

## Theoretical Study of Colorimetric Resonant Structures for Biosensing Applications

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In general, biosensors consist of a highly specific recognition element and a transducer that converts the molecular recognition event into a quantifiable signal. In the case of optically-based transduction methods, that do not require labelling of analytes with fluorescent compounds, they are of interest due to the relative assay simplicity and ability to study the interaction of small molecules and proteins that are not readily labelled. Direct optical methods include surface plasmon resonance (SPR) [1], evanescent wave devices [2], grating couplers [3] and others.

Optical Grating Couplers (OGC) are based in the highly dependence of the coupling angle in front of the local external refractive index. There are two main different modes of operation for monitoring refractive index changes in this type of optical biosensors: angular and spectral interrogation.

In angular interrogation there are different configurations: i) a monochromatic light is focused to create a range of illumination angles and directed into the waveguide grating. The reflected light is monitored with a CCD camera or other imaging detector. ii) It is also possible to measure the coupling angle rotating the sample and measuring the output light at the end of the waveguide; it is known as OWLS (Optical Waveguide Light-mode Spectroscopy) technique. iii) In our group we have developed an optical set-up for measuring the out-coupling angle in a two-grating configuration, without moving parts [4].

In spectral interrogation mode, a broadband spectrum light (white light) is sent on the grating surface and the reflected light is collected and monitored with a spectrometer. By observing the spectral location of the resonant peak wavelength value (PWV), one can monitor refractive index changes at or near the surface of the waveguide grating or, linking receptor molecules to the grating surface, complementary binding molecules can be detected without the use of any kind of fluorescent probe or particle label [5,6]. Laboratory equipment based in this technique is Corning Epic-system [7].

In this work we present optical design of diffraction gratings structures and spectral interrogation for biological applications. For our purpose we have used OptiFDTD 8.0 software. Figure 1 is a cross-section of the simulated structure: a glass substrate ( $n=1.46$ ) with 200nm silicon nitride layer ( $n=2.0$ ) working as a waveguide; a diffraction grating is etched on the surface with a period of  $\Lambda=500\text{nm}$ , 50% duty cycle. We use normal incidence and light polarized perpendicular to the grating period. The red layer represents any biolayer attached to the top surface in an external medium; we have used  $n=1.5$  as the refraction index.

Figure 2 shows i) the reflectance spectrum, showing the resonant behaviour of this type of structure and ii) the shift of Peak Wavelength (PWV) due to the growth of a thin layer in the range of nanometres on the grating. Also we see how the PWV doesn't shift for thick protein layers; this means that above 500nm of thickness, the biolayer behaves as the external medium, saturating the shift effect.

The location of the PWV depends strongly on the geometry of the structure and on material properties: refractive index, depth, duty cycle, and period. In figure 3 we show the linear dependence of PWV versus the refractive indices of liquid solutions, using water ( $n=1.333$ ), PBS ( $n=1.339$ ), acetone ( $n=1.36$ ), isopropyl alcohol ( $n=1.38$ ), and sodium chloride solution ( $n=1.4$ ) as standards.

For this structure we obtain a great theoretical sensitivity of  $S=\Delta\lambda/\Delta n = 130 \text{ nm}$ , higher than  $S = 87.5 \text{ nm}$  in [5]. Taking account that we can resolve variations  $\Delta\lambda=0.01\text{nm}$  for a standard spectrometer like the popular SD2000 (OCEAN OPTICS), we expect an approximately detection limit of  $7\cdot 10^{-5}$  RIU (Refractive Index Units), which is enough for applications of surface molecular recognition.

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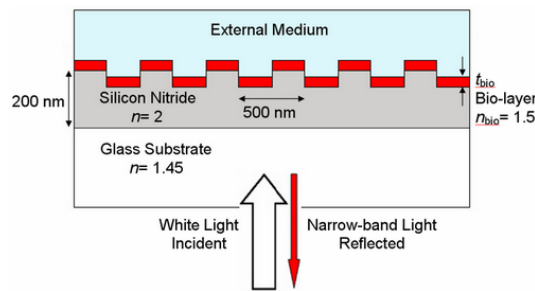


Figure 1. Cross section of the simulated structure: grating etched on a silicon nitride layer on a glass substrate. Grating period = 500nm

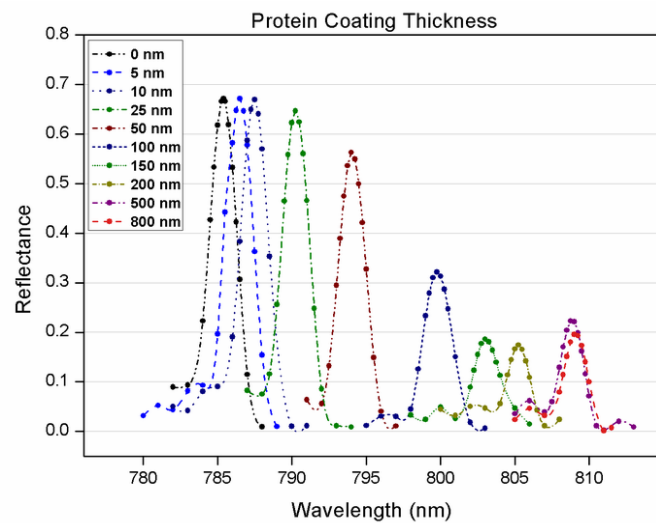


Figure 2. Peak Wavelength value shift in front to the thickness of the biolayer.

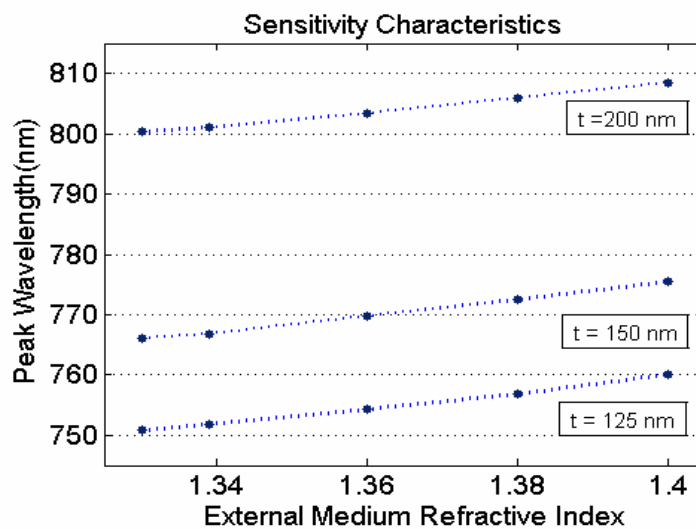


Figure 3. Peak Wavelength value shift for three values of thickness (t) of silicon nitride layer, in front of external refractive index.