High performance optical systems using MIM based plasmonic structures

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Abstract
In this paper, the design of high performance optical systems based on MIM based plasmonic structures is proposed. Using a design methodology based on optimization functions, two novel components are proposed: demultiplexer and gas sensor. Further optimization of these plasmonic systems, high performance optical demultiplexer is maintained with a narrow line-width down to 4 nm with acceptable power level around 30%. On the other side, highly sensitive optical sensor is proposed with sensitivity up to 2000 nm and a limit of detection down to $10^{-4}$.

1. Introduction
Surface plasmon polaritons (SPPs) are electromagnetic waves that have the ability to constrain and control the direction of light in dimensions which are smaller than the diffraction limit [1]. Therefore, SPPs are promising for many applications including nanoscale plasmonic filters [2]. On the other hand, the field intensity of SPPs decays rapidly with distance. This major problem calls for research to create smaller structures on the nanometer scale in order to decrease the effect of propagation loss on the total insertion loss of the plasmonic components. In addition, compact size is highly desirable to minimize the size mismatch between photonic and electronic components on the same chip.

Among several plasmonic waveguides, the MIM waveguide and its 3D counterpart, plasmonic slot waveguide, are thought to be the most appropriate configurations for highly dense integration and tight confinement of optical fields [3]. Unfortunately, nanoscale spatial distribution of the optical mode is challenging. However, hybrid junctions using orthogonal coupling scheme solved such problem [4, 5]. This method provides an effective, wideband, and non-resonant coupling scheme to and from a silicon rib waveguide. In order to ensure small size and low propagation loss, tight size limits in range of tens of nanometers were set. Various systems have been proposed to solve problems arising with the dimensions [4–13].

Plasmonic filters with sharp peaks have been extensively used for designing various division multiplexing/demultiplexing applications. In addition, the sharp transmitted signal through the filter can be used in sensing applications which require high figures of merit (FOM) and sensitivities [14].

Many plasmonic demultiplexers have been suggested with a trade-off between narrow line-width and high transmission [15–17]. For example, a demultiplexer based on nano-disk geometry was proposed with a large line-width of around 80 nm and high transmission levels at 85% [15]. Enhancing (narrowing down) the full width half-maximum (FWHM) comes on the expense of the transmission level as has been proposed. A plasmonic slot cavity-based wavelength filter shows a 65% transmission level with FWHM as wide as 50 nm [17]. A great contribution towards narrow line-widths was made when a demultiplexing device used an MIM configuration to achieve optical resolution as narrow as 18 nm [18] with a relatively low transmission level in the range of 50%.

Besides optical demultiplexing, optical sensing is considered a crucial process in many applications and several researches are still being done within this area. Optical sensing includes a huge range of applications, including environmental, biological, and medical applications. The quality of chemicals and edible products can be determined through the measurement of the refractive index of these synthetic materials. Such techniques...
can give a perceptive vision about the concentration and density of chemicals inside food products [19–22]. One of the common techniques is the detection of the spectral wavelength shift due to variation in the refractive index [23].

SPPs, which are a key feature in surface plasmon resonances plasmonic structures, enable strong interaction between the optical sensor and the environment, thus opening the door for a quite appealing technique for optical bio-molecular detection [23–33].

In principle, plasmonic structures shall show high performance in terms of optical sensing; this is due to the strong dependence of the optical properties of the surface plasmon wave on the metal/dielectric interface as discussed in [34]. However, due to the small area of interaction (owing to their miniature size) the maximum achievable sensitivity is not high. For example, A ring resonator based sensor was proposed with sensitivity up to 600 nm RIU \(^{-1}\) (i.e. RIU is abbreviation for refractive index unit) only at operating wavelength around 1550 nm [35]. An interferometer based sensor was proposed with a limited sensitivity of 250 nm RIU \(^{-1}\) [36]. On the other hand, a large scale bio-chemical sensor was proposed with sensitivity as high as \(-92\ 000\ \text{nm RIU}^{-1}\), however, the use of glass and non-complementary metal oxide semiconductor (CMOS) compatible materials lacks the possibility of being integrated with electronic chips [37]. Nano-particle based sensor with sensitivity 650 nm RIU \(^{-1}\) around \(\sim 1500\ \text{nm}\) was proposed [38]. Despite their small size, plasmonic structures—based on the architectural design—might achieve high sensitivity by intensity and low limit of detection as proposed by [39–41] where detection limit down to \(10^{−3}\) is achieved while a sensitivity by intensity in the range of \(10^5\ \text{RIU}^{-1}\).

