Numerical investigation of mode characteristics of nanoscale surface plasmon-polaritons using a pseudospectral scheme

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Abstract: This study uses a full vector pseudospectral scheme in the frequency domain to investigate the mode characteristics of surface plasmon-polariton (SPP) waveguides. The wave equations solved in this study are based on the transverse magnetic field components, and thus the spurious modes are removed due to the constraint of divergence-free magnetic vector. The waveguide dimension dependences on the mode confinement and propagation length of the dielectric-loaded surface plasmon-polariton waveguide (DLSPPW) are extensively studied and characterized. The numerical results of the DLSPPW show that the proposed scheme is highly efficient and yields accurate complex effective indices while requiring much less memory than the commonly used finite element method. This study also analyzes the propagation characteristics and figures of merit of an inverted metal slot waveguide (IMSW) in detail. The IMSW achieves a propagation loss an order of magnitude lower than nanoparticle chains with comparable degrees of lateral confinement.

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OCIS codes: (130.2790) Guided waves; (230.7370) Waveguides; (240.6680) Surface plasmons.

References and links


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1. Introduction

The ability for fabricating the integrated circuits is now at dimensions below 100nm. Further scaling the electronic circuits encounters some limitations such as operating bandwidth, signal delay, and energy dissipation [1,2]. For working with these problems, applying the photonic circuits offers an effective solution. However, using pure dielectrics to produce nanoscale photonic components is primarily restricted by the inherent diffraction limit. Therefore, it is difficult to make photonic integrated circuits fully compatible with the field of integrated electronic circuits. In recent years, exciting the surface plasmon polariton (SPP) is a promising way to squeeze the optical energy in nanometric cross section [3]. Theoretically, the SPP occurs at the interface between a dielectric and a metal due to the coupling of an electromagnetic wave and the free electrons of the metal [4]. Enlarging the SPP wavevector decreases the size of the resulting spatial confinement more than the conventional dielectric methods can. Many studies report various types of plasmonic structures to achieve the nanoguiding of light power [5–12]. The most essential characteristics of plasmonic waveguides include the dependences of mode confinement and propagation length on the geometric structure and the operating wavelength. Theoretically, the plasmonic waveguide structures need at least one interface composed of a dielectric and a metal to produce the SPP mode, and the SPP mode profile from the interface into the metal changes acutely (i.e., the penetration depth is only tens of nanometers). In numerical computations, an acute varying field is harder to be precisely captured than that in a pure, lossless dielectric waveguide.

Lately, many numerical schemes have been developed to analyze the SPP propagation characteristics and further to design various plasmonic integrated optical circuits. Previous published schemes include the finite-difference frequency domain (FDFD) [10,13–16], finite element method (FEM) [12,17–21], finite-difference time domain (FDTD) [8,22–25], method of lines [26–29], differential method [30,31], imaginary-distance beam propagation method [32], and density of states formulation [33]. The widely used FDFD and FEM use many discretization points to achieve accurate results, and thus lead to high memory and computation requirements. The FDTD approach is better suited to pulse propagation problems and dispersion characteristics because it scans a period of the bandwidth. Solving mode problems in a specific frequency is a time-consuming scheme that requires huge memory for three-dimensional structures. The method of lines discretizes all but one dimension to yield systems of coupled ordinary differential equations. These systems can be solved by choosing a time integrator as the time domain approach. The differential method based on the rigorous vector diffraction theories was originally dedicated to analyze periodic structures such as diffraction gratings. The unknown variables in this approach include the transverse electric and magnetic field components. Each field component is expanded by the Fourier basis. The Fourier coefficients are then substituted back to the spatial domain to find the field profiles. In the dielectric-loaded surface plasmon-polariton waveguides (DLSPPPWs) [17], the differential method needs 100 terms of Fourier harmonics in each field component to yield the convergent solutions. The transverse spatial discretizations in the imaginary-distance BPM are still based on the finite difference scheme. The density of states formulation, much like the electronic density of state in the presence of a localized electronic defect, computes a
Lorentzian shape near a guided wave-vector resonance. The density of states formulation also needs to calculate the Green’s dyad and using multiple-scattering description.

The pseudospectral scheme [34,35] with high-order accuracy and fast convergence was originally developed to solve fluid dynamics problems. In later years, the author combined the scheme with the multidomain approach to study the mode problems of lossless dielectric optical waveguides [36–39]. The calculated results of the multidomain pseudospectral scheme demonstrate that it is indeed reliable and efficient to find accurate effective indices and mode field profiles for various dielectric optical waveguides. Compared with the results calculated by the FDFD and FEM, the multidomain pseudospectral scheme achieves better accuracy and performance in reducing memory capacity because it requires fewer matrix equations [36–39]. This study is the first to use the multidomain pseudospectral scheme to investigate the SPP waveguide structures, including the DLSPPW and inverted metal slot waveguide (IMSW). In previous reports, the multidomain pseudospectral scheme require only 10 terms of basis functions in each subdomain to achieve high accuracy while calculating the lossless dielectric waveguides. In contrast, the plasmonic waveguide structures require extremely fine discretization points to capture the fast decay field within a narrow scale. For the FDFD and FEM approaches, the computational efforts increase significantly while solving the SPP problems. Consequently, this study aims to circumvent these massive computation requirements using the multidomain pseudospectral scheme, and offers an efficient and accurate approach to analyze the mode characteristics of nanoscale plasmonic structures. The remainder of this paper is organized as follows. Section II formulates the wave equations for the three-dimensional waveguide structures. Section III presents the related issues of the numerical scheme. Section IV calculates the numerical examples to demonstrate the accuracy of the proposed scheme, and discusses the mode characteristics of DLSPPW and IMSW in detail. Finally, Section V draws conclusions.

