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Simulation and analysis of Au-MgF_2 structure in plasmonic sensor in near infrared spectral region

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ABSTRACT

Plasmonic sensor based on metal-dielectric combination of gold and MgF_2 layers is studied in near infrared (NIR) spectral region. An emphasis is given on the effect of variable thickness of MgF_2 layer in combination with operating wavelength and gold layer thickness on the sensor's performance in NIR. It is established that the variation in MgF_2 thickness in connection with plasmon penetration depth leads to significant variation in sensor's performance. The analysis leads to a conclusion that taking smaller values of MgF_2 layer thickness and operating at longer NIR wavelength leads to enhanced sensing performance. Also, fluoride glass can provide better sensing performance than chalcogenide glass and silicon substrate.

1. Introduction

Plasmonics is one of the most widely applied areas of nanophotonics and possesses an exclusive setting for the manipulation of electromagnetic (EM) radiation *via* confinement of the corresponding EM field to the regions well below the diffraction limit. One particular domain where plasmonics has explored significant opportunities, and in which the sub-wavelength mode confines at nanoscale region, is the surface plasmon-based sensing technology. In simplest of the words, surface plasmons (SP) can be defined as quanta of coherent transverse magnetic (TM) oscillations of the surface charges at metal boundary [1]. SP-based optical sensors have been extensively used for highly sensitive and selective detection of various physical, chemical, and biological parameters [2–7].

The performance of any plasmonic sensor depends on the concerned metallic and dielectric media because they are the main drivers of how deep the SPs can be confined and how strongly they can interact with the incident EM field. In this view, there are ever-existing possibilities of improving performance of SPR-based sensors by, for example, introducing new materials, manipulating the light wavelength, and optimizing the thickness of media (primarily, metallic and dielectric) involved [8–10]. In this view, many two-dimensional (2D) dielectric materials with sub-atomic thickness and complex refractive index (*RI*) are being explored to enhance the performance of photonic devices by manipulating the depth and interaction of SPs [11–13]. However, these 2D materials (*e.g.*, graphene, MoS_2, $MoSe_2$) are still in the exploration stage and lot of information, such as dispersion relations in a large near infrared (NIR) spectral range (which is available in limited wavelength regions only [14,15]), is still to be produced for further implementation in SP-based devices and sensors, in particular.

In this context, other dielectric material layers such as SiO_2 [16] and MgF_2 [17] have been studied by exploring another similar phenomenon known as plasmon waveguide resonance (PWR) to enhance the sensitivity of plasmonic sensors. PWR is primarily defined as a method to enhance the evanescent field by increasing the thickness of dielectric layer (*e.g.*, SiO_2, MgF_2 *etc.*) in order to couple the waveguide mode of dielectric layer with surface plasmon wave (SPW). The above study determined that MgF_2-based plasmonic sensor provided significantly superior performance than SiO_2-based sensor [17]. However, there are a few aspects that are yet to be explored. First, the above MgF_2-based plasmonic sensor was operated at single visible wavelength (633 nm) whereas MgF_2 is a dielectric medium showing encouraging optical properties in NIR also, therefore, the MgF_2-based SPR sensor should be explored in as large NIR spectral range as possible. This point is important in terms of the application of MgF_2-based sensor in determination of biosamples due to their much smaller photodamage in NIR range compared with visible wavelengths [19]. Therefore, an important objective should be to study the MgF_2-based plasmonic sensor in NIR leading to the development of sensor probe for important practical applications such as biosensing.

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Apart from this, several key benefits can be achieved by moving into the IR regime like enhanced sensitivity, lower power requirements, and deeper penetration depth [20–22]. Second, because the penetration depth of SPW (which has a strong dependence on wavelength) is directly connected to the thicknesses of metallic and dielectric media involved, and strongly dictates the performance of plasmonic devices [23], the variation in thickness of dielectric MgF_2 layer should be explored in conjunction with metal layer thickness and operating wavelength in context of plasmonic sensor's performance. Furthermore, the role of different substrate materials active in NIR spectral region should also be investigated.

In this work, an Au-MgF_2 'metal-dielectric' configuration has been considered to analyze a plasmonic sensor in NIR spectral region. The sensed samples are taken as normal water (H_2O) and heavy water (D_2O) at room temperature. In order to optimize the sensor's performance, the analysis is carried out for a wide spectral range in NIR. As a very important performance tuning parameter, the effect of MgF_2 thickness is evaluated in combination with different thicknesses of Au layer. Further, the MgF_2-based sensor's performance is analyzed and compared for important glass materials (chalcogenide, fluoride, and silicon) possessing favorable optical properties in NIR.

2. Theory and background

Proposed plasmonic sensor is based on Kretschmann configuration [24] and comprises of four layers (shown in Fig. 1): (*i*) light coupling substrate, (*ii*) metal layer, (*iii*) MgF_2 layer, and (*iv*) analyte.