Previously, the authors proposed a CMOS compatible plasmonic structure that can reach high sensitivity values up to 3500 nm RIU \(^{-1}\) with acceptable FOM [42].

In this paper, MIM based plasmonic structures for high performance optical demultiplexing and sensing are proposed. The proposed optical demultiplexer shall represent the best compromise between FWHM, and maximum transmission peak. In addition, the plasmonic gas sensor achieved high performance sensing in terms of the lowest limit of detection, high sensitivity and narrow FWHM. Throughout the paper, design methodology is described in section 2, including the optimization functions, numerical simulation setup, proposed structures and initial results. Section 3 shows the further optimization processes on the optimization functions are performed to reach the best performance for the proposed structures, optimized results are shown. Finally, the paper is concluded.

2. Design methodology

The design problem is set as an optimization problem. This optimization problem can be written as

\[
\text{max} \ (\text{min})_p F
\]

Subject to \(p_{1\text{max}} < p_1 \leq p_{1\text{max}}, p_{2\text{min}} < p_2 < p_{2\text{max}}\),

(1)

where \(F\) is the objective function. \(\text{max}(\text{min})\) denotes maximizing (minimizing) the objective function according to the optical application. The vector of design parameters, \(p_1\), includes all the geometrical design parameters while \(p_2\) includes the allowed power limits in each channel. \(p_{1\text{min}}\) and \(p_{1\text{max}}\) in (1) are the lower and upper bounds for all the geometrical design parameters. These limits ensure realistic design parameters for the proposed structure. \(p_{1\text{min}}\) is chosen to avoid unrealistic dimensions that cannot be fabricated using the current technologies. \(p_{1\text{max}}\) ensures that a practical model is designed, therefore, it is crucial to pick a value for this limit in a way that guarantees that the structure does not occupy a considerable space within the whole optical system. For an optical demultiplexer, the optimization problem is solved iteratively to reach the narrowest FWHM. This iterative method includes the sweeping of all the design parameters independently until the best performance is maintained. In addition to the geometrical constraints, the optimization function is subjected to power level constraints vector which allows for sufficient power level for efficient optical applications. The upper bound of power level, \(p_{2\text{max}}\), should not exceed the input power level for stable bounded systems. An initial guess of the design parameters was made by building a structure similar to the optical filter proposed in [3] followed by studying the effect of varying the dimensions of each cavity resonator on the objective function, independently. The variation in the dimensions is done in small steps to maintain the best performance for the smallest practical structure. The optimization function is applied on the two components of interest; optical demultiplexers and optical sensors.

By applying the optimization function on an optical demultiplexer, it is assumed that the objective function is in the form \(F = \Delta \lambda\) where \(\Delta \lambda\) is the FWHM of the plasmonic demultiplexer.

The optimization problem takes the form

\[
\text{min}_p F
\]

Subject to \(p_{1\text{min}} < p_1 \leq p_{1\text{max}}, p_{2\text{min}} < p_2 < p_{2\text{max}}\).

(2)
Here, the $p_{1\text{ min}}$ constraints are taken to be 7 nm. An EO polymer with refractive index of 1.6 is used and the metal used is assumed to be silver utilized by FDTD Lumerical tool with its multi-coefficient Johnson and Christy silver model that highly fits silver experimental data. Simulation time of 1000 fs is set with a time stability factor of 0.7. The mesh accuracy is set to 6 to guarantee high accuracy. The minimum mesh step size is 0.25 nm to ensure that small dimensions are considered. Perfect matched layer (PML) boundaries are assumed to minimize the reflections back into the system to ensure higher accuracy. The schematic of the proposed design is shown in figure 1. The source is positioned on the left side while the monitor is placed on the right side with the arrows representing the propagation direction of the optical mode inside the MIM waveguide. The transverse magnetic mode is selected in which the magnetic field has only one component pointing out of the page. The proposed design parameters for the single channel demultiplexer are given as:

- $W_1 = 210$ nm,
- $W_2 = 68.5$ nm,
- $W_3 = 471.5$ nm,
- $W_4 = 261$ nm,
- $W_5 = 56.5$ nm,
- $W_6 = 16.5$ nm,
- $W_7 = 74$ nm,
- $L_2 = 150$ nm,
- $L_3 = 179$ nm,
- $L_4 = 140$ nm,
- $L_5 = 60$ nm,
- $L_6 = 119$ nm.

Minimum dimensions can be fabricated using electron beam (e-beam) lithography which can reach a feature size below 10 nm, however, with long exposure time. The intersecting cross sections between different cavities affects both the resonance wavelength as well as the FWHM of the multiplexing output. Aligned cross sections cause the output to be totally divergent from that of a resonator cavity. Such phenomenon can be analyzed using s-matrix model of intersecting junctions which can give an insight about the resonance peaks and the width of the output signal. There is slight shift between the cavities as shown in figure 1; for example a shift of around 50 nm exists between the right arm ($W_7^*L_6$) and the bridge, while another shift in the range of 7 nm exists between the left arm and the bridge. Also, a shift of 10 nm exists between the upper arm and the bridge.

In the proposed sensor design, 2 objective functions are studied; one for the line-width (FWHM) and the other for the structure sensitivity. The objective function of the FWHM is given by equation (2) while the objective function for the sensitivity is given by

$$\max_p F_2$$

Subject to $p_{1\text{ min}} \leq p_1 \leq p_{1\text{ max}}, p_{2\text{ min}} \leq p_2 \leq p_{2\text{ max}},$ \hspace{1cm} (3)

where $F_2 =$ Sensitivity is the objective function. Controlling the resonant wavelength depends on the cavity design lengths; where cascaded cavities might exist. A schematic of such design is shown in figure 2. Port 1 has a thickness of 210 nm to ensure single mode propagation. The gas here is assumed to be air, and sensitivity is calculated by changing the index of refraction by 0.01 and observing the wavelength shift. Thus, sensitivity can be defined as

$$S = \Delta \lambda / \Delta n .$$

The transmission for such design with resonant wavelength around 1500 nm is shown in figure 3.

The metal used is silver Johnson and Christy model built in Lumerical FDTD with the slot waveguides assumed to be air as the reference index. The main problem of the proposed design is the broad FWHM which is calculated to be around 50 nm; this will certainly affect the FOM (overall performance) of the design given by equation (5).

$$\text{FOM} = \frac{S}{\text{FWHM}} = \frac{\Delta \lambda / \Delta n}{\text{FWHM}} .$$
The resonance condition in the structure is given by
\[ m = 2\sum n_{\text{eff}} L_i, \quad (6) \]
where \( m \) is an integer representing the order of resonance, \( \lambda \) is the resonant wavelength, \( n_{\text{eff}} \) is the effective refractive index of each cavity, while \( L_i \) is the length of each cavity. It should be noticed that not all the cavities contribute to equation (6), owing to the structure design and cavity orientation. Another schematic for the gas sensor is shown in figure 4; the design is composed of 2 cavities with different lengths and widths, the alignment of the center offset affects the position and the width of the transmitted signal. The FWHM is enhanced as shown in figure 5 and is calculated to be 11 nm, and the sensitivity is in the range of 1540 nm RIU−1 yielding an FOM of...
1. Smaller changes in the refractive index of $5 \times 10^{-3}$ as in [39] were simulated and resulted in similar performance. Electric field distribution at both resonant wavelengths is shown in figure 6.

