NanoPhotonic structures for biosensing applications

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MSc Thesis Entitled

NanoPhotonic Structures for biosensing Applications

As a part of the Master’s Degree Fulfillment

Presented by

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Under the supervision of

Prof. Mohamed Abd Al-Azim Swillam
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Abstract

Photonics – science of optics – has become one of the emerging sciences in many applications nowadays. The study of light interaction with matter has opened a lot of interesting phenomena that differ in their applications including sensing, modulation, demultiplexing, etc.

Sensing applications represent a major part in the photonics field owing to their crucial role in the detecting and diagnosis of diseases in many medical applications. On the other hand, gas sensing is considered an important application in many industrial centers. During the manufacturing of several products, toxic gases may be generated and hence the ability to detect such types of gases becomes a necessity.

The first part of this thesis is concerned with sensing applications using plasmonic and photonic structures. Several plasmonic and photonic structures are proposed that are characterized by their ultimate sensitivity and high performance. Other parameters are taken into consideration like the CMOS compatibility of our design and the possibility of being integrated with electronic chips.

Beside optical sensing and their important role in biomedical and environmental applications, optical demultiplexers are considered from the main blocks in different communication systems that are based on wavelength division multiplexing (WDM). The need to highly select certain wavelength to carry the data during transmission is increasing.

In the second part of the thesis, the design methodology of an optical filter is discussed. The optical filter can fit into many applications including demultiplexing and sensing. An optical demultiplexer is proposed and characterized by its high selectivity of wavelength in the near-infrared range to fit with the telecommunication systems. In addition, the transmission levels are of an acceptable range to ensure high signal to noise ratio.
The third and the last part of the thesis is concerned with optical coupling from free-space to guided structures. In the last part, an optical grating coupler is proposed that is characterized by its high transmission levels. The grating coupler couples the light from free-space to a shallow waveguide with a narrow lateral dimension. Such system can fit in many applications including sensing and modulation applications.
Introduction

Overview

The Physics of light matter interaction has drawn increased worldwide attention since the evolution of Maxwell equations which describe precisely the propagation of electromagnetic (EM) waves in medium. By the beginning of 1950s, extensive research has been directed towards light-matter interaction phenomena and its involvement in applications that vary from free-space optics to optical integrated circuits. In 2016, many breakthroughs in optics were achieved in many branches of optics including lasers in which 2 groups in China and Denmark [1, 2] succeeded in making an efficient, high quality single-photon laser sources which is considered as a key element in many applications including quantum information technology, and optical quantum computing. In US, a research group has proposed and demonstrated the use of optical metamaterials to play the same role as the metallic structures but with less losses using only dielectrics; the work that can lead to no-losses plasmonics and can pave the way to many applications including guiding the light in small areas and other applications [3]. In this thesis, we propose interesting applications that mainly targets sensing applications. However, we believe that before going into deep technical details related to these applications, it is important to highlight some of the basic concepts in optics in which our work is based upon. A transverse electromagnetic wave is a wave that is composed of two components; electric and magnetic field components that propagate perpendicularly to each other. These two components are also perpendicular to the direction of propagation of the wave as indicated in figure 1 (a). However, if it is possible to polarize the light into certain direction, two types of electromagnetic waves can originate. The first of them is the polarized transverse-electric (TE) electromagnetic wave (in which the electric component is perpendicular to the plane of incidence and the magnetic component is parallel to plane of incidence as indicated in figure 1 (b) [4].
Figure 4. Different optical modes. (a) Transverse electromagnetic wave in which the electric and the magnetic field are perpendicular to each other and to the direction of propagation. (b) Transverse electric (TE) mode, in which the electric field is perpendicular to the plane of incidence and the magnetic field has 2 components (x and z) in the figure. (c) Transverse electric (TM) mode, in which the magnetic field is perpendicular to the plane of incidence and the electric field has 2 components (x and z) in the figure.

The other type is the transverse magnetic mode (TM) in which the electric component of EM wave is parallel to the plane of incidence while the magnetic component is perpendicular to plane of incidence as shown in figure 1(c). It is important to determine which of both components will interact with our proposed structures based on certain configuration as will be seen by the end of this chapter. When light is propagating through different media, it is governed by Snell’s law of refraction which is given as follows:

$$n_1 \sin \theta_1 = n_2 \sin \theta_2$$  \hspace{1cm} (1)

Where $n_1$ and $n_2$ are the refractive indices of two media. The refractive index of a material is a unique property that describe the speed of light in that particular material in which the speed of light in the material is the speed of light in free-space divided by the refractive index. $\theta_1$ is the angle of incidence in medium one which is measured from the normal to the incident beam while $\theta_2$ is the refraction angle in medium two which is measured from the normal to the refracted beam. Figure 2 shows a schematic for the two media and the corresponding angles. An interesting phenomenon happens when $\theta_1$ reaches a certain value (i.e. critical angle) through which $\theta_2$ becomes 90 degrees and almost all the incident field is reflected back within the same medium with almost zero transmitted (refracted) field. This phenomenon is called total internal reflection (TIR) and it is the basic idea behind guiding optical waves inside an optical waveguide [4, 5].
Figure 5. Schematic showing Snell’s law. $E_i$ is the incident field, $E_r$ is the reflected field while $E_t$ is the transmitted field. $n_1$ and $n_2$ are the refractive indices of the 2 media.

In the next section, the theory behind the guided modes will be explained through Maxwell’s equations and applying the continuity equation. In addition, a quantum mechanical description to this nature will be explained.

**Guided Modes**

According to Maxwell’s equations [6], the electric and magnetic fields are governed by the following set of equations

\[ \nabla \times E = -j\omega \mu H \]

\[ \nabla \times H = j\omega \varepsilon E \]

\[ \nabla \cdot E = \frac{\rho}{\varepsilon} \]

\[ \nabla \cdot H = 0 \]

Assuming a structure in which a medium with high index of refraction is sandwiched between two media with lower index of refraction as shown in figure 3 [4, 5].
Figure 6. Slab waveguide assuming infinite thicknesses for the outer media

Solving Maxwell’s equations in the Cartesian coordinates, and assuming the direction of propagation of the wave to be along the x-axis, and assuming a TE excitation (i.e. $E_x = 0$, $E_z = 0$, $H_x$ is non-zero and $H_y = 0$).

The following set of equations is revealed [4, 5]

\[
\left(-\frac{\partial E_y}{\partial z}\right) i + \left(\frac{\partial E_y}{\partial x}\right) k = -j\omega\mu (H_x i + H_z k)
\]

\[
\left(\frac{\partial H_z}{\partial y}\right) i + \left(\frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x}\right) j + \left(-\frac{\partial H_x}{\partial y}\right) k = j\omega\varepsilon (E_y j)
\]

Therefore,

\[
-\frac{\partial E_y}{\partial z} = -j\omega\mu H_x
\]

\[
\frac{\partial E_y}{\partial x} = -j\omega\mu H_z
\]

\[
\left(\frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x}\right) = j\omega\varepsilon E_y
\]
The above equations show the spatial dependence of the $E_y$ on the $z$-position inside the waveguide.

Combining the above 3 equations and assuming $E_y = E_y(z)e^{-i\beta x}$, we get

$$\frac{\partial^2 E_y}{\partial z^2} + \frac{\partial^2 E_y}{\partial x^2} = -w^2\mu\varepsilon E_y$$

Which yields

$$\frac{\partial^2 E_y}{\partial z^2} = (\beta^2 - w^2\mu\varepsilon)E_y$$

And knowing that $\varepsilon = \varepsilon_0 n^2$ and given the fact that the materials don’t possess magnetic property ($\mu = \mu_0$),

$$\frac{\partial^2 E_y}{\partial z^2} = (\beta^2 - k^2 n^2)E_y$$

Where $k = \frac{w}{\sqrt{\mu_0\varepsilon_0}} = \frac{2\pi}{\lambda}$ where $\lambda$ is the operating wavelength, and $\beta$ is the propagation vector and equals $\frac{2\pi}{\lambda} n_{\text{eff}}$, where $n_{\text{eff}}$ is the effective refractive index.

Solving for the 3 media (i.e. $n_1, n_s, n_0$) and applying the continuity equations for the magnetic and electric field, we get a sinusoidal shape inside the core (i.e. $n_1$) and exponential decay in each of the cladding ($n_0$) and the substrate ($n_s$). Figure 4, shows the mode profile of the fundamental TE mode inside the slab waveguide.
Similarly, for the TM mode (i.e. $H_x = 0$, $H_z = 0$, $E_x$ is non-zero and $E_y = 0$), we get \[4, 5\]

\[-\frac{\partial H_y}{\partial z} = -j\omega \mu E_x\]

\[\frac{\partial H_y}{\partial x} = -j\omega \mu E_z\]

\[\left(\frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x}\right) = j\omega \varepsilon H_y\]

Which finally yields

\[\frac{\partial^2 H_y}{\partial z^2} = (\beta^2 - k^2 n^2) H_y\]

**Plasmonics**

Although photonic waveguides are characterized by its lossless nature, however, one of its fundamental limitations is the diffraction limit \[7\]. Abbe diffraction limit law has described the relation between the incident wavelength and the minimum dimension in which the light can propagate through. In another
words, a wave guide with core thickness comparable to or smaller than the wavelength of interest could result in weak confinement inside the core waveguide and thus wave propagation will be impossible.

In order to overcome the diffraction limit restrictions, plasmonics are being employed as an ultimate solution to consider sub-wavelength core and cladding dimensions beyond the diffraction limit. Plasmonics is an important physical phenomenon which serves as a basic platform for the emerging field of nano photonics. Plasmonics are simply a form of light matter interaction that occurs in very small dimensions much smaller than the wavelength of light. The ability of plasmonics to confine light in very small volume allows for extreme sensitivity values for Bio and gas sensors [8]. Also, it allows more components to be integrated on a chip. The paradox between electronic circuits which are of small dimensions, however, they are limited in terms of speed processing. Whereas, on the other hand, the dielectric based photonic circuits are faster in terms of speed, however, they are large in dimensions. Plasmonics have bridged the gap between the necessity of small dimension and fast processing. They can achieve sub-wavelength confinement while photons can transmit the signal which by nature faster than electrons. Recently, many integrated electronic/photonic circuits are an active research field which mainly relies on plasmonics’ concept.

Plasmonics deal with the interaction between light and the electrons in the outer most shell of metals where electrons oscillate in phase with incident field with the field experiencing an attenuation with different coefficients as shown in figure 5. This interaction results in a surface wave on top of metal (and within certain skin depth inside the metal) called: Surface Plasmon Polariton (SPP). Plasmonics can be described by two possible optical properties, either propagating surface plasmon polariton or localized Surface Plasmon Resonance (LSPR). These two properties depend on the geometrical shape, material type, and the operating wavelength.
Figure 5. Schematic for the Metal/dielectric interface on which the SPP propagates

LSPR can be realized when dimension of metallic nano particle embedded inside a dielectric medium is smaller than wave length of light $d < \lambda$. This property can have interesting applications including antennas, resonance cavities, solar cells, and enhanced Raman scattering surfaces. On the other hand, propagating SPPs can be manipulated into other applications including interference effects, data transmission, etc [9]. In the rest of this section, we will be dealing with propagating SPPs as it is the main concern in the thesis topic.

