Bio-molecular sensors based on guided mode resonance filters

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Abstract. In this work a low surface roughness and homogenous, high refractive index, and amorphous TiO2 layer on corrugated structures of diffractive optical element is coated by Atomic Layer Deposition (ALD) for biosensors. The design of Guided Mode Resonance Filters (GMRFs) is based on refractive indices and thicknesses of the waveguide biomolecular layers. The designed spectral shifts are calculated by Fourier Modal Method (FMM) and depend on the magnitude of the variations in refractive index of the biomolecular layer on waveguide structures. Furthermore, the sensitivity of the biomolecular sensors depends on the thickness of biomolecular layer and periodicity of the structures. The waveguide structures designed for larger periods show an enhancement in the sensitivity (nm/RIU) of the biomolecular sensor at longer wavelengths. The periodicities of nanophotonic structures are varied from 300 to 500 nm in design calculations with predominance of increase in effective index of the structure to support leaky waveguide modes.

1. Introduction
Metamaterials encountered great interest in several applications of precise optical sensors and other elements. The development of perfectly tuned optical components is a result of highly efficient and sophisticated modeling tools and modern fabrication of nanostructures by accurate experimental lithographic, coating, and etching techniques. Metallic sub wavelength nanostructures show useful optical properties, Surface Plasmon Resonance (SPR) to measure minute changes in the refractive index of materials in regions of nanostructures referred as the refractive index of the cavity nc. The spectral shift of central resonance peak is a measure of the sensitivity of the sensor in nanometers per Refractive Index Unit (RIU) [1-4]. Generally, a high efficiency and spectral resolution optical sensor with larger figure of merit detects minor changes in refractive index of cavity [5].

The physics of metallic nanostructures is based on scattering phenomena while sub wave length dielectric nanostructures support Wood’s anomalies of Guided Mode Resonance Filters (GMRFs) [6]. Incident light couple to the excited leaky waveguide modes guided by the waveguide nanostructure under resonance conditions [7]. This results in narrowband of reflected or transmitted wavelengths through the sensor at resonance [8]. GMRFs are quite often used to target several promising applications such as pressure, humidity, or protein detections. The precise sensing with highest resolution of such sensor elements is achieved and facilitated by rapid and cost-effective productions through accurate control of structural and optical parameters at resonance wavelengths [9-11].

The practical realization of such sensors and corresponding nanostructures require precisely uniform depositing techniques compatible with the interacting wavelengths. Traditionally, optical
Coatings of metals and dielectrics are obtained by Physical Vapor Deposition (PVD) using solid source materials through resistive heating, electron-beam evaporation, sputtering, laser-assisted evaporation, or ion-assisted deposition at high enough deposition rates. To confine and smooth propagation of waveguide modes through dielectric films, the control of film homogeneity, composition, thickness uniformity, adhesion with underlying substrate, and better microstructure control can be achieved by Atomic Layer Deposition (ALD) [12]. ALD method exhibits angstrom level resolution, layer-by-layer growth of ultra-thin compound films on planar and high-aspect ratio nanostructures. ALD operates in cycles consisting of four steps: (1) exposure of first precursor material, (2) evacuation or purging of chamber, (3) exposure of second precursor material, and (4) evacuation or purging of reaction byproducts from the chamber [13-15].

In this paper we report on the design and optimization of optical properties of GMR bio-molecular sensors. The sensing properties of the sensors have been optimized theoretically with increase in the thickness of the analyte layer. The localized refractive index is tailored by the incremental increase in the thickness of analyte layer within the cavity. Figure 1 shows the structure of a TiO$_2$ based GMRF bio-molecular sensor. A polarized light (s and p) illuminates the replicated grating [16-17] at an angle of incidence $\phi_i$ with respect to the normal to the grating and outgoing light makes an angle $\phi_o$ with the normal to the grating.

**Figure 1.** Ideal grating profile of bio-molecular sensor functionalized with an analyte in the presence of coated TiO$_2$ and Al$_2$O$_3$ thin layers

### 2. Results and discussion
#### 2.1. Design and simulation

Consider 1D grating structure, the grating can couple light into and out of the waveguide by diffraction phenomena. The grating structure can slightly modify the envelope and propagation constant of the waveguide propagating mode. The height of the grating structure is typically much smaller than the incident wavelength $\lambda_o$. The grating period $d \approx \lambda_o/n_b$, where $n_b$ is refractive index of analyte, so the first diffracted orders into the structure are propagating, whereas rest of the higher diffracted orders are evanescent. The first order diffraction occurs at: $$\frac{2\pi}{d} = \pm n_i k_o \sin \phi_i + \beta_r,$$ where $k_o = \frac{2\pi}{\lambda_o}$ and $\beta_r$ is real part of propagation mode constant $\beta = \beta_r + i\beta_i$ [18].

