CHAPTER 2

Fluoride Glass based Surface Plasmon Resonance Sensor in Infrared region: Performance Evaluation

2.1 Introduction

Increasing research interests towards fluoride glasses are due to their excellent optical properties such as mean dispersion, special partial dispersion, low Rayleigh scattering, high threshold for laser damage, broad transparency, and low birefringence (Tran et al., 1984). They possess larger value of Abbe number than other types of glasses such as oxides and silicates (F. Gan, 1995). Abbe number represents the dispersion property of a material. Higher the value of Abbe number, the lower is the dispersion. Hygroscopic nature of fluoride glasses and their resistance to corrosion-causing agents (such as HF, F₂ gases) make them feasible under normal laboratory conditions (Tran et al., 1984).

In addition to above properties, the fluoride glasses also show low phonon energy and high transparency (Tran et al., 1984), which make them attractive materials for various photonic applications such as infrared (IR) imaging, laser power delivery, supercontinuum generation (Swiderski & Michalska, 2014), sensors (Herminjard et al., 2009), polarization rotating elements, and photonic crystal fiber for communication in mid-IR region (Tee et al., 2016). There are number of fluoride glasses available for operation in near infrared (NIR) region such as CaF₂, HBL (concentration of materials in mole %: BaF₂ = 33, LaF₃ = 5, HfF₄ = 62), ZBG (ZrF₄ =63%, BaF₂ = 33%, GdF₃ =4%), ABCY (AlF₃ =40%, BaF₂ = 22%, CaF₂ =22%, YF₃ = 16%), ZBLAN (ZrF₄=53%, BaF₂ = 20%, LaF₃=4%, AlF₃ = 3%, NaF = 20%) (Ghatak & Thyagarajan, 1998). Dispersion relation for fluoride glasses with λ₀ (μm) as operating wavelength of p-polarised (TM) incident light can be given as (Ghatak & Thyagarajan, 1998):

\[ n(\lambda_0) = A\lambda_0^{-4} + B\lambda_0^{-2} + C + D\lambda_0 + E\lambda_0^4 \]  (2.1)
where, the coefficients (A to E) have different constant values for different glass materials as shown in table 2.1 (Ghatak & Thyagarajan, 1998). Based on the above discussed dispersion relation, figure 2.1 shows the refractive index (RI) variation with wavelength for different fluoride glasses.

Table 2.1 Coefficients values for fluoride glass substrate

<table>
<thead>
<tr>
<th></th>
<th>A (µm$^4$)</th>
<th>B (µm$^2$)</th>
<th>C</th>
<th>D (µm$^{-4}$)</th>
<th>E (µm$^{-2}$) × 10$^{-6}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>HBL</td>
<td>28.61020 × 10$^{-6}$</td>
<td>3.11470 × 10$^{-3}$</td>
<td>1.509294</td>
<td>−1.17821 × 10$^{-3}$</td>
<td>2.64123</td>
</tr>
<tr>
<td>ZBG</td>
<td>93.67070 × 10$^{-6}$</td>
<td>2.94329 × 10$^{-3}$</td>
<td>1.51236</td>
<td>−1.25045 × 10$^{-3}$</td>
<td>4.01026</td>
</tr>
<tr>
<td>ZBLA</td>
<td>300.8037 × 10$^{-6}$</td>
<td>4.03214 × 10$^{-3}$</td>
<td>1.51272</td>
<td>−1.21921 × 10$^{-3}$</td>
<td>6.77630</td>
</tr>
<tr>
<td>ZBLAN</td>
<td>93.6707 × 10$^{-6}$</td>
<td>2.94329 × 10$^{-3}$</td>
<td>1.49136</td>
<td>−1.25045 × 10$^{-3}$</td>
<td>4.01026</td>
</tr>
<tr>
<td>ABCY</td>
<td>7.67742 × 10$^{-6}$</td>
<td>2.16195 × 10$^{-3}$</td>
<td>1.42969</td>
<td>−1.28304 × 10$^{-3}$</td>
<td>5.35487</td>
</tr>
</tbody>
</table>

For last few decades surface plasmon resonance (SPR), which is the resonant oscillation mode of electron density at a metal-dielectric interface, has been extensively used for photonic sensing in a broad spectral range including IR. In this context, optical sensors based on SPR have been developed in IR region that utilise
CaF$_2$ substrate/prism for gas sensing applications (Herminjard et al., 2009) and MgF$_2$ prism for biosensing (at 632 nm) application (Mishra & Mishra, 2017). There is a certain need of developing highly precise photonic sensors in NIR for detection of chemical and biological processes/parameters.