The dispersion relation for the metal-dielectric plasmonic structure can be obtained by solving Maxwell’s equations and following the same procedures as done for the photonic structures. Through a mathematical proof, it can be shown that a metal/dielectric interface cannot support TE modes and can only support TM modes. The electric field in this case is given by [7]

$$E_{z>0} = A_2 e^{i\beta x} e^{-k_2 z}$$

$$E_{z<0} = A_1 e^{i\beta x} e^{k_1 z}$$

By solving Laplacian equation: $\nabla^2 E = 0$, we get that $k_1 = k_2 = \beta$

The propagation vector is represented by [7]

$$\beta = \frac{2\pi}{\lambda} \sqrt{\frac{\varepsilon_m \varepsilon_d}{\varepsilon_m + \varepsilon_d}}$$
where $\varepsilon_m$ is the metal permittivity while $\varepsilon_d$ is the dielectric permittivity. From this equation it can be concluded that the effective index is given by

$$n_{\text{eff}} = \sqrt{\frac{\varepsilon_m \varepsilon_d}{\varepsilon_m + \varepsilon_d}}$$

Since $\varepsilon_m$ is a function of the wavelength, the effective index varies with changing the spectral range. $\varepsilon_m$ can be expressed by the following model [7]

$$\varepsilon(\omega) = \varepsilon_r(\omega) + i\varepsilon_i(\omega)$$

$$\varepsilon_r(\omega) = 1 - \frac{\omega_p^2}{\gamma^2 + \omega^2}$$

$$\varepsilon_i(\omega) = \frac{\gamma \omega_p^2}{\omega(\gamma^2 + \omega^2)}$$

Where $\varepsilon_r(\omega)$ and $\varepsilon_i(\omega)$ are the real and imaginary parts of the metal permittivity, $\omega_p$ is the plasma frequency, and $\gamma$ is the collision frequency.

To ensure the continuity of the field across the boundaries in which [7]

$$E_{z>0}(0) = E_{z<0}(0)$$

and [7]

$$\varepsilon_d(\partial E_{z>0}/\partial z) = \varepsilon_m(\partial E_{z<0}/\partial z),$$

we get: $\varepsilon_d + \varepsilon_m = 0$; hence, for the plasmonic effect to occur, and given that the real part of $\varepsilon_d$ is positive we conclude that the real part of $\varepsilon_m(\omega)$ must be negative.
Layered Plasmonic Structures

In most of the plasmonic systems, researchers mostly employ layered plasmonic structures in which layers of metals and dielectrics are stacked on each other. These metal-insulator stacks possess some interesting properties as discussed below.

One of the famous architectures in plasmonics is the 3-layered structure. For simplicity, we assume an MIM structure in which a dielectric with $\varepsilon > 0$ is sandwiched between two identical metal layers with $\varepsilon_r(\omega) < 0$. The dispersion relation, which relates the propagation vector to the angular frequency, is given by [7]

$$\tanh k_d \frac{d}{2} = - \frac{k_m \varepsilon_d}{k_d \varepsilon_m}$$

for fundamental even mode, and [7]

$$\coth k_d \frac{d}{2} = - \frac{k_m \varepsilon_d}{k_d \varepsilon_m}$$

for the fundamental odd mode.

Where $k_d = \sqrt{\beta^2 - \left(\frac{\omega}{c}\right)^2 \varepsilon_d}$, $k_m = \sqrt{\beta^2 - \left(\frac{\omega}{c}\right)^2 \varepsilon_m}$, and $d$ is the thickness of the middle layer. Similarly, for the IMI structures, the dispersion relation is given by [7]

$$\tanh k_m \frac{d}{2} = - \frac{k_d \varepsilon_m}{k_m \varepsilon_d}$$

for fundamental even mode, and [7]

$$\coth k_m \frac{d}{2} = - \frac{k_m \varepsilon_d}{k_d \varepsilon_m}$$
for the fundamental odd mode.

Figure 6 shows the dispersion relation for an MIM structure, the metal was assumed here to be lossless with the drude model [7]

\[ \varepsilon (\omega) = 1 - \frac{\omega_p^2}{\omega^2} \]

with \( \omega_p = 800\pi \) THz = 0.34 \( \frac{2\pi c}{d} \). The dielectric is assumed to have \( \varepsilon_m = 6.25 \) was assumed as the insulator. As shown in the figure, the propagation vector reaches a saturation level at the plasma frequency of the system. As shown from the figure, the propagation vector saturate at an angular frequency equal to 0.12 \( \frac{2\pi c}{d} \). Beyond this plasma frequency, no plasmonic modes exist.

![Figure 6. Dispersion relation for the MIM structure](image)

One of the limitations of the MIM structures is that although the field is confined at the interface between the metal and the dielectric, as the thickness of the insulator decreases, more of the field enters the metal layers and thus a huge amount of the field is lost. That’s why it is of great importance to consider this effect while designing MIM systems.
Insulator-Metal-Insulator (IMI) plays an important role in many applications that require having 2 surface plasmons waves that do not interfere with each other. Theoretically speaking, electric field cannot penetrate the metal layer. However, because of the collision frequency and the losses, some of the field penetrate the metal into a very small depth called the skin depth. However, if the metal is thick enough, the 2 surface plasmons waves can be decoupled.

**Brief on the thesis work**

In this work, optical sensing is the main concern. For optical plasmonic sensors, a design based on IMI plasmonic sensor has been introduced that has the capability of being integrated with electronic chips. This design is suitable for lab-on-chip (LoC) applications in which various sensors are integrated on one chip to perform different diagnosis, thus, saving time and area on chip. Different parameters have been considered to maintain high performance including the sensitivity of the sensor which describes how responsive is the sensor to minor chemical changes in the medium. The other branch in optical sensing applications is the environmental sensing. Environmental sensing is considered a crucial application and especially in industrial corporations in order to sense and detect the presence of toxic gases that may appear during the manufacturing of products. One of the ways of the detection of these gases is optical spectroscopy that helps is characterizing these gases by the detection of certain absorption peaks for them along the spectrum and especially in the mid-infrared region. For this, working on the design of optical sensors in the mid-infrared region to highly select different gases based on their absorption spectrum is crucial. Thus, as a part of the thesis, the design of an IMI plasmonic sensor at the infrared region has been performed to detect such gases.

The second part of the thesis focuses on large scale applications in which a design of a fiber-based optical liquid sensor that works in the near-infrared region (wavelength: 1200 nm –> 2000 nm) is proposed. The optical fiber achieved high performance in terms of the sensitivity. Being based on fiber can make it easier to fabricate than the integrated based optical sensors.
In the third part, in addition to the plasmonic sensor, a shallow waveguide photonic based optical sensor has been also studied which minimizes the losses associated with plasmonic structures. The shallow waveguide photonic optical sensor has higher performance in comparison with the conventional photonic sensor available nowadays. Therefore, can be a promising solution for applications that require the usage of high performance sensing applications.

In the last part of the thesis, a new computational technique based on the Beam Propagation method (BPM) is discussed. The new technique relies on using the leap-frog technique to solve the BPM equation by splitting real and the imaginary parts ahead. By doing so, less computational time was achieved. Different photonic structures are solved to prove the validity of the proposed method. Comparison with experimental data is done to check the accuracy and the proposed method is faster than the conventional way of solving the BPM equation by 200%.
References


Silicon Plasmonic Integrated Interferometer Sensor for Lab on chip Applications

Abstract. A novel sensing structure on a silicon platform is proposed with access silicon waveguide ports. The sensing mechanism is mainly based the interference effect between the SPP wave on both interferences. The sensing platform contains a metal channel deposited on silicon nitride base. The top and the bottom metal surfaces carry 2 decoupled SPP modes. The dimensions are optimized to maximize the coupling from the input silicon waveguide to the SPP wave at the top and bottom metal interfaces. High sensitivity and small foot print is achieved using this integrated simple plasmonic design. Full wave analysis is performed to examine the performance and optimize the dimensions and material. The optimized design and optimal material yield enhanced sensitivities of 19000 nm/RIU.

Introduction

The compact size of integrated sensor is an essential feature for lab on chip (LoC) applications. These applications require the sensor to be integrated, low-cost, compact, highly sensitive and selective for portable, and rapid bio-analytical applications. Among various types of optical sensors, plasmonic structures based sensors have been utilized increasingly in the design of LoC sensing applications [[1],[2],[3],[4]].

Surface plasmon waves are originated from the interaction of light with free electrons in the metal resulting in oscillatory surface plasmon polaritons at the dielectric-metal interface. Being sensitive to the optical properties of the environment (i.e. refractive index of the surroundings), surface plasmon waves and hence plasmonic structures can be an effective solution for building nano-scaled optical sensors. Aside from being a promising solution for optical sensing, this nature can help in different aspects of optical applications [[5] - [18]].

Being compactly integrated with micro-fluidic platforms, Nano-plasmonic biosensors could be a promising alternative in the development of portable biosensors in different biomedical applications [[19]-[23]]. Due to having the capability of being miniaturized and cost effective (i.e. depending on the materials used and their CMOS compatibility), plasmonic sensors can be used in the design of LoC sensor containing hundreds and may be thousands of sensors on the same chip [[3],[19]]. Among these LoC applications, an array of plasmonic sensors was designed with a footprint in the order of micrometer square and a multiplexing capacity in the order of 10 million sensors in 1 centimeter square [[24]] opening the door for effective and parallel processing and characterization [[23]].
Although many plasmonic based sensor have been proposed in the previous years and have proven to be of high sensitivity and good performance, most of them lack the possibility of being integrated with CMOS technology. In addition, many of sensors proposed before that have the integration capability suffer from low sensitivity as shown in the below sections. Furthermore, for MZI-based sensors, sensitivities and the overall performance are closely related to the arm length. However, due to the intrinsic propagation loss of metals, channel length of the metal/insulator is limited and hence the achievable optical performance doesn’t reach high levels. Through the recent years, many plasmonic-based MZI sensors were proposed [17, 25-26], however, the reported sensitivities were much smaller than those reported for photonic-based sensors [27, 28]. On the other hand, photonic-based MZI sensors require long structures and thus don’t fit into applications that require small size. That’s why plasmonic integrated based sensors are preferred for applications that require massive multiplexing for lab on chip applications.

For example, a large scale bio-chemical sensor was proposed with sensitivity as high as -92,000 nm/RIU, however, it lacks the possibility of being integrated with electronic chips [29].

Interferometric sensors have been among the efficient alternatives owing to their dependence on optical interference and can be utilized to monitor molecular interactions. Different interferometry techniques have been emerged in sensing applications including, but not limited to, fluorescence interferometry, Young and back-scattering interferometry [30-37]. Plasmonic interferometric sensors were proposed in [38, 39], and considered as an efficient platform for label-free based biomedical sensors [40].

Throughout this work, a compact, highly sensitive on chip sensor is proposed. The sensor is characterized by its high FOM. The proposed sensor can be fabricated using silicon photonic technology for large scale production of lab on chip systems. In order to achieve these objectives, the proposed design utilizes the advantages of plasmonic sensors in terms of compact size and high sensitivity along with the silicon access waveguides for coupling and integration with other silicon photonic devices on the same chip. High sensitivity in the range of 19000 nm/RIU is achieved which is higher than those previously reported [[15]-[18]]. The proposed design has higher FOM than in [29]. It also can be easily integrated with other silicon photonics structures on the same platform.
The paper is organized as follows; Section 2 describes the proposed sensor structure in addition to the materials used along with simulation results. In addition, section 2 provides a theoretical analysis of the proposed structure and compares its results with the simulation results. Section 3 shows the optimization processes of the performance of the proposed structure. Section 4 discusses some of the previously proposed results and compares between the proposed results and previous results in literature. Finally, section 5 concludes the paper.

1. Structure Analysis

This section describes the proposed design and the theoretical analysis for obtaining higher sensitivity and better performance for the sensing structure. A closed model that was already proposed in [38] is described and verified based on the recent results. The section is organized as follows; sub-section A describes the proposed design and sub-section B describes the theoretical model and the dependence of the sensitivity on different design parameters.

A. Proposed Design

The schematic of the sensing structure is illustrated in figure 1; the structure consists of two silicon ports with a plasmonic (IMI) channel in between. Each metal/dielectric interface can support an SPP mode with interference effect between the two branches. As can be seen from figure 1, the top surface represents the sensing arm while the dielectric beneath the metal represents the reference arm. In simulations, water (n=1.33) is assumed as the upper arm and "Johnson and Christy" models available in Lumerical are used [41]. The metal thickness is adjusted to be 30 nm, the silicon-dioxide thickness is 1 μm, and the two silicon ports are 0.22 μm thick while the base insulator layer to the metal is 60 nm thick. The depth is adjusted to be 0.40 μm. Both the insulator and metal type are varied in this work till reaching the best possible optimized results.