2. Mathematical formulations

Assuming a monochromatic optical wave with a time dependence of exp(iωt) and propagating along the $z$ direction in a medium with refractive index $n(x,y,z)$, the vector wave equation derived from Maxwell’s equations based on the magnetic field vector $\mathbf{H}$ is

$$\nabla^2 \mathbf{H} + k_0^2 n^2 \mathbf{H} + \frac{n^2}{n_{eff}^2} \times (\nabla \times \mathbf{H}) = 0$$  \hspace{1cm} (1)

where $k_0 = \frac{2\pi}{\lambda_0}$ and $\lambda_0$ the wavelength in vacuum. For solving a mode problem, the waveguide structure in the longitudinal propagation direction is invariant. The refractive index profile only depends on the transverse directions, that is, $n = n(x,y)$. Here, the wave with $z$ dependence of the form exp(-iβz) is considered, where $\beta = k_0 n_{eff}$ is the propagation constant and $n_{eff}$ is the mode effective index. The general waveguide structures involve distinct materials with a high-contrast refractive index in the computational domain, especially for the plasmonic waveguides consisting of a dielectric medium and a metal medium with negative permittivity. This approach partitions the computational domain into a few subdomains with a uniform refractive index. The last term of Eq. (1) equals zero due to the homogeneous refractive index profile in each subdomain. This reduces the vector wave equation to two decoupled wave equations for the transverse magnetic field components $H_x$ and $H_y$ as follows:

$$\frac{\partial^2 H_x}{\partial x^2} + \frac{\partial^2 H_y}{\partial y^2} + k_0^2 (n^2 - n_{eff}^2) H_s = 0, \hspace{1cm} (s = x, y).$$  \hspace{1cm} (2)

However, the polarization dependence and the coupling effect can be recovered by incorporating the interfacial boundary conditions. These boundary conditions include the continuous normal and tangential components of magnetic fields at each intra-element boundary. Moreover, the continuities of the longitudinal components $H_z$ and $E_z$ provide the
coupling effect of $H_x$ and $H_y$ through the relations $\nabla \times \mathbf{H} = j\omega \varepsilon_0 n^2(x,y) \mathbf{E}$ and $\nabla \cdot \mathbf{H} = 0$. For a horizontal interface, since the derivatives of $H_x$ and $H_y$ with respect to $x$ on both sides of the interface are equal, the continuity of $E_z$ yields

$$n_y^2 \frac{\partial H_x}{\partial y} |_{y_+} - n_y^2 \frac{\partial H_x}{\partial y} |_{y_-} = (n_x^2 - n_y^2) \frac{\partial H_y}{\partial x}$$

(3a)

and the continuity of $H_z$ yields

$$\frac{\partial H_x}{\partial y} |_{y_+} = \frac{\partial H_x}{\partial y} |_{y_-}$$

(3b)

where $y^+$ and $y^-$ refer to the locations infinitesimally above and below the horizontal interface, respectively. Likewise, for a vertical interface,

$$n_x^2 \frac{\partial H_y}{\partial x} |_{y_+} - n_x^2 \frac{\partial H_y}{\partial x} |_{y_-} = (n_x^2 - n_y^2) \frac{\partial H_x}{\partial y}$$

(3c)

and

$$\frac{\partial H_y}{\partial x} |_{x_+} = \frac{\partial H_y}{\partial x} |_{x_-}$$

(3d)

where $x^+$ and $x^-$ refer to the locations infinitesimally to the right and to the left of the vertical interface, respectively. Note that the spurious modes do not satisfy the divergence-free magnetic fields [40] and then the spurious modes are completely eliminated in [41] by imposing the constraint $\nabla \cdot \mathbf{H} = 0$. Importantly, the constraint $\nabla \cdot \mathbf{H} = 0$ is explicitly imposed by the proposed scheme to patch the subdomains to effectively prohibit the spurious modes.

