press, et. all. 1988) for lossless and argument principle method (APM) (Anemogiannis and Glytsis 1992, Kocabas, et all. 2009) for lossy structures can be utilized to have real and complex solutions of modes respectively. APM gives nearly accurate results but the main challenge is its computation time especially for structures supporting large number of modes.

There are also some other techniques which require exact programming defined for special problem and are not efficient in general (Press, et. all. 1988, Anemogiannis, et all. 1999, Zia, et all. 2004). For instance, high sensitivity to initial guesses provided by user is another important challenge of these methods. On the other hand, although full numerical solution like finite difference time domain (FDTD) method (Feigenbaum and Orenstein, 2007) can extract the parameters and physical picture of plasmonic waveguides but this method usually suffers from intensive computational cost. Scattering matrix (S-matrix) method along with finite difference frequency domain (FDFD) (Kocabas, et all. 2008) can be useful in modal analysis but commonly the form of the derivations are not suitable to handle the field distribution.

In this paper rational function fitting of spectral Green's function (SGF) is used for fast mode analysis of HPW of Figure. 1. Modified VECTFIT

Torabi, A.
Mode Analysis of Hybrid Plasmonic Waveguide Using Multilayer Spectral Green's Function and Rational Function Fitting Method.
DOI: 10.5220/0011647300003408
In *Proceedings of the 11th International Conference on Photonics, Optics and Laser Technology (PHOTOPTICS 2023)*, pages 28-33
ISBN: 978-989-758-632-3; ISSN: 2184-4364

algorithm is used for rational function fitting process extracting complex modes including surface plasmonic modes of the structure. The speed of the method allows us to evaluate the behaviour of the effective index and propagation length against thickness of the layers of the structure effectively. Advantages of simple implementation as well as accuracy of this method are shown and verified for HPW like Figure. 1.

This paper is organized as following. In section 2, rational function fitting of SGF for HPW is described. Numerical results and validations of the method are presented in section 3 while some concluding remarks are given in section 4.

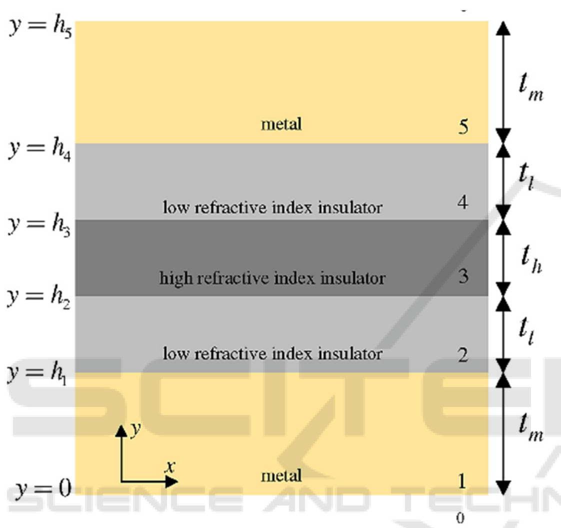

Figure 1: Schematic of HPW waveguide (MIM).

2 RATIONAL FUNCTION FITTING OF SGF FOR HPW

Consider a 2D (no variation in z direction) hybrid metal-insulator-metal layered plasmonic waveguide (Fig. 1) which has a dielectric region (#3) with high refractive index like Si with thickness t_h placed between two low refractive index dielectric regions (#2, 4) like SiO_2 with thickness t_l and two metal layers (#1, 5) like Ag with thickness t_m. We have z-axis propagation with x-y plane confinement.

We first derive the vector potential Green's function of a line source located in (x', y') and field point in (x, y) both in region 3 with usual spectral technique (Michalski and Mosig 1997):

(1)

$$G_A^m\left(y, y', \beta_x\right) = \frac{\left(1+R_{3,2}^m e^{-j2\beta_{y_3} y_<}\right)\left(1+R_{3,4}^m e^{-j2\beta_{y_3}(h_3-y_>)}\right)}{2j\beta_{y_3}\left(1-R_{3,2}^m e^{-j2\beta_{y_3} t_h}\right)} \quad (1)$$

where $R_{3,2}^m$ and $R_{3,4}^m$ can be found by recursive relations:

$$R_{i+1,i}^m = \frac{r_{i+1,i}^m + R_{i,i-1}^m e^{-j2\beta_{y_i} t_i}}{1 + r_{i+1,i}^m R_{i,i-1}^m e^{-j2\beta_{y_i} t_i}}, \quad r_{i+1,i}^m = \frac{\beta_{y_{i+1}}/\varepsilon_{i+1} - \beta_{y_i}/\varepsilon_i}{\beta_{y_{i+1}}/\varepsilon_{i+1} + \beta_{y_i}/\varepsilon_i} \qquad i = 1,2,3 \quad (2)$$

$$R_{i,i+1}^m = \frac{r_{i,i+1}^m + R_{i+1,i+2}^m e^{-j2\beta_{y_{i+1}} t_{i+1}}}{1 + r_{i,i+1}^m R_{i+1,i+2}^m e^{-j2\beta_{y_i} t_{i+1}}}, \quad r_{i,i+1}^m = \frac{\beta_{y_i}/\varepsilon_i - \beta_{y_{i+1}}/\varepsilon_{i+1}}{\beta_{y_i}/\varepsilon_i + \beta_{y_{i+1}}/\varepsilon_{i+1}} \qquad i = 3,4 \quad (3)$$

in (2) and (3), $\varepsilon_i = n_i^2$ is the relative dielectric constant of region i. in (1), $y_>$ and $y_<$ are the greater and smaller values of y and y' respectively. $\beta_{y_i} = \sqrt{n_i k_0^2 - \beta_x^2}$, $(i = 0,1,\ldots,6)$ where $k_0 = 2\pi/\lambda$ and λ is free space wavelength and β_x is the propagation constant of x direction. For $R_{1,0}^m$ and $R_{5,6}^m$, they are the reflection coefficients of light for semi-infinite layer of air, and we will have $R_{1,0}^m = r_{1,0}^m, R_{5,6}^m = r_{5,6}^m$. Relation (1) to (3) are general for 5 layered structures, while in our considered case, due to symmetry (similarity of two metal layers (regions 1 and 5) and two low refractive index insulator layers (regions 2 and 4)), we have $R_{3,2}^m = R_{3,4}^m, R_{2,1}^m = R_{4,5}^m, R_{1,0}^m = R_{5,6}^m$. G_A^m includes transverse magnetic (TM) SW and SP modes which are the zeros of denominator of SGF.

Modified version of VECTFIT algorithm has been successfully applied to SGF like (1) to fit it with rational form which corresponds to spectral form of surface modes. Indeed here we have an approximation below with total number of M poles (Torabi, *et. all*. 2013, Torabi and Shishegar 2015, Torabi 2019):

$$G_A^m\left(y, y', \beta_x\right) \simeq \sum_{p=1}^{M} \frac{R_p}{\beta_x^2 - \beta_{xp}^2} \quad (4)$$

that β_{xp} and R_p are p-th computed pole and its residue of G_A^m respectively. Sampling of β_x from straight line $[-\tau_{max} k_0 - j\delta, \tau_{max} k_0 + j\delta]$with

Table 1: Results of the proposed and APM (Anemogiannis and Glytsis 1992) for defined structure above.

Mode number	Real(n_{eff})		Imaginary(n_{eff})	
	Proposed method	APM (Anemogiannis and Glytsis 1992)	Proposed method	APM (Anemogiannis and Glytsis 1992)
TM_{00}	1.740200419	1.740200909	0.002165046	0.002165111
TM_{01}	1.124098123	1.124098306	0.003525932	0.003525802

appropriate values of τ_{max} and d is the first step of VECTFIT algorithm. Construction of auxiliary matrix for sample points $\left(\beta_{xi}, G_A^m(y, y', \beta_{xi})\right)$ in each iteration, is the next step where its eigenvalues are the approximate poles for the next step. Then using least square technique for a linear equation, R_p would be found for each pole. We can have criteria for relative error as (5) to control the accuracy and required number of poles. Modified VECTFIT algorithm is very fast and relative error of 10^{-9} for (5) can be obtained with $10 \sim 15$ poles typically less than 0.5 second.

$$Err = \sum_i \frac{\left| G_A^m\left(y, y', \beta_{xi}\right) - \sum_{p=1}^{M} \frac{R_p}{\beta_{xi}^2 - \beta_{xp}^2} \right|}{\left| G_A^m\left(y, y', \beta_{xi}\right) \right|} \tag{5}$$

Extracted poles of modified VECTFIT algorithm includes all SW and SP modes (solution of the dispersion equations or in other words the zeros of the denominator of SGF) as well as some other poles which are representatives of continuous spectrum contributions called radiation modes. SW and SP modes of the SGF are independent of the source (y') and filed point (y) location. On the other hand radiation modes re perfectly dependent to y and y'. This fact comes from construction of continuous spectrum of radiation modes which depends on the location of excitation and observation points (Torabi, *et. all*. 2013). Each pole that makes the denominator of G_A^m zero belongs to group of SP and SW modes otherwise it belongs to group of radiation modes.