Detection by SPR based sensor in IR region is more beneficial than detection in the visible region because longer IR wavelength provides larger penetration depth of surface plasmons into sensing medium (Golosovsky et al., 2009). Visible radiation can cause photo-damage or photo-toxicity to biosamples but this is not the case with IR radiation. Apart from significantly different optical properties of surface plasmons, the choice of substrate material also becomes very crucial in SPR based photonic sensor in IR. Many research in the area of SPR based sensors have been done with different glass substrate/prism as a medium to provide ATR, such as SF10 (Choi et al., 2011), BK7 (Maharana, Padhy, et al., 2013), 2S2G (Jha & Sharma, 2009), SiO$_2$ (Sharma, 2013) etc. in visible and in NIR region. Transparency of glass substrate plays an important role in performance of the SPR based sensor in IR. Among available fluoride glasses, HBL has remarkable optical properties in NIR region. Good chemical and mechanical characteristics with glass forming ability have been shown by HBL glasses (Bendow et al., 1982).

Fluorohafnate glasses are suitable candidates for various photonic devices requiring low dispersion and high transparency in infrared region due to their vibrational edge properties (Bendow et al., 1982). Zero dispersion wavelength of HBL was reported at 1.7 µm, which shows much smaller dispersion than silica (Bendow et al., 1981). Thus, HBL can be a suitable candidate for plasmonic sensing applications in IR spectral region.

This chapter presents performance evaluation of SPR based sensor in NIR region for the detection of NaCl concentrations in water. Sensing in IR region and favourable optical properties of HBL glass are beneficial for precise and accurate sensing. Performance evaluation is done in terms of two performance parameters i.e., detection accuracy (D.A.) and signal-to-noise ratio (SNR). The performance of proposed scheme is also compared with the SPR sensor operated in visible with SF10 glass substrate and in corresponding NIR region with silica glass. The overall performance of sensor with HBL substrate is found to be better than aforementioned counterparts.
(i.e., SF10 in visible and silica in NIR). The results are explained in terms of well-established phenomena related to plasmonic excitation.

2.2 Theory

In order to take advantage of SPR in photonic sensors, an important step of excitation of surface plasmons at metal-dielectric interface has to be fulfilled. In this context, two light coupling schemes (Otto and Kretschmann configurations), based on attenuated total internal reflection (ATR), are generally followed. Our proposed design of sensor is based on Kretschmann configuration, which is one of the simplest and the most widely used scheme (as shown in figure 2.2).

![Kretschmann configuration for SPR based sensor](image)

As per the above configuration, the SPR is achieved when the following resonance condition is fulfilled (Sharma et al., 2007):

$$\frac{\omega}{c} n_p \sin \theta_{spr} = \text{real} \left( \frac{\omega}{c} \sqrt{\frac{\varepsilon_m \varepsilon_s}{\varepsilon_m + \varepsilon_s}} \right)$$

(2.2)

Where $n_p > 1$, is the refractive index of the dielectric substrate medium (glass/prism), $\omega$ is the angular frequency of the incident light, $c$ is the velocity of light in vacuum, $\theta_{spr}$ is the angle at which SPR occurs (always greater than critical angle), $\varepsilon_m$ is the metal dielectric constant and $\varepsilon_s$ is the dielectric constant of the sensing medium (analyte).

Left hand side of the above equation represents propagation constant ($k_x$) of the incident light at the metal-substrate interface. Right hand side of equation (2.2) represents real part of surface plasmon propagation constant ($k_{sp}$) at metal-analyte interface. At the occurrence of SPR (i.e., $\theta = \theta_{spr}$), the reflected light intensity $R$
reaches a minimum value (as shown in figure 2.2). This curve is highly sensitive to a small change in dielectric constant of sensing medium.