3. Numerical approaches

The pseudospectral approach first expands the dependent variables in each subdomain using a set of orthogonal basis functions [34,35]. The product of basis functions and Fourier coefficients are then transferred to the individual Lagrange-type interpolation functions and the grid points of fields. This process transforms the unknown Fourier coefficients in the frequency domain to the field points in the physical domain to obtain the mode profiles directly. The pseudospectral scheme requires that the wave equations must be satisfied exactly at specific collocation points depending on the basis functions. The differential equations are then converted to a system of linear equations. For the mode problems, the effective refractive index is found by solving a matrix eigenvalue equation. To preserve the exponential convergence behavior of the pseudospectral scheme, the computational window is partitioned into several subdomains with homogeneous refractive indices. Finally, the subdomains are assembled by patching the physical interfacial boundary conditions to the entire computational domain.

In subdomain $r$, the transverse magnetic fields ($H_x$ and $H_y$) are represented as a product of suitable (described in the next subsection) basis function $\theta(x)$ in the $x$-direction, the basis function $\psi(y)$ in the $y$-direction, and the $H_x$ and $H_y$ field values denoted as $H'_{x,p,q}$ and $H'_{y,p,q}$ at $(n_x+1) \times (n_y+1)$ collocation points associated by the corresponding basis functions as follows:

$$H'_s(x, y) = \sum_{p=0}^{n_x} \sum_{q=0}^{n_y} \theta'_p(x) \psi'_q(y) H'_{s,p,q}, \ (s = x, y)$$

(4)

where $\theta'_p(x_m) = \delta_{mp}$, $\psi'_q(y_n) = \delta_{qn}$, and $\delta_{np}$ denotes the Kronecker delta. Note that the number of terms of basis function expanded and collocation point is identical. Substituting Eq. (4) into
Eq. (2), and then Eq. (2) perfectly satisfies these \((n_r-1) \times (n_r-1)\) collocation points in subdomain \(r\). The differential equations are then converted to a matrix eigenvalue equation

\[
\begin{bmatrix}
P' & 0 \\
0 & P'
\end{bmatrix}
\begin{bmatrix}
H'_x \\
H'_y
\end{bmatrix} = (k_{0,\text{eff}})^2 \begin{bmatrix}
H'_x \\
H'_y
\end{bmatrix},
\]

(5)

where the operator \(P'\) is

\[
P'H'_s = \left[\frac{\partial^2 H'_s}{\partial x^2} + \frac{\partial^2 H'_s}{\partial y^2} + k^2_n n^2 H'_s\right]_{x=x_{r,x},y_{r,y}}, (s = x, y)
\]

\[
= \sum_{i=1}^{n_{r,x}-1} \sum_{j=1}^{n_{r,y}-1} \left[\sum_{p=0}^{n_{r,x}} \left(\theta_p^{(k)}(x)\psi_q^{(k)}(y) + \theta_p^{(k)}(x)\psi_q^{(2,k)}(y) + k^2_n n^2 \theta_p^{(k)}(x,y)\psi_q^{(2,k)}(y)\right)\right]_{x=x_{r,x},y_{r,y}} \{H'_s\}
\]

(6)

and \(\theta_p^{(k)}(x)\) and \(\psi_q^{(k)}(y)\) indicate the \(h\)-th order derivatives of \(\theta_p(x)\) to \(x\) and \(\psi_q(y)\) to \(y\), respectively. After obtaining the matrix eigenvalue equation in Eq. (5) for each subdomain, the next step is to assemble all the matrix elements into a global computational domain. If the computational domain is divided into \(m\) subdomains, the pattern distribution of the matrix elements forms the following block diagonal matrix equation:

\[
\begin{bmatrix}
Q_1 & 0 & 0 & 0 \\
0 & Q_2 & 0 & 0 \\
0 & 0 & \ddots & 0 \\
0 & 0 & 0 & Q_m
\end{bmatrix}
\begin{bmatrix}
H_1 \\
H_2 \\
\vdots \\
H_m
\end{bmatrix} = (k_{0,\text{eff}})^2 \begin{bmatrix}
H_1 \\
H_2 \\
\vdots \\
H_m
\end{bmatrix},
\]

(7)

where

\[
Q' = \begin{bmatrix}
P' & 0 \\
0 & P'
\end{bmatrix}, \quad H' = \begin{bmatrix}
H'_x \\
H'_y
\end{bmatrix}, \quad (r = 1, 2, 3...m).
\]

(8)

In addition to the elements inside each subdomain, the final matrix must include other contributions at interfacial boundary points (remainder collocation points) satisfying the physical conditions in Eq. (3)a)-(3d) between different materials. Enforcing the boundary conditions from Eq. (3)a)-(3d) recovers the exponential convergence rate of pseudospectral scheme [35]. After adding the interfacial boundary conditions Eq. (3)a)-(3d), the pattern of the final matrix is no longer a block diagonal form, but remains a moderate sparse matrix. For SPP mode problems, \(n_{\text{eff}}\) is complex. The real part characterizes the wave vector (which is approximately inversely proportional to the mode size) and the imaginary part represents the propagation length (the power drops to \(1/e\) with respect to the input power) of the SPP mode.