To start the algorithm, poles (β_{xp}) and their related residuals (R_p s) should be initially set. It is obvious that, if the initial poles are close to the exact answers, then the algorithm will converge fast. Therefore, in each iteration of the VECTFIT algorithm, the poles extracted in the previous step are used as initial poles. It should be noted that one of the main advantages of the proposed RFF-SGF method is that the used modified VECTFIT algorithm does not depend on the first starting the initial guesses of the poles. In other words, the modified VECTFIT algorithm is robust enough that its convergence does not depend on the first initial guess (Gustavsen and Semlyen 1999). Therefore, in all simulations, one can choose random N_p values in region $[-\tau_{max}k_0 - jd, \tau_{max}k_0 + jd]$ as first initial guesses (first iteration) of poles.

3 RESULTS

In Fig. 1, suppose regions 1 and 5 as Ag with $\varepsilon_r = -143.5 - j9.5$, $t_m = 300nm$, region 2 and 4 as SiO_2 with $\varepsilon_r = 2.1$, $t_l = 100nm$ and region 3 as Si with $\varepsilon_r = 12.2$, $t_h = 100nm$. Table. 1 shows effective indices of the first two TM modes of this structure at $\lambda = 1.55\mu m$. Results are compared with Argument Principle Method (APM) (Anemogiannis and Glytsis 1992, Kocabas, et all. 2009) and excellent agreements can be seen for computed results. Also the total time of (4) is nearly 1/30of the APM (proposed method: 2 sec and APM: 1 min). High speed of the VECTFIT algorithm help us to have mode analysis of HMIM. The real and imaginary part of effective refractive index are related to modal index and the propagation length ($Pl = \lambda/(4\pi\, Im(n_{eff}))$) respectively. Propagation length of a mode is defined as a distance over which the guided power is reduced to nearly 37 %of the initial power. It is desired that by increasing the thickness of high index region (region 3-Si), the resulted HPW would be similar to a dielectric waveguide. Moreover it can be seen that the first mode (TM_{00}) results in stronger light confinement than the second mode (Figure. 2). Moreover, Figure. 2 shows increasing in propagation length by increasing Si thickness (t_h). Reversely it is desired that by increasing the low refractive index regions (region 2 and 4) the nature of HPW turns towards to plasmonic waveguide. Figure. 3 shows decreasing in real part of effective index and increasing of propagation length for TM_{00} with increasing of t_l.

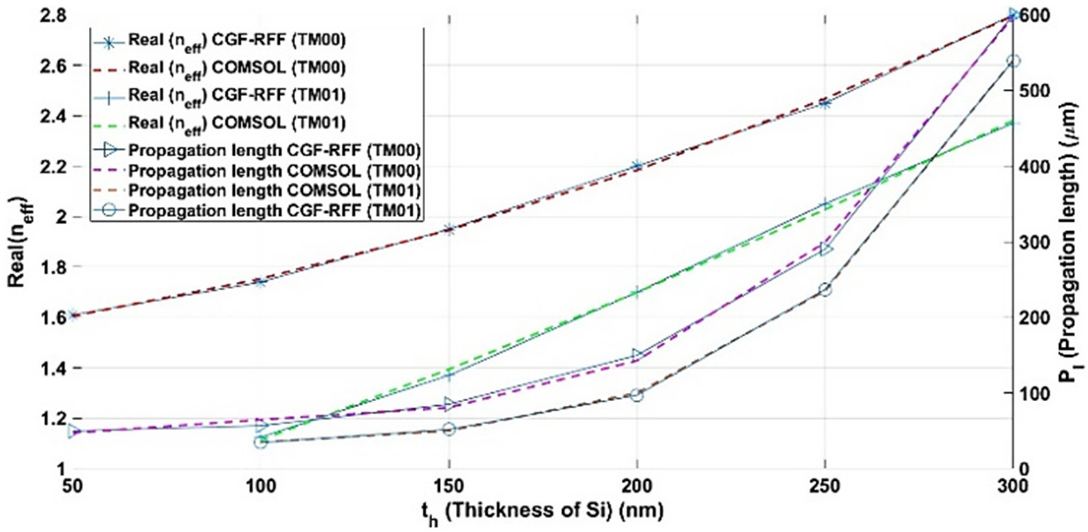

Figure 2: Real part of effective index and propagation length versus t_h .Regions 1, 5 as Ag with $\varepsilon_r = -143.5 - j9.5$, $t_m = 300nm$, region 2, 4 as SiO2 with $\varepsilon_r = 2.1$, $t_l = 100nm$, region 3 as Si with $\varepsilon_r = 12.2$.

