Design and analysis of near infrared high sensitive metal-insulator-metal plasmonic bio-sensor

H Ben salah 1,2, A Hocini1,* N Melouki1 and D Khedrouche1

1Laboratoire d’Analyse des Signaux et Systèmes, Department of Electronics, University of M’Sila BP.166, Route Ichebilia, M’Sila, 28000, Algeria.

2Université Yahia fares Médéa, Algeria.

*E-mail: abdesselam.hocini@univ-msila.dz

Abstract. In this paper, a high sensitivity metal-insulator-metal (MIM) waveguide based plasmonic sensor, coupled by a hexagonal ring resonator is proposed. The sensing characteristics of the device are analyzed by the finite-difference time-domain (FDTD) method embedded in the commercial simulator R-Soft. From results, there is a linear relation between the material’s refractive index and its wavelength resonances. Moreover, the maximum linear sensitivity is $S = 1743 \text{ nm/RIU}$ for the second mode and it is $S = 836 \text{ nm/RIU}$ for the first mode, its corresponding sensing resolution is $5.73 \times 10^{-6} \text{ RIU}$ for mode 2 and $1.19 \times 10^{-5} \text{ RIU}$ for mode 1. The proposed sensor can be implemented in high performance nano-sensors and bio-sensing devices. The positions of transmission peaks can be easily manipulated by adjusting the inner side lengths of the hexagonal ring resonator, making this structure a dynamically controllable band pass filter. In addition, introducing another small hexagonal ring within the base resonator decreased the full width of half maximum (FWHM) of the resonance peak.

1. Introduction
The Surface Plasmon Polaritons SPPs are electromagnetic fields which travel along the metal-insulator interface. The capability to modulate nano-scale light and to break the diffraction limit takes the interest of many researchers over several decades [1]. Furthermore, as its volume is so tiny several applications will be realizable such as, optical processing and manipulation in nanoscale optical communication [2,3]. SPP-based waveguide designs, for instance, filters [4], diodes [5], optical switches and sensors [6,7] have been thoroughly tested for optical instrumentation. Sensors based on Surface Plasmon Resonance (SPR) have been developed for a variety of applications such as proteins [8], DNA [9] and drugs [10] in the biomedical and clinical research sector. SPR instruments are commonly utilized to analyze and assess the index of refraction for a variety of substances because of their high sensitivity, easy production and nanoscale size [11,12]. Among different plasmonic structures, metal-insulator–metal (MIM) based structure is one of the most promising choices for realization of the mentioned requirements [13]. The confinement of light in sub-wavelength insulator regions is highly achievable, so a prominent transmission efficiency and simplicity in fabrication procedure, made the MIM-based devices a good candidate in nanoscale photonic devices [14]. As one of the most innovating devices in optical circuits, MIM waveguide based plasmonic sensors and filters for wavelength selection has been investigated numerically and experimentally, and different types of the plasmonic sensors and filters such as nanodisk resonators [15], ring resonators [16,17,18,19] and tooth-shaped waveguide [7-20].
In integrated circuits, plasmonic ring resonators are key elements. Owing to their compact size, excellent efficiency, and ease of production, they have gained interest in latest years [21]. Besides, wavelengths of resonance may be finely tuned by changing the ring geometric parameters [22, 23].

Sensitivity of the sensor is among the most critical merit for evaluating the sensor functionality for various substances according to the variation in the index of refraction. The aim is to enhance the sensitivity aspect by using various designs in a limited space and to evaluate the efficient sensitivity and transmission features.

In this work, a MIM waveguide with structures based on stub and hexagonal resonators are used as a refractive index based plasmonic nano-sensor. In order to determine the impact on the sensor functionality and refractive index sensibility, we have varied the inner side length of the hexagonal resonator with the distance between the hexagonal ring resonator and the waveguide. The boundary condition of absorbing perfectly matched layers (PML) is imposed and computed using the FDTD algorithm which is implemented in the commercial software R-SOFT.

2. Structural and theoretical analysis

The proposed MIM based plasmonic structure is depicted in figure 1. It consists of a slit (waveguide) with w =50 nm as a width and fixed to that value so the only excited mode is (TM$_0$) in the MIM waveguides [24], and a hexagonal ring resonator (HRR), with L$_1$=200nm and L$_2$=125nm as an outer and inner side lengths respectively, g =10 nm, is the distance between the HRR and the waveguide. The gray area represents the silver layer, and the white one represents the dielectric material.

The frequency dependent dielectric constant of silver is calculated and expressed by Lorentz–Drude model [25]:

$$\varepsilon_m(\omega) = \varepsilon_\infty - \frac{\omega_p^2}{\omega(\omega + i\gamma)}$$

where $\varepsilon_\infty$ is the dielectric constant at the infinite angular frequency with a value of 3.7, $\omega_p$ is the bulk plasma frequency ($\omega_p$=1.38 x 10$^{16}$Hz), and $\gamma$ is the electron collision frequency ($\gamma$=2.73 x 10$^{13}$Hz) and $\omega$ is the angular frequency of the incident wave in vacuum [26].

