FDTD Analysis on Geometrical Parameters of Bimetallic Localized Surface Plasmon Resonance-Based Sensor

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Abstract—The localized surface plasmon resonance (LSPR) properties are numerically analyzed using finite-difference time domain (FDTD) method, which is a reliable technique in solving Maxwell’s equations in dispersive medium. Optical properties and LSPR characteristics were analyzed with Titanium Nitride (TiN) as an adhesion layer at gold(Au)/silver(Ag) interface. The reflection spectra of bimetallic layer nano-holes was compared with various metallic layer thicknesses of Au and Ag, hole radii and lattice period. When compared between single and bimetallic Ag/TiN/Au nano-hole layers, it showed that the layer with 70nm-thick Ag/5nm-thick TiN/50nm-thick Au (Ag70/TiN5/Au50) gave greater LSPR-based sensor performance with narrower plasmonic line width and better full width at half maximum (FWHM). Change in geometrical parameters such as lattice period and hole radii was affected the sensitivity and detection accuracy of Ag70/TiN5/Au50 nano-hole layer; which maximum of 90.9% reflection intensity and minimum of 18nm FWHM were obtained.

Keywords-component; localized surface plasmon resonance, finite-difference time domain, single nano-hole layer, TiN adhesion layer, bimetallic

I. INTRODUCTION

Localized surface plasmon resonance (LSPR) method with nano-structures is widely used in countless applications in the field of sensing such as detection of pesticides, proteins, enzymes and so forth. It is a physical phenomenon which involves optical excitation of surface plasmon waves (SPW) at the interface between a dielectric and a metal. The excitation of SPW is enhanced by changing the angle of incident (angular interrogation) or operating wavelength (wavelength interrogation) of a light source in order to obtain a resonance condition, which is observed as a sharp dip in the optical reflection spectrum. When the refractive index of the metal-dielectric medium is modified due to adsorption of bio-molecules on the surface, the sharp dip is shifted [1].

LSPR-based optical sensors are highly sensitive to variation in the refractive index of the surrounding medium which enables them to be highly efficient for sensing application. Common metallic material layers that offer better sensitivity is Au and Ag but well known problems with these two materials are Ag is easily oxidized whereas Au peels off easily. Au is mostly opted for LSPR applications as it has good resistance to oxidation and corrosion in different environment. In this work, we propose introducing Titanium Nitride (TiN) as an adhesion improvement layer for Au meanwhile Au is proposed to be a protective layer for Ag from being oxidized. Kim et al. reported an experimental study on TiN as an adhesion layer of Au/substrate. They observed that TiN layer could give sufficient adhesion strength at the substrate/TiN and TiN/Au interface and its performance is comparable with that of Titanium (Ti) layer [2]. It has been found that Au/TiN plasmonic stack showed higher peak transmittance, had lower damping and narrower line width than gold with conventional adhesion layer such as Ti.

The optical reflectance properties of single and bimetallic layer nano-hole array with different geometrical parameters were also numerically investigated. The LSPR capability depends on parameters such as metallic layer thickness, the geometry of nano-holes and dielectric properties of both material and local environment surrounding the nano-holes. Change in geometrical properties of the nano-holes and the metallic layer affected the transmission/reflection light intensity while change in the substrate material and metallic layer coating resulted in a spectrum shift [3]. In previous work on multi-hole (three dissimilar hole chain array) nanostructures in Au metallic film, they obtained minimum FWHM of 29nm with hole radii of 80nm, side-hole radii of 25nm and periodicity of 550nm [4].

In order to study the phenomenon associated with LSPR interaction, one of the important parameter of interest is Attenuated Total Reflection (ATR). It gives a measure of the length scale over which the LSPR mode is sensitive to changes in the sensing layer’s refractive index and in turn the performance of the LSPR sensor. Full width at half maximum (FWHM) is the spectral width or the difference between the two extreme values of the operating wavelength at which the reflection intensity is equal to half of the maximum value. A smaller FWHM is desired in the LSPR sensor because a deeper and narrower resonance peak allows detecting the resonance shift effectively. The performance of the sensor is analyzed in terms of the operating wavelength range, reflection intensity (sensitivity) and FWHM (inversely proportional to detection accuracy).

II. FDTD FRAMEWORK

Numerical study of sub-wavelength metallic nano-hole layer has been carried out using commercial software package from Lumerical Solutions to analyze and design the LSPR-based sensor. It uses a finite-difference time domain...
(FDTD) technique, which is one of the major computational electromagnetic modeling method. This method solves the problem by providing a full-wave solution and solve Maxwell's curl equation in time domain. The FDTD method is faster than multiple-multipole method and Green's dynamic method, but its applicability is limited by a requirement of small grid size to produce rapid spatial variation of electromagnetic fields at metallic-dielectric interfaces [4].