The other issue of the proposed scheme is to determine the basis functions to represent the mode fields. Distinct basis functions depending on the field behaviors are chosen for different subdomains in this work. Chebyshev polynomials are suitable to expand the optical fields in interior subdomains with finite boundaries because of their robustness to non-periodic structures. In contrast, Laguerre-Gaussian functions (LGFs) expand the exponential field profiles of guided modes in exterior subdomains with a semi-infinite boundary. For Chebyshev polynomials, the explicit form of the Lagrange-type interpolation function is as follows [35],

\[
\theta_p(x) = \frac{(-1)^{p+1}(1-x^2)T_p(x)}{c_p n^2 (x-x_p)}, \quad c_p = \begin{cases} 
2, & \text{if } p=0,N \\
1, & \text{if } 1 \leq p \leq N-1
\end{cases}
\]

(9)
where $T_v(x)$ is the general Chebyshev polynomial of order $v$ and $x_p$’s are the collocation points for Chebyshev polynomials. For LGFs, the explicit form is as follows [35],

$$
\theta_p(\alpha x) = \frac{xL_v(\alpha x)}{\alpha(x - x_p)[xL_v(\alpha x)]}_{|x=x_p} e^{-\alpha(x-x_p)^2},
$$

where $L_v(\alpha x)$ is the Laguerre polynomial of order $v$ and $x_p$’s are the collocation points for LGFs. Parameter $\alpha$, called the scaling factor, and affects the accuracy for a given term of LGFs. The definite procedure to determine $\alpha$ has been derived in earlier research [37].

4. Simulation results and discussion

This section investigates two plasmonic waveguides. First, the SPP modes in a DLSPPW structure are solved to demonstrate the computational merits of the proposed scheme compared with those of two reliable numerical schemes, the FEM [17] and differential method (DM) [30]. The mode confinement and figure of merit for DLSPPWs have also already been extensively studied in [42] by combining numerical simulations and leakage radiation microscopy. Moreover, the dependences of the mode confinement and propagation length by varying the geometric parameters of DLSPPW are extensively investigated. Secondly, this section studies the mode characteristics of a low-loss IMSW [43] applied to nanoscale circuits in detail, and discusses the figure of merit (FOM) [44].

4.1 The dielectric-loaded surface plasmon-polariton waveguide (DLSPPW)

The mode characteristics of DLSPPW have been verified experimentally by near-field optical microscopy and leakage radiation microscopy, which are able to guide efficiently the SPP modes [45]. A variety of photonic components based on the DLSPPW structure involving ring resonators [46], multimode interference splitter [47], active Bragg reflector [48], and thermo-optics control Mach-Zehnder interferometers [49] have been successively reported because the advantages including high localization, moderate propagation length (tens of micrometers), thermo-, electro-, all-optical functionalities, and easily integrated to optoelectronic devices. For the conventional integrated optics components; however, the efficiency of coupling has not been investigated yet. It would be useful to provide examples of more complex plasmonic circuits. The DLSPPW is constructed by depositing a dielectric polymer ridge with thickness $t$ and width $w$ on a gold film with thickness $h$ covering a semi-infinite dielectric substrate. Figure 1(a) depicts the cross section of the DLSPPW. The refractive indices of materials are air $n_a = 1$, core $n_p = 1.535$, gold film $n_g = 0.55-11.5i$ (the form of complex refractive index depends on the plane-wave solution form chosen [50], and this study uses the $\exp(i(\omega t - \beta z))$ solution), and substrate $n_d = 1.6$ at an excitation wavelength of optical communication $\lambda = 1.55\mu m$. This study investigates the mode characteristics by varying the width and thickness of the polymer ridge at a fixed thickness of gold film $h = 0.1\mu m$, and then analyzes the wavelength dependence.

![Fig. 1. (a) The cross section of DLSPPW with refractive indices of core $n_p$, gold film $n_g$, substrate $n_d$, and air $n_a$. (b) The division of computational domain for the DLSPPW structure.](image)

The DLSPPW at $w = 0.6\mu m$ and $t = 0.6\mu m$ was first calculated to demonstrate the convergence of the proposed scheme. The proposed scheme divides the computational domain into 12 subdomains as illustrated in Fig. 1(b), and then expands the unknown fields in each subdomain using appropriate basis functions. This study uses LGFs and Chebyshev polynomials to represent the mode fields for subdomains with semi-infinite (exterior
subdomains) and finite (interior subdomains) extents, respectively. For example, the transverse magnetic field components in the $x$- and $y$-directions of the subdomains 1, 3, 10, and 12 with infinite extents are both expanded by LGFs. For subdomains 2 and 11, Chebyshev polynomials expand the mode fields in the $x$-direction, and LGFs expand those in the $y$-direction. The proposed scheme requires no extra boundary conditions at the computational boundaries due to the well-matched profiles of the guided-modes and the mathematical exponential decay of LGFs. Compared with other numerical approaches dealing with boundary conditions, the proposed scheme is simple while considering the guided SPP mode problems. For the scaling factor $\alpha$ adjusting the exponential rate of LGFs, previous research [37] has presented a definite procedure for determining it. After assembling all subdomains, the Arnoldi iteration method is used to efficiently solve the generalized eigenvalue problem [51]. Table 1 and 2 show the convergences of the real part of the effective index and propagation length $L_c$ of the fundamental SPP ($\text{TM}_{00}$) mode, respectively. Note that the same terms of basis functions are used to expand mode fields in the $x$- and $y$-directions.