2.3 Design Considerations

There are three main components of the SPR sensors’ structure as shown in figure 2.2. These components are discussed as follows:

2.3.1 Substrate Material

In the proposed design, the light coupling substrate is taken as HBL. Dispersion relation for HBL glass can be given by equation (2.1). The values of coefficients (A to E) used in equation (2.1) for calculation of refractive index of HBL glass substrate are mentioned in table 2.1 (Ghatak & Thyagarajan, 1998).

For SPR based sensor configuration in visible, SF10 glass substrate is widely used. SF10 glass prism has good transmission window in visible region. Many works have been reported so far with SF10 glass prism as a substrate to couple incident radiation (Luňáček et al., 2016), (El-Gohary et al., 2013). In this context, mercuric ion detection using SPR based sensing utilising SF10 prism was demonstrated by (Chah et al., 2004). The application of graphene as interacting layer with analyte was theoretically examined by (Choi et al., 2011) with SF10 as coupling substrate. RI value of 1.7267 is taken at 600 nm for SF10 glass (Palik, 1985). In NIR region (nearly 1 μm-2 μm), silica substrate is usually preferred due to its physical and optical properties. RI of SiO\(_2\) at λ=1.7 μm is calculated using Sellmeier relation as following (Ghatak and Thyagarajan, 1998).

\[
n^2(\lambda) = 1 + \frac{b_1\lambda^2}{\lambda^2 - a_1} + \frac{b_2\lambda^2}{\lambda^2 - a_2} + \frac{b_3\lambda^2}{\lambda^2 - a_3}
\]

(2.3)

In eq (2.3), \(a_1, a_2, a_3\) and \(b_1, b_2, b_3\) are Sellmeier coefficients (Ghatak & Thyagarajan, 1998).

2.3.2 Metal Layer

Glass substrate is coated with gold (Au) layer which is sandwiched between the HBL substrate and sensing layer. Au is the best suited metal due to its stability against oxidation and its biocompatible nature. Values of dielectric constant for Au at different wavelengths are taken from a previous work (Olmon et al., 2012). For experimental realisation, deposition of metal layer can be accomplished using electron beam
deposition or thermal vapour deposition technique. Large sensing region can be covered when the evanescent field is stronger, this can be achieved by thickness optimization of metal layer. Metal layer thickness should be chosen such that the value of R is as close to zero as possible (Ong et al., 2006). For calculation, 40 nm is the optimized Au layer thickness. A summary of refractive index values is presented in table 2.2.

Table 2.2: Refractive index values for different materials

<table>
<thead>
<tr>
<th>Material</th>
<th>Refractive index</th>
</tr>
</thead>
<tbody>
<tr>
<td>SF10 (at (\lambda=660) nm)</td>
<td>1.7267</td>
</tr>
<tr>
<td>Silica (at (\lambda=1700) nm)</td>
<td>1.4422</td>
</tr>
<tr>
<td>HBL (at (\lambda=1700) nm)</td>
<td>1.5069</td>
</tr>
<tr>
<td>Au at (\lambda=660) nm</td>
<td>0.14870+3.7460i</td>
</tr>
<tr>
<td>Au at (\lambda=1700) nm</td>
<td>0.3770+11.6401i</td>
</tr>
</tbody>
</table>

### 2.3.3 Sensing Medium

For this study, the sensing medium is considered to be water solution with different concentrations of NaCl at room temperature. Experimental values of refractive index of NaCl mixed water solutions at visible and NIR wavelengths are taken (X. Li et al., 2015).

### 2.3.4 Calculation of R

Transfer matrix method (TMM) is used to calculate the precise values of R at different angles (\(\theta\)) and wavelengths (\(\lambda\)) as it has no approximations (Sharma & Gupta, 2013). The detailed explanation about TMM has been provided in appendix section. For a particular angle of incidence, a sharp dip is observed in SPR curve. This curve is sensitive to change in dielectric constant of sensing layer. Small change in refractive index of analyte causes shift of SPR curve. Position sensitive detector (PSD) is one of the method used for measurement of angular shift of monochromatic beam (Cui & Soh, 2010).
2.4 Results and Discussions

Performance analysis is based on analytical modelling of sensor’s structure and mathematical calculation of performance parameters.