The proposed design is similar to the work proposed in [38] in the way of having 2 media on the top and bottom of the metal layer (i.e. and hence the name vertical). The 2 SPP waves will propagate independently till they interfere at the output waveguide. Although the method of excitation is different, however, the same technique of operation (propagation of 2 SPP modes and interference) is the same in both designs.
The sensitivity is controlled by the dimensions and the optical properties of the materials [29]; it was proposed that having a dielectric with an index of refraction close to that of the upper arm will lead to an enhanced sensitivity. However, such materials shall have refractive index large than that for the substrate, otherwise the SPP may find a leaky way to the substrate.

Initially, silicon layer was used as the lower sided dielectric layer. Longer channel helps in increasing the sensitivity as expected from [(29)]. A limited sensitivity of 300 nm/RIU was recorded for a 30 µm long plasmonic channel at wavelength about 1.55 µm. Higher sensitivity through longer plasmonic channels can be achieved with a degradation in power level.

To enhance the sensitivity, different materials with lower refractive indices than silicon are tested to achieve higher sensitivities for the same device length. Silicon nitride is found to be the best choice to use since its index of refraction has a value of 2.1 which is closer to water (background index of the sensing material) than silicon. In addition, silicon nitride is characterized by its CMOS compatibility and thus can be used in the fabrication of silicon photonics. Hence, no complex processes will be involved during the fabrication of the proposed sensor [(42), (43)].

A sensitivity of 3881 nm/RIU is achieved using this platform which is ~10 times higher than that recorded for silicon for the same channel length (L=30 µm).

For the rest of this paper, silicon nitride is used as the dielectric layer beneath the metal layer. The rest of the paper will study the effect of using different metal types and its effect on the sensitivity, the line-width (i.e. full-width half maximum FWHM) and the Figure of Merit (FOM).

\[
\text{FOM} = \frac{S}{\text{FWHM}} = \frac{\Delta \lambda/\Delta n}{\text{FWHM}} \quad (1)
\]

Assuming silver as the metal layer, figure 2 and 3 show the output transmission as a function of wavelength through the FDTD simulations. Figures 2 and 3 correspond to the transmission intensities for a refractive index change of 0.01.
(from 1.33 to 1.34) for channel length of 40µm and 60µm, respectively. Assuming light propagation from left to right side, the transmission intensity is detected at the right silicon photonic waveguide. To be more precise in evaluating the sensors performance, the figure of merit is calculated and found to be 132 with a FWHM in the range of 27.87 nm.

By replacing silver by gold, figure 4 and 5 show the transmission pattern as a function of wavelength in the FDTD simulations.

*Figure 1.* 3D Design of the proposed plasmonic sensor, d1=d4=0.4µm, d2=0.22µm, d3=2µm, d6=60nm, d7=1µm. d5 as well as the length of the channel are varied according to the metal and dielectric used.

The inset shows electric field profile distribution on the (IMI) interface. In addition, the inset shows the electric field exponential decay along the metal depth and the propagation path as shown by the lower exponential curve. Background refers here to the sensing arm.

*Figure 2.* Transmission as a function of the wavelength; Lch=40µm, d6=60nm, and d5=100nm.
Red and blue lines in figures 4 and 5 correspond to the transmission intensities for slightly different refractive indices of the environment with different design parameters. For channel length of 40μm, it is found that the sensitivity is around -3,600 nm/RIU for gold thickness of 50nm at $\lambda_0 \sim 1.55$μm. The minus sign "-" expresses that the shift is a blue shift towards smaller wavelength.

Increasing the channel length from 30μm to 40μm affects both the sensitivity and the FWHM. As shown in figure 6, the sensitivity is around -2900 nm/RIU at $\lambda_0 \sim 1.55$μm. For the proposed sensor, it is found that the structure yields a sensitivity of -3691 nm/RIU at a channel length of 40μm at $\lambda_0 \sim 1.55$μm. The FOM of this plasmonic MZI (for L = 40 μm) is around 37.2 with FWHM of 77.88 nm.

Figure 3. Transmission as a function of the wavelength; Lch=60μm, d6=60nm, and d5=100nm

Figure 4. Transmission as a function of the wavelength; Lch=40μm, d6=60nm, and d5=100nm
**B. Theoretical Analysis**

The explicit relation between sensitivity and each of the effective index as well as the operating wavelength was explicitly proposed in [31] and given by the following equations

\[
S = \frac{\frac{\lambda}{nu^3} \left(\frac{\epsilon_m(\lambda)nu^2}{\epsilon_m(\lambda)+nu^2}\right)^{\frac{3}{2}}}{\left(\frac{\epsilon_m(\lambda)nu^2}{\epsilon_m(\lambda)+nu^2}\right)^{\frac{1}{2}} - (neff)^{\frac{1}{2}}} \tag{2}
\]

\[
FOM = \frac{2Lch}{\lambda} \left(\frac{\epsilon_m(\lambda)nu^2}{\epsilon_m(\lambda)+nu^2}\right)^{\frac{1}{2}} \frac{1}{nu} \tag{3}
\]

Where \(\epsilon_m\) is the permittivity of the metal, \(nu\) is the refractive index of the upper layer (water), \(neff\) is the effective index of the lower plasmonic interface which is calculated from the FDTD simulator, and \(Lch\) is the plasmonic
channel length. The effective index of the lower channel is calculated using the FDTD simulator since the dielectric is not thick enough to use the common formula to calculate the plasmonic effective index, therefore, it's measured using the FDTD tool. Equation (2) shows the relation between the sensitivity and the difference between the effective indices of each metal dielectric interface. From such expression, it can be concluded that having upper and lower arm (i.e. in this case the two dielectric interfaces) with close refractive indices results in achieving higher sensitivity. In addition, equation 2 describes the dependence of the sensitivity on the operating wavelength. Based on equation (2), working at higher optical wavelengths leads to higher sensitivity values keeping in mind water absorption at near infrared [33]. Equation (3) interprets the relation between the figure of merit, and each of the channel length, wavelength and the ratio between the effective index and the background index.

From equations 2 and 3, longer plasmonic channels leads to better FOM. Such good matching between this model and the simulation results would help in further enhancing the closed form model in a way that can fit with the results in the near-infrared region.

Although equation 2 predicted that enhanced sensitivity is achieved by having a slight difference in the refractive index between the lower arm (dielectric beneath metal) and the surrounding medium. However, on the other hand, making the index smaller than that of silicon nitride makes its value closer to that of the substrate (i.e. silicon dioxide) and hence the SPP wave can find a leaky path towards the substrate and the interference pattern will be affected negatively. Figure 7 shows the transmission in case of using aluminum oxide instead of silicon nitride; as can be seen, the FWHM is greatly widened, resulting in very low FOM. This output is extracted for the same design parameters as those in figure 5 but using aluminum oxide (n=1.7) instead of silicon nitride and hence has a worse interference pattern as stated above.
As stated in [29], it was shown through theoretical equation that the design sensitivity is affected by the background index, the channel effective index and the channel length. Although the proposed design and design previously proposed in [29] differ in some points, both have the same overall schematic. It is shown through simulations that silicon nitride has better performance in terms of sensitivity and FOM than silicon. Increasing the length of the channel affects the figure of merit and the sensitivity of the plasmonic sensor. Changing the metal type affects the sensitivity and hence the FOM.

The relation between the FOM and the channel length using silver in 2D simulations at specific dimensions is showed in figure 8. As expected from the theory, having an approximately increasing sensitivity with increasing the channel length and a narrower FWHM with increasing the channel length (since more peaks and valleys exist in the same wavelengths range) will result in an increasing FOM as shown in equation 1. However, this comes on the expense of the output power level. The relation between the thickness and the FOM doesn't follow a certain trend; it
takes an oscillatory pattern as shown in figure 9. The change in the FOM is not significant which minimizes the effect of fabrication tolerance on the performance of the structure. The effect of the metal thickness on the FOM is lower than the effect of the channel length owing to the fact of having a weak dependence of the effective refractive index on the metal thickness. Therefore, with keeping the channel length constant and having almost no change in the effective index, the FOM will vary within a small range.

The relation between changing the channel length and the FWHM of the transmission is shown in figure 10. Increasing the channel length will strongly enhance the interference effect which results in increasing the number of peaks and valleys of the signal and hence decreasing the FWHM. Due to the fact of being inversely proportional to the FOM, this leads to increasing the FOM as shown in figure 7.

**Figure 9.** Figure of Merit versus different metal thicknesses using Gold – 2D; Lch=30µm, d6=60nm

According to the theory of plasmonic structures, when a metal sheet is interfacing with an insulator, there exists a surface plasmon wave that is referred to as the plasmonic mode. However, for the case of MIM/IMI structure where the metal thickness is large, the two plasmonic modes become decoupled.

**Figure 10.** FWHM versus different channel lengths using Silver – 2D
In such case, each plasmonic mode can be dealt with as an isolated metal/insulator interface in which the effective index is given by the relation

\[ n_{\text{eff}} = \sqrt{\frac{\varepsilon_1 \varepsilon_2}{\varepsilon_1 + \varepsilon_2}}, \varepsilon_1 > 0 \quad (4) \]

where \( \varepsilon_1 \) and \( \varepsilon_2 \) are the, dielectric and metal permittivity, respectively. According to modal analysis using FDTD simulations, it is concluded that the minimum metal thickness required to have 2 decoupled modes (i.e. the metal thickness in the IMI channel) shall be in the range of 50nm. Variations in the metal thicknesses are made in the 2D simulations ranging from 50nm to around 100nm to study the effect of these thicknesses on the overall performance as shown in figure 9.

In order to gain knowledge on the coupling efficiency, a comparison between the effective indices of the input waveguide and the insulator/metal/insulator plasmonic waveguide is made. The effective index of the input waveguide is calculated to be 1.73 while the effective index of the water/metal/SiN is found to be 1.64, 1.65, and 1.76 for silver, gold, and copper, respectively. These close values predict efficient coupling between the photonic and plasmonic modes. In addition, the propagation losses of copper, gold, and silver are calculated and found to be 1.54 dB/\( \mu \)m, 0.54 dB/\( \mu \)m, and 0.13 dB/\( \mu \)m, respectively. Although the propagation loss of copper plasmonic channel is high, smaller lengths can be employed while still maintaining high optical sensitivity.

The fabrication of the optical structure can be performed in a sequence of fabrication procedures as follows: (1) depositing poly silicon at approximately 700 degree Celsius on the silicon dioxide substrate, (2) using positive dry etchant to etch the silicon everywhere except at the designated places at the input and output ports; the use of dry etching will guarantee anisotropic etching in the vertical direction only, (3) depositing silicon nitride along the structure including the silicon waveguide, (4) depositing the metal layer along the structure covering the silicon and silicon nitride, (5) use negative wet etchant to etch the metal and the silicon nitride everywhere except along the plasmonic waveguide in design. Although the wet etching can etch in 2 directions, the small thickness of the metal
and the silicon nitride will guarantee that the horizontal etching is minimized in a way that does not affect the design functionality. By using positive and negative etchant, it is possible to use the same lithography techniques.

A similar structure to this sensor was proposed in [29]. Nearly, perfect matching of transmission patterns between the simulation and the experimental results was achieved. This gives a motivation to suggest that the proposed design will not have crucial problems in terms of the reproducibility of the results experimentally. The proposed design is characterized by its ease of fabrication due to the absence of complex shapes in the design. Therefore, a prediction that simulation results will match the experimental results is valid.

2. 3D Analysis

Utilizing gold as the metal layer, figures 11, 12 and 13 show the relation between the output transmission and the wavelength from the FDTD simulations. For 3D simulations, a sensitivity of -1500 nm/RIU for channel length 40μm is achieved while it is around -1900 nm/RIU for channel lengths 60μm and 80μm with different FWHM at \( \lambda_0 \sim 1.55 \mu \text{m} \). The design yields a sensitivity of -1660 nm/RIU at channel length about 80μm at \( \lambda_0 \sim 1.55 \mu \text{m} \) with a FOM of 60.68.

