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Photonic Crystal Design for Bloch Surface Wave Sensing

Bernardo Dias[1,2], José M. M. M. de Almeida[1,3], Luís C. C. Coelho[1,2]

[1]INESC TEC–Institute for Systems and Computer Engineering, Technology and Science, Faculty of Sciences, University of Porto, 4169-007 Porto, Portugal
[2]Department of Physics and Astronomy, Faculty of Sciences, University of Porto, 4169-007 Porto, Portugal
[3]Department of Physics, School of Science and Technology, University of Trás-os-Montes e Alto Douro, 5001-801 Vila Real, Portugal
bernardo.s.dias@inesctec.pt

Abstract. Bloch Surface Waves (BSW) consist of electromagnetic modes generated at the interface between a photonic crystal and an isotropic dielectric. This type of surface mode displays sharp resonances and high sensitivity to external refractive index variations, and thus appears to be an ideal candidate for usage in optical sensors. Nevertheless, design and optimization of photonic crystals is not a trivial task and constitutes an ongoing field of research. The sensitivity of BSW in both refractometric and adsorption sensing is calculated analytically using first-order perturbation theory for TE modes, allowing the understanding of how several physical parameters of the photonic crystal influence the sensitivity. Preliminary experimental results are presented, which aim to use the analytical calculations to allow for both refractometric and adsorption sensing in a single photonic crystal structure.

1. Introduction

Electromagnetic surface wave (ESW) sensors have become one of the most preeminent fields of research in optical sensors, especially since the popularization of surface plasmon resonance (SPR) and the demonstration of its application in many contexts, such as refractometric and affinity sensing[1]. While these modes display high sensitivities, they also have some drawbacks such as large linewidths, poor mechanical stability and possibility of oxidation, depending on the metal considered[2]. In the past years, Bloch Surface Waves (BSW) sensors have emerged as a possible candidate for applications where conventional SPR sensors may not perform optimally[3].

BSW's are generated at the interface between a photonic crystal (PhC) and a uniform dielectric, and display sharp resonances, possibility of multiple modes in both light polarizations[3] and very good mechanical and chemical stability, especially if oxide materials are used[4]. These ESW are created due to the symmetry breaking of the periodic modulation of the refractive index (RI) inside of the PhC, generating a mode which propagates at the interface and decays exponentially to both sides[5]. This interface confinement of the mode makes it highly sensitive to variations of the external medium, which is ideal for optical sensor applications.

The sensitivity of ESWs can be characterized by changes in the effective index associated with a specific mode due to two different phenomena: variations of the RI of the external medium (refractometric sensitivity) and adsorption of molecules by the device surface (adsorption sensitivity)[6]. This second phenomenon is particularly important in optical sensors which have been functionalized for specific molecule detection (affinity sensing), in which a measurable change in the mode's spectrum can be verified due to molecule binding, which causes a variation of the thickness of the functionalized layer[6]. This mechanism is the principle associated with conventional biosensing applications of ESW based sensors, and has been thoroughly explored in SPR sensors, both theoretically[6] and experimentally[3]. Nevertheless, while there have already been a few publications tackling the optimization of BSW design[7,8], much research is still needed to fully understand the role of the design parameters of the PhC in the final BSW performance.

Following similar procedures applied previously in SPR sensors[6], the sensitivity of BSW modes to both refractometric and adsorption cases is calculated for TE modes using first-order perturbation theory. Following this calculation, preliminary experimental results are demonstrated by analyzing the peak wavelength sensitivity to RI variations of the external medium. In section 2, the basic theory behind the electric field (for TE modes) in BSWs is presented, which allows for the calculation of the refractometric and adsorption sensitivities. In section 3 the experimental methods and setup are presented, along with the simulation routines used to calculate the PhC spectra. Section 4 discusses the experimental and simulation results obtained, along with commenting shortly regarding further work needed. Section 5 presents a short conclusion of the work here presented.