In the next few sub-sections (2.4.1 to 2.4.4), the simulation results are discussed in a systematic fashion to comprehensively analyse the performance of proposed sensor scheme.

2.4.1 Plasmon Resonance Condition

One of the most important and foremost tasks is to ensure the occurrence of SPR with proposed sensor scheme having HBL glass as substrate and NaCl solution as sensing medium. Fundamentally, the occurrence of SPR is nothing but the fulfilment of bulk resonance condition as mentioned in equation (2.2). Figure 2.3 represents the variation of propagation constants of (i) light incident through HBL, and (ii) surface plasmon wave (SPW) at metal-sensing medium interface for three different concentrations of NaCl (0 gm/lt, 18 gm/lt, and 36 gm/lt) in water solution at room temperature and at an operating wavelength of 1.7 µm.

Figure 2.3 Simulated variation of propagation constants of incident light and of SPW (for three different NaCl concentrations) to show the fulfilment of bulk SPR condition ($\lambda = 1.7 \, \mu m$).

The intersection of curves (at points A, B, and C) represents the fulfilment of resonance condition (equation (2.1) when LHS and RHS are equal) with the present scheme. Three discrete values of $\theta_{spr}$ (61.743°, 64.127°, and 66.092°) are obtained for three different concentrations (0 gm/l, 18 gm/l, and 36 gm/l), which confirms that the occurrence of SPR can definitely be ensured by using HBL glass as a substrate.
Since, the above resonance condition is for bulk gold, therefore, for a thin gold layer, the values of $\theta_{spr}$ will be slightly different.

### 2.4.2 SPR Curves and Performance Evaluation

After ensuring the occurrence of SPR with the proposed sensor scheme, figure 2.4 shows simulated SPR curves ($R$ vs. $\theta$) at $\lambda = 1.7 \, \mu$m for four different NaCl concentrations in water at room temperature. The upper inset shows the corresponding C-$\theta_{spr}$ curve and the lower inset shows the C-FWHM curve for concentrations ranging from 0 to 36 gm/l.

As mentioned earlier, an optimised thickness of Au layer (40 nm at 1.7 µm) has been utilised to obtain nearly zero value of $R$ at resonance. Condition at which zero R value obtained is called critical coupling (intrinsic losses are equal to radiation losses). More precisely, a discrete set of $\theta_{spr}$ values ($61.743^0, 63.451^0, 64.534^0$, and $66.092^0$) is obtained for the corresponding set of NaCl concentrations (0 gm/l, 12 gm/l, 24 gm/l, and 36 gm/l) in aqueous solution (as shown in upper inset of figure 2.4).

Shift in resonance angle ($\delta \theta_{spr}$) for a small change in the sensing medium properties and FWHM (full width at half maximum) of the SPR curve are the prime indicators of the performance of a SPR sensor. $\delta \theta_{spr}$ should be as large as large possible for a small change ($\delta C$) in the concentration of sensing medium. As, it is apparent from figure 2.4, there is a significant shift in the values of $\delta \theta_{spr}$ with change in NaCl concentra...
concentration. For instance, increasing the concentration of NaCl from 0 gm/lt to 12 gm/lt, the shift in $\theta_{SPR}$ is found to be $1.707^\circ$. This results in achieving high sensitivity ($\frac{\delta \theta_{SPR}}{\delta C}$) of measuring NaCl concentration with the proposed sensor scheme.

The Minimum angular shift that can be detected is $0.001^\circ$ (Kolomenskii et al., 1997), therefore, above values also suggest that extremely small changes in the concentration values of NaCl in water can be detected with high sensitivity. Assuming a near-linear variation of $\theta_{spr}$ for any small change in NaCl concentration, the resolution (defined as: smallest variation in NaCl concentration measurable), denoted as $R_C$ and mathematically defined as $R_C = \frac{\delta C}{\delta \theta_{SPR}} \times 0.001^\circ$, comes out to be nearly 0.007 gm/lt, which is a significant value in terms of SPR sensor’s performance. Here, it is to be mentioned that even if the variation of $\theta_{spr}$ with NaCl concentration is not perfectly linear, the average resolution, as calculated at different concentrations, remains of the same order (0.007 gm/lt) for small variation in NaCl concentration.