Using copper instead of gold, figure 14 shows the relation between the output transmission and wavelength in the FDTD simulations. For 3D simulations, it is found that the structure yields a sensitivity of -19400 nm/RIU at channel length of 80μm at \( \lambda_0 \sim 1.55 \mu \text{m} \) with FOM of 143 (FWHM=135 nm) which is the greatest to our knowledge among all the previously proposed sensors.
Figure 11. Transmission as a function of the wavelength; Lch~40µm, d6=60nm, and d5=50nm

Referring to equation (2), closer effective indices of the upper and lower arms leads to higher sensitivity. The high sensitivity value for using copper may be due to the fact that the lower plasmonic interface has an effective refractive index closer to the effective refractive index of the upper plasmonic channel. By calculating the plasmonic modes effective indices, it was found that Cu/SiN interface has an effective index of 2.35 compared to 2.29 for Au/SiN. Given that the effective index of the Cu/water is 2.45 and that for Au/water is 2.41 it can be found that copper experience a better sensitivity as compared to gold. The same technique of calculating the effective index using the FDTD tool was used in validating the sensitivity ratio between Si and SiN in the case of using silver; ratio was found to be 20/1.6 which is close to 10 times as found through simulations.

Using equations (1) and (2) for 3D analysis and taking into consideration the change in the effective refractive index from 2D to 3D transition, an insight about the results can be estimated. The variations of the effective refractive index between 2D and 3D analysis affect the mode coupling and effective index matching between the plasmonic and photonic waveguides. Thus, the detected power levels vary.

Figure 12. Transmission as a function of wavelength; Lch~60µm, d6=60nm, and d5=50nm
3. Discussion of The Results

Recently, a fiber-optic waveguide-based SPR plasmonic sensor was proposed with a sensitivity of 4400 nm/RIU [44]. Despite the high sensitivity value as compared to the silver and gold proposed in this paper, the FOM is calculated and found to be 41 which is less than the reported values in this paper even at short lengths as can be seen from figure 8. A young-interferometer based chemical sensor was proposed with a length of 4 mm and a sensitivity equivalent to -3300 nm/RIU [45]. Although the sensitivity reported was high, however, no information on the FWHM or the FOM was discussed.

An SOI photonic crystal based gas sensor that has sensitivity of 510 nm/RIU with cavity length of 2 µm was proposed in [14]. An SOI chemical sensor with sensitivity 2,169 nm/RIU around $\lambda_0$=1.5µm and size of 200 × 70 µm$^2$ was proposed in [15]. High sensitivity was achieved through the design of an interferometric based bio-chemical sensor with sensitivity up to −92000 nm/RIU and FOM around 122 in the visible range [29]. Various sensors are compared in Table 1.
### TABLE 1. Calculated Sensor Sensitivities, Full Width Half Maximum (FWHM), and FOMs for Different Sensor Structures

<table>
<thead>
<tr>
<th>Architecture</th>
<th>Operating Wavelength (µm)</th>
<th>Sensitivity (nm, RIU⁻¹)</th>
<th>FWHM (nm)</th>
<th>FOM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Proposed Design</td>
<td>~1.550</td>
<td>-19,400</td>
<td>135</td>
<td>143</td>
</tr>
<tr>
<td>Interferometer Based Sensor [29]</td>
<td>~0.400-0.800</td>
<td>-92,000</td>
<td>--</td>
<td>122</td>
</tr>
<tr>
<td>EOT Based Sensor [16]</td>
<td>1.520-1.570</td>
<td>1,100-1,570</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>Interferometer Based Sensor [17]</td>
<td>~1.550</td>
<td>250</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>Ring Resonator Based Sensor-Disk [18]</td>
<td>~1.460</td>
<td>600</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>Ring Resonator Based Sensor-Triangular [18]</td>
<td>~1.555</td>
<td>600</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>Fiber based plasmonic sensor [44]</td>
<td>~0.400-0.800</td>
<td>4400</td>
<td>~107</td>
<td>41</td>
</tr>
<tr>
<td>Young interferometer based sensor [45]</td>
<td>~0.400-0.800</td>
<td>-3300</td>
<td>--</td>
<td>--</td>
</tr>
</tbody>
</table>
4. Conclusion

In this paper, a plasmonic MZI based sensor that is suitable for LoC sensing applications is proposed. 2D simulations showed that the combination of sensitive interferometric techniques with Nano-plasmonic architectures can yield an enhanced sensitivity up to 3000 nm/RIU and high FOM in order of 130. Additionally, the 3D simulation yields sensitivity around 1660 nm/RIU and FOM of 61. Using copper instead of gold yields sensitivity of 19317 nm/RIU and FOM of 143 which is the greatest to our knowledge. The study of generalizing the sensor functionality to work in biomedical applications related to measuring the concentration of different species like proteins or viruses will be studied given the fact of the high adhesion of gold to these species.

References


Silicon Plasmonics On-Chip Mid-IR Gas Sensor

**Abstract.** A novel all silicon plasmonic structure is proposed with silicon access waveguides. In principle, a highly doped silicon which acts as a plasmonic like media carries two surface waves on each surface that interfere at the output waveguide. The top surface is considered as the sensing arm of this plasmonic Mach-Zehnder interferometer (MZI). The bottom surface is considered as the reference arm of the sensor. High sensitivity and small footprint is achieved using this integrated simple all silicon based plasmonic design. The optimization process of the design and the material yields enhanced sensitivities up to 6000 nm/RIU at operating wavelength of 5300 nm. The proposed on Chip sensor has been utilized for different carbon gas. This study shows the capability of the proposed sensor to characterize of different gases. Being built of CMOS compatible materials, it is believed that the proposed design could be fabricated without altering the conventional fabrication steps in the CMOS foundry.

**Keywords:** interference, sensor, mach-zehnder, plasmonics, selectivity, Kramers-Kronig.

**INTRODUCTION**

LAB-ON-CHIP (LoC) applications are considered as one of the promising application in the field of optical sensors. However, these applications require building optical sensors that possess small intrinsic size, with high sensitivity and selectivity. Fortunately, Nano-plasmonic sensors are an emerging platform that can fit with LoC applications [1]-[9].

Mid-Infrared (Mid-IR) range offers a promising alternative to detect various gases whose absorption peaks exist within the mid-IR region. In this region, many gases absorb the incident optical field in a unique way and thus the absorption peaks act like a fingerprint for each gas in the mid-infrared region and this would therefore help in the design of highly selective optical sensors. The absorption peaks affect the overall transmission pattern of the system and the gas could be easily detected [10].

Nano-plasmonic sensors employ nanoparticles or nanostructured metallic films to couple incident light directly into Surface Plasmons (SPs). This optical property at the metal-insulator interface highly affects their sensitivities to changes in the refractive index at the metal interface. This attractive property of SPs is the basis for Surface Plasmon Resonance (SPR) sensing, modulation, and other applications [11]-[21].

On the other hand, plasmonic based sensors suffer in terms of the optical losses due to the intrinsic optical loss characteristic nature of metals [22] which puts a stringent limit on the dimensions of the structure to minimize the propagation loss effect. Therefore, by employing their high sensitivity, and the necessity of having small-sized plasmonic structures, such structures are considered promising candidates for LoC applications. Consequently, by
employing plasmonic optical structures with both potentially high selectivity, through working in the mid-infrared range, and high sensitivity owing to the SPs confinement, an efficient LOC based sensor easily achieved.

Although many plasmonic based sensors have been proposed in the previous years and have proven to be of high sensitivity and good performance, most of them lack the possibility of being integrated for on-Chip applications [23]-[27]. Varying between their bulky sizes or the complex design pattern including plasmonic nanoparticles made the process of integration with chip technology not feasible. Through the recent years, many plasmonic-based MZI sensors were proposed [23]-[25], however, the reported sensitivities were much smaller than those reported for photonic-based sensors [28][29]. Through this work, an MZI based plasmonic integrated sensor is proposed that have high sensitivity that out performs the performance of previously reported counterparts. By having a high sensitivity along with high selectivity, it is believed that this design topology could result in an efficient LOC based sensor.

In general, plasmonic structures utilize Nobel metals such as silver and gold to achieve the surface wave in the optical regime. However, these metals suffer from the lack of CMOS compatibility. In addition, metal-dielectric structures in MIR range suffer from low field localization at the interface which leads to low sensitivity [18]. Recently, doped silicon is proposed as a suitable plasmonic material in the Mid-IR range with high field localization and CMOS compatibility [18]-[20]. In addition, the doping level can be easily exploited to control the working wavelength range, confinement and losses [18]-[20].

In this paper, an integrated plasmonic sensor design is proposed. This sensor is based on interface effect and can be easily fabricated using the conventional silicon fabrication techniques. It leads to a highly compact sensing system in terms of high density associated with a high sensitivity and selectivity.

**Structure Design**

The schematic of the sensing structure is illustrated Fig. 1; the structure consists of two silicon ports with a plasmonic (IMI) channel in between; each interface can support an SPP mode with interference effect between the two branches. As can be seen from Fig. 1, the top surface represents the sensing arm while the dielectric beneath the metal represents the reference arm. Different gases are assumed in the simulations. In sensitivity calculations, air was assumed as the gas being sensed while doped silicon is assumed as the metal layer. The permittivity of the doped silicon is calculated based on the doping concentration. The use of doped silicon will help on controlling the tunability
of the plasma frequency and hence the response of the optical structure.

In the proposed model, magnesium fluoride (MgF$_2$) is used as the dielectric layer beneath the doped silicon layer. MgF$_2$ is a CMOS compatible material [30] that has a good transmission spectrum in the MIR range (2000nm-6000nm) besides being a low-cost material, and a material with wide usage in many industrial applications. Sensitivity is affected by the dimensions as well as the materials used. After rigorous analysis as shown in [31], it could be found that increasing the sensitivity is achieved by using an insulating layer beneath metal with refractive index closer to the refractive index of the upper arm and greater than the substrate index (Al$_2$O$_3$) which is considered a CMOS compatible material in transistors fabrication [32]-[33]. In addition, increasing the length will increase sensitivity value on the expense of the transmission power level.

![Fig. 1. 3D Design of the proposed plasmonic MZI, $d_1=d_4=1.4\mu m$, $d_2=0.8\mu m$, $d_7=1\mu m$. The inset shows electric field profile distribution on the (IMI) interface. In addition, the inset shows the electric field exponential decay along the metal (doped silicon) depth and the propagation path as shown by the lower exponential curve. Background refers here to the sensing arm. $d_5$ and $d_6$ are varied.](image)

The doped silicon permittivity is defined by the Drude model

$$
\varepsilon_m(\omega) = \varepsilon_\infty - \frac{\omega_p^2}{\omega^2 + j\Gamma},
$$

(1)

$$
\omega_p = \sqrt{\frac{N_e q^2}{\varepsilon_0 m}}, \quad m^* = 0.25 m, \quad \text{and} \quad \Gamma = \frac{q}{m^* \mu}
$$

where $\omega_p$ is the plasma frequency, $q$ is the electron charge, $m^*$ is the electron effective mass, $N_e$ is the doping concentration, $r$ is the collision frequency, and $\mu$ is the electron mobility. The sapphire substrate thickness is assumed to be of $1 \mu m$ through simulations, the two silicon ports are $0.8 \mu m$ thickness while the doped silicon layer thickness
and the base insulator layer thickness to the doped silicon layer are varied to get the best performance. The doped silicon is designed to have minimal losses at the mid-infrared range to ensure proper power levels at the output port. The effect of different doping concentrations on the doped silicon permittivity is shown in Figs. 2 and 3. Increasing the doping concentration increases the plasmonic effect of the doped silicon whose real part tends to have a more negative value with an increasing imaginary term which amplify the intrinsic losses. Both the plasma wavelength, and the collision frequency are dependent on the doping concentration. The collision frequency dependence on the doping concentration owes to the dependence of the mobility on the doping concentration in which the relation is inversely proportional. For doping concentration of $5 \times 10^{20} \text{cm}^{-3}$ of boron, the plasma wavelength is approximately $2.56 \mu \text{m}$ and the mobility is approximately $46.5 \text{cm}^2/\text{V.s}$. The rest of the results are evaluated at doping concentration of $5 \times 10^{20} \text{cm}^{-3}$ of boron with plasma wavelength around 2550 nm. The plasma wavelength is determined by plotting the real part of the doped silicon permittivity shown in Eq. (1) and calculating the plasma frequency at which the real part equals zero. From the plasma frequency, the plasma wavelength could be easily calculated. The effect of the real part of the permittivity of doped silicon on the effective index of the Insulator-Metal-Insulator (IMI) plasmonic channel is shown in Fig. 4. The optical properties of the doped silicon shall not be confused with the optical properties IMI plasmonic channel. On the contrary of the increased losses along the wavelength for doped silicon, by solving the IMI dispersion relation [22], the IMI plasmonic structure tends to have increasing losses (the imaginary part of propagation vector) as the frequency keeps increasing and thus decreasing losses as the wavelength increases as shown in Fig. 5.