2. Bloch Surface Wave Sensitivity

2.1. Application of Perturbation Theory to Bloch Surface Waves

Consider an experimental setup for BSW excitation in the Kretschmann configuration[1], composed of a prism with RI n_0, a PhC made of two dielectric materials with RI n_1 and n_2 (with $n_1 > n_2$) and thicknesses d_1 and d_2, a cap layer of RI n_1 and thickness d_3 and an external medium with RI n_3. In the case of adsorption sensing, consider also a layer with RI n_A and thickness d_A. Light in the TE polarization is incident on the interface between the prism and the PhC at an angle θ. This configuration in both refractometric and adsorption sensing is illustrated in Fig. 1.

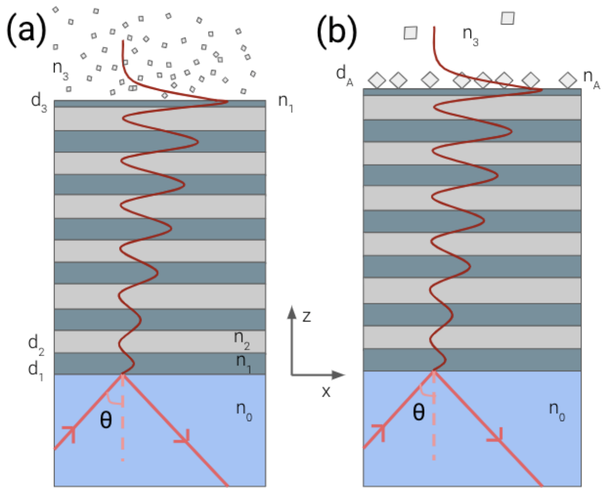

Figure 1 – Setup of a BSW sensor in the Kretschmann configuration: (a) Refractometric sensing; (b) Adsorption sensing.

Inside the PhC, the transverse component of the electric field is given by[5]:

$$E(z) = E_K(z)e^{-iKz} \quad (1)$$

where $E_k(z)$ is a function with the periodicity of the optical lattice and K is the Bloch number, which is complex inside the forbidden bands of the PhC, thus allowing an exponential decay of the field, which is a characteristic of ESW's. Outside of the PhC, resonant tunneling of the total internal reflection is verified[5], and the electric field is given by:

$$\mathrm{E(z)} = a_0 \mathrm{e}^{qz} \ (2)$$

where a_0 is the electric field amplitude and $q = \frac{2\pi}{\lambda}\sqrt{N^2 - \mathrm{n_3}^2}$, where λ is the free space wavelength of light and $N = n_0 \sin\theta$ is the effective index associated with the BSW mode. Equations (1) and (2) allow for a complete description of the electric field associated with the TE BSW modes. In order to calculate the refractometric and adsorption sensitivities, an approach based on first order perturbation theory was chosen. For TE modes, an expression for the change in the effective index caused by a small perturbation in the RI profile can be written as[6]:

$$\Delta(N^2) = \int_{-\infty}^{+\infty} \Delta\varepsilon(z)|E(z)|^2 dz \cdot \left(\int_{-\infty}^{+\infty} |E(z)|^2 dz\right)^{-1} \ (3)$$

By inserting the field configurations of Equations (1) and (2) into Equation (3), along with the correct permittivity variation profile $\Delta\varepsilon(z)$, both the refractometric and adsorption sensitivities can be calculated. In the case of the refractometric sensitivity, $\Delta\varepsilon(z) = 2n_3\Delta n_3$ in the external dielectric region. For the adsorption sensitivity, the permittivity perturbation is $\Delta\varepsilon(z) = n_A^2 - n_3^2$ [6] in the adlayer on top of the PhC. Based on these expressions, both the refractometric $\left(\frac{\partial N}{\partial n_3}\right)$ and adsorption $\left(\frac{\partial N}{\partial d_A}\right)$ sensitivities can be calculated.