### Table 1. The convergence of the real parts of effective index calculated by the proposed scheme for different widths $w$ of ridge at $t = 0.6\mu$m versus the terms of basis functions.

<table>
<thead>
<tr>
<th>$n_c (= n_r)$</th>
<th>0.8</th>
<th>0.7</th>
<th>0.6</th>
<th>0.5</th>
<th>0.4</th>
<th>0.3</th>
<th>0.2</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>1.34830</td>
<td>1.32360</td>
<td>1.29197</td>
<td>1.25117</td>
<td>1.19885</td>
<td>1.13447</td>
<td>1.06509</td>
</tr>
<tr>
<td>10</td>
<td>1.34787</td>
<td>1.32287</td>
<td>1.29111</td>
<td>1.25038</td>
<td>1.19851</td>
<td>1.13485</td>
<td>1.06606</td>
</tr>
<tr>
<td>15</td>
<td>1.34741</td>
<td>1.32226</td>
<td>1.29036</td>
<td>1.24954</td>
<td>1.19754</td>
<td>1.13395</td>
<td>1.06647</td>
</tr>
<tr>
<td>20</td>
<td>1.34742</td>
<td>1.32237</td>
<td>1.29850</td>
<td>1.24974</td>
<td>1.19782</td>
<td>1.13434</td>
<td>1.06582</td>
</tr>
</tbody>
</table>

### Table 2. The convergence of the propagation lengths $L_c(\mu$m) calculated by the proposed scheme for different widths $w$ of ridge at $t = 0.6\mu$m versus the terms of basis functions.

<table>
<thead>
<tr>
<th>$n_c (= n_r)$</th>
<th>0.8</th>
<th>0.7</th>
<th>0.6</th>
<th>0.5</th>
<th>0.4</th>
<th>0.3</th>
<th>0.2</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
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<td>39.8</td>
<td>40.7</td>
<td>42.5</td>
<td>46.0</td>
<td>53.9</td>
<td>74.4</td>
</tr>
<tr>
<td>10</td>
<td>42.2</td>
<td>42.9</td>
<td>43.9</td>
<td>46.0</td>
<td>49.6</td>
<td>58.1</td>
<td>79.4</td>
</tr>
<tr>
<td>15</td>
<td>42.9</td>
<td>43.3</td>
<td>44.7</td>
<td>46.2</td>
<td>50.1</td>
<td>58.6</td>
<td>80.3</td>
</tr>
<tr>
<td>20</td>
<td>42.2</td>
<td>43.1</td>
<td>44.4</td>
<td>46.1</td>
<td>50.2</td>
<td>58.2</td>
<td>80.2</td>
</tr>
</tbody>
</table>

In previous report analyzing optical waveguides with pure dielectrics [37], the relative difference of $n_{eff}$ is achieved by the order of $10^{-6}$ while one increases the terms of basis functions from $n_r = 10$ to 15 terms. In contrast, the plasmonic waveguides with a high-contrast index degrades the convergence behavior. In Table 1, the results of the real parts of $n_{eff}$ show that only the order of $10^{-2}$ is achieved even if the number of basis functions exceeds 30 terms in each subdomain. This consequence means that the acute field profiles of the SPP modes at metal-dielectric interfaces are more difficult to accurately capture. This phenomenon also appears in other reliable numerical approaches, such as the FDFD and FEM schemes. The results listed in Table 2 were obtained by converting the imaginary parts of $n_{eff}$ (the convergent rates are the same order as those of the real parts) to the propagation length $L_c$ by the formula of $L_c = 1/(2k_0 \times \text{imag}(n_{eff}))$. This reveals that the numerical convergences of $L_c$ calculated by the proposed scheme are about the order of $10^{-4}\mu$m. From a computational point of view, the computational effort (the number of unknowns) is four times that of the waveguide structures with only dielectrics involved [37], but the stable values of the real parts of $n_{eff}$ are only achieved at the fourth place of decimals. The computations were performed on a PC with an Intel Core 2 Quad Q8200 2.33GHz CPU, and the computational times and memory capacities versus the number of unknown are shown in Fig. 2(a) and (b), respectively. The total number of unknowns in the proposed scheme with $n_r$ in each subdomain is $(3 \times n_r - 2) \times (4 \times n_r - 3) \times 2$. The four points in Fig. 2(a) and (b) are $n_r = 5$, 10, 15, and 20 in order from left to right sides.
Fig. 2. (a) The computational time and (b) the memory capacity versus the number of unknown of the proposed scheme.

To compare the accuracy, Fig. 3(a) and (b) show the relative errors of the real parts of $n_{ef}$ and $L_c$'s obtained by the proposed scheme using $n_x = 20$ for various widths, respectively, relative to the reference values obtained by the FEM [17].