The incident light for excitation in our simulation process of the SPP Mode is TM-polarized; this led to the magnetic field being parallel to y axis [27].

The resonance wavelength $\lambda_m$ of the single plasmonic hexagonal cavity can be obtained theoretically by [28]:

$$\lambda_m = \frac{(6L_{eff})}{m - \varphi 2\pi} \Re(n_{eff})$$

Where L$_{eff}$ is side lengths of hexagonal cavity, Re (n$_{eff}$) is the real part of the effective refraction index of the hexagonal shaped cavity. The positive integer m represents the order of the standing SPP wave in the cavity; $\varphi$ also presents the total phase shift in the corners of the hexagonal cavity.

3. Simulation results and discussion

The commercial simulator R-Soft, is used in all carried out simulations, it’s based on the FDTD method [29]. The Perfectly Matched Layers (PML) is imposed and applied on the structure to simulate its transmission characteristics, as the absorbing boundary condition for all sides of the computational window to absorb outgoing waves.

The grid size in both the x and z directions was chosen as $\Delta x = \Delta z = 5$ nm [7], with a continuous TM polarized Gaussian modulated wave based input type. The transmitted light was collected at the right side of the waveguide which is defined as $T = P_{out}/P_{in}$. The incident power P$_{in}$ and the transmitted power P$_{out}$ are observed at positions A and B respectively. Initially, both the insulator in the dielectric core and the cavities have a refractive index n of 1. Figure 2(a) Shows the transmission spectra of both the hexagonal based cavity (side length L$_1$=200nm) and the proposed hexagonal ring resonator (L$_1$=200nm and L$_2$=125nm).
**Figure 1.** Schematic diagram of the proposed MIM Based plasmonic structure.

(a)

**Figure 2.** (a) The transmission spectra of MIM plasmonic structure with $n = 1$, $L_1=200\,\text{nm}$, $L_2=125\,\text{nm}$ and $g=10\,\text{nm}$. (b) Magnetic field patterns of the MIM plasmonic structure at resonance wavelengths of 742.6 nm (center), 1388.4 nm (right) and at wavelength 1200nm (left).

The structure with hexagonal shaped cavity exhibits a low transmission peak at the resonance wavelengths of 742.6 nm, whereas the case of the MIM waveguide is coupled with the HRR, the two transmission peaks is observed at the resonance wavelengths of 742.6 nm and 1388.4 nm, corresponding to the first and second resonance modes of the HRR. Figure 2(b) depict the field distributions of $|H_y|$ for the on and off resonance wavelengths of the proposed structure. It’s clearly noticed that the incident
light within the wavelengths of both 742.6 nm and 1388.4 nm, couples to the HRRs resonance wavelengths, so it’s prohibited to pass through the waveguide, contrary to the rest of the wavelengths which are transmitted to the output.

To investigate the influence of the coupling distance \( g \) on the transmission spectra of the proposed MIM based plasmonic structure, the distance \( g \) is set as a state variable from 10 nm to 20 nm with a step of 5 nm, while keeping the other structural parameters fixed (\( L_1=200\text{nm}, L_2=125\text{nm}, \text{and } n = 1.0 \)). From figure 3, it’s noted that when the coupling distance \( g \) is increased, the wavelengths of the peaks shift slowly towards short wavelengths and the bandwidth become narrower. In the other hand, the maximum transmittances are reduced accordingly, due to the fact that the MIM coupler losses are increased also with increasing of the distance \( g \) [30].

![Figure 3. The transmission spectrum of the structure versus wavelength with different coupling distance \( g \) at \( n = 1 \), \( L_1=200\text{nm}, \text{and } L_2=125\text{nm} \).](image)

Figure 4(a) illustrates the transmission spectra of the proposed structure for different refractive indices varying from 1 to 1.2 in steps of 0.05. Increasing the refractive index \( n \), results in a red-shift of resonance wavelengths of the transmitted spectra, with a larger shift in mode 2 in comparison to mode

![Figure 4. (a) The transmission spectrum of the structure for different refractive index \( n \), at \( g = 10\text{nm}, L_1=200\text{nm}, \text{and } L_2=125\text{nm} \). (b) The resonance wavelength versus the refractive index \( n \) of the material under sensing.](image)
1. Figure 4(b) represents the maintained linearity relation between the resonance wavelengths and the refractive indices for both the first and the second modes.

Sensitivity (S), is an important aspect in the designing and analyzing of the SPR based sensors, it can be calculated as \( S = \frac{\Delta \lambda}{\Delta n} \) (nanometer per refractive index (nm/RIU))[31], where \( \Delta \lambda \) denotes the shifting rate of resonant peak wavelength of transmittance, and \( \Delta n \) represents the changing rate in the refraction index in the plasmonic sensor structure. Keeping the other existing parameters fixed, and increasing the refraction index between \( n = 1 \) and \( n = 1.2 \), the sensitivity for the first mode is around 670 nm/RIU and for the second mode is around 1380 nm/RIU.