2.2. *Sensitivity analysis of Bloch Surface Waves*

2.2.1. Refractometric Sensitivity. Based on the procedure described in the previous section, the refractometric sensitivity of TE BSW modes can be calculated, yielding:

$$\frac{\partial N}{\partial n_3} = \frac{1}{N} \cdot \frac{n_3}{1 + 2q\frac{P}{a_0{}^2}} \ (4)$$

where $P = \int_{-\infty}^{+\infty} |E(z)|^2 dz$, which can be calculated numerically using matrix method methods[7]. Analysis of Equation (4) reveals some interesting properties of the refractometric sensitivity, in particular of the dependence with the incident angle. Given that when approaching the critical angle, N tends to n_3 making q tend to zero, which greatly increases the sensitivity, as seen in Equation (4). This result is in agreement with previously published theoretical work [8] and justifies why many BSW sensor applications use experimental setups near the critical angle[9].

2.2.2. Adsorption Sensitivity. Considering a thin layer of varying thickness d_F and RI n_F, the adsorption sensitivity can be calculated using Equation (3):

$$\frac{\partial \mathrm{N}}{\partial \mathrm{d_F}} = \frac{1}{N} \cdot \frac{\mathrm{n_F^2} - \mathrm{n_3^2}}{\frac{1}{q} + 2\frac{\mathrm{P}}{a_0{}^2}} \ (5)$$

Equation (5) displays interesting similarities with Equation (4), with the major difference being the dependence on the penetration depth 1/q. In this case, when approaching the critical angle, again q will tend to zero, but the sensitivity will also tend to infinity, as opposed to what is seen in the refractometric sensitivity. Thus, it can be seen that a higher sensitivity to thickness variations of the adlayer is attained at higher angles, in opposition to what is verified in the refractometric sensitivity. Further research is needed in order to demonstrate if this increase in sensitivity is verified and how experimental sensor setups can be designed to maximize sensitivity to molecule binding events.

3. Materials and Methods

In order to allow for RI variation measurements, an experimental setup based on the Kretschmann configuration in spectral mode was devised, which is illustrated in Fig. 2.

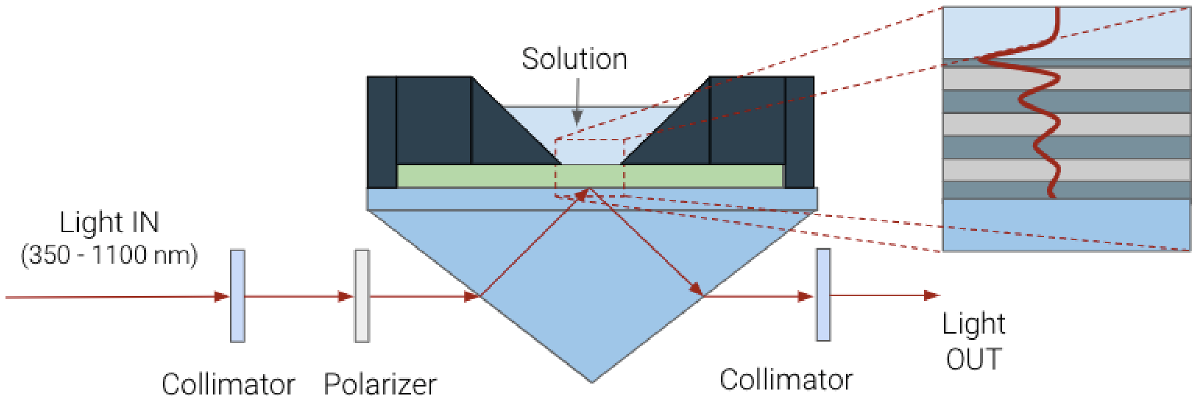

Figure 2 – Experimental setup for BSW sensor measurement using the Kretschmann configuration in the spectral mode. The dielectric on top of the BSW can be changed to allow for RI characterization.