The relation between the design parameters and the location of the resonant wavelength is shown in figure 7. Small change in the upper cavity length can affect the position of the resonant wavelength significantly as shown in figure 7(a). However, for more precise control on the resonant wavelength, the width of the upper cavity shall be engineered as shown in figure 7(b). The original length and width of the upper cavity are 3518 nm and 190 nm, respectively. Better FOM is reached by having a rectangular cavity with low aspect ratio as shown in figure 8. Such design yields an FOM about 150 RIU$^{-1}$ with sensitivity about 1500 nm RIU$^{-1}$.

### 3. Design optimization

This section proposes the optimized results of the different optical structures described in the previous section. The section also presents the dependence of the behavior of the system on different design parameters. The section includes two sub-sections; the first describes the optimum design and results for the optical demultiplexer, the second sub-section describes those for the gas sensor.

#### 3.1. Optical demultiplexer

In this sub-section, single and double channel demultiplexers are discussed along with the optimized results. The dependence of the performance on the dimensions is shown.
3.1.1. Single channel demultiplexer

The proposed design of the single channel demultiplexer that is mentioned in previous section is used with minor changes in the dimensions. More optimized design parameters for the single channel demultiplexer are given as: \( W_1 = 210 \text{ nm} \), \( W_2 = 69 \text{ nm} \), \( W_3 = 472 \text{ nm} \), \( W_4 = 261 \text{ nm} \), \( W_5 = 57 \text{ nm} \), \( W_6 = 17 \text{ nm} \), \( W_7 = 74 \text{ nm} \), \( L_2 = 150 \text{ nm} \), \( L_3 = 179 \text{ nm} \), \( L_4 = 150 \text{ nm} \), \( L_5 = 60 \text{ nm} \), \( L_6 = 119 \text{ nm} \). The dimensions are changed to count for the ease of fabrication of such structures instead of precision as small as 0.5 nm. The output power from port 1 is shown in figure 9. The proposed design is tunable, and has FWHM—the line width of the transmission peak—(FWHM) of 8.15 nm, and peak transmission ratio of 30% with resonance around 1340 nm.

The effect of the design parameters, including the upper cavity width’s and height’s effect, on the peak power are studied in details and shown in figure 10. The dependence of the resonance wavelength on these parameters is shown. Figures 10(a) and (c) show how the dimensions of the upper cavity affect the resonant wavelength value. The interesting part in these graphs is that the position of the resonant wavelength is not changing abruptly which can be useful during the fabrication in a way that can minimize the effect of fabrication tolerance on the performance. On the other hand, these changes can affect the output transmission. However, it is important to mention that such fabrication tolerances in the current manufacturing foundry are in the range of ± 2 nm which would not affect either the resonant wavelength or the transmission level dramatically.

In addition, studying the effect of sweeping the dimensions on the FWHM (i.e. the second optimization parameter) is performed and shown in figure 11. The tradeoff is between the narrowest FWHM and the maximum transmission maintained. As can be shown from figures 10 and 11, increasing \( L_4 \) in the interval from 150 to 170 nm results in more enhancement in the FWHM while lowering the maximum transmission.
However, a good tradeoff between FWHM and maximum transmission is achieved at $L_4$ of 160 nm as shown in figure 11(b) in which the FWHM is in the range of 4 nm with transmission peak of 0.3 at resonant wavelength around 1370 nm. On the other hand, increasing $W_4$ results in a broader transmission signal and hence keeping $W_4$ at 261 nm is the best choice. From the above discussion, it is obvious that dimensions of $L_4$ of 160 nm and $W_4$ of 261 nm achieve the best tradeoff between FWHM and the maximum transmission.
3.1.2. Double channel demultiplexer

Two identical single channel demultiplexers with a slight central mismatch between them are used to design the double channel demultiplexer. A non-zero central mismatching ‘D’ was initially assumed. Applying the optimization identity, and setting a maximum and minimum limits for the wavelength, high resolution is achieved down to 25 nm. The center offset ‘D’ affects both the line-width (FWHM) and the resonant wavelength value [3]. Two resonant peaks with wavelength shift of 15 nm were observed through the simulation of the double channel demultiplexer as shown in figure 12. The final optimization reached is for having two aligned single channel demultiplexer (i.e. no center offset) with the spectrum as shown in figure 13. The full width half maximum is considered to be the smallest FWHM reported with a value of 9.8 nm.