Fig. 3. The relative errors of (a) the real parts of $n_{ef}$ and (b) the propagation lengths $L_c$(μm) of the proposed scheme at $t = 0.6μm$ versus different width $t$. The reference values are obtained by the FEM [17].

Tables 3 also lists the precise real parts of $n_{ef}$ obtained by the proposed scheme using $n_x = 20$ along with the FEM [17] and DM [30], and the $L_c$'s are shown in Table 4.

| Table 3. Comparisons of the real parts of effective index obtained by the Finite Element Method (FEM), the differential method (DM), and the proposed scheme (this work) for different widths $w$ of ridge at $t = 0.6μm$. |
|------------------|-----|-----|-----|-----|-----|-----|-----|
| $w$(μm)          | 0.8 | 0.7 | 0.6 | 0.5 | 0.4 | 0.3 | 0.2 |
| FEM              | 1.348 | 1.323 | 1.291 | 1.250 | 1.198 | 1.133 | 1.064 |
| DM               | 1.348 | 1.323 | 1.291 | 1.250 | 1.198 | 1.133 | 1.064 |
| This work        | 1.3474 | 1.3224 | 1.2905 | 1.2497 | 1.1978 | 1.1343 | 1.0658 |

| Table 4. Comparisons of the propagation lengths $L_c$(μm) obtained by Finite Element Method (FEM), the differential method (DM), and the proposed scheme (this work) for different widths $w$ of ridge at $t = 0.6μm$. |
|------------------|-----|-----|-----|-----|-----|-----|-----|
| $w$(μm)          | 0.8 | 0.7 | 0.6 | 0.5 | 0.4 | 0.3 | 0.2 |
| FEM              | 42.2 | 42.8 | 44.4 | 46.4 | 50.1 | 59.1 | 81.3 |
| DM               | 42.2 | 42.8 | 44.0 | 46.0 | 50.1 | 59.1 | 80.4 |
| This work        | 42.2 | 43.1 | 44.4 | 46.1 | 50.2 | 58.2 | 80.2 |

Table 3 and 4 show good agreement of the mode characteristics between these approaches. The total number of unknowns in the proposed scheme with $n_x = 20$ is in the order of $10^3$. In contrast, the FEM [17] requires much more unknowns with the order of $10^5$. As a result, the proposed scheme shows higher computational efficiency (much less memory)
than that of FEM. This study also computes the results of varying the thickness of the ridge at width \( w = 0.5 \mu m \). Figure 4(a) and (b) show the relative errors of the real parts of \( n_{eff} \) and \( L_c \)'s of the proposed scheme for various thicknesses, respectively, relative to the FEM [17]. These calculated results by the proposed scheme and the FEM exhibit good agreement.

![Fig. 4. The relative errors of (a) the real parts of \( n_{eff} \) and (b) the propagation lengths \( L_c \) of the proposed scheme at \( w = 0.5 \mu m \) versus different thicknesses \( t \). The reference values are obtained by the FEM [17].](image)

To study the mode characteristics of DLSPPW in detail, Fig. 5(a) and (b) show the effective indices and the propagation lengths of the fundamental TM\(_{00}\) mode for various waveguide dimensions.

![Fig. 5. (a) The real parts of effective index and (b) the propagation lengths of DLSPPW versus the ridge width \( w \) for several thicknesses \( t \).](image)

Figure 5(a) shows the real parts of effective index increase monotonously with the increase of the ridge width and thickness. A smaller thickness makes the mode characteristics approach the SPP mode at a metal-air interface. Considering the dependences of \( L_c \) and the waveguide dimensions, \( L_c \) increases monotonously as \( w \) decreases as shown in Fig. 5(b) because more power is confined in the ridge region. However, the dependence of \( L_c \) and \( t \) is somewhat complicated. For the condition \( t<0.4 \mu m \), \( L_c \) increases as \( t \) decreases for all \( w \)'s, but the reverse relations between \( L_c \) and \( t \) are observed while \( t \) is greater than 0.4 \( \mu m \). In addition, the occurrence of cross points is resulted from the various relations between \( L_c \) and the \( t \). The result makes the optimum choice of the trade off between the confinement and propagation length. This study discusses two definitions of mode confinement. The first one is the lateral mode extent proposed in [17] (where the mode width is measured by the \( 1/e \) of peak value of power). The lateral mode extents are computed by the effective index method (EIM), which is a simple approximate approach but only accurate for the strongly guided mode. Here, the results calculated by the proposed scheme and those by the EIM (indicated as the dash lines) are shown in Fig. 6(a).
The significant deviations of the width size for achieving the minimum lateral mode extents are found between the EIM and the proposed scheme. For instance, the minimum width size obtained are $w = 0.35\mu m$ by the proposed scheme but that are $w = 0.5\mu m$ by the EIM for the conditions $t = 0.4\mu m$ and $t = 0.6\mu m$. More deviations are found for $t = 0.2\mu m$ and $t = 0.3\mu m$. These results show that an accurate numerical scheme is vital to design photonic devices. Different from the lateral mode extent, this study proposes a simple and intuitive definition to evaluate the confinement area of DLSPPW. The new definition computes the area of a rectangle consisted of the lateral and vertical mode extents. Figure 6(b) shows the calculated results. Except for $t = 0.2\mu m$, the dependence between confinement area and thickness in Fig. 6(b) show opposite tendency relative to those in Fig. 6(a). That is, increasing the ridge thickness should theoretically shrink the lateral mode extent, but instead stretches the vertical one. The degree of stretching in the vertical dimension is greater than the shrunken degree in the lateral dimension. Figure 7 shows the mode intensity profiles $|H_x|^2$ of the fundamental SPP modes at $w = 0.8\mu m$ for different $t$'s, and verifies the opposite tendency between the lateral mode extent and the confinement area. Note that the SPP mode contour plots shown in Fig. 7(a)-(c) indicate that the peak values in each plot are normalized to 1 and the outermost contour lines denote the $1/e$ of the peak value.