Light is injected into the system via fiber optics and passes through a collimator (Avantes COL-UV/VIS) and a polarizer (Thorlabs LPNIR050-MP2), which was set to allow passage of s-polarized light only. A silica substrate in which the PhC was deposited was placed on top of the prism with an index matching fluid in between. Light inside the prism suffers total internal reflection (with an incidence angle of 74º) and a BSW is created at the top interface, between the PhC and the dielectric. After passing again through a collimator, a spectrometer (Avantes AvaSpec-ULS2048CL-EVO) records the spectrum for each RI value. Various solutions of calibrated RI (using an Abbe refractometer – Atago DR-A1 at 589.3nm) were fabricated using mixtures of water and sucrose with different ratios. These solutions can be exchanged as seen in Figure 2, allowing the spectrometer software to register the different spectra associated with each RI value.

Numerical simulations of the PhC spectra and sensitivity performance were made using the transfer matrix method[5,10], on a home-made Python based code. By performing matrix multiplication of the different transfer and interface matrices, the reflectivity spectrum can be calculated, and the RI sensitivity can be estimated.

In order to perform preliminary tests regarding the refractometric sensitivity, a PhC was deposited via RF Magnetron Sputtering, consisting of 2 bilayers of TiO_2 and SiO_2 (with thicknesses 150 and 140 nm, respectively), and a TiO_2 cap layer 95nm thick. The PhC was deposited on an SiO_2 substrate which matches the RI of the prism. The thicknesses of the layers were chosen to allow the appearance of BSW modes in the ultraviolet and infrared range, using the proportionality between the penetration depth and the wavelength to allow for a large difference in sensitivity between the two modes.

4. Simulation and Experimental Results

Using the configuration mentioned previously, after deposition the PhC was characterized under RI variations. Figure 3 displays the simulated and experimental spectra obtained.

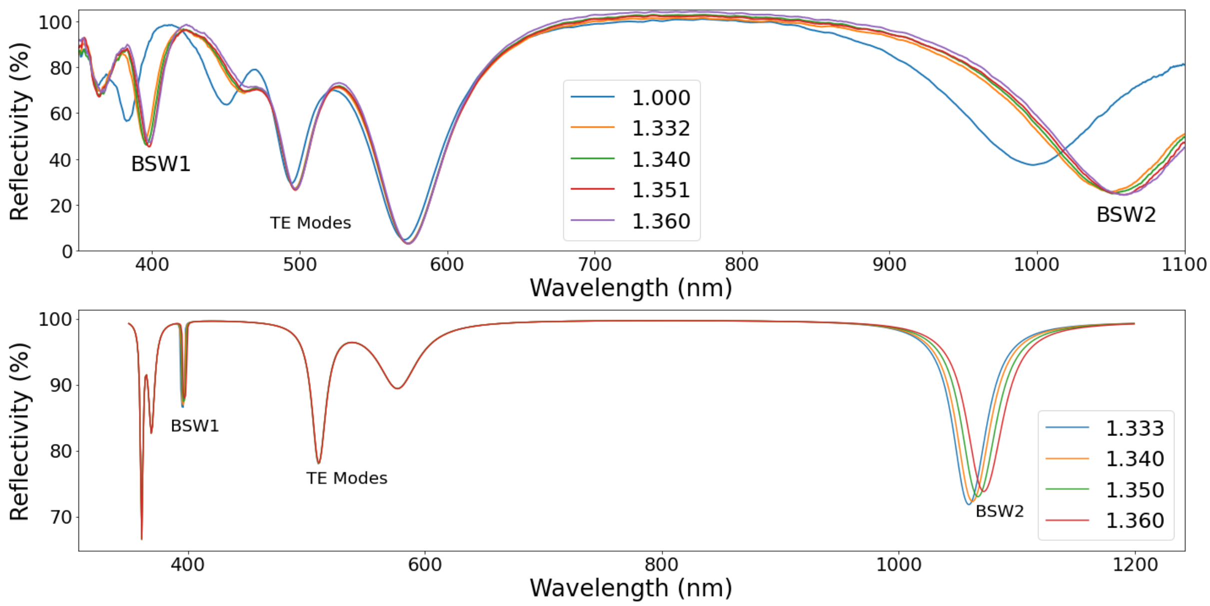

Figure 3 – Spectra of the PhC under the Kretschmann configuration: (a) Spectra simulated with transfer matrix methods; (b) Experimental results.

