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Dispersion characteristics of plasmonic waveguides for THz waves

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ABSTRACT

Today there is an increasing surge in Surface Plasmon based research and recent studies have shown that a wide range of plasmon-based optical elements and techniques have led to the development of a variety of active switches, passive waveguides, biosensors, lithography masks, to name just a few. The Terahertz (THz) frequency region of the electromagnetic spectrum is located between the traditional microwave spectrum and the optical frequencies, and offers a significant scientific and technological potential in many fields, such as in sensing, in imaging and in spectroscopy. Waveguiding in this intermediate spectral region is a major challenge. Amongst the various THz waveguides suggested, the metal-clad waveguides supporting surface plasmon modes waves and specifically hollow core structures, coated with insulating material are showing the greatest promise as low-loss waveguides for their use in active components and as well as passive waveguides. The H-field finite element method (FEM) based full-vector formulation is used to study the vectorial modal field properties and the complex propagation characteristics of Surface Plasmon modes of a hollow-core dielectric coated rectangular waveguide structure. Additionally, the finite difference time domain (FDTD) method is used to estimate the dispersion parameters and the propagation loss of the rectangular waveguide.

Keywords: Finite-element method (FEM), finite-difference time-domain method (FDTD), surface plasmon, THz waveguide, dielectric coated guide

1. INTRODUCTION

A remarkable expansion of technology to a wide range of components, instruments and applications, carried out in the terahertz portion of the electromagnetic spectrum (loosely defined as the frequencies from 0.3 THz to 10 THz), has been witnesses in recent years. These advances in Terahertz applications depend on the transmission properties of Terahertz sources, the penetration of Terahertz radiation through dielectric materials and the high sensitivity of Terahertz sensors. The unique properties of Terahertz radiation and spectroscopic sensing have lead to new fields of interest and significant advances in astrophysics and atmospheric science, biological and medical sciences, security screening and illicit material detection, non-destructive evaluation (NDE), communications technology, and ultrafast spectroscopy. Terahertz radiation exhibits good balance between good resolution and penetration as well as good selectivity (fingerprint) in many materials.

At present the techniques for generating Terahertz radiation are based on optically pumped lasers (OPTL), time-domain system sources, backward wave oscillators, direct multiplied sources, and frequency mixing. The introduction of quantum-cascade lasers (QCL) has proved more successful for terahertz generation and recently new techniques have revealed that that the performance of terahertz QCLs can be greatly improved by the use of spoof surface plasmon (SP) for active photonic devices.

Moreover significant research is carried out on the development of Terahertz waveguides in order to expand on current applications. Due to the absorption of THz radiation of dielectrics and metals, an outstanding problem has been the development of efficient waveguide structures with minimal transmission loss and minimal dispersion. Several waveguide designs have been proposed, including photonic crystal fibers, cylindrical hollow waveguides with dielectric coating, on-chip terahertz circuits, metallic slit, and microstrip circuits.

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Among various approaches considered, a metal clad guide which supports surface Plasmon modes (SPMs) is one of the most promising because of low loss in both active components and passive waveguides. Surface plasmon polaritons (SPPs) are transverse magnetic (TM) waves that propagate along the interface between a metal and a dielectric and decay evanescently on both sides of the interface. They are created because of the resonant interaction of the free electrons of the metal with the electromagnetic field of incident light wave. Recently, it has been shown that a dielectric-coated metal-clad hollow core circular waveguide yields low loss at THz frequencies. Such flexible guides are more suitable to deliver high power electromagnetic waves to a target, instead of using free space transmission.

In the present work the full-vectorial H-field formulation of the Finite Element Method (FEM) and the Finite Difference Time Domain (FDTD) approach have been used to analyze the modal and propagation properties of plasmonic waveguides, as well as the dispersion characteristics of such structures.

2. THEORY

A surface plasmon mode may be defined as the fundamental electromagnetic mode at the interface between a material with negative permittivity and a material with positive permittivity, where at a specific frequency electron surface-charge oscillations occur. Surface plasmon modes are confined to the surfaces where there is a strong interaction of the electromagnetic waves at the interface of the bounding materials. Surface plasmon modes couple with the free electromagnetic field along the interface between a metal and a dielectric. The interaction of the free electrons with the electromagnetic field causes surface plasmon polaritons that propagate along the interface of the materials and decay evanescently on both sides of the material.

The nature of surface plasmons (SP) can be expressed in terms of their respective field distributions, wavevectors, and the key characteristic of the electric field propagation along the interface and decay away from both the conducting and dielectric media. Thus the surface plasmon condition of the 2D wavevector $k_{sp}$ along an optically thick conducting sheet is defined by:

$$k_{sp}(\omega) = \frac{\omega}{c} \sqrt{\frac{\varepsilon_m \varepsilon_d}{\varepsilon_m + \varepsilon_d}}$$

in which the wavevector is determined by the permittivity of the thin conducting sheet ($\varepsilon_m$) and the dielectric coating ($\varepsilon_d$), where $\omega/c$ is the free space wavevector.