In particular, the confinement areas for the condition $t = 0.2\mu m$ increases significantly while the width $w$ was smaller than $0.4\mu m$ as shown in Fig. 6(b). The result can be observed in Fig. 8, which shows the mode intensity profiles at $w = 0.2\mu m$ for different values of $t$. In Fig. 8(c), the largest mode spreading is observed at the condition $t = 0.2\mu m$. 

![Fig. 6. (a) The lateral mode extents and (b) the confinement areas of DLSPPW versus the ridge width $w$ for several thicknesses $t$.](image)

![Fig. 7. The mode intensity profiles $|H_x|^2$ of DLSPPW at $w = 0.8\mu m$ for (a) $t = 0.6\mu m$ (b) $t = 0.4\mu m$ (c) $t = 0.3\mu m$.](image)
From these results, some conclusions are given. In general, the smaller thickness and width allow the longer propagation length, and the confinement area decreases with the thickness decreases except the condition \( w < 0.4\mu m \) for \( t = 0.2\mu m \). Consequently, for obtaining the large values of FOM, the thin thickness and modest wide width around \( w = 0.4\mu m \) of the dielectric load are suitable for the optical communication wavelength \( \lambda = 1.55\mu m \). In addition, the lateral mode extent as defined only provides the measurement of the bend angle with accepted bend losses. In contrast, the confinement area proposed in this study is to calculate the mode spreading along both the lateral and vertical extents. The confinement area can be used to evaluate the performances of the active plasmonics and to measure the cross-talk of powers while constructing the compact three-dimensional photonic components. This study also analyzes the dependence of the mode characteristics and excitation wavelength. The three wavelengths of \( \lambda = 1.55\mu m (n_g = 0.55-11.5i), \lambda = 1.22\mu m (n_g = 0.36-8.60i), \) and \( \lambda = 0.893\mu m (n_g = 0.21-5.94i) \) at \( t = 0.3\mu m \) and \( w = 0.4\mu m \) are calculated, and Fig. 9 shows the resulting mode profiles. The smaller wavelength \( \lambda = 0.893\mu m \) yields better confinement areas, and therefore results in shorter \( L_c \) due to a longer penetration depth (with high material loss) of the field into the gold film.

**4.2 The inverted metal slot waveguide**

Recently, Chen et al. [43] reported experimentally that the IMSW can be efficiently coupled to a standard silicon dielectric waveguide with a high coupling efficiency of approximately 2.5dB per facet. In addition, compared with the degrees of mode confinement of nanoparticle chains, which achieve approximately \( \lambda/5 \) with losses of 30dB/\( \mu m \) (propagation length \( L_c = 0.15\mu m \)) [52], the IMSW achieves a propagation loss one order of magnitude lower. However, the geometry and wavelength dependences of the propagation characteristics are not well defined or understood. Therefore, this study investigates in detail the dependences for this waveguide. Figure 10 depicts the cross section of this waveguide structure. To conveniently integrate with a silicon wire waveguide, this design used silicon (Si) as the core and gold (Au) as the cladding. To reduce the power loss produced by a metal, a thin silica (SiO\(_2\)) layer was deposited on the top of silicon to isolate the optical field from the gold. SiO\(_2\) was also used as the substrate below the core region.
Fig. 10. The cross section of the IMSW with refractive indices of core $n_{Si}$, gold cladding $n_{Au}$, substrate $n_{SiO2}$, and silica cladding $n_{SiO2}$.

The refractive indices of Si and SiO$_2$ are $n_{Si} = 3.48$ and $n_{SiO2} = 1.44$, respectively, while that of gold is $n_{Au} = 0.55-11.5i$ under the excitation wavelength $\lambda = 1.55\mu$m. Figures 11(a) and 11(b) show the real parts of $n_{eff}$ and propagation lengths $L_c$ calculated by the proposed scheme as a function of core width $w$ for several different thicknesses $t$ for a SiO$_2$ layer with a thickness of $h = 80$nm.