In Figure 5, the increase in the value of \( L_2 \) from 125 to 145 nm with a step of 5 nm is associated with an increase in the resonance wavelength. Meaning, the value of \( L_2 \) causes a shift in resonance wavelength, and the shift for mode 2 is larger than that for mode 1 as shown in figure 5(a). According to figure 5(b) the linearity of wavelength resonances versus the refractive indices is maintained in spite of the increase in the value of \( L_2 \). Moreover, an enhancement of the sensor’s sensitivity is achieved by increasing the value of \( L_2 \), for mode 1 the sensitivity is 836 nm/RIU whereas in the case of mode 2, the sensitivity was 1743 nm/RIU, i.e. sensing resolution of \( 1.19 \times 10^{-5} \) RIU for mode1 and \( 5.73 \times 10^{-6} \) RIU for mode2, is achieved corresponding to value of \( L_2 =145 \) nm, in comparison to sensitivity of 670 nm/RIU for mode1 and 1380 nm/RIU for mode2 where the value of \( L_2 \) was 125 nm. In figure 5(c) it is clearly shown that the greater the value of \( L_2 \) is, the better the sensor’s performance.

**Figure 5.** Sensing properties as functions of \( L_2 \). (a) Transmission spectra of index 1 for \( L_2 \) varying from 125 to 145 nm. (b) The resonance wavelengths versus the refractive index for different \( L_2 \). (c) Sensitivities of the plasmonic sensors for \( L_2 \) varying from 125 to 145 nm.

For a better characterization of a plasmonic sensor’s performances, both the sensitivity (S) and figure of merit (FOM=\( S/\Delta \lambda_{FWHM} \)) are considered to be the most important parameters, and preferably being as high as possible for a better performing sensor [32].

By using a secondary hexagonal ring inside the main one, as illustrated in figure 6, the proposed design with double-ring resonator where \( L_1 =200 \) nm, \( L_2 =145 \) nm, \( L_3=100\)nm, \( L_4=70\)nm and \( g=10\)nm
are the main parameters of this structure, narrowed down the bandwidth, hence the higher FOM as illustrated in figure 6(b) at the resonance wavelength of 1701 nm, where the FWHM when using the proposed design decreased from 112 nm to 55 nm, in addition to the results from both the sensitivity and the FOM value for the first proposed design (single hexagonal ring resonator (S = 1743 nm/RIU, FOM=15.6 (mode2)), and the second proposed MIM based plasmonic sensor with double hexagonal ring resonator (S = 1743 nm/RIU, FOM=31.7 (mode2)), shows a promising results for enhancing the FOM, and consequently the sensor’s performance.

Figure 6(c) depict the field distributions of $|H_y|$ for the on and off resonance wavelengths states of the proposed structure. It’s clearly observed that the incident light within the wavelength of 841.5 nm and 1701 nm, couples the hexagonal shaped double-ring resonator and it’s prohibited to pass through the waveguide, while the rest of the wavelengths are transmitted to the output freely. Table 1 compares the sensitivity (S) for different reported MIM plasmonic sensors in literatures with our present work.

Figure 6. (a) schematic of the proposed structure with double-hexagonal ring resonators, (b) transmission of the structure proposed with double-hexagonal rings with corresponding FWHM, (c) Magnetic-field patterns of the structure proposed at resonance wavelengths of 841.5 nm (center), 1701 nm (right) and at wavelength 1200nm (left).
Table 1. Sensitivity comparison of different sensor structures.

| Reference   | Sensitivity | Year |
|-------------|-------------|------|
| [33]        | 1125        | 2017 |
| [22]        | 1540 for mode 1 and 1010 for mode 2 | 2018 |
| [18]        | 1160        | 2018 |
| [7]         | 2602.5      | 2019 |
| This work   | 1743 for mode 2 and 836 for mode 1 | 2019 |

4. Conclusion

An MIM based waveguide slab coupled by a hexagonal shaped ring resonator for a near-infrared refractive index sensor is proposed. The finite-difference time-domain (FDTD) method embedded in the commercial simulator R-Soft is used to characterize all design variations. The positions of transmission peaks are of a linear nature in respect to the refractive index of the material under sensing, and can be easily manipulated by adjusting the inner side length of HRR. In this proposed structure, the maximum linear sensitivity is $S = 1743 \text{ nm/RIU}$ and $S = 836 \text{ nm/RIU}$ for both mode 2 and mode 1 respectively, after optimizing the structural parameters. In addition, when introducing another hexagonal shaped ring inside the main one, the figure of merit (FOM) is enhanced, which makes our proposed design an attractive candidate for a good performing bio-sensor.

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