The performance of SPR sensor is evaluated not only in terms of sensitivity and resolution but also in terms of detection accuracy, which demands that the FWHM of SPR curve should be as small as possible. Detection accuracy (D.A.) of a sensor is defined as the reciprocal of the FWHM of the SPR curve:

$$D.A. = \frac{1}{FWHM}$$

(2.4)

In above context, the FWHM of the SPR curves simulated for different NaCl concentration values is also analysed. From figure 2.4, a discrete set of FWHM values ($0.240^\circ$, $0.269^\circ$, $0.298^\circ$, and $0.338^\circ$) is obtained for the corresponding set of NaCl concentrations (0 gm/lt, 12 gm/lt, 24 gm/lt, and 36 gm/lt) in aqueous solution (as shown in the lower inset in figure 2.4). The above FWHM values are clearly separated from one another. The above FWHM values are in a fairly reasonable range compared to high-performance SPR sensor curves obtained in theoretical (Sharma, 2013) (Mishra et al., 2015) and experimental results (Person et al., 2008). It suggests that the proposed sensor should be able to provide the high detection accuracy for the determination of NaCl concentration in water. It is also worth-mentioning that smaller the NaCl concentration, the better the D.A. (as defined in equation (2.4)) because FWHM of SPR curve increases, although the extent of variation is not significantly large, with an increase in NaCl concentration in water.
2.4.3 Comparative Analysis (HBL vs conventional glass substrates)

In sub-section 4.2, it was established that the SPR sensor with HBL substrate operated at an NIR wavelength (1.7 µm) is able to provide good sensitivity, resolution, and detection accuracy of measuring the NaCl concentration in water. However, at this point it becomes necessary to compare the performance of HBL-based SPR sensor with the one based on conventional glass substrates operated in different spectral regions. When the $R$ vs $\theta$ curves are analyzed for SF10 glass based SPR sensor (operated at 0.6 µm) and HBL-based SPR sensor (operated at 1.7 µm) with pure water as sensing medium, it is found that the width of SPR curve in case of HBL glass (0.240°) is significantly smaller (almost 28 times) than that of SF10 (6.684°) due to less lossy behaviour of Au at lower optical frequencies (i.e., IR wavelengths). At larger wavelengths, ohmic losses in noble metal are reduced, therefore, sharper SPR curve (i.e., smaller FWHM) is obtained than at a visible wavelength (Golosovsky et al., 2009). For a NIR wavelength, resonance angle is close to critical angle but for a visible wavelength, resonance angle is far away from critical angle. This closeness of critical angle to resonance angle is a key feature while designing SPR sensor because it is directly related with the occurrence of SPR (when the incident angle crosses critical angle). In effect, sharper SPR curve will lead to better detection accuracy of the sensor in NIR region. Although, shift in SPR curves may be almost similar in both cases for any given small change in concentration, sharpness of SPR curve is a unique advantage of using HBL over conventional glass substrate. Going another step ahead, variation of D.A. with NaCl concentration for SPR sensors based on three different substrates (HBL at 1.7 µm, SF10 at 0.6 µm, and SiO$_2$ at 1.7 µm) are shown in figure 2.5.

It is clearly evident that HBL substrate-based SPR sensor provides greater value of D.A. at any concentration of NaCl (in water) compared with SiO$_2$ and SF10 substrates. Throughout the concentration range, HBL-based SPR sensor provides almost 40% better detection accuracy than SiO$_2$-based one.
Figure 2.5 Variation of D.A. with concentration for SPR sensors based on different substrate materials and operated in different spectral regions.