In this paper, we demonstrate an analysis and numerical modeling of bimetallic layer nano-hole for LSPR-based sensor with varied geometrical parameters using FDTD method. The simulation is one unit cell but it correctly represents an infinite periodic nano-hole illuminated by a plane wave source. Figure 1 shows schematic diagram of single and bimetallic nano-hole with TiN as an adhesion layer of Au and Au as coating layer of Ag.

a) 

b) 

c) 

Figure 1. Schematic diagram of single and bimetallic nano-hole with TiN as an adhesion layer (a) single metallic layer in periodic lattice array, (b) cross section of Au with TiN nano-hole layer and Ag nano-hole layer and (c) cross section of bimetallic Ag/TiN/Au nano-hole layer.

The three-dimensional (3-D) FDTD was carried with plane wave source injection in z-axis with wavelength range of 400nm to 1000nm. Surface Plasmon Polariton (SPP) excitation is performed using a wavelength interrogation technique. The periodic boundary condition was used in x and y directions and Perfectly Matched Layer (PML) boundary in z direction as the absorbing boundary condition. Simulation time was set to 100fs and reflection intensity was calculated using x-y monitor at 200nm away from dielectric medium/metal nano-hole interface. The simulation background and filling of nano-hole were taken as air (n=1.00) and the substrate material was set to Silicon Dioxide (SiO₂) with thickness of 950nm. The bimetallic nano-hole was investigated in conditions of fixed 50nm-thick Au with varied Ag layer thicknesses of 40nm, 70nm and 90nm and fixed 50nm-thick Ag with varied Au layer thicknesses of 40nm, 70nm and 90nm. Beneath the Au nano-hole layer, a 5nm-thick TiN nano-hole layer is used to enhance adhesion between the Au/Ag interface. The reflection intensity of bimetallic Ag70/TiN5/Au50 nano-hole was then studied with different lattice period (p) and hole radii (r). Calculation on percentage of reflectivity, FWHM and resonance wavelength were taken into consideration.

III. RESULTS AND DISCUSSIONS

The FDTD results for reflectance spectra of varied bimetallic layer thickness, nano-hole radii and periodicities are discussed. The output from numerical investigation (LSPR response curve) is plotted as the normalized reflected power versus operating wavelength. The resonance condition is achieved when phase matching occurs between the fundamental mode of Ag/TiN/Au nano-hole and the localized surface plasmon mode. When the resonance condition is achieved, a dip in LSPR response curve appears. The detection accuracy and sensitivity are two important performance parameters that can be defined from the LSPR response curves. The detection accuracy is inversely proportional to the width(FWHM) of the LSPR curve, the narrower(smaller) the width(FWHM) the higher the detection accuracy. However, the sensor sensitivity is proportional to the LSPR curve depth which means the deeper the depth, the higher the sensitivity.

In Figure 2, a comparison of metallic layer nano-hole of TiN5/Au100, Ag100 and Ag70/TiN5/Au50 were studied. The geometrical parameters used were nano-hole radii (r) of 100nm and periodicity(p) of 400nm. Other than solving the Ag oxidation problem, Table 1 shows that the Ag70/TiN5/Au50 performs better than the pure Ag100 and TiN5/Au100 nano-hole layer with reflection intensity of 88.5% and FWHM of 24nm.

![Figure 2. Reflection spectra of TiN5/Au100, Ag100 and Ag70/TiN5/Au50 bimetallic nano-hole layer (fixed r=100nm and p=400nm).](image)

<table>
<thead>
<tr>
<th>Metallic nano-hole layer configuration</th>
<th>Reflection intensity (%)</th>
<th>FWHM (nm)</th>
<th>Resonance wavelength (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>TiN5/Au100</td>
<td>80.5</td>
<td>36</td>
<td>679</td>
</tr>
<tr>
<td>Ag100</td>
<td>85.2</td>
<td>37</td>
<td>648</td>
</tr>
<tr>
<td>Ag70/TiN5/Au50</td>
<td>88.5</td>
<td>24</td>
<td>655</td>
</tr>
</tbody>
</table>
A. Bimetallic Layer Thickness (r=100nm, p=400nm)

LSPR sensor performance is influenced by the metal layer thickness. Figure 3 demonstrates the optical reflectivity intensity over wavelength of Ag50/TiN5/Au(x) nano-hole layer with fixed Ag thickness of 50nm, 5nm-thick TiN and varied Au thickness (x) of 40nm, 70nm and 90nm.