Due to the different frequency components travelling in the medium, the material dispersion properties are also taken under consideration. In this case, the group velocity dispersion parameter (GVD) is expressed as the temporal spread (ps) per unit propagation distance (km), per unit pulse spectral width (nm) and it is measured in ps/nm-km. The GVD parameter is associated with the second derivative of the propagation constant $\beta$, thus:

$$D = \frac{2\pi c}{v_g^2 \lambda^2} \frac{d v_g}{d\omega}$$

where $\lambda$ is the free space wavelength, $v_g$ is the group velocity, and $d v_g/d\omega$ is the rate of change of the group velocity with respect to the angular frequency $\omega$.

3. NUMERICAL ANALYSIS

The Finite Element method has emerged as one of the most powerful and successful numerical methods. A wide range of devices can be modeled from the formulations used in the FEM. The FEM offers accurate, versatile and flexible numerical analysis of optical waveguides and structures with arbitrary shapes, index profiles and anisotropies. In the present study a full vectorial H-field formulation utilizing the perturbation technique including a penalty function has been successfully applied for the modal analysis of the waveguide structure to characterize a wide range of plasmonic structure devices, at optical and Terahertz frequencies. The full vectorial approach improves the accuracy of highly localized modes, thus exploiting the irregular size elements. The full vectorial formulation, in terms of the nodal values of the full H-field vector, is based on the minimization of the of the following functional:
\[
\omega^2 = \frac{\int \left[ (\nabla \times \mathbf{H})^* \cdot \varepsilon^{-1} (\nabla \times \mathbf{H}) + p (\nabla \cdot \mathbf{H})^* (\nabla \times \mathbf{H}) \right] dx \, dy}{\int \mathbf{H}^* \cdot \mu \mathbf{H} \, dx \, dy}
\]

where \( \omega^2 \) is the eigenvalue and \( \omega \) is the angular frequency of the wave, \( \mathbf{H} \) is the full vectorial magnetic field, \(^*\) (asterisk) is the complex conjugate and its transpose, \( \varepsilon \) and \( \mu \) are the permittivity and permeability respectively, and \( p \) is the dimensionless penalty function\(^6\).

The Finite Difference Time Domain method (FDTD) has been regarded as versatile, useful and widely used electromagnetic tool. The performance of the FDTD is embellished with the development of new algorithms to cope with a wide variety of EM problems as well as ABCs\(^7\). The 2D FDTD has been widely used as a highly efficient method for solving Maxwell’s equations. In order to determine the frequency dependent dielectric properties of the metal, the Drude model has been incorporated in the leapfrog algorithm of the FDTD method. The dielectric function \( \varepsilon(\omega) \) of the Drude model is dependent on the plasma frequency \( \omega_{pd} \), and the damping coefficient \( \Gamma_D \), with well know values over a wide range of frequencies\(^8,9\):

\[
\varepsilon(\omega) = \varepsilon_r - \frac{\omega_{pd}}{\omega(\omega - i\Gamma_D)}
\]

4. RESULTS

At Terahertz frequencies most systems and applications consider free-space propagation due to lack of low-loss waveguides. Earlier work has reported on the optimization of a metal-clad circular hollow waveguide\(^10\) by adjusting the polystyrene (PS) coating, a minimum loss can be achieved. In this work, a hollow core rectangular waveguide for Terahertz propagation is presented. The structure illustrated in Fig 1 is composed of a thin gold clad (\( t_m \)) silicon waveguide with air core. The width and height of the rectangular waveguide is 1mm and the length (L) is 4.3mm. The thickness of the thin gold clad (\( t_m \)) was set to 1\( \mu \)m. A thin layer of 1\( \mu \)m of Teflon (\( t_d \)) was deposited in the inner surface of the cladding with a complex refractive index 1.445 + j0.00119 at 2.5THz. Although the structure of the waveguide supports many modes only the profile of the fundamental mode \( H_{10}^x \) and first quasi-order TM mode \( H_{20}^x \) are considered, with low loss of 10.22db/m at 2.5THz, for 1\( \mu \)m of Teflon coating.

![Waveguide Structure](image)

The effects in terms of changes in effective index and losses by changing parameters in guide dimensions, metal cladding thickness, and varying thickness of the dielectric have been reported elsewhere\(^11\). The waveguide structure presented here supports SPMs at the two interfaces between the metal/dielectric (gold/silica), and the metal/dielectric (gold/Teflon). However, since the decay length of the inner interface (gold-air) is much longer than the outer, the electromagnetic field at the silica-gold interface will decay much faster. Thus, the SPP modes formed in the inner
interface (metal/air) couple to form supermodes. An air-guided mode is formed when two supermodes are coupled. The $H^s$ field profiles are presented in Figs 2 and 3 for the fundamental $H^s_{10}$ mode along the vertical and horizontal directions using the FEM. In Fig 2 the field profile indicates the concentration of the field on the upper and lower interface of the waveguide. The SP modes on the top and bottom metal-dielectric interface couple together to form a supermode along the y-axis, as illustrated in Fig 3. A half-Gaussian wave curve along the centre axis is formed due to the boundary conditions of the side walls, which force $H^s$ to zero.

Similarly, in Fig 4 the $H^s_{20}$ higher mode field distribution also illustrates a field concentration along the upper and lower interfaces, as well a propagating field in the centre of the waveguide. The contour plot of the field profile in Fig 5 shows the rapid change of field profile at the metal/dielectric interface along the vertical direction, thus illustrating the plasmonic nature of the waveguide. The deposition of Teflon coating can minimize the negative lobes (Fig 5), thus allowing a Gaussian shaped pulse to be launched in the waveguide.

Moreover, the FDTD method is used to obtain the dispersion characteristics of the waveguide. A 2D formulation of the FDTD method with PML ABCs is used to study the electric field distribution along the axis of propagation of the waveguide. A Gaussian pulse was launched into the waveguide and the electric field at various points along the direction of propagation was monitored. The electric field distribution for a spot size of 80% and 90% of the width of the rectangular waveguide is illustrated in Figs 6 and 7 respectively, sampled at 2.5THz using DFT. The waveguide supports
a propagating fundamental mode along the centre of the waveguide with high field concentration, based on the electric field distribution. The propagating fundamental mode can be supported with minor losses as the spot size of the input pulse is decreased to 90% and 80% of the width of the waveguide. After that threshold, as the spot size decreases there is a rapid decay in the electric field with significant losses and the plasmonic behavior of the waveguide rapidly deteriorates.

In Fig 8 the normalized electric field is plotted for a source spot size of 90% the width of the waveguide (0.9mm) along the direction of propagation at two different points. The normalized electric field presents the difference in amplitude of the electric field with respect to the position of the monitor along the direction of propagation.

The dispersion parameters of the plasmonic waveguide can be calculated based on the GVD equation given earlier. Given the time-domain values of the normalized electric fields, the full-width half-maximum (FWHM) pulse width in ps for each of the monitors can be determined. The FWHM pulse spread is calculated at various points along the direction of propagation of the waveguide. In Fig 9 the FWHM pulse spread with propagation distance for different input pulse spot sizes (85-95%) is plotted. As the propagation distance increases the FWHM pulse spread increases exponentially as an indication of the dispersion that the electric field undergoes as it travels though the waveguide. The FWHM pulse spread is plotted in Fig 10 for different widths of the waveguide and for a fixed spot size of 90% the width of the waveguide. As the waveguide width decreases from 0.85mm to 0.7mm, the FWHM pulse spread increases. Whereas the plasmonic waveguide behavior in terms of the FWHM pulse spread changes in the case of 0.9mm and 0.95mm where the
FWHM pulse spread significantly decreases compared to the other values, indicating that for these values the waveguide dispersion is significantly low.

![Figure 9](image1.png)  ![Figure 10](image2.png)

**Figure 9.** Full Wave Half Maximum pulse spread with propagation distance for different input pulse spot size.

**Figure 10.** Full Wave Half Maximum pulse spread with propagation distance for different input pulse spot size.

The plasmonic waveguide dispersion per unit length (ps/mm) is illustrated in Figure 11 for various widths of the waveguide and for spot sizes of 90% and 95% of the width. As the waveguide width is decreased the dispersion per unit length is increased reaching a maximum for a waveguide width of 0.75mm and a spot size of 95% of the width of the waveguide. Similarly, the waveguide dispersion is reaching a maximum for a waveguide width of 0.76mm for a spot size of 90% of the width. As the width is decreased further down to 0.7mm the waveguide dispersion is also decreasing but at a much lower rate, compared with the minimum waveguide dispersion values obtained for a 0.9mm waveguide width and spot size 90% and 95% of the width.

![Figure 11](image3.png)

**Figure 11.** Full Wave Half Maximum pulse spread with propagation distance for different input pulse spot size.

### 5. CONCLUSIONS

A low-loss hollow-core rectangular plasmonic waveguide structure is presented with Teflon dielectric coating for Terahertz propagation. The plasmonic behavior of the waveguide is analyzed using the full vectorial FEM and the modal properties of the waveguide with emphasis on the SPM. Moreover, the FDTD method has been used as a numerical analysis tool for evaluating the electric field distribution and determining the dispersion characteristics of the plasmonic waveguide. The parameters that have been taken under consideration are the width of the waveguide, and the spot size of
the source. It has been shown that the structure of the waveguide is at optimum (minimum dispersion) when the width of the waveguide is 0.9mm with 1μm of Teflon coating, and a spot size of 95% of the width of the waveguide. The optimisation of the plasmonic waveguide is an important feature for Terahertz wave guided-applications.

REFERENCES