Now, it is worth-mentioning that $\delta \theta_{SPR}$ and FWHM are the indicators of two opposite features of sensor’s performance. The value of $\delta \theta_{SPR}$ must be as large as possible for sensitive measurements and on the contrary, FWHM of SPR curve must be as small as possible for the measurement error to be minimum. In this view, many literatures define a combined SPR performance parameter, normally known as signal-to-noise ratio (SNR), as the ratio of $\delta \theta_{SPR}$ and FWHM (Zynio et al., 2002). As a matter of fact, SNR, a unitless quantity, is a critical parameter in determining the overall performance of any instrument. Thus, by the virtue of its above definition, the overall SNR of SPR sensor should be as large as possible. In the present performance analysis, SNR is also calculated for above discussed structures at different NaCl concentration values (figure 2.6). It is found that for all concentration values, the SNR of HBL-based sensor is considerably higher than that of SF10-based sensor and the difference between the SNR of HBL and SF10 based sensors keeps on increasing with an increase in NaCl concentration. For lower concentrations, the SNR of SiO$_2$-based structure is comparable with the HBL-based structure but as the concentration increases, SNR of HBL-based sensor structure keeps getting better than that of SiO$_2$-based one. The gap between the SNR of HBL- and SiO$_2$-based sensors goes on widening with an increase in NaCl concentration. It clearly indicates that for further higher concentration values, the performance of HBL-based SPR sensor is bound to become even better compared with the conventional substrates. Moreover, HBL has greater refractive index and much higher optical transmission than silica in the NIR spectral region. These added
advantages make HBL even more preferable substrate material to design SPR-based sensors in NIR for highly accurate and sensitive detection of other sensing media such as biosamples and gases.

![SNR Variation with Concentration](image)

Figure 2.6 Variation of SNR with concentration for SPR sensors based on different substrate materials and operated in different spectral regions.

2.4.4 Performance Analysis of Proposed Sensor Scheme for more Samples

Since SPR based sensors have been reported for alcohol sensing application (Srivastava et al., 2011; Zhao et al., 2016) plus biocompatibility nature of gold and chemical stability of fluoride glasses, the performance of our proposed sensor is analysed for following samples also (shown in table 2.3).

Table 2.3 Refractive index values of samples at two different wavelengths

<table>
<thead>
<tr>
<th>Tag</th>
<th>Sample</th>
<th>Refractive index at 600 nm</th>
<th>Refractive index at 1.7 µm</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>n1</td>
<td>Pure water</td>
<td>$1.332 + 1.09 \times 10^{-8}i$</td>
<td>$1.3145 + 1.02 \times 10^{-4}i$</td>
<td>(Hale &amp; Querry, 1973)</td>
</tr>
<tr>
<td>n2</td>
<td>Ethanol</td>
<td>$1.3640 + 8.36 \times 10^{-8}i$</td>
<td>$1.3498 + 1.13 \times 10^{-4}i$</td>
<td>(Sani &amp; Dell’Oro, 2016)</td>
</tr>
<tr>
<td>n3</td>
<td>Propanol</td>
<td>$1.3768 + 6.51 \times 10^{-8}i$</td>
<td>$1.3668 + 1.01 \times 10^{-4}i$</td>
<td>(Sani &amp; Dell’Oro, 2016)</td>
</tr>
<tr>
<td>n4</td>
<td>Ethylene glycol</td>
<td>$1.4311 + 5.0 \times 10^{-8}i$</td>
<td>$1.4192 + 1.11 \times 10^{-4}i$</td>
<td>(Sani &amp; Dell’Oro, 2014)</td>
</tr>
</tbody>
</table>
For above four different samples, D.A. and SNR are calculated and are shown in figure 2.07. From figure 2.7, it is observed that the same trend of higher SNR and D.A. values for HBL at 1.7 µm wavelength is obtained for above four samples as well. The other substrates (i.e., silica at 1.7 µm and SF10 at 0.6 µm) provide inferior performance compared with HBL. This result reaffirms the better performance of HBL-based SPR sensor operated at 1.7 µm compared with other substrates.

![Graph showing SNR and D.A. for four different samples](image)

Figure 2.7 Variation of SNR and D.A. for four different samples simulated for SPR sensors based on different substrate materials and operated in different spectral regions. The SNR is calculated with reference to an arbitrary liquid refractive index of 1.21.