![Figure 3. Reflection spectra of bimetallic nano-hole layer with fixed 50nm-thick Ag, 5nm-thick TiN and varied Au thickness.](image)

As shown in Table 2, bimetallic nano-hole layer of Ag50/TiN5/Au70 gives greater results with FWHM of 31nm and reflection intensity of 85.0% compared to others.

<table>
<thead>
<tr>
<th>Au nano-hole thickness, x (nm)</th>
<th>Reflection intensity (%)</th>
<th>FWHM (nm)</th>
<th>Resonance wavelength (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>40</td>
<td>85.0</td>
<td>43</td>
<td>661</td>
</tr>
<tr>
<td>70</td>
<td>85.0</td>
<td>31</td>
<td>655</td>
</tr>
<tr>
<td>90</td>
<td>84.8</td>
<td>31</td>
<td>650</td>
</tr>
</tbody>
</table>

Figure 4 presents reflection spectra of bimetallic nano-hole with fixed 50nm-thick Au, 5nm-thick TiN and varied Ag thickness (y) of 40nm, 70nm and 90nm.

![Figure 4. Reflection spectra of Ag(y)/TiN5/Au50 with fixed 50nm-thick Au, 5nm-thick TiN and varied Ag thickness.](image)

Table 3 shows that bimetallic nano-hole of Ag70/TiN5/Au50 gives greater results with FWHM of 24nm and reflection intensity of 88.5% compared to others. Reflection intensity of 40nm and 70nm-thick Ag is similar but the thinner layer has a broader FWHM, hence results in low detection accuracy.

B. Variation of Hole Radii and Lattice Period

In order to find the effects of geometrical parameters on the bimetallic nano-hole structure on the reflection depth, FWHM and resonance wavelength, the nano-hole radii (r) and lattice period (p) of Ag70/TiN5/Au50 was varied as illustrated in Fig. 5.

![Figure 5. Reflection spectra of Ag70/TiN5/Au50 with varied hole radius.](image)

![Figure 6. Reflection spectra of Ag70/TiN5/Au50 with varied lattice period.](image)

Table 3 shows the optical reflection intensity, FWHM and resonance wavelength for Ag(y)/TiN5/Au50 nano-hole.

<table>
<thead>
<tr>
<th>Ag nano-hole thickness, y (nm)</th>
<th>Reflection intensity (%)</th>
<th>FWHM (nm)</th>
<th>Resonance wavelength (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>40</td>
<td>88.1</td>
<td>43</td>
<td>661</td>
</tr>
<tr>
<td>70</td>
<td>88.5</td>
<td>24</td>
<td>655</td>
</tr>
<tr>
<td>90</td>
<td>79.2</td>
<td>24</td>
<td>650</td>
</tr>
</tbody>
</table>
increases with the increment in lattice periodicity. Resonance wavelength was red-shifted as lattice period was increased. The maximum optical reflection intensity of 90.9% was observed at resonance wavelength of 642nm, period of 400nm, and hole radii of 80nm. Whereas the minimum FWHM was recorded as small as 18nm for hole radii of 100nm and periodicity of 500nm, which is considered very desirable for high sensitivity LSPR sensor. The SPP excitation did not occur for nano-hole radii of 40nm with lattice period of 500nm. Ag70/TiN5/Au50 nano-hole configuration with lattice period of 300nm and hole radii above 120nm results in low detection accuracy due to the wide LSPR curves. It offers low sensitivity with shallow LSPR curves that are attributed to the decay of the evanescent waves which makes the LSPR sensor unable to detect changes in the refractive index.

### IV. CONCLUSIONS

In summary, LSPR-based sensor with Ag/TiN/Au nano-hole was investigated using 3D-FDTD simulation. The detection accuracy and sensitivity of the LSPR sensor are affected by their geometrical properties. In this paper, spectra of reflectivity, FWHM and resonance wavelength of Ag/TiN/Au with varied lattice period, nano-hole radii, metallic nano-hole layer thickness has been demonstrated.

As an adhesion layer, TiN is applicable in Au nano-hole based sensor whereas Au layer is desirable as a coating layer of Ag. For high sensitivity sensor application, Ag70/TiN5/Au50 with hole radii of 80nm and lattice period of 400nm can be chosen due to its greater reflection intensity of 90.9%. However periodicity of 500nm with nano-hole radii of 100nm is desirable for high accuracy sensor with narrower FWHM of 18nm. Using these proposed LSPR-based sensor design that provides larger reflection intensity and greater detection accuracy suggest promising applications in bio-sensing and nano-photonics application.

### ACKNOWLEDGMENT

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