Following equation represents the plasmon resonance condition:

$$\frac{2\pi}{\lambda} n_p \sin\theta_{SPR} = real\left(\frac{2\pi}{\lambda}\sqrt{\frac{\varepsilon_m \varepsilon_s}{\varepsilon_m + \varepsilon_s}}\right) \tag{1}$$

The left hand and right hand sides of Eq. (1) represent the wave vectors (along the interface) of incident TM light (monochromatic) and SPW, respectively. In above equation, ε_m and ε_s are, respectively, the dielectric constants of metallic and dielectric (analyte) media; n_p is *RI* of the light coupling substrate material; θ_{SPR} is the resonance angle of incidence; and λ is the wavelength of incident light. On coupling of SPs with incident light, a narrow dip in resonance curve is obtained at the output having minimum (near zero) reflectance (R_{min}) at resonance angle (θ_{SPR}) as shown in Fig. 1. In the following sub-sections, different components of the sensor along with their properties and selection criteria are discussed:

2.1. Layer 1: Light coupling substrate

SPR-based structures in IR region have substantially different excitation parameters and support advantages for sensing applications in terms of high probe depth [20] and more precise determination of SPR dip [25]. For that matter, chalcogenide glasses based on the Group VI chalcogen elements (sulfur, selenium, and tellurium) have generated significant interest due to their transparent behavior in the IR region [26]. Substrates based on chalcogenide glass have advantage over silica glass owing to its higher thermal and chemical stability [26]. For the present study, $As_{40}Se_{60}$ chalcogenide glass has been considered as light coupling substrate. The wavelength-dependent *RI* of $As_{40}Se_{60}$ is taken into account [27].

2.2. Layer 2: Thin metal layer

Gold and silver encompass extraordinary optical properties supporting plasmonic devices due to strong free electron behavior [28]. Au is chosen as SPR active metal in the present study due to its high stability against oxidation, more efficient bonding with biochemical layers (*e.g.*, thiol *etc.*) in comparison to silver [29], and the largest $\delta\theta_{SPR}$ among the other SPR active metals, *e.g.*, Ag, Al and Cu [30,31]. Also, Au is preferred because highly polarized SPW is generated with enhanced evanescent wave [32]. For the present study, 40–65 nm thickness of Au layer is considered. The wavelength dependent dielectric constant of gold in NIR is considered for sensor simulations [33].

2.3. Layer 3: MgF_2 layer

An MgF_2 layer is considered to be sandwiched between Au layer and analyte sample. The previous studies show that MgF_2 is almost entirely immune to radiation damage in NIR [34]. This feature can

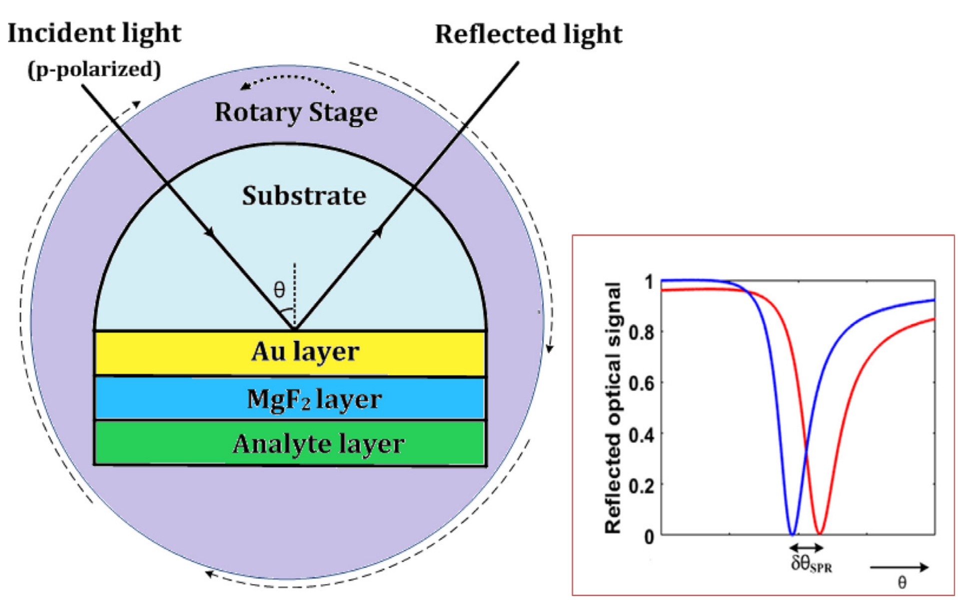

Fig. 1. Schematic of 4-layer Kretschmann configuration as an Au-MgF_2 'metal-dielectric' configuration based plasmonic sensor. The sensor structure is usually fixed on a rotary stage in order to carry out the sensing procedure under angular interrogation method. On the right hand, the corresponding resonance curve is depicted in which the reflected optical signal encounters a sharp dip at the resonance angle (θ_{SPR}), which shifts to some other angle value upon change in analyte. The angular shift in resonance curve is represented as $\delta\theta_{SPR}$.