### 2.4.5 Field Enhancement at Resonance (θ_{SPR})

COMSOL Multiphysics software which is based on finite element method (FEM) has been used to study the variation of magnetic field intensity at the corresponding interface joined with the analyte. Flow chart in figure 2.8 presents a brief description to study reflectance and field properties for SPR based sensors (Kretschmann configuration). In the present analysis a three layered structure having HBL substrate, Au (40 nm) and pure water as an analyte are taken into account. Electromagnetic wave frequency domain analysis is used. The wavelength of incident TM light is taken as 1.70 µm (for present study). In simulation, for TM wave, plane of incidence is taken as X-Y plane (\(H_x = H_y = 0\) and \(E_z = 0\)). Input port is considered at the substrate side and output port assignment is done at the sensing layer side. The variation of incident angle (auxiliary sweep) with an interval of 0.05° is done under frequency stationary study. The interval is chosen such that the accuracy is maintained with less time consumed in solving. The inbuilt expression for reflectance is given as:

\[
R = \frac{\sin^2 (\theta_{SPR})}{1 + \sin^2 (\theta_{SPR})}
\]
$abs(ewfd \cdot S11)^2$, where, $abs$ and $ewfd$ stand for absolute and electromagnetic wave frequency domain analysis, respectively. $S11$ is the reflection coefficient.

![Flow chart for device simulation using FEM analysis](image)

Figure 2.8 Flow chart for device simulation using FEM analysis (COMSOL Multiphysics).

Field enhancement at resonance plays an important role in deciding the performance of the SPR based sensor. Sensitivity of the sensor can be maximized by maximizing the overlap integral, which is proportional to the interaction volume (Shalabney & Abdulhalim, 2010). Interaction volume can be increased by increasing penetration depth or field enhancement into analyte region. When $R$ value reaches its minimum value, there is enhancement in field at the metal-analyte interface due to maximum absorption of incident radiation. This denotes the interaction of field with sensing layer. Figure 2.9 clearly indicates that the highest field enhancement occurs at resonance condition.
2.4.6 Gas Sensing behaviour of Proposed Scheme

Gas sensing in IR spectral region is more advantageous than that in visible due to absorption bands of gases in IR region. A large number of vibration modes are possessed by molecules which are responsible for absorption bands. Spectral distribution of the incident radiation is responsible for absorption of light by molecules. Other factors such as temperature and pressure are assumed to be constant which play a crucial role in narrowing or broadening of absorption spectrum. The refractive index range of gaseous analyte is taken between 1.000 and 1.004. In this context, figure 2.10 shows the variation of SPR curves with incident angle for different RI values of gaseous analyte. The calculated average FWHM value is found to be 0.0516° which indicate towards a high D.A. of 19.37. A SNR value of 3.998 is calculated for small change in gaseous analyte (δn_s=0.004) from its reference value (n_s=1.000).
Figure 2.10 Variation of SPR curves with incident angle at $\lambda=1.7$ µm for different refractive index of gaseous analyte (in case of proposed scheme 40 nm Au over HBL).

2.5 Conclusion

HBL fluoride glass-based SPR sensor is simulated and analysed in near infrared for reliable and accurate detection of NaCl concentration in water as well as for sensing of other samples such as ethanol, propanol, and ethylene glycol. Based on the detailed analysis of simulation results in terms of different performance parameters (e.g., sensitivity, resolution, detection accuracy, and SNR), it is found that HBL-based SPR sensor is able to provide significantly enhanced sensing performance compared with other conventional glass substrates operated in different spectral regions (SF10 in visible and SiO$_2$ in NIR). Due to greater refractive index and higher optical transmission than above-mentioned conventional glasses in visible and NIR, it can be a preferred material as substrate for SPR based sensors in NIR for biosensing and gaseous sensing. Enhanced performance at IR wavelength may also lead to fiber optic SPR sensor probe in future for different biological and chemical sensing applications. The proposed sensor probe can also be used as a reusable one by using an appropriate buffer solution between Au layer and the sensing medium.