The scope of this work is to develop highly sensitive and efficient GMR structures for bio-molecular sensors. For this purpose, we systematically calculated the spectral shift in resonance wavelength by gradually increasing the analyte thickness. A schematic presentation of such sensors is shown in Figure 1. Design was carried out using rigorous coupled wave analysis through Fourier Modal Method (FMM). Design was performed for both TE- and TM-polarized lights. Figure 1 shows...
a three-layered structure of TiO$_2$/Al$_2$O$_3$/analyte layers on a replicated grating in polycarbonate substrate. Film thicknesses of TiO$_2$ and Al$_2$O$_3$ materials are kept fixed at 40 and 20 nm, respectively while the thickness of analyte layer varies from 5 nm onward. Structural parameters of the grating are: periodicity $d = 325$ nm, line width $w = 205$ nm, ridge height $h = 100$ nm, angle of incidence $\phi_i = 18^\circ$ using both TE- and TM-polarized light. Refractive indices of: air $n_1 = 1$, polycarbonate $n_3 = 1.53$, bio-molecule $n_b = 2.2$, Al$_2$O$_3$ $n_a = 1.67$, and TiO$_2$ $n_t = 2.4$.

Figure 2. Transmittance/reflectance spectra of GMR sensor with peak positions at 662 nm and 668 nm at 5 and 15 nm thickness of analyte layers, respectively

2.2. Wavelength shift of bio-molecular sensor with incremental increase in analyte thickness

Figure 2 shows transmittance/reflectance spectra of GMR sensor for TE-mode with resonance wavelength peak positions at 662 nm and 668 nm for analyte layer thicknesses of 5 nm and 15 nm, respectively. Resonance peaks show a shift around 6 nm on increasing analyte thickness by 10 nm. Figure 3 shows calculated reflectance spectra for TE-mode of bio-molecular sensor with 5 nm increase in analyte thickness in each spectral calculation. The wavelength shifts towards longer wavelengths by 3 nm on increasing analyte thickness by 5 nm as shown in each spectral image. As a result, peak shifts from 662 nm to 684 nm by increasing analyte thickness from 5 to 40 nm. The shift in peak wavelength results in due to increase in effective index of analyte layer owing to the increase in the optical thickness of analyte layer. One can estimate a linear change in the wavelength shift as a function of analyte thickness with low sidebands and almost a symmetric spectral profile. It shows an average shift of 0.6 nm per nm increase in analyte thickness.
Figure 3. Wavelength shift of a TE-polarized light on increasing the thickness of the analyte layer.
Figure 4. Wavelength shift of a TM-polarized light on increasing the thickness of the analyte layer.
Figure 4 shows calculated reflectance spectra for TM-mode by increasing the analyte layer thickness from 5 to 40 nm. It is evident from the spectra that narrow line width of spectral waveform with lower sidebands and symmetric profile appears at relative low analyte thicknesses (5 to 15 nm). However, more waveguide modes appear on increasing the thickness beyond 15 nm. In the context of ultra-thin layers, we introduce the spectral shifts in response to the thickness of the analyte layer. For simplicity in the calculations, the thickness of the analyte layer is considered; however, a detailed analysis can be made using optical thickness. For TM-modes the peak shifts are not linear with the thickness of the analyte layer which shows that the sensor is more efficient with layer thicknesses around 5 to 15 nm rather than with thicker layers.

The designed biomolecular sensor is also optimized in a flow cell configuration to investigate the kinetics of a chemical reaction for which such sensors can be used in microfluidic applications. Figure 5 shows TE- and TM-polarized reflectance spectra calculated in a flow cell arrangement filled with either air (refractive index: $n_1 = 1$) or water (refractive index $n_3 = 1.33$). In the case of structure with air filling scheme, the calculated spectra for TE- and TM-polarized lights shows resonance peak positions at 662 and 614 nm, respectively. However, all spectra show shifts towards longer wavelengths once the refractive index of the cavity is changed with water. The TE- and TM-shifted resonance peaks show spectral positions at 694 and 651 nm, respectively. The calculated long-range sensitivities obtained for TE- and TM-modes are 97 and 82 nm/RIU, respectively. It is worthwhile to describe that the peaks in water environment are much narrower than those calculated for air which facilitate to design sensors at higher figure of merit value due to low refractive index contrast between the cavity and optical materials (polycarbonate, TiO$_2$, Al$_2$O$_3$ etc.).

![Figure 5. Reflectance spectra in a flow cell configuration of (a) TE-Mode and (b) TM-Mode](image)

### 3. Conclusion

Guided mode resonance biomolecular sensors have been designed with respect to the thickness layer of the analyte. The 3-layer structure design is made for a replicated grating in polycarbonate, with thin films of metallic oxides (TiO$_2$ and Al$_2$O$_3$) and analyte layer as bio-molecule. The calculated TE-polarized spectra showed a linear shift in resonance peak wavelength with the increase in analyte layer thickness from 5 to 40 nm while TM spectra followed linearity only for very thin layers (5 to 15 nm) of analyte and showed generation of new modes with more narrowed peaks. The sensitivities of TE- and TM-modes are calculated in a flow cell configuration filled with either air or water. In the case of cavity filled with water, significant peak shifts have been observed for both TE- and TM-modes which resulted in long range high sensitivities of 97 and 82 nm/RIU, respectively. The calculated high sensitivities are attributed to low refractive index contrast between the cavity and grating’s optical materials.
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