3.2. Optimized gas sensor

Schematic of the optimized gas sensor is shown in figure 14. The sensor design is inspired by the design of the optical demultiplexer described above. The sensor is composed of multiple cavities which contribute to the position of the resonant wavelength as well as the width of the resonant peak. This structure could be thought of as the superposition of the initially proposed design in figures 2, 4, and 8. (i.e. the input nozzles and vertical cavities superimposed with the square cavity.) The alignment of the cavities affects the resonance effect. A shift of around 25 nm exists between the right arm (W7L6) and the bridge. The optimized sensor parameters are as follows: W1 = 60 nm, W2 = 17 nm, W3 = 261 nm, W4 = 144 nm, W5 = 88 nm, W6 = 55 nm, L1 = 329 nm, L2 = 60 nm, L3 = 150 nm, L4 = 90 nm, L5 = 179 nm, L6 = 144 nm. Such design yields a sensitivity of 1521 nm RIU$^{-1}$ and FWHM of 9 nm resulting in FOM of 169 RIU$^{-1}$ which is the greatest among sensing applications to our knowledge. The FOM of the proposed design exceeds that for the large-scale plasmonic based sensor previously proposed in [38] with sensitivity up to 92 000 nm RIU$^{-1}$ and FOM of only 122 RIU$^{-1}$. The transmission for different background index and its effect on the transmission is shown in figure 15. To test the limit of detection of the proposed gas sensor, refractive index change of 10$^{-4}$ is made. This
refractive index change achieved a wavelength shift in the range of 0.2 nm resulting in a sensitivity around 2000 nm RIU$^{-1}$. Effect of changing the refractive index by $10^{-3}$ on the wavelength shift is shown in figure 16. As can be observed, a sensitivity up to 2000 nm RIU$^{-1}$ is achieved resulting in a figure of merit of 222 RIU$^{-1}$.

Another metric that affects the sensor performance is the sensitivity by intensity. This metric relates the change in the power level to the change of the refractive index and is given by equation (7) as defined in [39–41].
ΔR refers to the change in power level, Δn refers to the small change in the refractive index of the surrounding. For the proposed sensor, the maximum value for sensitivity by intensity is around 300 RIU\(^{-1}\) which is two orders of magnitude smaller when compared to \(3.2 \times 10^4\) RIU\(^{-1}\) reported in [39] and 1.4 \(\times\) 10\(^7\) RIU\(^{-1}\) reported in [41]. On the other hand, for the proposed sensor in this paper, an angular sensitivity of 120° RIU\(^{-1}\) is maintained compared to 30° RIU\(^{-1}\) reported in [39] and 16° RIU\(^{-1}\) reported in [41], which is four times greater than that reported in [39, 41].

4. Conclusion

Design methodology for the design of MIM based plasmonic structures is proposed in this paper. Different optical systems are proposed based on this design methodology including optical demultiplexers and optical sensors. A novel optimized design for a plasmonic demultiplexer is proposed. Fabrication of this structure can be maintained using E-beam lithography with adequate exposure time. The plasmonic MIM demultiplexer can also be fabricated using the focused ion beam technique to mimic the small foot prints in the design. This design is utilized as a good starting point for a large number of channel demultiplexing through the optimization of channel spacing only. The optimal design for a single channel demultiplexer results in a FWHM down to 4 nm with output transmission of 30% at resonant wavelength of 1370 nm. This design opens the door for more functionality towards efficient and dense plasmonic circuits. In addition, a gas sensor based on MIM architecture is proposed. The gas sensor is characterized by its narrow FWHM of 9 nm, high sensitivity of 4 and high figure of merit of 222 which is greatest to our knowledge. Further work could be done to increase sensitivity by intensity of the proposed sensor which could help to increase the sensitivity by intensity by more than one order of magnitude. In conclusion, in this work, optical systems based on MIM plasmonic structures were proposed that could compromise different tradeoffs in the design of optical systems. Such proposed designs shall contribute in building an MIM optical interconnect to be coupled to silicon waveguides using conventional coupling techniques.

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