![Fig. 2. Doped silicon real permittivity as a function of wavelength and doping concentration](image-url)
Fig. 3. Doped silicon imaginary permittivity as a function of wavelength and doping concentration.

Fig. 4. Dispersion relation of the IMI plasmonic structure. The slope decreases until it reaches zero as $\beta_{\text{real}}$ increases until it almost reaches zero which corresponds to zero group velocity.

Fig. 5. Dispersion relation of the IMI plasmonic structure. The losses increase as the frequency (wavelength) increases (decreases). This is on the contrary to the optical properties of the doped silicon in which the losses increase as the wavelength decreases.

Results And Discussions

The relation between the transmission and the optical spectrum is shown in Fig. 6 with $d_5$ of 300 nm and $d_6$ of 200 nm. As expected from the MZI theory of constructive and destructive interference, the transmission pattern takes an oscillatory shape with more obvious oscillations as the wavelength is shifted further from the plasma wavelength and therefore better unfolding between the two SPP waves is achieved. The increased transmission level with wavelength is due to the increase in the phase velocity as the wavelength increase and hence the system-losses are minimized. From the dispersion relation of the IMI structure as shown in Figs. 4 and 5, the confinement of the surface plasmons become maximum as the slope tends to zero (zero group velocity) which corresponds also to greater losses as depicted.
in [22], and hence lowering the angular frequency (increasing the wavelength) results in lower losses and thus increased transmission. Thus shall not contradict the results plotted in Fig. 3 which describe the properties of the doped silicon solely not the IMI structure. Figs. 7 and 8 show the transmission versus the wavelength for doped silicon thickness of 400 nm and 500 nm, respectively, while keeping the MgF$_2$ thickness fixed at 200 nm. The red and the blue curves represent the transmission curves for background index of 1 and 1.01, respectively. Such incremental change in the background is assumed just to show the shift in the peaks and not limited to it.

**Fig. 6.** Transmission Versus wavelength for different background index with $d_5$ of 300 nm and $d_6$ of 200 nm.

**Fig. 7.** Transmission Versus wavelength for different background index with $d_5$ of 400 nm and $d_6$ of 200 nm.

**Fig. 8.** Transmission Versus wavelength for different background index with $d_5$ of 500 nm and $d_6$ of 200 nm.

Figs. 9 to 11 show the transmission versus the wavelength for doped silicon thickness of 300 nm, 400 nm and 500 nm, respectively, while keeping the MgF$_2$ thickness fixed at 100 nm.
Fig. 9. Transmission Versus wavelength for different background index with d₅ of 300 nm and d₆ of 100 nm.

Fig. 10. Transmission Versus wavelength for different background index with d₅ of 400 nm and d₆ of 100 nm.

Fig. 11. Transmission Versus wavelength for different background index with d₅ of 500 nm and d₆ of 100 nm.

The performance of these structures is listed in table (1) as a function of the design parameters (i.e. d₅ and d₆). From the table, sensitivity increases as the thickness of the MgF₂ decreases allowing more interaction with the surrounding along the plasmonic channel, this could be the cause for better sensitivity as the MgF₂ thickness shrank.

<table>
<thead>
<tr>
<th>d₅ (nm)</th>
<th>d₆ (nm)</th>
<th>Sensitivity (nm/RIU)</th>
<th>λ₀ (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>300</td>
<td>100</td>
<td>10700</td>
<td>5081</td>
</tr>
<tr>
<td>400</td>
<td>100</td>
<td>10800</td>
<td>5070</td>
</tr>
<tr>
<td>500</td>
<td>100</td>
<td>10100</td>
<td>5070</td>
</tr>
<tr>
<td>300</td>
<td>200</td>
<td>6000</td>
<td>5300</td>
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<tr>
<td>400</td>
<td>200</td>
<td>4900</td>
<td>4918</td>
</tr>
<tr>
<td>500</td>
<td>200</td>
<td>4700</td>
<td>4944</td>
</tr>
</tbody>
</table>

To evaluate the performance of plasmonic sensors more precisely, the Figure Of Merit (FOM) is calculated by
Here FWHM is the full width at half-maximum (FWHM) of the sensing peak. Highest FOM achieved is for \( d_3 \) and \( d_6 \) of 300 nm and 200 nm, respectively in which the FWHM is as narrow as possible. The FOM of the plasmonic MZI (for \( L = 80 \, \mu\text{m} \)) is found through simulations to be 35.

The explicit relation between sensitivity and each of the effective index as well as the operating wavelength was explicitly proposed in [35] and given by

\[
S = \lambda \left( \frac{\varepsilon_m(\lambda) n_u^2}{\varepsilon_m(\lambda) + n_u^2} \right)^{3/2} \left( \frac{\varepsilon_m(\lambda) n_l^2}{\varepsilon_m(\lambda) + n_l^2} \right)^{1/2}, \tag{3}
\]

\[
FOM = \frac{2 L \lambda}{\Delta} \frac{\varepsilon_m(\lambda) n_l^2}{\varepsilon_m(\lambda) + n_l^2}, \tag{4}
\]

where \( \varepsilon_m \) is the permittivity of the metal, \( n_u \) is the refractive index of the upper layer (air), \( n_l \) is the refractive index of the lower layer, and \( L_{ch} \) is the plasmonic channel length. Referring to equation (3), closer effective indices of the upper and lower arms leads to higher sensitivity. For the proposed design, magnesium fluoride is considered an efficient material to use in the mid-infrared range in addition to its low refractive index of 1.413. Higher FOMs could be reached by expanding the arm length as governed by equation 4 on the expense of the transmission level.

Different gases that are IR active are used to test the selectivity of the design. Methane and octane are used where each one of them has an absorption peak between 3000nm-4000nm. In the selectivity analysis the plasmonic channel length need not be large as long as selectivity calculations are concerned. Fig. 5 and Fig. 6 show the transmission when using methane and octane as the analyzed gas, respectively. The real and imaginary part of the refractive index of each gas was calculated using the Kramers-Kronig relation [34]

\[
n(\lambda_o) = n(\lambda) + P \int_0^\infty \frac{\lambda^2 k(\lambda) d\lambda}{\pi \left( \lambda_0^2 - \lambda^2 \right)} \left( \frac{\lambda_o^2 - \lambda^2}{\lambda^2 - \lambda^2} \right), \tag{5}
\]

\[
\alpha(\lambda) = \frac{4\pi k(\lambda)}{\lambda}, \tag{6}
\]
The refractive index, \( n \), is estimated from \( k \) using the kramers-kronig relation in equation (5), where \( n(\lambda_1) \) is a known refractive index of the analyte at wavelength \( \lambda_1 \), and \( P \) is the Cauchy principal value of the integral. The extinction coefficient, \( k \), was be obtained from absorption, \( \alpha \), through the relation in equation (6).

![Graph of Normalized Transmission vs Wavelength](image.png)

**Fig. 12.** Transmission spectrum for methane gas. The inset show the absorption peaks of methane as a function of the wavenumber.

The resonance effect in the output transmission corresponds to the absorption properties of the methane at selected wavelengths. The insets show the absorption peaks of methane and octane with respect to wavelength, which corresponds to wavelength around 3300nm and 3400 nm, respectively. The transmission shown in Fig. 12 and 13 are the transmission patterns for methane and octane being subtracted from the transmission pattern of air and then normalized. Despite that transmission doesn't match exactly with the absorption spectrum, this can be related to the way that the FDTD simulator use in calculating the real and imaginary value of the permittivity using the Kramers-Kronig relation and therefore 2 resonance peaks appear in the transmission not only one in addition to being shifted from the original position of the peak. As a result, the transmission pattern matches the fitted model of the methane and octane which is calculated using FDTD simulations. Although the selectivity analysis is performed at different wavelength, however, it could be expanded to operate at operating wavelength near 5300 nm. Methane and octane are used here as a proof of concept of the capability to detect the absorption peaks and hence detect specific gases. It worth mention that this analysis is not limited to methane and/or octane. The FOM is usually defined in the vicinity of certain wavelength around which the device is operating. It differs from vicinity of wavelength to other depending on the material properties especially for metals whose optical properties changes across the spectral range.
The power coupling efficiency between the photonic and plasmonic modes is calculated using Mode solver commercial tool, coupling efficiency of 0.60 is calculated at $d_5$ and $d_6$ of 300 nm and 200 nm, respectively, while coupling efficiency of 0.69 is calculated at $d_5$ and $d_6$ of 400 nm and 200 nm, respectively, as shown in Fig. 14.

To measure the detection limit of the proposed sensor, minimum limit of detection (LOD) of $5 \times 10^{-3}$ RIU is achieved for design parameters of $d_5$ and $d_6$ of 300 nm and 100 nm, respectively, as shown in Fig. 15. Such LOD is considered high when compared to other structures proposed in [36-38] with LODs down to $1 \times 10^{-7}$, however, the advantage of this work lies in its integration capability, CMOS computability, and acceptable performance in the MIR range.
The fabrication of the optical structure can be performed in a sequence of fabrication procedures as follows; (1) depositing poly silicon on the aluminum oxide (Sapphire) substrate, then (2) using positive dry etchant to etch the silicon everywhere except at the designated places at the input and output ports; the use of dry etching will guarantee anisotropic etching in the vertical direction only, (3) depositing magnesium fluoride along the structure including the silicon waveguide, (4) depositing the doped silicon layer along the structure covering the silicon and magnesium fluoride, (5) use negative wet etchant to etch the metal and the magnesium fluoride everywhere except along the plasmonic waveguide in design. Although the wet etching can etch in 2 directions, the small thickness of the metal and the magnesium fluoride will guarantee that the horizontal etching is minimized in a way that does not affect the design functionality. By using positive and negative etchant, it is possible to use the same lithography techniques.

Conclusions
Silicon plasmonic-integrated MZI for miniaturized and ultrasensitive optical bio-sensing is proposed. The plasmonic-integrated interferometer sensor can be easily fabricated using the conventional CMOS fabrication techniques. For the simulations, the combination of sensitive interferometric techniques with Nano-plasmonic architectures yields enhanced sensitivities up to 10000 nm/RIU for an arm length of 80μm. Best FOM of 35 is achieved at λ0~5.3μm using doped silicon. Higher FOMs could be maintained by expanding the arm length. High selectivity was validated by using specific gases with absorption peaks in the MIR range 3000 nm-4000 nm; however, it is extended along longer wavelength. This proposed design could open the door towards CMOS integrated optical sensors.

REFERENCES


**Fiber-optic-based interferometric sensor**

**Abstract.** A fiber based plasmonic sensor design is proposed. In principle, both the top surface insulator/metal interface and bottom surface can support SPP decoupled modes. The combination of sensitive interferometric techniques and the optimization process of the design and the material yields to enhanced sensitivities in range of 11000 nm/RIU.