The mode behaviors of the IMSW are consistent with the physics of the coupled SPP mode at vertical metal-dielectric interfaces, indicating that the optical power has better confinement (larger real part of $n_{eff}$) and yields a shorter $L_c$ (more power penetrates into metal leading to higher material loss) as the core width decreases. Figure 12 illustrates the mode intensity profiles $|H_y|^2$ at $t = 250$nm for several widths.
The mode sizes in both the lateral and vertical directions shrink as the width $w$ decreases due to the stronger coupling of the two SPP modes at metal-dielectric interfaces. Accordingly, the spot size shrinks to several tens of nanometers while the cost is the decrease of $L_c$ to several hundreds of nanometers. In particular, the $L_c$'s for the case of $t = 10$nm increase markedly as the width increases. Figure 13 illustrates the mode intensity profiles at $w = 150$nm for several different thicknesses. The effect of decreasing the thickness to the case of $t = 10$nm leads to a fairly strong spreading (less confinement) in the field from the core region to the silica regions, but the propagation length is much longer than those of the thicker core. This effect exists in pure dielectric waveguides as shown in Fig. 13(d) because the fundamental guided mode becomes a plane wave in the thin SiO$_2$ layer.

![Mode intensity profiles](image)

Note that the coupled SPP mode of the two SPP modes determines the subwavelength confinement. Consequently, the mode characteristics are analogous while reducing the core width to $w = 10$nm with the strong coupling as Fig. 12(d). For further illustrating dependences between the mode characteristics and waveguide dimensions, Fig. 14(a) and 11(b) also show the real parts of $n_{ef}$ and $L_c$'s versus the thickness $t$ for three different widths. The $L_c$'s are several tens of micrometers, while the thickness is smaller than 30nm for the case of $w>100$nm, as Fig. 14(b) shows. Beyond the width of $w = 100$nm, the differences of the mode characteristics are small.

![Mode characteristics](image)

In the IMSW, the confinement area is determined mainly by the beam height in vertical direction, and thus the degree of spreading produced by the index guiding in the $y$-direction is
also analyzed. Figure 15(a) shows the beam heights as a function of the thickness for several different widths. The minimum beam heights (about 60nm) for the cases \( w = 50\)nm and \( w = 100\)nm are both approximately at \( t = 40\)nm. The beam height is further reduced to 30nm while decreasing the width to \( w = 10\)nm. Compared to a nanoparticle plasmon waveguide with about \( L_c = 0.15\)μm \([52]\), the IMSW achieves several tens of micrometers \( L_c \) for a mode size of approximately \( \lambda/5 \) (here, \( \sim 310\)nm). In addition, this study adopts the definition of \( M_2 \) as a “benefit-to-cost” ratio of confinement and propagation length \((M_2 = (\text{real}(n_{\text{eff}}) - n_{\text{Si}})/\text{imag}(n_{\text{eff}}))\) as proposed by Berini \([44]\) to investigate the FOM of the IMSW. Figure 15(b) shows the resulting FOMs versus the \( w \) for several thicknesses \( t \). The optimum values of FOMs are between 20 and 30, revealing a trade-off between the mode confinement and propagation distance.

Figure 16 illustrates the mode intensity profiles \( |H_y|^2 \) at four optimum FOMs. Figure 16(d) clearly shows a strong spreading of the field resulting from the diffraction limit, yielding a longer \( L_c \).

Finally, this study analyzes dependence of the mode characteristics and excitation wavelength. Figure 17 shows the mode profiles for the two wavelengths, \( \lambda = 1.22\)μm and \( \lambda = 0.893\)μm, at \( t = 250\)nm and \( w = 150\)nm. The wavelength \( \lambda = 1.55\)μm has been shown in Fig. 12(a). The same conclusion as the DLSPPW is obtained, namely, a shorter wavelength yields shorter \( L_c \), due to the longer penetration depth of the mode field into the gold cladding.
5. Conclusion

This study has presented a full vector multidomain pseudospectral method to investigate the mode characteristics of nanoscale surface plasmon-polaritons (SPPs), including the dielectric-loaded surface plasmon-polariton waveguide (DLSPPW) and the inverted metal slot waveguide (IMSW). The proposed scheme prevents the spurious modes from implicitly enforcing the divergence-free condition of magnetic vector. This study has studied the waveguide dimension and wavelength dependences on the mode confinement and propagation length of the DLSPPW and IMSW structures in detail. On the other hand, for the previous confinement factor, it encounters a difficulty in integrating the power inside the core while the field decays acutely at corner and thus shows an oscillatory phenomenon even if the finer grid point distribution is applied. Accordingly, a new confinement, which calculates the area of rectangle by a product of lateral and vertical mode extents, has been proposed to evaluate the mode confinement. The confinement area shows the physical mode spreading and also evades the numerical instability produced in the previous confinement factor. Numerical results have shown that the proposed scheme is efficient and accurate for investigating the SPP mode problems compared with the generally used finite element method. The proposed scheme offers an efficient and reliable modeling approach to study various complex nanoscale plasmonic components.

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