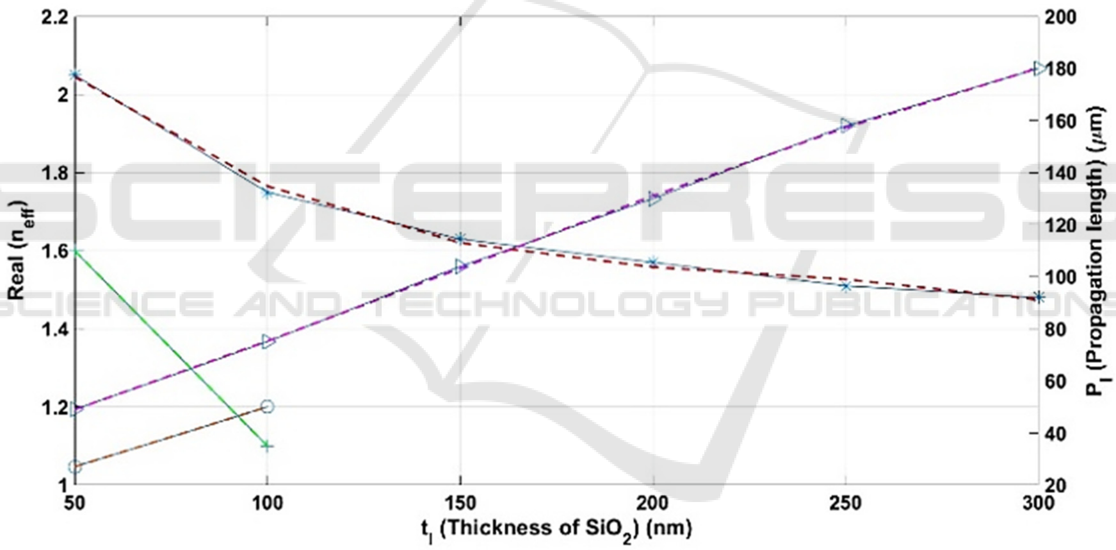

Figure 3: Real part of effective index and propagation length versus t_l .Regions 1, 5 as Ag with $\varepsilon_r = -143.5 - j9.5$,$t_m = 300nm$, region 2, 4 as SiO2 with $\varepsilon_r = 2.1$, region 3 as Si with$\varepsilon_r = 12.2$,$t_h = 100nm$ (Legends are similar to Fig. 2).

For $t_l < 100nm$we will have TM_{01} mode. Results of COMSOL simulations (dashed lines) are also shown in Figure. 2 and 3. Excellent agreement can be seen.

4 CONCLUSIONS

A new approach for SP modes evaluation and modal analysis of hybrid plasmonic waveguide is presented in this paper. The method is based on the rational function fitting of the spectral Green's function of the desired multilayered plasmonic structure. Modified VECTFIT algorithm is used to rational function fitting process and related SP modes of the structure would be extracted. The main requirement of this method is derivation of the spectral Green's function of the structure once which have a closed form relation. Simple and fast implementation while preserving accuracy are the main advantages of the proposed method which are validated by exact rigorous results of COMSOL (finite element method).

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APPENDIX

Modified Vectfit Algorithm

Suppose that the samples of $G_A^m(y, y', \beta_x)$ at β_{xi}^s , $i = 1,2,\dots,L$ are provided and are shown by $G_A^m(\beta_{xi}^s)$ (ignoring y and $y¢$ for simplicity). If $\beta_{xp}, p = 1,2,\dots,M$ be an initial guess for the poles of (4), then for every β_{xi} one can form

$$\boldsymbol{E}_i \boldsymbol{r} = g_i \tag{6}$$

Where

$$\mathbf{E}_i = \left[\frac{1}{{\beta_{xi}^s}^2 - \beta_{x1}^2} \cdots \frac{1}{{\beta_{xi}^s}^2 - \beta_{xM}^2} \frac{-G_A^m(\beta_{xi}^s)}{{\beta_{xi}^s}^2 - \beta_{x1}^2} \cdots \frac{-G_A^m(\beta_{xi}^s)}{{\beta_{xi}^s}^2 - \beta_{xM}^2}\right] \tag{7}$$