**Keywords:** interference, sensor, mach-zehnder, plasmonics, fiber-optic

**Introduction**

Surface Plasmon Wave is originated through the coherent oscillations of the excited charges at the metal-dielectric interface. This optical property highly affects their sensitivities to changes in the refractive index which might originates due to the Kerr effect, or those induced by surface bio molecular binding events. This attractive property of SPs is the basis for surface plasmon resonance (SPR) bio sensing [1-4].

In recent years, periodic Nano-plasmonic structures have been successfully employed in bio sensing applications. However, the sensitivities for these Nano-plasmonic structures reported to date are much lower (two to three orders of magnitude) than other sensitive optical sensing technologies [1, 5-16]. For example, an SPR Nano-structured sensor with sensitivity 7,000 nm/RIU around $\lambda_0\sim1.5\text{mm}$ was proposed in [17], another Nano-particle based sensor with sensitivity 650 nm/RIU around $\lambda_0\sim1.5\text{mm}$ was proposed in [18].

Compared to the non-plasmonic interferometer based bio-chemical sensor with $-92000$ nm/RIU sensitivity, these sensors suffer a lot in terms of the recorded sensitivity [19].

Another type of SPR sensors is a waveguide based SPR sensor such as a fiber-optic SPR sensor. Optical fibers as SPR sensor bodies have been extensively studied in recent years. Fiber-optic SPR sensors have some advantages compared to other sensors, which include their capability of miniaturization, simplified optical design, and remote sensing using fibers and a high sensitivity due to SPR [20]. In a previous study, an optimized sensitivity of about 4000 nm/RIU was achieved by coating the fiber with Au metal film [17].

In this paper, a fiber-optic interferometer sensor design is proposed. The plasmonic interferometer sensor can be easily fabricated. It leads to high-performance bio-sensing in terms of high sensitivity and high figure
of merit. The fiber-optic based interferometer sensor helps more in remote sensing, solving the problem of low power level recorded in the silicon-integrated sensor. Due to its large length, it’s characterized by its high sensitivity and figure of merit to our knowledge than other fiber-optic based sensors. It is also characterized by its easy fabrication process.

**FDTD SIMULATIONS**

**Design Structure**

A fiber-optic based sensor that is manageable to be used in experimental work is proposed and hence is characterized by its low cost, and ease of fabrication. Figure 1 shows a schematic diagram for the fiber sensor. Once the SPP modes excited input fiber input port, the SPP signals from the two optical branches (the top and bottom interfaces) propagate to the output optical fiber. At the output waveguide both branches interfere with each other and modulate the far-field scattering. The top surface is considered as the sensing arm of this plasmonic Mach-Zehnder interferometer (MZI). The surrounding is considered as the sensing media of the sensor. High sensitivity and small footprint is achieved using this integrated simple plasmonic design. The single mode fiber is 9 µm /125 µm with core refractive index equals 1.4390 and cladding refractive index equals 1.4370. Single mode optical fiber (SMF) can serve as an efficient optical transport highway for multifunctional sensing when integrated with optical probes and diagnostic devices. Such fiber sensing provides advantages over conventional electronic sensors due to their immunity to electromagnetic interference [21], compact size, light weight, mechanical flexibility, robustness, chemical inertness, low auto-fluorescence, biocompatibility, high wettability, and high thermal conductivity that underpin diverse applications for embedded, remote, or distributed sensing in extreme, long distance, or biological environments [22,23]. Hence, the prospect of developing lab-on-fiber (LOF) has recently emerged with label-free chemical and biological sensing [24, 25], acoustic pressure wave analysis [26], and trace TNT explosive detection [27]. While performing the FDTD simulation it is assumed to have the cladding of
infinite size since there will be almost no field outside the cladding. The plasmonic effect happens in the intermediate channel in which the cladding of the fiber is etched followed by etching the core until 3.5 µm are remaining from the core, this can be done using HF acid [28-30] or potassium hydroxide etching [31]. Coating the 3.5 µm core with 100 nm of silver enables the plasmonic mode to propagate along the channel.

Figure 1. Fiber based plasmonic sensor

The sensor is designed to have 80 µm channel length. However, longer channels will yield higher sensitivities and hence greater FOM. Figure 2 shows the transmission versus the wavelength for different refractive indices, the sensitivity was calculated to be

$$s = \frac{\Delta \lambda}{\Delta n} = \frac{(1.47015 - 1.58861) \times 1000}{0.01} = 11,864 \text{ nm RIU}$$

@\(\lambda \sim 1.58 \text{um}\)

Which is the greatest sensitivity for a fiber-optic based sensor to our knowledge. The FOM was calculated to be around 140 (fwhm=85 nm). However, longer channel will lead us to higher sensitivity and higher FOM. Still, the power level difference between the peak and the valley needs to be maximized. Some simulations efforts were done in an attempt to increase the difference, however, this was done on the expense of both sensitivity and FOM.
Wavelength (μm)

**Figure 2.** Transmission levels for different refractive indices

**Conclusion**

A plasmonic fiber MZI for ultrasensitive optical bio-sensing is proposed. The combination of sensitive interferometric techniques with plasmonic architectures yields enhanced sensitivities up to 11000 nm/RIU and record high FOM in order of 140 nm/RIU/nm in a simple sensor platform. This sensor design opens the door for sensing applications that require highly sensitive optical devices.

**References**


High Performance Photonic Structures using Ultra Thin Silicon Waveguide in SOI technology

Abstract. A new platform for the design of photonic structures is proposed in this work. The platform is based on the design of an ultra thin waveguide with narrow lateral thickness with low confined field inside the core waveguide which enables using this waveguide for building high performance photonic based sensors and modulators. By employing this waveguide into Mach-Zehnder based sensor, a sensitivity of 5000 nm/RIU is achieved. This value resulted in high performance photonic structures as compared to the conventional waveguide based structures delimiting some of the constraints when using photonic structures.

Keywords: interference, modulation, sensing, MZI

INTRODUCTION

Silicon Photonics is the most efficient platform for applications that require low power consumption, high bandwidth, and compatibility with CMOS fabrication techniques [1]. Eventually, the integration between electronic and photonic integrated circuits became a huge demand and the need for systems with higher bandwidth becomes a necessity for many applications and especially data-centers [1]. This integration resulted in systems with both the ease of fabrication of electronic circuits, and the high speed and low loss of photonic circuits [2]. Photonic integrated circuits have been employed in different applications including optical modulation, and sensing [1, 3].

A major application for such devices is optical sensing. Different types of optical sensors based on resonating structures [4] and interference effects have been demonstrated through the past years. Although resonant structures are characterized by their high quality factors, MZI based sensors are widely used in various applications requiring optical/thermal stability.

Mach-Zehnder interferometric structures (MZIs) are commonly used in many sensing applications including chemical sensing [5-7]. However, due to their large size in the milli-scale, they are not suitable for many applications that require relatively smaller sizes. Different design schemes were proposed to overcome this limitation including the usage of spiral paths with diameters in order of few hundreds of micrometers, however, this requires complex fabrication procedures.

In the recent years, different optical sensors were demonstrated with high performance but long arms. An interferometric SIO based sensor with sensitivity up to 4930 Rad/RIU was demonstrated [5]. Another bio-chemical sensor was proposed with sensitivity up to 1730 Rad/RIU with arm length in the millimeter range [6]. Recently, an
interferometric based sensor with sensitivity as large as 6552 \text{\pi} \text{ Rad/RIU} was demonstrated in the visible range with an arm length as long as 10 mm [7].

From the previous examples it is observed that achieving high performance photonic structure is considered a tradeoff with size and loss. Therefore, the need for a new scheme in designing optical photonic structures is needed. In such scheme, the objective function is to enhance the performance (i.e. the extinction ratio, sensor overall performance) under limitations on the upper and lower bounds of the dimensions and the loss. In this work, a new design for MZI based modulators with optimized dimensions other than the conventional dimensions for silicon waveguide is proposed, resulting in an enhanced performance for different photonic structures including sensors and modulators. The paper is organized as follows: section (2) describes the proposed waveguide which is considered the new platform for different photonic application, section (3) describes the optical sensor employing the proposed waveguide, finally section (4) concludes the paper.

ULTRA THIN WAVEGUIDE PROPERTIES

The proposed structures are designed based on silicon waveguide with different cross sectional area while supporting the fundamental mode as in the conventional silicon waveguide. The proposed silicon waveguide has a narrow lateral side with thickness of only 50 nm, as shown in figure 1(a) and thus in the rest of the manuscript it will be referred as “Ultra thin waveguide”. Owing to the small thickness, only one type of modes is supported in which the electric field major component is along the plane of incidence (TM mode). In addition, due to the narrow thickness, the mode experiences low confinement in the core waveguide as shown in figure 1(b) [8, 9], the fact that makes this waveguide a suitable platform for different applications, including sensing applications. This is in contrast with the conventional waveguide in which the mode is highly confined in the core which limits the possibility of having a high performance optical sensor. The cross sectional area is varied to see its effect on the optical properties of the ultra thin waveguide.

The effect of changing the width of the waveguide on the effective refractive index of the structure while keeping the thickness of 50nm is shown in figure 2. In the figure, it’s assumed that the surrounding is air while the substrate is silicon dioxide (SiO$_2$). Although the figure shows the effect of changing the width on a large span, only the first fundamental mode is supported between 700 nm and 2000 nm, no modes are supported when the width is below 700 nm, on the other hand, multi-modes are supported when the width exceeds 2000 nm. The proposed waveguide can be
fabrication using the standard fabrication process for the conventional waveguide. The fabrication steps are performed in the following sequence: (1) Having the SOI wafer from the Foundry (2) Doing partial etching to get the required thickness (i.e. 50 nm thickness) (3) Performing mask lithography (4) Development of the wafer (5) Performing the DRIE etching process to etch the unneeded Si layer (6) Removing the etchant to reach the final structure. Fabrication tolerance will not affect the overall performance as seen in figure 2 in which the $n_{eff}$ is not varying abruptly with changing the different thickness, the fact that compensates the fabrication tolerances.

![Figure 1](image1.png)

**Fig. 1** SOI ultra thin waveguide structure. (a) Schematic for the physical dimensions of the ultra thin waveguide. (b) Mode profile for the ultra thin waveguide.

The ultra thin waveguide properties enable it to be employed in different applications to obtain enhanced performance as compared to applications employing the conventional waveguide (220 nm X 400 nm).

The propagation loss is calculated for the waveguide in order to know the limitations on the arm length. A propagation loss of 70 dB/cm is considered an acceptable value for the design of long-arm modulators. Other losses other than that from the waveguide will affect the transmission, such as the bending loss of curved structures. However, for large bending radii, bending losses can be minimized.

In the next two section, two applications are discussed which are optical sensing, and optical modulation. In the two sections, comparison with the conventional waveguide based system is performed. Simulation are done using Beam Propagation Method (BPM) [10]. Simulation results are shown to highly match the expected theoretical results.
Fig. 2 The effect of changing the waveguide width on the effective index. The substrate is assumed to be SiO$_2$ with air as the surrounding.

ULTRA THIN WAVEGUIDE BASED PHOTONIC SENSOR

MZI based Photonic Sensor

A schematic for the Mach-Zhender (MZI) based sensor in SOI technology is shown in figure 3. The MZI structure is based on having the ultra thin waveguide as the core waveguide. As can be seen from the mode profile in figure 2, the mode is highly affected by the surrounding media since a considerable portion of the field is outside the waveguide and hence high performance can be achieved with much lower arm lengths results in small-sized optical sensor, making it a promising platform for many optical sensing structures in photonic integrated circuits. The low effective refractive index reflects the fact that the field is not highly confined inside the core waveguide as can be seen from figure 1. In the rest of the paper, ultra thin waveguide with cross-sectional area 2000 nm X 50 nm whose effective refractive index equals 1.57 is used.