From Fig. 3 the simulated and experimental results are in agreement regarding the wavelength position associated with each mode. Nevertheless, a large increase is seen in the full width at half maximum of the modes, especially the mode marked with BSW2 in Fig. 5. This broader resonance could be explained by uncertainties associated with the deposition method, in particular if some of the PhC layers do not have the same exact thickness. This effect is more intense because only two bilayers were deposited, making the lattice periodicity less defined.

Using the data from both simulations and experimental results, the refractometric sensitivity of the PhC can be evaluated, which is done in Fig. 4.

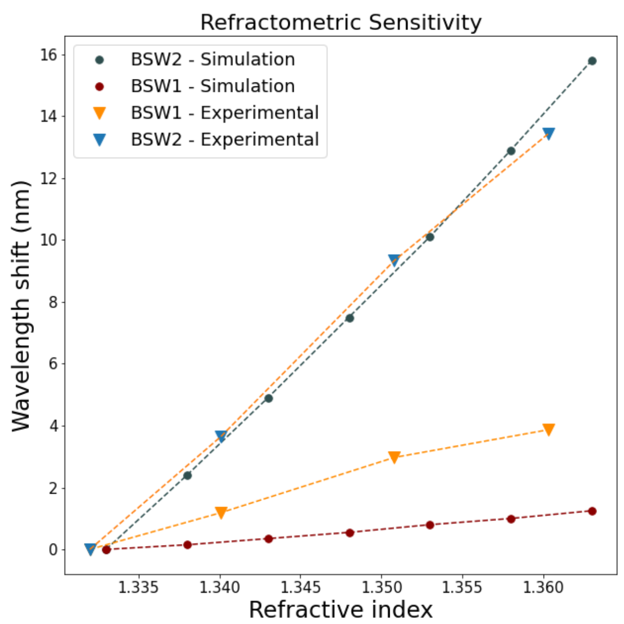

Figure 4– Experimental and simulation results for the refractometric sensitivity of the two BSW modes of the deposited PhC.

Figure 4 shows good agreement between experimental and simulation results, especially for the BSW mode in the infrared region (BSW2), which displays a sensitivity of 525nm/RIU (RIU - refractive index units). In the case of the BSW1 mode, the sensitivity is considerably lower, with the simulation results showing a sensitivity of 42 nm/RIU and the experimental results a sensitivity of 60 nm/RIU. The difference between the sensitivity of the two modes is as expected from the Equation (4), since 1/q is proportional to the wavelength, meaning that the lower the wavelength, the lower the sensitivity (considering the P/a_0^2 ratio approximately the same).

The obtained results show considerable interest for real-world application in optical biosensors. Considering that the response of the BSW1 to RI variations is almost negligible (especially when the objective is the detection of specific molecules dissolved in water), the sensor shows promise for allowing both refractometric and adsorption monitoring using both BSW TE modes. Further work is needed in order to experimentally test the response of both modes to adsorption effects, meaning that the PhC should be functionalized for specific molecule binding and tested in the laboratory.

5. Conclusion

The sensitivity of BSW to RI variations and adsorption was studied for TE modes using first-order perturbation theory. A simple analysis of the dependence of the sensitivities with the incidence angle is made, which revealed that for refractometric variations the sensitivity is higher near the critical angle, and for adsorption sensitivity higher angles should be used. Preliminary experimental results regarding the usage of two different BSW modes in TE polarization are presented, which were characterized under different external RI values. The results revealed good agreement with both analytic and numerical analysis, establishing the path for future work in the study of BSW sensors.

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