and

$$\mathbf{r} = \left[R_1 \dots R_M \ \widetilde{R_1} \dots \widetilde{R_M}\right]^T, \quad g_i = G_A^m(\beta_{xi}^s) \tag{8}$$

where sign “%” and “T ” denotes complex conjugate and transpose operator. For all β_{xi} points, we reach to a linear and over determined system like the following:

$$\boldsymbol{Er} = \boldsymbol{g} \tag{9}$$

where $\mathbf{E}$ is a $L \times (2M)$ matrix which its ith row is given by (7) and $\mathbf{g}$ is a column vector of g_i .

$$\mathbf{E} = \begin{bmatrix} \frac{1}{{\beta_{x1}^s}^2 - \beta_{x1}^2} \cdots \frac{1}{{\beta_{x1}^s}^2 - \beta_{xM}^2} \frac{-G_A^m(\beta_{x1}^s)}{{\beta_{x1}^s}^2 - \beta_{x1}^2} \cdots \frac{-G_A^m(\beta_{x1}^s)}{{\beta_{x1}^s}^2 - \beta_{xM}^2} \\ \frac{1}{{\beta_{x2}^s}^2 - \beta_{x1}^2} \cdots \frac{1}{{\beta_{x2}^s}^2 - \beta_{xM}^2} \frac{-G_A^m(\beta_{x2}^s)}{{\beta_{x2}^s}^2 - \beta_{x1}^2} \cdots \frac{-G_A^m(\beta_{x2}^s)}{{\beta_{x2}^s}^2 - \beta_{xM}^2} \\ . \\ . \\ . \\ \frac{1}{{\beta_{xL}^s}^2 - \beta_{x1}^2} \cdots \frac{1}{{\beta_{xL}^s}^2 - \beta_{xM}^2} \frac{-G_A^m(\beta_{xL}^s)}{{\beta_{xL}^s}^2 - \beta_{x1}^2} \cdots \frac{-G_A^m(\beta_{xL}^s)}{{\beta_{xL}^s}^2 - \beta_{xM}^2} \end{bmatrix} \tag{10}$$

$$\boldsymbol{g} = [G_A^m(\beta_{x1}^s), \dots, G_A^m(\beta_{xL}^s)]^T \tag{11}$$

By solving (9), a new set of poles which are closed to the poles of G_A^m can be obtained as the eigenvalues of a $\mathbf{Q}$ matrix defined as following:

$$\mathbf{Q} = \begin{bmatrix} \beta_{x1}^2 & 0 & \cdots & 0 \\ 0 & \beta_{x2}^2 & & 0 \\ \cdot & & & \cdot \\ \cdot & & \cdot & \cdot \\ \cdot & & & \cdot \\ 0 & 0 & \cdots & \beta_{xM}^2 \end{bmatrix} - \begin{bmatrix} 1 \\ 1 \\ \cdot \\ \cdot \\ \cdot \\ 1 \end{bmatrix} \left[\widetilde{R_1}, \widetilde{R_2}, \ldots \widetilde{R_M} \right] \quad (12)$$

Then by applying the iteration form, poles of the last iteration would be utilized as the starting poles of the next iteration. After a good convergence, $R_p s$ can be found by solving a linear system as following:

$$\mathbf{E}'\mathbf{r}' = \mathbf{g} \quad (13)$$

where $\boldsymbol{E}'$ is $L \times M$ matrix and $\boldsymbol{r}'$ is vector given below:

$$\mathbf{E}' = \begin{bmatrix} \dfrac{1}{{\beta_{x1}^{s}}^2 - \beta_{x1}^2} & \cdots & \dfrac{1}{{\beta_{x1}^{s}}^2 - \beta_{xM}^2} \\ \dfrac{1}{{\beta_{x2}^{s}}^2 - \beta_{x1}^2} & \cdots & \dfrac{1}{{\beta_{x2}^{s}}^2 - \beta_{xM}^2} \\ \cdot & & \\ \cdot & & \\ \cdot & & \\ \dfrac{1}{{\beta_{xL}^{s}}^2 - \beta_{x1}^2} & \cdots & \dfrac{1}{{\beta_{xL}^{s}}^2 - \beta_{xM}^2} \end{bmatrix} \quad (14)$$

$$\mathbf{r}' = \left[R_1 \ldots R_M \right]^T \quad (15)$$

Vector $\mathbf{g}$ is given by (11).