Fig. 3 Schematic of the MZI based photonic sensor
Sensor Results

During the computational analysis, bending radii of 80 µm is assumed. A microfluidic channel is assumed to be on one arm (i.e. the sensing arm) while keeping the other arm unchanged (i.e. the reference arm), by changing the liquid inside the microfluidic, the effective index of upper arm will change causing a phase shift in the optical mode in the upper arm, which in turns will affect the interaction between the two optical modes at the output port constructively and destructively. The transmission pattern at the output port is shown in figure 4. With an arm length of 350 µm and by changing the refractive index of the medium from 1.33 to 1.34, the transmission pattern experience a positive wavelength shift (red shift) from 1560 nm to 1610 nm. The sensitivity of the optical structure is calculated to be 5000 nm/RIU. To better evaluate the performance of the proposed sensor, a new parameter is defined as the Figure of Merit (FOM) which represents the overall performance of the sensor [11-12] and is defined by

$$FOM = \frac{\text{Sensitivity}}{\text{FWHM}} = \frac{\Delta \lambda / \Delta n}{\text{FWHM}}$$

where FWHM is the full width at half maximum of the transmission pattern. FOM is calculated to be around 150 for arm length of 350 µm. Such values out perform any other MZI photonic based sensors. The effect of changing the arm length on the FOM is shown in figure 5. This increase in the FOM reflects the narrowing in the full width at half maximum of the transmission signal since the sensitivity is weakly affected by the arm length and tends to have the same value of 5000 nm/RIU. This design is characterized by its ability to be used in other optical applications including optical modulators in which it can increases the modulation index (extinction ratio) ultimately as compared to conventional silicon single mode based MZI structures with cross-sectional area of 220nm*400nm as discussed in the next section.

![Fig. 4 Transmission versus wavelength for different refractive indices at an arm length of 350 µm](image-url)
Following figure 5, the FOM is around 84 [8] with a FWHM of around 60 nm at an arm length of 215 $\mu$m. Using the conventional waveguide results in an FOM of 34 only at an arm length of 215 $\mu$m. By comparing this value with the FOM at the same arm length using the ultra thin waveguide, it will be concluded that the ultra thin waveguide based sensor offers an FOM which is more than a factor of 2 as compared to the conventional waveguide based sensor. This enhanced FOM is owing to the improved quality factor in the case of the ultra thin waveguide which arises from having a much higher resonance order in the case of the ultra thin waveguide than in the case of the conventional waveguide which leads to a narrower full width at half maximum (FWHM). This can be easily verified by solving the resonance equation given by [13]

$$\Delta \beta L = 2m\pi ,$$

(2)

Where $\Delta \beta = \frac{2\pi}{\lambda_0} (n_{effu} - n_{effl})$ where $n_{effu}$ and $n_{effl}$ are the effective index of the upper and lower arm, respectively. Thus equation 1 can be simplified to

$$L = \frac{n_0^2}{2(n_{effu} - n_{effl})} ,$$

(3)

For the case of the ultra thin waveguide, $n_{effu} = 1.666$ and 1.669 when using water and salt water, respectively, while $n_{effl}$ equals 1.57. Thus, for L=215 $\mu$m, n=26 with $\lambda_0$ of 1580 nm and 1630 nm for water (n=1.33) and salt water (n=1.34), respectively. Doing the same analysis for the conventional waveguide for L=215 $\mu$m resulted in having n=4 with $\lambda_0$ of 1500 nm and 1610 nm for water (n=1.33) and salt water (n=1.34), respectively. Although the sensitivity
of the conventional waveguide seems to be much greater than that recorded for the ultra thin waveguide based sensor, the small n in the conventional waveguide based sensor reflects the wide FWHM which is calculated to be 290 nm as compared to 60 nm for the ultra thin waveguide based MZI sensor which owes to its large n.

CONCLUSION
New architecture of photonic MZI –based sensor is proposed. The sensor can help in having a high FOM with small arm lengths as compared to conventional MZI-based modulators. We reported an ultimately high sensitivity of 5000 nm/RIU and FOM around 150 at arm length of 350 μm. Such device can help in minimizing the size of photonic integrated circuits and maintaining the high performance in terms of sensitivity, figure of merit, and CMOS compatibility.

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Abstract. In this paper, a novel and efficient approach to solve the BPM equation is proposed. The approach is based on reformulating the BPM equation to solve only real system matrices at each propagation step. The updated equation exploits leapfrog technique to couple the real and imaginary parts of the field in an iterative way. The method is proved to be at least 30% faster than the conventional BPM in solving waveguide problems. To test the validity of the proposed LF-BPM method, different photonic structures including directional couplers, and multi-mode interferometers (MMI) are simulated. The simulation results highly match the theoretical results with a negligible computational error. In addition, results have been experimentally verified by comparing it to results measured for fabricated nanophotonic structures. The proposed LF-BPM approach is considered as a promising technique for efficient solution of optical structures.

Index Terms— BPM, numerical methods, computational techniques, photonics, Leap-frog.

INTRODUCTION

Integrated Photonics is the most efficient platform for applications that require low power consumption, high bandwidth, and compatibility with CMOS fabrication techniques [1]. Eventually, the integration between electronic and photonic integrated circuits became a huge demand and the need for systems with higher bandwidth becomes a necessity for many applications and especially data-centers [1]. This integration resulted in systems with both the ease of fabrication of electronic circuits, and the high speed and low loss of photonic circuits [3]. Photonic integrated circuits have been employed in different applications including optical modulation, sensing, etc.

To efficiently define the behavior of photonic circuits, various computational algorithms are being employed to solve Maxwell’s equations including finite difference time domain method (FDTD method), finite element method (FEM), and beam propagation method (BPM method). Although most of these methods are utilized in various commercial computational tools, many of them suffer in terms of the computational speed and memory allocation. As an example, although FDTD method is considered the most famous computational algorithm used, it suffers from high latency when used for solving long structures (i.e. hundreds of micrometers and few millimeters) and could results in numerical dispersion errors. On the other side, FEM method is considered a competing solution owing to its unconditional stability and hence no constraints are applied on the mesh sizes. BPM method is considered the most efficient algorithm for solving long simple structures with no numerical dispersion errors but it may suffer from conditional stability [4]-[9]. Although BPM method is considered the most powerful and fastest computational method for solving long structures, boosting the computational speed further could help in enhancing the overall computational performance.
In this paper, a new numerical method is proposed that highly fits with long photonic integrated systems and results in boosting the computational speed. In section II, the computational algorithm is discussed. In section III, simulation results for various photonic structures are shown. In section IV, experimental validation of the results is shown. In Section V, stability analysis is performed for the proposed LP-BPM method. Finally, section VI concludes the paper.

**Computational Algorithm**

The BPM equation can be expressed by [4]:

\[
2 j k n_0 \frac{\partial \varphi}{\partial z} = \frac{\partial^2 \varphi}{\partial x^2} + k^2 (n^2 - n_0^2) \varphi \tag{1}
\]

By assuming \( \varphi \) to be a complex function; it can be written as:

\[
\varphi = \varphi_r + i \varphi_i
\]

Therefore, equation 1 can be reformulated into two equations as follows:

\[
2 kn_0 \frac{\partial \varphi_r}{\partial z} = \frac{\partial^2 \varphi_r}{\partial x^2} + k^2 (n^2 - n_0^2) \varphi_i \tag{2-a}
\]

\[
-2 kn_0 \frac{\partial \varphi_i}{\partial z} = \frac{\partial^2 \varphi_i}{\partial x^2} + k^2 (n^2 - n_0^2) \varphi_r \tag{2-b}
\]

Using the finite difference method, the first derivative with respect to space can be approximated by:

\[
\frac{\partial \varphi}{\partial z} = \frac{\varphi_{k+1} - \varphi_{k-1}}{2 \Delta z} \tag{3}
\]

The second derivate can be rewritten in the following form:

\[
\frac{\partial^2 \varphi}{\partial x^2} = \frac{\varphi_{k+1}^{m+1} - 2 \varphi_{k+1}^m + \varphi_{k+1}^{m-1}}{\Delta x^2}
\]

Therefore, equations (2-a) and (2-b) are formulated as follows:

\[
2 kn_0 \frac{\varphi_{k+1}^{m+1} - \varphi_{k+1}^{m-1}}{2 \Delta z} = \frac{\varphi_{k+1}^m - 2 \varphi_{k+1}^m + \varphi_{k+1}^{m-1}}{\Delta x^2} + k^2 (n^2 - n_0^2) \varphi_{k+1}^m \tag{5}
\]

\[
-2 kn_0 \frac{\varphi_{k+1}^{m+1} - \varphi_{k+1}^{m-1}}{2 \Delta z} = \frac{\varphi_{k+1}^m - 2 \varphi_{k+1}^m + \varphi_{k+1}^{m-1}}{\Delta x^2} + k^2 (n^2 - n_0^2) \varphi_{k+1}^m \tag{6}
\]

Letting \( d_1 = \frac{2 \Delta z}{2 kn_0 \Delta x^2} \), \( d_2 = \frac{2 \Delta z}{2 kn_0} \) equation 5 becomes
\[ \phi_{k+1}^{m} = \phi_{k}^{m} + d_{1}(\phi_{k}^{m+1} - 2\phi_{k}^{m} + \phi_{k}^{m-1}) + d_{2}k^{2}(n^{2} - n_{0}^{2})\phi_{k}^{m} \]  \hspace{1cm} (7)

On the other hand, equation 6 becomes

\[ \phi_{k+1}^{m} = \phi_{k-1}^{m} - d_{1}(\phi_{k}^{m+1} - 2\phi_{k}^{m} + \phi_{k}^{m-1}) - d_{2}k^{2}(n^{2} - n_{0}^{2})\phi_{k}^{m} \]  \hspace{1cm} (8)

Equations (7) and (8) are solved iteratively in which \( \varphi_{i} \) is evaluated at k=odd and then be used in the next iteration (i.e. k=even integer) to evaluate \( \varphi_{r} \) and keep iterating until all the iteration are evaluated (k=Nz). Such iterative algorithm is called the leap frog method [16]. Since each term of \( \varphi_{i} \) (\( \varphi_{r} \)) is linked to the previous and next iteration of \( \varphi_{r} \) (\( \varphi_{i} \)), the absolute value of \( \varphi \) at each iteration is given by

\[ \varphi_{k} = \sqrt{\varphi_{k}^{2} + \varphi_{k-1}^{*}\varphi_{k+1}} , \]  \hspace{1cm} (9)

For k=even integer.

While for k=odd integer,

\[ \varphi_{k} = \sqrt{\varphi_{k}^{2} + \varphi_{k-1}^{*}\varphi_{k+1}} \]  \hspace{1cm} (10)

**RESULTS AND DISCUSSIONS**

Both the conventional BPM method, that is based on solving the wave-function as one whole complex term, and the proposed LF-BPM method reached close results in terms of the optical properties of the system (i.e. mode profile). However, the proposed method achieved better computational performance where the computational speed was boosted by a factor of 30% [17]. The schematic and the mode profile is shown in figures 1 and 2, respectively.

![Fig. 1 Schematic for the SOI based straight waveguide](image-url)
To further study the validity of the proposed computational technique, we solved a directional coupler problem. The access waveguides are assumed to have thickness of 220nm and effective index $n_c$ of 2.95 surrounded with silicon dioxide ($n=1.4$) with gap width of 200 nm. Theoretically, a coupling length of 3.875 $\mu$m should be concluded. The mode profile of the electric field in the second waveguide is monitored. According to the proposed technique, a coupling length of 4.1 $\mu$m is calculated with a computational error of 5.8% exists. Schematic and Field profile inside the directional coupler structure is shown in figures 3 and 4, respectively, with a coupling length of 4.1 $\mu$m.

To evaluate the performance of the proposed LF-BPM method for directional couplers, several simulations are performed with different gap width between the 2 parallel plate waveguides as shown in figure 5. From the figure, it can be observed that the results extracted from the proposed technique are close to the simulation results obtained.
from FDTD tool [18] with a negligible error. In the proposed technique, effective indices of the single mode SOI waveguide is substituted with a core effective index \( n_c = 2.95 \), substrate index \( n_s = 1.45 \) and \( n_0 = 2.2 \).

Extending the concept of optical coupling, a 3-parallel waveguides system is simulated. As expected based on the coupling theory, 50% of the power is coupled to the other 2 waveguides at a coupling length equal to 2 \( \mu \text{m} \) which is the length at which 50% of the field is coupled to the second waveguide in the case of the simple directional coupler. Schematic and simulation result at a gap width of 0.2 \( \mu \text{m} \) are shown in figures 6 and 7, respectively.

Finally, an SOI multi-mode interferometer (MMI) system is simulated as shown in figure 8. Effective index of the core is assumed to be \( n_c = 1.6 \), substrate index \( n_s = 1.45 \) and \( n_0 = 1.54 \).

Theoretically, the input field will have a mirror image at an MMI length of 118 \( \mu \text{m} \). Using the proposed LF-BPM technique, a mirror image is formed at an MMI section length of 120 \( \mu \text{m} \) with an error not exceeding 2%. Field profile in the MMI structure is shown in figure 9.
To validate the results of the MMI structure, an MMI structure with half the length of the previously discussed MMI is simulated. As expected, 2 half mirror-images are created at half the length of the MMI structure previously simulated. Schematic of the MMI structure is shown in figure 10 with an MMI section length of around half the MMI length in figure 8. The field is distributed on the 2 output ports as expected from the theory. The field profile is shown in figure 11.
EXPERIMENTAL VERIFICATION

To further validate the accuracy of the proposed LF-BPM technique, the coupling length of the TE\(_0\) mode for a single mode SOI structure with the Si core (220 nm * 400 nm) surrounded by SiO\(_2\) cladding is calculated and compared with the measured results from fabrication. Table 1 shows both the calculated coupling length using the proposed technique versus the measured coupling length for the single mode conventional SOI with SiO\(_2\) as cladding. It is obvious from the table of results that the calculated results are in a good match with the measured results with a minimum calculation error less than 0.5%.

Table 2. Comparison between the measured results and the calculated results using the proposed LF-BPM technique for a single mode SOI surrounded by SiO\(_2\) at operating wavelength of 1550 nm. \(\Delta Z\) is assumed to be 1 nm and \(\Delta X\) is assumed to be 20 nm. TE\(_0\) mode is assumed.

<table>
<thead>
<tr>
<th>Separation Distance ((\mu m))</th>
<th>Measured Coupling Length ((\mu m))</th>
<th>Calculated Coupling Length ((\mu m))</th>
<th>Error Percentage (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>9.23</td>
<td>9.19</td>
<td>0.44</td>
</tr>
<tr>
<td>0.3</td>
<td>31.4</td>
<td>30.5</td>
<td>2.8</td>
</tr>
<tr>
<td>0.4</td>
<td>39.4</td>
<td>39</td>
<td>1.02</td>
</tr>
</tbody>
</table>

Figure 12 shows the SEM image for the directional coupler (DC) fabricated using SOI technology with separation of 400 nm. The fabricated optical coupler shown in the figure yields an optical coupling coefficient of 0.04\(\mu m^{-1}\) resulting in a coupling length of 39.4 \(\mu m\). The measured output power for this DC is shown in figure 13. The low output power counts for the grating coupler to the directional coupler which suppresses the final output power by around 20 dBm power loss. Port 1 and 2 represent the power in each arm. Calculated results for several DCs are shown in figure 14 along with measured results at an operating wavelength of 1.55 \(\mu m\).
**STABILITY ANALYSIS**

To fully study the newly proposed computational technique, a stability analysis is performed. From the matrix form expressed above, it can be seen that the modulus of the diagonal element (i.e. \(-d_2 k^2(n(m,k)^2-n_0^2)+2d_1\)) is a key factor in the stability analysis. To ensure a stable process, this diagonal should have a magnitude less than 1, therefore, reaching the following equation:
\[
\max \left| \frac{2\Delta z}{2kn_0} (-k^2 (n^2 - n_0^2) + 2d_z) \right| < 1 \tag{11}
\]

\[
\max \left| \frac{2\Delta z}{2kn_0} (-k^2 (n^2 - n_0^2) + 2d_z) \right| < 1 \tag{12}
\]

\[
\left| \frac{2\Delta z}{2kn_0} (-k^2 (n^2 - n_0^2) + \frac{2}{\Delta x^2}) \right| < 1 \tag{13}
\]

From here, it can be proved than smaller step size along the propagation direction (\(\Delta z\)) results in higher stability on the expense of the simulation time.

Another factor that decides the stability is \(d_z = \frac{2\Delta z}{2kn_0\Delta x^2}\) which represent the off-diagonal elements in the matrix.

Since stability is concerned, all the elements must have a magnitude smaller than 1 and hence, larger step size in the transverse direction (\(\Delta x\)) leads to higher stability on the expense of the field distribution accuracy. The effect of changing the step size along the transverse and propagation direction on the diagonal element (which is given the name stability factor) is shown in figure 15 and 16, respectively.

**Fig. 15** Effect of changing the step size in the transverse direction on the stability factor

**Fig. 16** Effect of changing the step size along the propagation direction on the stability factor
On the other hand, the conventional BPM technique is based on using the Cranck-Nickleson method for the second derivative with respect to the transverse axis which helps on having an unconditionally stable system on the expense of the time taken per situation and thus taking more time than the proposed BPM based leapfrog technique.

The effect of changing the mesh steps on the simulation results for the directional coupler is shown in Table 2. It can be observed that sweeping over the mesh steps affects the accuracy of the results. However, fine changes of the mesh steps are necessary to ensure numerical stability of the computational technique. The table shows how changing the transverse step size changes the condition for stability validating the results shown in figures 15 and 16. From table 2, minimum step size for the optical structure could be detected to ensure stability.

The effect of changing the mesh steps on the simulation time is shown in Table 3. As shown in the table, smaller mesh steps result in longer simulation time and thus the choice of the mesh steps should be carefully done by the designer in order to compromise each of the accuracy, simulation time and the numerical stability. The time saving factor (TSF) is defined as

\[
TSF = \frac{t_{\text{Conv-BPM}} - t_{\text{LF-BPM}}}{t_{\text{Conv-BPM}}} \times 100\% \tag{14}
\]

where \( t_{\text{Conv-BPM}} \) is the simulation time for conventional BPM technique, and \( t_{\text{LF-BPM}} \) is the simulation time for the LF-BPM proposed technique.

Table 2. The effect of changing the mesh step on the accuracy of the calculated results. The propagation mesh step (\( \Delta Z \)) is fixed to be 1 nm. Calculations are done at operating wavelength of 1550 nm with a measured coupling length of 9.23 \( \mu \)m and separation distance of 200 nm. TE\(_0\) mode is assumed.

<table>
<thead>
<tr>
<th>Transverse Step Size (nm)</th>
<th>Stability Factor ((S))</th>
<th>Calculated Coupling Length ((\mu)m)</th>
<th>Error Percentage (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>Unstable ((S&gt;1))</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>20</td>
<td>0.56</td>
<td>9.19</td>
<td>0.44</td>
</tr>
<tr>
<td>30</td>
<td>0.24</td>
<td>8.23</td>
<td>10.83</td>
</tr>
<tr>
<td>40</td>
<td>0.13</td>
<td>7.54</td>
<td>18.31</td>
</tr>
</tbody>
</table>

Table 3. Relation between the transverse mesh step size (\(\Delta X\)) and the simulation time for the proposed computational technique for a directional coupler structure with total length of 70 \(\mu\)m and spacing of 200 nm.
<table>
<thead>
<tr>
<th>20</th>
<th>140</th>
<th>448</th>
<th>220%</th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>97</td>
<td>196</td>
<td>102%</td>
</tr>
<tr>
<td>40</td>
<td>80</td>
<td>136</td>
<td>70%</td>
</tr>
<tr>
<td>50</td>
<td>64</td>
<td>84</td>
<td>30%</td>
</tr>
</tbody>
</table>

It should be mentioned here that for small propagation step sizes (\( \Delta Z \)), the conventional BPM technique is taking more computational time as compared to the proposed LF-BPM technique; the proposed LF-BPM technique is faster than the conventional technique by a minimum TSF of 30\% in this case. In addition, the accuracy is degraded for the conventional technique as an effect of increasing the transverse step size.

**CONCLUSION**

LF-BPM for solving photonic structures (SOI technology based structures) is proposed in this work. The new technique shows higher computational speed with a minimum time saving factor of 30\% of the conventional BPM method. To test the validity of the proposed method, different photonic structures including directional couplers, and multi-mode interferometers (MMI) are simulated. The simulation results highly match the theoretical results calculated by commercial simulators with a negligible computational error. In addition, an almost perfect match is shown between the calculated results using the proposed technique and the measured results for the fabricated structures. This proposed LF-BPM method opens the door for an efficient fast computational algorithm for modeling of optical structures.

**REFERENCES**


[18] FDTD tools: (https://lumerical.com/)
Conclusion and Future Work

In this thesis, light interaction with matter was the main concern of the Master’s thesis. In this work, study of optical sensors and its involvement in biomedical and environmental applications was the main target. Several architectures including photonic and plasmonic structures were proposed that aimed at enhancing the performance of the optical sensors in terms of the sensitivity, full width at half maximum and hence the figure of merit. In the design process of biomedical sensors, different factors were taken into consideration including the CMOS compatibility of the design and the capability of being integrated with electronic devices. To ensure this, silicon platform represents the preferred platform to work on in a way that makes photonic circuits integrated with silicon based electronic chips. In addition, the new technology of lab on chip becomes a necessity to maintain high throughput in the diagnosis process in such a way that various sensors are built on the same chip to test various samples with different functionalities. So, in this work on biomedical sensors, a platform for an optical sensor that is characterized by its CMOS compatibility, integration capability, high performance in terms of the sensitivity and the figure of merit is proposed. Such platform can help in the Lab on Chip (LoC) technology that would help in the diagnosis of many diseases. High performance is achieved by having sensitivities up to 19000 nm/RIU for liquid sensors with FOM up to 150. In addition to liquid sensors (i.e. biomedical sensors), gases sensors are crucial elements in many industrial corporations to detect toxic gases during the manufacturing processes. So, as a part of the thesis, a gases sensor based on the IMI architecture I proposed with sensitivity up to 6000 nm/RIU and with high selectivity of gases based on their absorption peaks at the mid-infrared regime.

Despite the importance of small scale integrated circuits (ICs) in LoC applications, large scale optical devices are characterized by their ease of fabrication as compared to small scale optical ICs. In addition, large scale ICs can be more feasible for testing microfluidic channels with different liquid concentrations. So, as a part of the thesis work, the design of a fiber-optic based liquid sensor is proposed. The design
achieves sensitivity up to approximately 12000 nm/RIU which shows the high performance of the proposed design.

In a way to avoid the optical losses associated with plasmonic structures, a photonic based MZI optical sensor is proposed. The MZI is based on a photonic waveguide with cross-sectional area of 2μm*50nm, these dimensions allowed the field to interact with the cladding more than the conventional waveguide. The design maintained sensitivity up to 5000 nm/RIU with FOM up to 85 for an arm length of 215 μm which is 4 times the FOM of the MZI with conventional waveguide dimensions.

Finally, a computational algorithm for the design of photonic structures is proposed. The computational technique is based on the BPM method using leap-frog technique. Using this algorithm, high computational speed could be reached with a time saving factor more than 200% with high accuracy.

Future works includes working in several directions:

- For the plasmonic MZI sensors; using different materials could help in achieving better performance while maintaining CMOS compatibility.
- For the ultra-thin waveguide based sensor; using different architecture such as suspended ring resonators or MMIs could help for achieving better FWHM and hence better FOM.
- For the LF-BPM Computational technique; perhaps by utilizing different way to formulate the BPM method, a better computational speed with time saving factor much greater 200%.
List of Publications

Conference Papers:


5. Ahmad B. Ayoub, Abdelrahman Abdelhamid, Mai Saad, and Mohamed A. Swillam, “Fiber-optic based interferometric sensor,” SPIE Photonics West, 2017


Submitted Journal Papers:


