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Bloch mode engineering for photonic biosensors

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Bloch mode engineering for photonic biosensors

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ABSTRACT

ARRUDA, G. **Bloch mode engineering for photonic biosensors**. 2021. 97f.

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Point-of-care (PoC) devices are an important technology in the field of medicine, playing a crucial role in healthcare by providing real time and in situ diagnostics, thus being especially suitable for regions with inadequate traditional healthcare and clinical laboratories. Photonic biosensors have advanced this area over the last few years, enabling high sensitivity, miniaturisation and mass production capability. Various configurations of these sensors have been explored, using different types of materials, such as metals and dielectrics. One of the most promising photonic biosensor configurations is the silicon waveguide based on Quasi Guided Mode Resonances (GMR), which uses a simple detection setup, and is compatible with the Silicon on Insulator (SOI) fabrication technology, thus being suitable for mass production, which is crucial for PoC devices. However, their performances are still hindered by lower sensitivities, as compared to other photonic biosensors, such as sensors based on plasmonic resonances and Subwavelength Gratings (SWGs). This dissertation proposes to find design strategies to enhance the performance of GMR sensors, without significant addition of complexity. The first step was to understand the behaviour of the silicon GMRs and SWGs for optimized structures of different geometric complexities, where the less complex is a 2D structure and the most complex is a 3D structure, typically associated with the state-of-the art devices. Using simulations in COMSOL Multiphysics, the relationship between the waveguide's mode confinement and sensing performance was analysed and it was realized that, depending on the light polarization, a less complex structure can achieve a performance close to the state-of-art more complex structures. A design strategy to take advantage of the high sensitivity of the SWG and simplicity of the GMR is presented. The strategy essentially perturbs the SWG period to allow coupling of guided modes with radiation modes, which greatly simplify the system, while exhibiting resonances with arbitrarily large quality factors (only limited by fabrication imperfections). The sensing performances of these new perturbed SWGs were analysed and their tolerance to fabrication deviation was estimated.

Keywords: Point-of-care devices, photonic biosensors, waveguides, subwavelength gratings, quasi guided mode resonances.

RESUMO

ARRUDA, G. **Engenharia de modos Bloch para biosensores fotônicos**. 2021. 97f. Dissertação (Mestrado) - Escola de Engenharia de São Carlos, Universidade de São Paulo, São Carlos, 2021.

Dispositivos de uso local (*PoC*) constituem uma tecnologia importante para a medicina, apresentando um papel crucial na área de saúde, uma vez que propocionam diagnóstico em tempo real e *in situ*, sendo assim especialmente indicados para regiões com sistemas de saúde e laboratórios clínicos precários. Biosensores fotônicos contribuíram para o avanço dessa tecnologia nos últimos anos, permitindo altas sensibilidades e potencial para miniaturização e produção em massa. Diversas configurações desse tipo de sensor foram estudadas, feitas de diferentes materiais, tais como metais e dielétricos. Uma das configurações mais promissoras é a do guia de onda de silício baseada em *Quasi Guided Mode Resonances - GMRs*, que apresenta um sistema de detecção simples, além de ser compatível com a tecnologia de fabricação Silício-sobre-Isolador (*SOI*), a qual é compatível com produção em massa, condição crítica para os dispositivos *PoC*. Entretanto, suas performances são limitadas por baixas sensibilidades, quando comparadas a outros biosensores fotônicos, como os feitos com metais e até mesmo os de mesmo material, porém de diferentes configurações, tal qual é o caso das redes de difração sub-comprimento de onda (*Subwavelength Gratings - SWGs*). Esta dissertação procura por novas estratégias de engenharia do sensor GMR com o propósito de melhorar a sua performance. O primeiro passo é entender o comportamento das estruturas GMRs e SWGs de silício com diferentes complexidades geométricas, sendo a de menor complexidade uma estrutura 2D e a mais complexa 3D, tipicamente associada com os dispositivos do estado-da-arte. Usando simulações no COMSOL Multiphysics, a relação entre o confinamento do modo do guia de onda e sua capacidade de sensoriamento foi averiguada e foi visto que, dependendo da polarização da luz, uma estrutura menos complexa pode sim atingir uma performance próxima daquela reportada para estruturas mais complexas do estado-da-arte. Uma estratégia de engenharia é implementada para combinar a alta sensibilidade das SWGs com a simplicidade das GMRs. Ela consiste essencialmente em perturbar o período de uma SWG para permitir o acomplamento de modos guiados com modos radiantes, simplificando, assim, o sistema de sensoriamento dessas estruturas, enquanto mantém ressonâncias com fatores de qualidade arbitrariamente altos (teoricamente limitados por imperfeições do processo de fabricação). A performance de sensoriamento dessas novas SWGs perturbadas foi analisada e sua tolerância a erros no processo de fabricação foi estimada.

Palavras-chave: Dispositivos de uso local, biosensores fotônicos, guias de onda, redes de difração sub-comprimento de onda, *quasi guided mode resonances*.

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LIST OF ABBREVIATIONS AND ACRONYMS

ELISA	Enzyme-linked immunosorbent assay
EBEAM	Electron-beam
<i>FOM</i>	Figure of Merit
LED	Light Emitting Diode
LSP	Localized Surface Plasmon
LSPR	Localized Surface Plasmon Resonance
PoC	Point-of-care
PSP	Propagating Surface Plasmon
QGM	Quasi Guided Mode
RCWA	Rigorous Coupled Wave Analysis
RIE	Reactive Ion Etching
SPR	Surface Plasmon Resonance
SLR	Surface Lattice Resonance
SWG	Subwavelength Grating
TIR	Total Internal Reflection

LIST OF SYMBOLS

β	Mode's propagation constant
ϵ	Relative permittivity
FF	Fill Factor
$\mathbf{k}$	Wavevector
n	Refractive index
m	Integer number
Q	Quality Factor
S	Sensitivity
λ	Wavelength
Λ	Period
H	Height
W	Width

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1 INTRODUCTION

Few technologies in our modern life have such importance as sensors. Unlocking the smartphone screen with your finger or face, unlocking doors with a simple plastic card, giving voice commands to a computer to calculate the optimal traffic route and turning on/off the lights of the room when someone goes in/out are some of the many applications of sensors in our daily lives.

A sensor is a device responsible for detecting an event or change in its environment, such as a change in temperature, pressure or light intensity. This change is then translated into a signal, usually electrical¹, read by another gadget that will use this information, e.g. turning on the lights. The thermostat is one of the first sensors to have ever appeared, dating back to 1883². Its sensing mechanism is based on the expansion of metals with the increase of temperature.

Technology advancements led to smaller, cheaper and more accurate sensors, giving birth to new areas of development. Autonomous robots, self-driven automobiles, smart houses and the whole concept of Internet of Things exists today due to the enormous development of sensors³. Most important for this work, biosensors have emerged from this new wide range of uses.

Biosensors are devices capable of detecting chemical and biological reactions⁴. As seen in figure 1, they are typically composed of the following components: the analyte is the substance to be detected; the bioreceptor is a molecule or biological function that will react with the analyte; the transducer is the element responsible for converting the aforementioned reaction into some sort of signal; the electronics is responsible to process the output of the transducer into readable data, which can then be displayed to the user.

Figure 1 – Schematic of the components of a biosensor.

This new class of sensors aims to address the lack of medical diagnostics in regions with inadequate healthcare facilities and clinical laboratories. These diagnostics play a crucial role in healthcare by providing early detection of disease⁵, improving timely and appropriate care⁶, protecting the safety of medical products (such as blood for transfusion)⁷ and reducing healthcare costs⁸.

Biosensors are not the only way of getting good medical diagnostics, the enzyme-linked immunosorbent assay (ELISA), for example, is a method of detection able to distinguish concentrations as low as 1 pM⁸. However, it requires labeling the sample with a biomarker, which delays results, adds costs due to specialized reagent requirements and requires complex micro-evaluations using large, automated analysers⁹. Therefore, the development of affordable and well performing techniques of analysis for point-of-care (PoC) diagnostics is mandatory to provide access to cost-effective healthcare technologies all around the world. Biosensors are one of the most promising solutions to this problem,¹⁰ and it is expected that their market value will reach US \$31.5 billion by 2024¹¹.

The first biosensor was demonstrated in 1956. It was a system based on an oxygen electrode, designed to detect the levels of oxygen in blood, water and other samples¹². However, it was photonics that brought the most recent advance to biosensors¹³. Analogous to electronics, which deals with control and confinement of electrons, photonics deals with control and confinement of photons. Optoelectronics, for example, is a field of photonics characterized by the correlation between light and electricity. Lasers, Light Emitting Diodes (LEDs), solar cells and photodiodes are common examples of optoelectronic devices¹⁴.

For sensing applications, optical waveguides, such as fiber optics, play a crucial role. Optical waveguides are structures that guide light through its confinement inside a given region of space. They can assume various forms and be made of different types of materials, such as metals and dielectrics. A distribution of electric and magnetic field propagating in a waveguide is called a “mode”, and it may be highly dependent on the surrounding media¹⁵; it is the latter property that makes waveguides interesting for sensing.

The use of photonic waveguides in biosensing dates back to 1983, when it exploited the modes propagating on the surface of a thin film of silver as a sensing mechanism¹⁶. These modes are associated with Surface Plasmon Resonances (SPRs) and the biosensor based on this phenomenon showed a capability of detecting a concentration of 2ug/ml of antibodies in aqueous solution¹⁶. It is the equivalent of detecting a single grain of sugar in one liter of water.

In this dissertation, I begin by presenting the theoretical background of photonic waveguide biosensors, before discussing the current state of the art of this technology. A complete review of these sensors, including metals and dielectrics, will be done subsequently in this dissertation. But first, in this section, I briefly present the lay of the land of photonic biosensors.

At the present time, metallic sensors based on SPRs and other type of plasmonic resonances, such as Localized Surface Plasmon Resonance (LSPR) and Surface Lattice Resonances (SLRs)^{17,18}, have already reported the detection of concentrations on the order of pg/ml. Despite of the advances of these metallic waveguide-based biosensors, they still typically require complex equipment and trained personnel^{4,19,20}. Thus, they do not come in an easy-to-use integrated form, which is a basic requirement for PoC devices.

Dielectric waveguide-based biosensors, on the other hand, are potentially better candidates as PoC devices, especially those based on silicon, which is a material compatible with mass production²¹. Silicon waveguides also support Quasi Guided Modes (QGMs)¹⁴ which are easily accessed by illumination with external light sources, due to the fact that these modes may naturally couple to out-of-propagation-plane direction, meaning that the detection method of any sensor based on this waveguide should also be simple and practical, ideal for PoC devices.

However, the ease of use brought by the QGMs-based sensors come with a major drawback: a decrease of the sensor's sensitivity to changes in the surrounding medium²². This capability of the sensor is deeply related to the mode's sensitivity, which is a parameter that represents how well it can detect the change of refractive index of the surrounding medium, while the Quality Factor (Q) is related to the ease of the detection method. Both parameters will be properly defined in section 2.5. This means that the QGM-waveguide based sensors, that possess a high Q mode, cannot detect very small changes in the surrounding medium as, for example, the ones based on SPRs and SLRs. They also cannot, most of times, match the sensitivity of sensors made of the same material but based on a different type of propagating mode, such as Subwavelength Gratings (SWGs)²⁰.

1.1 Objectives

It is well known that perturbations of the waveguide's geometry influence the mode's characteristics²³. Therefore, this dissertation proposes to study the effects of perturbations in the architecture of silicon-based waveguides over their modes sensing parameters, aiming to achieve a balance between a good sensitivity and quality factor, contributing, then, to their use as PoC devices.

The investigation focuses on and compares waveguides with structures in 2 and 3 dimensions. In particular, the study aims to assess whether the higher complexity of 3D structures ensues in meaningful gain in performance. The performance is quantified in terms of Q and sensitivities.

1.2 Structure of this dissertation

This dissertation is divided into six chapters. The second chapter introduces the relevant theoretical background. In the third chapter, the state-of-the art of photonic biosensing devices is reviewed and the motivation of the project is further discussed in the light of the state-of-the-art. The fourth chapter contains the study relating the confinement of the electric field inside the periodic waveguides and their sensing performance. The fifth chapter shows the effects of the perturbation of the geometry of periodic waveguides on their sensing parameters. Finally, the sixth chapter presents the conclusion of this work.

2 SENSOR INTERROGATION MECHANISMS

In this chapter, I lay out the theoretical background necessary to understand the interrogation mechanism of the photonic sensor.

2.1 Fundamentals of resonant photonic sensors

A photonic sensor is typically based on an optical resonance²⁰. Such resonances can be obtained by trapping the light in a cavity that will exhibit strongly wavelength dependent parameters. The optical cavity is the most fundamental building block of a photonic sensor.

The most paradigmatic example of an optical cavity is formed by two perpendicular mirrors immersed in a dielectric medium, also known as a Fabry-Perot cavity, as illustrated in figure 2. Light introduced in this cavity undergoes multiple reflections inside the cavity. Each time it gets reflected, some small portion of the light also escapes. The part of the light that escapes into the same medium of the injected light gives the reflectance of the cavity, while the part that escapes into the other medium gives the transmission (see figure 1). As the reflected and transmitted waves build up from multiple interference arising from the multiple propagation inside the cavity, the reflection and transmission will be strongly dependent on the phase accumulation in a single round-trip inside the cavity^{24,25}. This is the origin of the wavelength-dependent nature of the cavity parameters.

Figure 2 – Two mirrors, in black, acting as a light cavity. The injected light (yellow arrow) undergoes multiple reflections between the two mirrors (black arrows). The red and blue arrows indicate the reflection and transmission of the cavity. In a) the phase accumulation inside the cavity is such that the reflected light interferes destructively with itself, while the transmitted light interferes constructively with itself. In b) it is the other way around.

The reflection and transmission spectra of a cavity will therefore consist of a sequence of resonance peaks. As an example, figure 3 shows the typical transmission of a Fabry-Perot cavity. Assuming a π phase shift upon reflectance from the mirrors and normal light incidence, the wavelengths of the transmission peaks are given by the condition²⁶ :

$$\frac{\lambda}{n}m = 2d \quad (2.1)$$

where λ is the free space wavelength, n is the refractive index of the medium between the mirror (λ/n is therefore the wavelength inside the medium), m is an integer and d is the distance between the mirrors. This condition expresses the fact that a peak of transmission is obtained when the phase accumulated in a full round trip is a multiple of 2π , thus resulting in constructive interference in transmission.

Figure 3 – Transmission spectrum of a cavity immersed in vacuum ($n = 1$). The distance between the mirrors is $1\mu m$ and their reflectance is 85%.

Now suppose that we want to use this cavity as a sensor. The cavity can be designed to show one of the peaks in a given wavelength of interest (usually the resonant wavelength is chosen by the designer according to constraints in the light sources and detectors), as illustrated in figure 4a. The peak occurs for the wavelength λ_0 that fulfills exactly the condition described in the last paragraph. But this condition depends on the refractive index of the medium, which can be altered by the presence of an analyte. Therefore, the change in the refractive index caused by the analyte is translated to a change $\Delta\lambda$ of resonant wavelength, as shown in figure 4b. This is the basic interrogation mechanism of a photonic sensor.

It is important to notice that the example of the Fabry-Perot cavity is only to illustrate the main interrogation principle of a photonic cavity: an analyte changes the refractive index, which alters the spectrum of the cavity. As shown later in this dissertation,

Figure 4 – Transmittance or reflectance spectrum of a sensing device with (a) and without (b) an analyte. The Y-axis denotes the transmittance/reflectance (Amplitude) and the X-axis the wavelength (λ).

a photonic sensor will typically rely on the modification of the refractive index of a thin layer of material.

In the next sections of this chapter the reader can find a discussion of the photonic structures relevant for this work, that act similarly as a resonant cavity, for sensing purposes, and are commonly used as sensors. For simplicity, we also assume our media are isotropic and absent from free charges or currents.

2.2 Optical Waveguides

Optical waveguides are media that propagate light confined inside a specific region of space. Coaxial lines (radio-frequency components connector), microstrip lines (microwave integrated circuits), rectangular waveguides (large amount of microwave power transfer) and optical fibers (optical and infrared frequencies) are a few of the many examples of commonly employed waveguides¹⁵. Figure 5 shows some typical waveguides.

Figure 5 – Typical waveguiding structures. The wave propagates confined in the grey region.

Given a certain waveguide geometry, the propagating wave solution to Maxwell's equations that satisfies the boundary conditions imposed by the waveguide is referred to as a waveguide mode. These modes are susceptible to changes of the surrounding media refractive indexes and, therefore, can be used for sensing applications.

2.2.1 Slab Waveguides

The type of waveguide most relevant to this dissertation is the slab waveguide, illustrated in figure 6a. The slab waveguide is formed by a slab of high refractive index material, which is the medium where the wave is guided, and is also termed “the waveguide core”. It provides confinement in only one direction (the $\mathbf{z}$ direction in figure 6a, and so the medium is assumed to extend indefinitely along the $\mathbf{x}$ and $\mathbf{y}$ directions).

Perhaps the most straightforward way to understand the propagation of the mode inside the slab is using a combination of ray optics with wave optics, whereby the ray direction is parallel to the propagation wavevector $\mathbf{k}$, as represented in figure 6b. In this description, there are two conditions the rays must fulfil: total internal reflection (TIR) and phase matching.

The first condition comes directly from Snell’s law²⁷. Once the light ray hits one of the interfaces, the incoming angle of incidence (θ_i) must be higher or equal than the critical angle (θ_c), so in this way light is totally internally reflected and no energy escapes the waveguide. One must notice that this condition is met only if $n_1 > n_2$ (see figure 6).

The second condition arises from the fact that the light beam bounces back and forth inside the waveguide, accumulating a round-trip phase along the $\mathbf{z}$ direction. The condition of existence of a mode requires that the light that comes back on itself interferes constructively. This condition will be satisfied when the phase accumulated in a round trip is a multiple of 2π . Therefore, this requirement sets a restriction on the allowed wavevector directions inside the waveguide, k_z in this case.

The restrictions on the allowed wavevector direction can be seen by imposing the requirement of constructive interference in a round-trip propagation. The phase accumulated in a wave cycle is due to the vertical propagation and to the phase picked up upon reflection on the interfaces. If the slab thickness is d , the round-trip propagation accumulates a phase of $2k_z d$. Denoting the phase picked up on the top and bottom reflections by ϕ_1 and ϕ_2 , the requirement of constructive interference is expressed as:

$$2k_z d + \phi_1 + \phi_2 = m2\pi \quad (2.2)$$

where m is an integer. Since the magnitude of the wavevector is fixed by the wavelength, for each wavelength there will exist only a discrete number of propagation directions allowed in the waveguide, each direction corresponding to the value of k_z that solves equation 2.2 for a given value of m . The longitudinal component (parallel to the interface n_2/n_1) of the wavevector is called the propagation constant β . In the example of figure 6, this component is along $\mathbf{y}$.

Figure 6 – a) Basic schematic of a slab waveguide. A slab of a uniform material (red), characterized by its refractive index n_1 , is immersed in a dielectric medium of refractive index n_2 . b) Drawing of a propagating mode along y axis. Meeting the conditions for both total internal reflection and phase matching requires some discrete values of k_z . Once k_z is known, β can be determined from the magnitude of the wave vector, which is fixed by the wavelength.

Due to the symmetry of the slab waveguide, the solutions to Maxwell's equations can be divided into a Transverse Electric (TE) polarized plane wave and Transverse Magnetic (TM) polarized plane wave. A TE polarized wave implies that there is no component of the electric field ($\mathbf{E}$) in the plane containing the wave vector ($\mathbf{k}$ is parallel to the Z-Y plane), while the TM polarization implies no magnetic component in the wave vector plane. In the example illustrated in figure 6, the TE polarization has its electric field only towards $\mathbf{x}$ (out of the paper), while the TM has its magnetic field only towards $\mathbf{x}$.

Coming back to the waveguide, the relation between the wavelength of the mode and its propagation constant is referred to as dispersion. It is different for TE and TM polarized plane waves, since the phase accumulation from the interfaces is different from one to another (the phase can be directly obtained from the Fresnel coefficients)²⁵. Once the dependence along y is known, one can write the electric and magnetic field as:

$$\mathbf{E} = \mathbf{E}(z, x)e^{-i\beta y} \quad \mathbf{H} = \mathbf{H}(z, x)e^{-i\beta y} \quad (2.3)$$

In order to find the remaining electric and magnetic field spatial distribution of this mode, one must solve Maxwell's equations, with the appropriate boundary conditions. The electric field $\mathbf{E}$ and magnetic field $\mathbf{H}$ components parallel to the interface n_2/n_1 must be continuous across the interface. The perpendicular components of the electric displacement field $\mathbf{D}$ and magnetic field flux density $\mathbf{B}$ are also continuous. Lastly, one must add the requirement of an oscillating vertical field inside the waveguide (high refractive index material) and decaying field outside it¹⁵.

For the slab waveguide, there are well known solutions capable of finding both the fields distributions and β values¹⁵. However, one can also use numerical tools, such as COMSOL Multiphysics or FDTD simulations. Figure 7a illustrates TE and TM polarized modes propagating in a 600 nm thick glass waveguide surrounded by air, while Figure 7b shows the dispersion curve of multiple TE modes.

Figure 7 – Modes propagating in a 600 nm thick glass ($n = 1.5$) waveguide surrounded by air with $\lambda=1500$ nm. The normalized electric and magnetic field intensity distribution of both TE and TM modes are shown in a). The dispersion curves of the modes are shown in b). The modes' distribution was computed using COMSOL and the dispersion curve with an implemented code on MATLAB.

The evanescent part of a mode (outside the waveguide core) plays an important role in photonic sensors. It can be applied to several different sensing approaches including evanescent fluorescence detection, monitoring of refractive index changes or detecting spectroscopic shifts²⁸. Since the mode is strongly dependent on the surrounding media, any change of the material above the surface perturbs the mode.

It is thus important to comment on the difference between TE and TM polarizations concerning sensing applications. It is easy to see that TM modes have an advantage over TE modes for sensing purposes. As seen in Figure 7a) the electric field of the TM modes has its energy partially concentrated outside the waveguide, while in the TE mode the energy is heavily concentrated inside the waveguide. This occurs due to the strong discontinuity of the normal component of the TM mode electric field at the top and bottom interfaces between the silicon core and the surrounding medium, which does not exist for TE modes.²⁹

Since most biosensing applications deal with variations of the dielectric constant, the electric field is the most affected by the presence of an analyte, and, therefore, TM modes are the most sensitive to variations of the surrounding media. This characteristic of

TM modes is not exclusive to slab waveguides and are also present in the other waveguide configurations discussed in this chapter.

2.2.2 Subwavelength Gratings (SWGs) Waveguides

Subwavelength gratings waveguides are periodic structures, as shown in figure 8, where the period is denoted by Λ . These structures might support waveguide modes when the period is smaller than the wavelength of the wave in all media²⁰.

Figure 8 – Schematic of a 2D SWG waveguide of period Λ and height H . The mode propagates from block to block (yellow material with refractive index n_{wv}). The blocks are attached to the surface of a substrate material of refractive index n_s and immersed in the cover material of refractive index n_c . The Fill Factor (FF) is a parameter that expresses the amount of core material (n_{wv}) in one period.

For simplicity, let's use the 2D periodic waveguide illustrated in figure 8 as an example for understanding the physics of SWG. Differently from the slab waveguide, there is a periodic modulation of the refractive index inside the waveguide core. The electric permittivity of the core of the waveguide can thus be written as a Fourier Series:

$$\epsilon(y) = \sum_m \epsilon^m e^{-i\frac{2\pi}{\Lambda}y} \quad (2.4)$$

Where m is an integer and acts as an index for the Fourier components ϵ^m , which can be calculated by the Fourier Transformation:

$$\epsilon^m = \frac{1}{\Lambda} \int_0^\Lambda \epsilon(y) e^{i\frac{2\pi m}{\Lambda}y} dy \quad (2.5)$$

The periodic symmetry condition of SWG waveguides leads to the conservation of the wave vector component parallel to the interface between the core and the cover ($\mathbf{k}_{||}$) up to an addition of a reciprocal lattice vector, following Bloch's theorem³⁰:

$$\mathbf{k}_{m||} = \mathbf{k}_{||} + m \frac{2\pi}{\Lambda} \mathbf{y} = \mathbf{k}_{||} + m G_y \mathbf{y} \quad (2.6)$$

where $\mathbf{k}_{m\parallel}$ is the new propagation constant, m is an integer number and G_y is the lattice vector component along $\mathbf{y}$. Notice that the SWG is periodic only in the $\mathbf{y}$ direction. Knowing the propagation constant of the mode, one can write the spatial distribution of the electric field as a sum of plane waves of the form:

$$\mathbf{E}(\mathbf{r}_{\parallel}, z) = \sum_m \Phi(z)^m e^{i(\mathbf{k}_{\parallel} + mG_y\mathbf{y}) \cdot \mathbf{r}_{\parallel}} \quad (2.7)$$

where $\Phi(z)^m$ are complex vectors and $\mathbf{r}_{\parallel}$ denotes the direction parallel to the x-y plane. The magnetic field component can also be described as the sum of plane waves and has its form analogous to the electric field. The field distributions along $\mathbf{z}$ of the plane waves, $\Phi(z)^m$, are calculated by applying boundary conditions to Maxwell's equations over the interfaces. This problem, however, involves solving an eigenvalue problem, which can be done using a numeric Eigensolver software, such as COMSOL, or implementing a solver method using a computer programming language, such as the Rigorous Coupled Wave Analysis (RCWA)³¹.

It is important to distinguish four very important operation regimes of periodic waveguides, depending on the size of the period Λ compared to the wavelength of the wave:

- **Diffraction:** When the period is larger than the wavelength at the free space. The structure acts as a conventional diffraction grating. The waveguide modes are fundamentally leaky.
- **Subwavelength:** The period is small enough to forbid diffraction in the cover and substrate. The structure might couple incoming light to the mode inside the waveguide. The waveguide modes are fundamentally leaky.
- **Deep-Subwavelength:** The period is small enough to forbid diffraction in all media. The structure behaves as a lossless waveguide and the core can be modelled as a uniform anisotropic material.
- **Photonic band gap:** Any incoming light is completely reflected to the cover. There is no propagation allowed inside the periodic structure.

The SWG waveguides are periodic structures operating in the deep-subwavelength regime. This condition is achieved for periods respecting the following relation, derived from Bragg's phase matching condition²⁹:

$$\Lambda < \frac{\lambda_0}{2n_{eff}} \quad (2.8)$$

Where λ_0 is the free space wavelength and n_{eff} is the mode's effective index, defined as the ratio between the mode's propagation constant β and the free space wavevector k_0 :

$$n_{eff} = \frac{\beta}{k_0} = \frac{\beta}{2\pi/\lambda_0} \quad (2.9)$$

Figure 9a illustrates the electric field intensity distribution of a 3D SWG obtained using COMSOL. The geometry parameters were taken from the literature²⁰. It is clear from the Poynting vector $\mathbf{S}$ (figure 9b) that the mode is indeed confined in the periodic structure. There is also evanescent field all around the blocks, which is desired for sensing purposes.

Figure 9 – 3D SWG waveguide (qTE mode). The parameters are as follows: width $W = 350$ nm, height $H = 220$ nm, period $\Lambda = 250$ nm, cover made of water $n_c = 1.33$, waveguide blocks (yellow) made of silicon $n_{sw} = 3.5$ and substrate made of SiO_2 $n_s = 1.44$. The electric field intensity distribution of the mode can be seen in a), while the Poynting vector intensity is found in b).

The operation in the deep-subwavelength regime is attractive to photonics because it allows the engineering of the Bloch mode (name given to the solution of equation 2.6) and consequently the propagation constant of the waveguide, by merely controlling the structure's geometry parameters. The mode wavelength dependence, or dispersion,

and even its birefringence can be tailored to specific applications²⁰. Ultra-narrowband filters,³² ultra-broadband couplers³³, ultra-broadband mode converter and de/multiplexer³⁴, polarization management structures³⁵ or highly efficient fiber-to-chip couplers³⁶ are but a few of the many recent devices using this concept³⁷.

SWGs are interesting for sensing because they allow a greater interaction of the field with the surrounding medium, when compared to slab waveguides, thus potentially leading to higher sensitivities. Such a comparison will be shown later in this dissertation. The main drawback of the SWG when applied to biosensing devices operating in the visible/near infrared band is the fabrication technology, since the device's dimension typically requires feature sizes of about 150 nm^{20,29}. However, with the advance of lithographic processes, already capable of achieving sub 100 nm patterns, their fabrication becomes progressively more viable³⁸.

2.3 Photonic Crystals, diffraction gratings and Quasi Guided Modes

The waveguide modes discussed so far are fully guided, meaning that the energy is trapped, in principle, for an infinite time in the waveguide. Quasi-guided modes, in contrast, are leaky modes, i.e., part of the energy escapes out of the waveguide. Their immediate advantage as compared to fully guided modes is the fact that they can be conveniently excited by a plane wave light source outside the waveguide, hence providing an easier coupling mechanism than guided modes. Quasi guided modes work under the subwavelength regime.

In order to understand the basic principles of quasi guided modes, consider the incidence of light onto the periodic structure in figure 10a), with a period of 500 nm, which guarantee a subwavelength operation regime for most wavelengths of the visible spectrum. It is a waveguide that consists of a slab of glass ($n = 1.5$) with a periodic perturbation, also made of glass, of height = 100 nm above it.

When the incoming light hits the periodic structure, new plane waves will be generated according to equation 2.6. Each value of m that solves that equation results in a diffractive wave with a wave vector component parallel ($k_{m||}$) to the plane of incidence (parallel to the y axis in the figure 10b), having their m_{th} values referred as the diffractive order, as in figure 10b. For the sake of simplicity, let's assume a normal incidence ($\theta = 0$) of the light. Applying equation 2.6 leads to:

$$\mathbf{k}_m \cdot \mathbf{y} = k_{m||} = \mathbf{k}'_0 \cdot \mathbf{y} + m \frac{2\pi}{\Lambda} = mG_y \quad (2.10)$$

Whenever one of these plane waves have their parallel wave vector matching the propagation constant of the waveguide ($mG_y = \beta$), a mode will be excited, and light will propagate horizontally, producing a fast phase accumulation, typical of resonant

Figure 10 – Schematic of a periodic waveguide upon excitation of plane wave a). The period $\Lambda = 500nm$ guarantees that the waveguide is operating in the subwavelength regime for most wavelengths of the visible spectrum. The structure (blue) is made of glass ($n = 1.5$) and it is immersed in air. The periodic perturbation above the glass slab is 100 nm thick. The phase matching requirement between the diffractive order and the waveguide mode is shown in b): the grey arrow represents a mode inside the waveguide with its propagation constant β ; $\mathbf{k}'_0$ is the wave vector of the incident wave (with incident angle θ) and $\mathbf{k}_m$ represents the diffracted waves, calculated using equation 2.6.

behaviours. In order to be confined inside the core, the wave vector of the mode must be higher than the wave vector of the wave in the cover (n_c) and substrate (n_s), which can be expressed as:

$$\beta = mG_y = m\frac{2\pi}{\Lambda} > \frac{2\pi}{\lambda}n \iff \Lambda < \frac{m\lambda_0}{n} \quad (2.11)$$

where λ_0 is the free space wavelength and n represents the highest value of refractive index between the cover and substrate media. The lowest value of m , apart from 0, that respects relation 2.11 tell us that the period of the waveguide must be smaller than the wavelength of the light in both cover and substrate media. Therefore, it must operate in the subwavelength regime.

One must also notice that the 0_{th} order corresponds to a plane wave in the same direction as the normal component of the incoming light, and it does contribute to the Bloch mode. This means that the original light source won't couple entirely to the waveguide mode, with some part of its original energy going to the 0_{th} order, hence the name quasi guided mode.

By sweeping through the external light source's incident angle and wavelength, i.e. altering the direction and magnitude of the $\mathbf{k}'_0$ in figure 10b, it is possible to identify the quasi guided modes resonances, as shown in figure 11, which illustrates the external source excitation method to find the modes of the waveguide of figure 10a using COMSOL and RCWA for numeric simulations (please tend to appendix A for a brief overview of the

numeric methods).

Figure 11 – Simulated reflectance spectrum of the structure of figure 10 obtained using RCWA. The plane wave was TE polarized and had a 10° angle of incidence. Each peak corresponds to the excitation of one waveguide mode, which has its electric field (E_x - out of paper plane) intensity distribution shown (calculated using COMSOL) at the right side of each peak (in plane cross section view). Red denotes high values and blue low ones.

Structures that operate with quasi guided modes are commonly referred to as diffraction gratings or photonic crystals. Although both terms are commonly used interchangeably in the literature, it is important to distinguish between them.¹⁴ The difference can be conveniently expressed in terms of the degree of perturbation. The perturbation of diffractive gratings is weak, mainly because of the small height of the periodic blocks and/or the small difference in refractive index between the periodic core and the slab. Their modes profile strongly resemble the purely guided modes and tend to be confined inside the slab, as seen in the electric fields of figure 11. That means that the mode is very similar to the un-perturbed structure and the blocks act essentially as a grating coupler.

Photonic crystals, on the other hand, exhibit a strong perturbation, meaning that the height and the refractive index contrast between the periodic core and substrate are high enough to deeply perturbate the original slab mode. Their modes are confined almost entirely inside the periodic blocks, much like the ones from a SWG. Figure 12 illustrates the difference in the geometry of photonic crystals and diffraction gratings.

Quasi guided modes have been present in a variety of applications, as optical filters,^{39,40} mirrors,⁴¹ bio-sensors^{42,43} and, as the most important feature to this dissertation, to inject and extract light from waveguides.^{44,45} Due to being larger than SWG waveguides, sensing devices based on photonic crystals are easier to fabricate. EBEAM lithography⁴⁶ is commonly used for writing the mask on the surface of the desired surface, while Reactive Ion Etching⁴⁷ (RIE) is used for the etching. For large scale fabrication, nano-imprinting

Figure 12 – Difference of the perturbation geometry of Diffraction Gratings and Photonic Crystals.

should be used.⁴⁸

2.4 Plasmonics

The waveguides discussed so far are made of dielectrics. However, there is a variety of resonant sensors that use metals in their composition. Plasmonics is the field of study that exploits the collective motion of conduction electrons in metals, making possible the coupling of light with nano-objects, providing a new range of optical effects at the nanoscale⁴⁹. It emerged from the conjunction of photonics, electronics and nanotechnology.⁵⁰

Plasmon modes come in two forms: localized surface plasmons and propagating surface plasmons. Both will be discussed in the next sections. Although they are not the main topic of interest in this work, their use in biosensing is of great importance and their performance will be extensively used for future comparisons. From now on, a plasmon mode shall be referred just as a plasmon, for simplicity.

2.4.1 Localized Surface Plasmons

Localized surface plasmons (LSP), are a result of the combined oscillation of the free electrons in a metallic nanoparticle and the oscillation of the surrounding electromagnetic field. For a single metallic particle surrounded by vacuum and radiated by an electromagnetic field, a dipole moment $\mathbf{p}$ will be induced, proportional to the applied electric field $\mathbf{E}$ ⁵¹. Figure 13 depicts this phenomenon.

Figure 13 – Induced dipole ($\mathbf{p}$) inside a sphere from an external electric field surrounded by vacuum. ($\mathbf{E}$).

Using a quasi-static approach, which implies assuming the particle size to be much smaller than the wavelength of the exciting wave, one can determine the value of $\mathbf{p}$, as given by⁵¹ :

$$\mathbf{p} = \alpha \mathbf{E}; \quad \alpha = 4\pi a^3 \frac{\epsilon(\omega) - 1}{\epsilon(\omega) + 2} \quad (2.12)$$

Where α is known as the polarizability, $\epsilon(\omega)$ is the frequency dependant relative permittivity of the sphere, and a is the sphere's radius. There is a dramatic increase in the polarizability, consequently the dipole moment, when the denominator of equation 2.12 approaches zero. At the point of $Re\{\epsilon(\omega)\} = -2$ a resonance occurs: the so-called localized surface plasmon resonance (LSPR). Note that for metallic spheres operating below the plasma frequency $\epsilon(\omega)$ will always have an imaginary part, so the denominator of equation 2.12 never gets to zero.²⁶ Figure 14 illustrates the resonance effect of a gold nanosphere of $a = 15$ nm, as well as the electric field dependence on the wavelength of the external field.

From figure 14a one can check the induced $\mathbf{p}$ by seeing the field enhancement outside the sphere, resultant of the attraction of the electrons caused by the incident field $\mathbf{E}_i$. The resultant electric distribution of this interaction is referred to as the scattered field pattern.

It is clear from figure 14b that the resonance peak is dozens of nanometers wide, so the resonance peak is not sharp. Indeed, this parameter depends mostly on the relative permittivity of the sphere at the plasmon frequency⁵². Little can be done to the geometry in order to increase this sharpness. The resonance frequency, however, depends on the size, shape, composition and, most important for sensing applications, the surrounding medium refractive index. As discussed in section 2.5.2, the peak sharpness is related to

Figure 14 – Simulation of a LSPR mode on resonance using COMSOL Multiphysics. A gold nano sphere of radius 15 nm is illuminated by a plane wave of wavelength 510 nm. The electric field intensity distribution is displayed a). The black arrows denote the incident electric field $[\mathbf{E}_i]$. The normalized dependence of the electric field intensity $|E|$ near the sphere on the wavelength of the external field is shown in b).

the sensitivity of the sensor. The broad resonance peak of the LSP is the main drawback for sensing applications.

Since no light coupling is necessary to excite these modes, differently from quasi-guided modes, LSPRs sensing devices can be very interesting for applications with coupling limitations. Metal nanoparticles also have simple fabrication procedures, such as colloidal chemistry based on reduction of metal salts⁵³ and even nanosphere lithography⁵⁴.

Besides sensing applications, these structures possess unique properties that allow their use in light manipulation and transformation at the nanoscale level^{55–60}, subwavelength imaging,^{61–63} nanolensing,^{56,61} nanolasing,^{64,65} field concentrators,⁶⁶ nanotweezers,⁶⁷ active optical elements⁶⁸ and many more⁴⁹.

2.4.2 Propagating Surface Plasmons

Differently from localized plasmons, the propagating surface plasmons (PSPs), propagate confined to the metal surface, hence the name. The waveguide can be either a uniform planar metal surface or an array of metal particles. Both configurations are discussed in the next sections.

2.4.2.1 Surface Plasmons Resonances

Surface plasmons resonances (SPRs) appear for structures very similar to the slab waveguide, the main difference being that a metal will take the place of one of the dielectric media. Consider an interface between a metal and a dielectric media, as shown in figure 15. The boundary conditions of Maxwell's equations for the electric and magnetic fields between the two media leads to an evanescent profile of the wave on both media; therefore, the wave propagates just at the surface of the metal. This condition, however, can be

achieved only for TM polarized waves, once there must be an electric field component parallel to the propagation constant β of the mode⁶⁹.

Figure 15 – Surface wave. The sub-indexes “d” and “m” denote, respectively, the metal and the dielectric; ϵ is the relative permittivity of the materials; k_y and k_z correspond to the wave vector components in the y and z direction, respectively; β is the propagation constant of the surface mode and the blue curve represents the decay of the field outside the interface.

Since the waves are evanescent outside the interface, it is not possible to couple light directly by external excitation, as is the case for LSPRs. Nanohole arrays can be etched in the metals surface in order to act as a grating coupler,^{70–72} similarly to the situation discussed in section 2.3. Also, the Turbadar-Kretschmann-Raether prism geometry^{73,74} can be used, in which light is directed into a glass prism with a thin (~ 50 nm) metal film on its surface. The reflected light from this film will generate SPRs on the far (opposite to the prism faces) side of the metal film.

As seen in figure 15, these modes have their field distribution all outside the waveguide (the surface/interface), meaning that they are highly sensitive to the surrounding environment. They are responsible for greatly advancing the development of biosensing methods, being a state-of-the-art technology for the study of biomolecular binding events^{75,76}. The main drawback of SPRs, in general, is the portability of the instruments based on this concept (e.g requiring a glass prism for light coupling)⁷⁷ and the expensive commercial products, that do not meet the affordability requirements of PoC to invest⁷⁸.

2.4.2.2 Surface Lattice Plasmons Resonances

The sharpness problem of the LSPRs can be overcome by arranging nanostructures in periodic arrays. The individual LSP mode of one particle may influence the response of the surrounding particles. If the period of the array is comparable to the incident light wavelength and under appropriate geometry and incident angle conditions, the individual scattered fields of the particles inside the array can be in phase with the incoming light.

Of course, any wave propagating through a periodic media must obey Bloch's equation (equation 2.6), meaning that the combined scattered fields correspond to the diffraction of the incident light in the plane of array, forming a diffractively coupled localized surface plasmon resonance⁴⁹, or just surface lattice resonance – SLR – for short. Just by tuning the array period, one can greatly improve the mode resonance width and, consequently, its sharpness. Figure 16 illustrates this effect.

Figure 16 – Comparison between LSPR (a) and SLR (b) in transmission spectra. The structure that originates the LSPR is an 80 nm radius gold sphere surrounded by air. The SLR is the result of an array of 1000 of these same metal spheres, with period of 620 nm. The inset shows a schematic of the particles arrangement. The electric field of the incident wave was perpendicular to the direction of the array.

Source: Image reproduced with permission from the American Chemical Society (see annex A). The article containing the image can be found at <https://pubs.acs.org/doi/10.1021/acs.chemrev.8b00243>⁴⁹. Any further use of this image should be requested to the rightful owners.

2.5 Main parameters of a photonic sensor

The dependence of the resonant wavelength on the medium refractive index is, therefore, the main interrogation mechanism of resonant optical sensors. These resonances are characterized by their bulk and surface sensitivities (S_b and S_s , respectively), quality factor (Q) and Figure of Merit (FOM). In this section I define these parameters.

2.5.1 Sensitivity

The sensitivity is the ratio between the resonant shift $\Delta\lambda$ to the refractive index variation Δn :

$$S = \frac{\Delta\lambda}{\Delta n} \quad (2.13)$$

I differentiate between bulk and surface sensitivities: the former is related to the resonance shift caused by a refractive index change of the entire cover material, while the

surface relates to a change of only the region near the sensing device's surface (see figure 17). For this dissertation, I assumed 10 nm as the height of this surface sensing region. This value relates to the size of the *Escherichia Coli* bacteria, which is typically used by our experimental partners. The surface sensitivity is more suitable for biosensors, due to the small dimensions of the analytes.

Figure 17 – Difference between bulk sensitivity (S_b) and surface sensitivity (S_s). The case is illustrated for both uniform and periodic waveguides. The difference is in the region of refractive index variation (Δn) considered, S_b assumes that the variation happens all over the cover while S_s assumes that it happens only near the waveguide surface. Since the dimensions of the features are very small, I do not take in account any refractive index variation between periodic blocks, assuming the analytes will not “fit” inside.

2.5.2 Quality Factor

The quality factor (Q) is a dimensionless variable defined as the ratio of the time-averaged energy stored in a cavity to the energy loss per cycle of propagation⁷⁹:

$$Q = \omega_r \frac{U}{P_d} \quad (2.14)$$

Where U denotes the stored energy, P_d is the dissipated power and ω_r is the particle's angular frequency, which is also the resonance frequency of the cavity. From equation 2.14 it is possible to derive two other alternative forms for Q ⁸⁰:

$$Q = \omega_r \frac{\tau}{2} \quad (2.15)$$

$$Q = \frac{\lambda_r}{\Delta_{FWHM}} \quad (2.16)$$

The τ parameter of equation 2.15 is the number of cycles necessary for the energy inside the cavity to decay by a factor of $e^{2\pi}$. Equation 2.16, however, comes directly from the frequency response of the cavity and is the most common expression for the quality factor. λ_r is the resonance wavelength and Δ_{FWHM} the fullwidth half maximum (FWHM) of the frequency response, the Lorentzian curve, as in figure 4.

Despite being defined for a mode confined in a light cavity, the quality factor concept can be expanded for quasi guided modes as well. In this context this parameter expresses the sharpness of the resonance peak observed in the response spectrum of the waveguide. The higher it gets, the easier the detection of a change in the mode's frequency, since the response shift becomes more evident.

Metal-based waveguide's modes, like the LSPR and even the SLRs, usually exhibit smaller Q (broader resonances) compared to dielectric quasi guided modes, due to their high absorption (large negative part of the electric permittivity). This way, dielectric based sensors tend to be an easier to use detection tool than their metal counterparts.

2.5.3 Figure of Merit

A good sensitivity allows to detect very small variations of refractive index, while a good Q allows to distinguish very small variations of the resonance wavelength. If a sensor has a very high sensitivity but small Q , the resonance shift will not be noticed. If it has very high Q and small sensitivity, the resonance will barely shift. The FOM captures both effects by dividing the mode sensitivity by the resonance width, representing a good balance between both factors⁸¹:

$$FOM = \frac{S}{\Delta_{FWHM}} \quad (2.17)$$

This parameter relates both the resonance sensitivity and its sharpness, this way, the FOM is a very important parameter to compare different sensor's architectures.

3 STATE OF THE ART OF PHOTONIC BIOSENSING DEVICES

In this section I review the current state of the art of photonic biosensors, which are a powerful tool for many applications in biomedical research, healthcare, pharmaceuticals, environmental monitoring, homeland security and the battlefield⁸². They offer advantages over other sensing technologies such as electrochemical, thermometric, piezoelectric or magnetic biosensors, exhibiting lower noise and being less susceptible to electromagnetic interference⁸³.

More specifically, silicon photonic biosensors can detect and monitor in real time trace amounts of biomolecules (antibodies and proteins), without needing to label the molecules (label-free operation)^{84,85}. They detect the variation of the refractive index caused by the analyte (the molecules, in this case) binding to the receptor biomolecules on the surface of the sensor. This method of interrogation is one of the most successful and commonly used up to this date, due to its ease of use and low cost.⁸⁶ They also have good mass scale production potential and can be integrated with electronic devices due to being compatible with the silicon-on-insulator (SOI) technology⁸⁷.

There are multiple aspects in biosensing, such as transduction signal generation (analyte recognition quality), fluidics design (sample injection and drainage), surface immobilization chemistry (analyte capture efficiency), analyte detection format and data analysis⁸⁷. The focus of this dissertation is on the first aspect, more specifically, the optical structures and their interactions with the analyte.

A lot of recent effort has been dedicated to improving the sensitivity of the biosensor, leading to various sensing architectures and optical structures⁸⁸. The architectures can be broadly grouped into two distinct configurations: interferometric and resonant. In the interferometric architecture one detects an optical phase shift between a reference wave and the wave propagating through the medium exposed by an analyte, e.g by evanescent sensing⁸⁶. Resonant architectures detect the wavelength shift of the mode after contacting the analyte and are more suitable for applications that require simultaneous measurement of many different reactions⁸⁹ or that work with small concentration of analyte, such as in single molecule detection⁹⁰. Their sensing mechanism is similar to an optical cavity, as discussed in the last chapter. They are the most relevant type for this dissertation and will be reviewed in the next paragraphs.

I begin by showing a review of sensors based on silicon waveguides, which have been extensively studied over the last decade,^{77,78,91,92} in table 1. The reader must notice that these modes are fully guided, meaning that they are not accessible by a simple normal external plane wave excitation. This is an important drawback of these systems, as the

mode excitation require fine waveguide alignment, thus resulting in higher complexity.

Table 1 – Different basic silicon waveguide geometries used in resonant biosensors architectures. The resonant frequency is around 1550 nm for all the given sensitivities. The bulk waveguide sensitivity is a theoretical value used mostly as a reference parameter.

Architecture	Sensing Mechanism	Sensing Data Sb in [nm/RIU]
<p>Bulk Waveguide</p>	<p>Simplest form of a waveguide. The evanescent field senses the change of refractive index. Mostly used as a reference parameter.</p>	<p>Sb = 340⁹¹ $Q = \infty$ FOM = N/A</p>
<p>SWG Waveguide</p>	<p>Periodic structures operating in the subwavelength regime. The evanescent field around the periodic yellow blocks senses the change in the refractive index</p>	<p>Sb = 579⁹³ $Q = 1500$ FOM = 556</p>
<p>Bragg gratings</p>	<p>The grating acts as a Fabry Perot cavity. The presence of the analyte changes the refractive index of the system, changing the response peak/dip of the transmission/reflectance spectrum.</p>	<p>Sb = 182⁹⁴ $Q = N/A$ FOM = N/A</p>
<p>Disk and Ring Resonators</p>	<p>The waveguide interacts with a cavity through evanescent coupling. The cavity senses the presence of the analyte, changing the waveguide mode.</p>	<p>Ring Sb: 270⁹¹ $Q = 4500$ FOM = 784 Disk Sb: 142⁹⁵ $Q = 16000$ FOM = 1465</p>

Small changes to the architectures also improve the mode sensitivity. In slot

waveguides, for example, the waveguide core is separated into two rails by a low index slot⁹⁶. The mode's electric field concentrates within the slot, instead of being spread around the waveguide, and has the potential to offer a greater sensitivity than of its single rail counterpart. A slotted Bragg grating, for example, has a sensitivity of 340 nm/RIU,⁹⁷ 1.86 times greater than the conventional structure (182 nm/RIU).

Suspended waveguides substitute the substrate for a lower index material, such as water or air,⁹ with remaining pillars, from the former substrate material, "holding" the waveguide in its original position. This method has been reported to slightly increase the sensitivity of ring resonators^{91,98} and SWGs.²⁰

More advanced configurations have been extensively studied and mixed models have emerged. For example, SWG silicon waveguides shaped as a ring resonator achieves a sensitivity of 490 nm/RIU,⁹⁹ higher than the former simple strip ring resonator (270 nm/RIU).

Although not necessarily made of silicon, SPR-based biosensors are worth mentioning since they offer the greatest sensitivities, typically thousands of nm/RIU^{78,92} and remain the state-of-the art technology up to date.⁷⁷ The reader must also keep in mind that any metal-based biosensor will be susceptible to ohmic losses, intrinsic to the metals.

Even though the aforementioned sensors do possess higher Q values as compared to QGMs (as will be seen further in the text), they still require waveguide coupling. The coupling methods are usually complex²⁰, hampering the transition from laboratory to commercial applications. Dielectric QGMs, LSPRs and SLRs, on the other hand, can be accessed by external plane wave excitation and thus require a much simpler setup.

Despite of the myriad of configurations already suggested for LSPR waveguides such as spheres, rods, stars and prisms, there are still some challenges yet to be surpassed, mainly regarding the low Q and poor spectrum of these modes.^{100–102} Even grating-coupled SPRs, which can sense single cell secretion¹⁰³ and perform simultaneous detection of two distinct analyses¹⁰⁴ with a sensitivity of 671 nm/RIU are still hindered by a signal amplitude of less than 10% of the source and a poor Q of only 30⁷².

This poor performance of the Q is partially improved with the use of SLRs, which have already reported Q s dozens of times greater than those of SPRs and LSPRs¹⁰⁵. This improvement, however comes at the expense of reduced sensitivity, which tend to scale inversely with the Q ²². When the electric field of the mode is well confined within the metal grating, the Q is high. However, the evanescent part of the field outside the core is small and, consequently, its sensitivity is also low. If the electric field has a high evanescent field outside the block, it is the other way around.

Quasi guided mode resonances, also referred to as Guided Mode Resonances (GMRs) in the literature, show promising performance, in terms of the resonance quality factor,

over the plasmonic resonances. They have been extensively studied, with different materials being used to fabricate these structures, such as silicon (Si), silicon nitride (SiN_3), silicon dioxide (SiO_2), and Epoxy (EP)^{22,106–112}. The reported quality factor of these waveguide's modes are hundreds of times greater than those of LSPRs and SPRs and one order of magnitude greater than those of SLRs (see table 2).

Silicon GMRs, in special, are already a promising technology, offering cost-effective fabrication process, easy integration on a chip and capacity to control the resonant wavelength by design (e.g. going from visible to near infrared regime). They also offer competitive sensing parameters compared to those of LSPRs, SPRs, SLRs and even GMRs of other dielectrics⁹¹.

Unfortunately, most of the dielectric GMRs, as the SLRs, up to date show either a high Q or high sensitivity, but not both²². The exception to this limitation is the slotted photonic crystal¹⁰⁶. However, due to the small slot size (200 nm), the detection speed is compromised as a result of the slow mass transport rate of the analytes diffusing through the channel. Besides adding another step of fabrication (making the slot), they also require delicate alignment from the free space to in-plane waveguide²².

Table 2 summarizes the comparison of the performance of biosensors based on waveguides with modes accessible to external wave excitation, along with their pros and cons.

Table 2 – Reported performance of waveguides with modes accessible to external plane wave excitation. The sensitivity is measured by following the resonance shift of the reflectance spectrum after the addition of an analyte.

Architecture	Sensing Parameters	Pros and Cons
<p>LSPR</p> <p>Au. nanostar immersed in water</p>	<p>Sb: 665 nm/RIU</p> <p>Q: 6.2</p> <p>FOM:54</p> <p>^{102,113}</p>	<p>PROS:</p> <p>High sensitivity; Low Fabrication cost; Easy Integration</p> <p>CONS:</p> <p>Low amplitude of signal; The bigger the particle, the lower the sensitivity.</p>

Table 2 continued from previous page

SPR (Grating coupling) Holes in Au. film on hybrid SiN and Glass substrate	Sb: 671 nm/RIU Q: 30 FOM: 42 ⁷²		PROS: High Sensitivity; Easy fabrication techniques. CONS: Low Q; Low amplitude of signal.
SLR (Metallic grating) 2D: 1D:	Case 1 (2D) Au. Grating on Glass Sb: 320 nm/RIU Q: 517 FOM: 184 ¹⁰⁵	Case 2 (1D) Au. Grating on SiO_2 Sb: 481 nm/RIU Q:68 FOM:36 ¹¹⁴	PROS: Higher Q than LSRPs and SPRs; Great sensitivities when coupled to interferometric architectures. ¹⁰⁵ CONS: Lower Sensitivities than LSPRs and SPRs; Q tends to scale inversely with the sensitivity.
GMR (Dielectric Grating) 2D:	Case 1 (2D) Si. Grating on SiO_2 Sb: 264 nm/RIU Q: 2828 FOM: 486 ²²	Case 2 (1D) Si_3N_4 Grating on SiO_2 Sb: 147 nm/RIU Q:1100 FOM: 192 ²¹	PROS: Cost effective fabrication process; Possibility of very high Q; Mass scale fabrication potential (SOI only).

Table 2 continued from previous page

<p>1D:</p>	Case 3 (1D)	Case 4 (2D)	<p>CONS:</p> <p>Quality factor tends to scale inversely with the sensitivity.</p>
	EP. Grating on EP. w/ TiO_2 coating	Suspended SiN_x Grating on Glass	
	Sb: 290 nm/RIU	Sb: 571 nm/RIU	
	Q: 300	Q: 126.5	
	FOM:101	FOM: 85	
	107	112	

Silicon GMRs are particularly interesting due to their potential to contribute to the improvement of both quality and affordability of label free PoC devices. They are easy to use, robust, and compatible to SOI fabrication. This process has already shown potential to mass fabrication of GMR sensors costing less than US \$1 per 1mmx1mm chip²¹. It is, therefore, a suitable technology even for undeveloped countries. It also exhibits the greatest FOM compared to the other dielectric biosensors with modes accessible to a simple normal external wave excitation.

However, silicon GMRs overall sensing properties are still lower than their fully guided versions and the metal-based waveguides. Therefore, it is of utmost importance to enhance the sensitivity of these modes, without compromising their main advantage over the others, which is the ease of detection, deeply related to the quality factor.

3.1 Motivation of the research project

The main motivation of this project is to find design strategies to improve the performance of GMR structures, especially its Q factor. The option of the GMR is due to its simplicity and compatibility with low-cost systems. The central idea is to design structures that benefit from the high performance of fully guided modes and yet can be easily assessed by external plane waves. The main idea is outlined in this section.

It has been shown that perturbations on the SWG period opens diffraction channels²³. This can be done by grouping up two consecutive blocks, thus creating a new periodic pattern, as seen in figure 18.

Figure 18 – Example of perturbation of the periodic of a 2D SWG. Just the cross section is showed. The period of the new structure is doubled, compared to the previous one.

The diffraction pattern is dependent on the Fourier Series of the periodic structure, which is perturbed in the new configuration, thus generating new components. These new Fourier components relate to new propagating waves inside the periodic structure (Bloch modes) that might be eventually excited by external light. Hence, by perturbing a SWG, one can, in theory, access its modes externally. They will remain similar to the non-perturbed modes, as long as the modification to the geometry is small, meaning they will maintain their high sensitivity.

This process can be easily understood by simply analyzing the mathematical form of a mode at the band edge of its band diagram (which relates the Bloch modes' propagation constants to their frequencies), as shown in figure 19a. According to equation 2.7, this mode will have its main modal field component A of the following form:

$$A(y, z) = A(z)_{-1}e^{-i\frac{G}{2}y} + A(z)_1e^{i\frac{G}{2}y} \quad (3.1)$$

where $G = \frac{2\pi}{\Lambda}$ denotes the structure's periodicity and the Fourier Series was truncated at $m = 1$ for simplicity's sake. The perturbation essentially doubles the period, thus folding the band-edge point into the $k = 0$ (gamma point)²³ of the band diagram, as shown in figure 19b. The band-folding now introduces a radiating component in the Bloch mode, labelled by the sub-index 0 below:

$$A'(y, z) = A'(z)_{-1}e^{-iG'y} + A'(z)_0e^{-i0y} + A'(z)_1e^{iG'y} \quad (3.2)$$

where $G' = \frac{2\pi}{2\Lambda} = \frac{G}{2}$ is the new periodicity. Notice that, apart from the $A'(z)_0$ term, equations 3.1 and 3.2 are exactly the same. Therefore, the band-folding couples the fully-guided Bloch mode to radiating modes, thus providing access by external plane wave excitation. Notice that the amplitude of the $A'(z)_0$ is dependent on the degree of perturbation, which allows a convenient design path to control the coupling and, hence the Q .

Figure 19 – Band diagram of a single period (a) and perturbed (b) SWG structure. The y-axis represents the frequency and the x-axis the propagation constant. The lightline (straight blue line), which separates the coupled modes (above region) and the fully guided modes (below region), is shown for better analysis. The band folding, or simply the duplication of the period, “brings” the mode within the guided zone at the band’s edge to the central axis ($k = 0$, the gamma point), where it couples to radiating modes. The dashed lines on (b) represents the band diagram of the unperturbed mode.

This work proposes to study the relationship between the perturbation of SWG structures and their modes' sensing characteristics, always comparing it to the unmodified version. In particular, the relationship between the Q and spatial perturbation will be quantified, thus shedding light on the feasibility of the design strategy. Furthermore, 2D and 3D structures are also compared, to determine whether there is any meaningful gain in using 3D structures over their simpler 2D versions.

4 IMPACT OF THE FIELD CONFINEMENT ON THE MODE'S SENSING PERFORMANCE

In this chapter I investigate the performances of both 2D and 3D silicon based periodic waveguides, aiming to understand the properties of both configurations. I focused mainly on the performances' analyses of SWGs, since their modes promise high sensitivities. I also compare these modes with 2D GMRs, aiming to critically compare performance and complexity of these two systems. The spatial distributions of the modes' fields contained in the next sections were computed using COMSOL Multiphysics Eigensolver.

4.1 2D SWG AND GMR

I begin by characterizing the sensitivity of both TE and TM modes of a 2D silicon SWG and GMR. The structure consists of a silicon ($n = 3.5$) periodic core on a SiO_2 substrate ($n = 1.45$) immersed in water (cover $n = 1.33$), as seen in figure 20, with geometric parameters labeled as follows: height (H), period (Λ) and Fill Factor (FF).

Figure 20 – Schematic of a 2D silicon periodic waveguide.

The parameters of analysis were chosen based on previous results in the literature for a mode wavelength of 1550 nm, common for mid-infrared applications²⁰. Two typical heights were chosen for analysis: 156 nm and 260 nm. Both values were taken from the literature, the first one is found for GMRs²¹ and the second one for SWGs²⁹. The periods were adjusted to guarantee operations in the two different regimes: deep-subwavelength (characterising SWG regime) and subwavelength (characterising GMR regime). For the SWG, a period $\Lambda = 250$ nm was chosen, following^{20,29,93}.

The period for the GMR is chosen from the dispersion curve of the equivalent slab waveguide ($FF = 1$) in order to maintain the mode wavelength at 1550 nm. Assuming a normal incidence of light on the surface to excite the quasi guided mode, one can set the

period of the grating using equation 2.6 from chapter 2:

$$\Lambda = \frac{2\pi}{\beta_s} \quad (4.1)$$

where β_s is the value of the propagation constant of the slab waveguide mode at the desired wavelength. Figure 21 shows the dispersion curve of both TM and TE modes for the chosen heights, along with the necessary period of the periodic waveguide to excite a QGM at 1550 nm under normal light incidence. The curves were generated by solving the transcendental equation of the slab waveguide¹⁵ using MATLAB.

Figure 21 – Dispersion curve of the equivalent slab waveguide of the periodic structure of figure 20. The abrupt decayment of the blue curve of the TM mode graph (right) is due to the disappearance of the guided mode for higher wavelengths.

After setting the waveguides' parameters, I compared the sensitivities of their modes. To compute the sensitivity of the mode, one must find the associated wavelengths of the modes for different cover media, and then analyze the relation between the change of the mode's wavelength and cover's refractive index. The computational window used in the simulations is illustrated in figure 22, along with its boundary condition.

Three Eigenfrequency simulations are necessary to calculate the mode's bulk and surface sensitivity of a given geometry: the first one gives the wavelength of the mode with an unaltered cover medium (water $n_c = 1.33$); the second one provides the new resonant wavelength assuming a change of $\Delta n = 0.01$ of the entire cover medium, while the last one assumes this variation just inside the surface area. With this data, one can calculate both bulk and surface sensitivities of the mode using equation 2.13. From the simulations, the mode sensitivity dependence on the structure's FF was extracted, as shown in figure 23 .

Figure 22 – Computational widow used in the 2D SWG and GMR simulations. The periodic boundary condition was used on its side walls, and the scattering boundary condition on the top and bottom limits. The region of the refractive index change for the surface sensitivity calculation is highlighted.

Figure 23 – Sensitivity of the mode of different 2D SWGs and GMRs. The legend informs the parameters of the simulation, in nanometers. The type of sensitivity (bulk or surface) is detailed at each title.

Both SWG and GMR TM and TE modes presented higher sensitivities than their

uniform ($FF = 1$) counterparts for at least some values of FF , confirming that there is an advantage in using a periodic waveguide. The SWG TM mode sensitivity dependence exhibited an inversed U-shaped like curve, with maximum bulk sensitivity of 455.7 nm/RIU ($FF = 0.4$ of red-asterisk curve) and surface sensitivity of 27.41 nm/RIU ($FF = 0.6$ of the red-asterisk curve). The first one is just a bit short of the greatest sensitivities reported for SWGs, which are around 500 nm/RIU⁹³ (the sensitivity of 575 nm/RIU reported in chapter 3 is from a more complex over-etched version). Notice an interesting feature for TM SWG modes: the bulk and surface sensitivities peaked for the taller structures (260 nm compared to 156 nm), which is somehow unexpected, since a taller structure has a more strongly confined mode.

The TE modes, however, exhibited the highest sensitivity for the smallest FF , with an inverse relation between both parameters, achieving maximum bulk sensitivity of 367.7 nm/RIU ($FF = 0.2$ red-asterisk curve) and surface sensitivity of 12.11 nm/RIU ($FF = 0.5$ green-cross curve), smaller than the TM modes' highest sensitivities. The curves of the GMR TE modes stop at $FF = 0.5$, this happens because there is no propagating mode at the wavelength of 1550 nm for the geometries with smaller FF s.

It is important to notice that the curves of the GMRs followed the trend of the SWGs, with smaller sensitivities for TM modes and, surprisingly, even higher surface sensitivities for TE modes. However, despite exhibiting higher surface sensitivities than their fully guided version, the TE GMRs' sensitivities are still more than two times smaller than those found for TM modes. The surface and bulk sensitivities' curves exhibited slightly different patterns, especially for the TM modes. The maximum value of the bulk sensitivity of the red curve, for example, occurs for $FF = 0.4$ while the surface sensitivity has its maxima at $FF = 0.6$. This happens because the surface sensitivity does not consider a difference of refractive index on its side walls, differently from the bulk sensitivity, as showed in figure 17.

In order to understand better the behaviour of the sensitivities, the electric field intensity distribution is displayed for both TM and TE SWGs, as seen in figure 24. The SWG was chosen in this analysis because their fully guided nature offers a cleaner interpretation.

Figure 24 – Normalized electric field intensity distribution of some of the 2D SWG modes.

For the TE modes, it becomes clear that the spreading of the electric field intensity outside the silicon core, as the FF shrinks, is responsible for the increase of the sensitivity. However, they remain highly concentrated inside the silicon core, even for low FF s, which limits their sensitivities. TM modes, however, exhibit highly concentrated electric field on the surface of the silicon core for all FF s. When the FF shrinks, there is a decrease of the field intensity inside the core, meaning that the electric becomes more confined on the top and bottom surface of the silicon core, explaining the surface sensitivity increase for FF s lower than 1. However, it starts to decrease for $FF < 0.6$, because the surface of the silicon core also shrinks, resulting in a smaller highly concentrated electric field area in contact with the sensing area. Thus, the highest sensitivity is achieved by balancing the energy of the electric field outside the core and the size of its surface.

The TM SWG showed higher bulk and surface sensitivities than their respective QGMs, while the TE SWG exhibited higher bulk sensitivity, but a slightly lower surface sensitivity. This overall better performance in terms of sensibility of the SWGs over the GMRs is in accordance with the literature, as seen in tables 1 and 2.

4.2 3D SWG

In this section I proceed to characterise the sensitivity of 3D SWG, as represented in figure 25. The 3D SWG can be intuitively contrasted with the 2D SWG by noticing that, while the latter is formed by corrugating a slab waveguide, the former is formed by corrugating a ridge waveguide. The simulations necessary for the 3D SWG are already very time-consuming and, therefore, I did not characterize any 3D GMR (which, due to the longer period, would be prohibitively time-consuming). The waveguides are the

3D versions of the previous study: a silicon ($n = 3.5$) periodic core on a semi-infinite SiO_2 substrate ($n = 1.45$) immersed in water (cover $n = 1.33$), as seen in figure 25, with geometric parameters as follows: height (H), period (Λ), Fill Factor (FF) and width (W).

Figure 25 – Schematic of a 3D silicon SWG.

The period chosen for analysis was of $\Lambda = 250$ nm. As before, it follows the literature^{20,29,93} and guarantees a deep-subwavelength regime for a wavelength of 1550 nm. The used height values were the same as in the last section: $H = 260$ nm and $H = 156$ nm. As for the width, I chose, at first, 250 nm and 350 nm, also based on the literature.^{29,93} Just like in the last section, the sensitivities of the modes of these structures were determined by analysing the difference of their wavelengths with the change of the cover's refractive index (first water, and then a $\Delta n = 0.01$ of refractive index). The computational window for these simulations is illustrated in figure 26. The surface sensing area is the region, above the periodic blocks, as seen in figure 26.

Figure 26 – Computational window used in the 3D SWG simulation.

Although the symmetry of the problem does not allow pure TE and TM modes,

the mode's field distributions can be grouped in two distinct groups: quasi-TE (qTE) and quasi-TM (qTM) modes (analogous to ridge waveguides). These modes maintain some similarities to their 2D counterparts. A qTE mode propagating in the Z-Y plane in the waveguide of figure 25, for example, would have its electric field intensity mostly concentrated in the x component, while the qTM mode would have its magnetic field intensity mostly concentrated in the x component. Figure 27 shows the dependence of the sensitivities of these modes on the FF for different geometry configurations.

Figure 27 – Sensitivity of the mode of different 3D SWGs. The legend informs the parameters of the simulation, in nanometers.

Comparison between figure 23 and figure 27 manifests an important feature, which has not been noticed in the literature yet: it shows that the sensitivity is enhanced in the 3D SWG with respect to the 2D only for TE modes. Indeed, one would expect that the increased surface area of 3D SWG would improve the sensitivity for both modes. The results show, however, that TM modes do not benefit from the more complex 3D structures. This happens because the electric field of the TM mode is already concentrated on the waveguide's surface.

These results also reinforce the need of analysing the sensing performance of the modes in terms of both bulk sensitivity and surface sensitivities. Differently from the 2D SWG, in 3D SWG the geometry that offers the highest bulk sensitivity is not translated into the highest surface sensitivity. This happens due to the region that suffers the refractive index change for both situations and can be better understood by analysing the qTM modes of the 3D SWG represented by the green-cross curve and black-diamond curve of the graphs presented in figure 27, as illustrated in figure 28.

Figure 28 – Normalized electric field intensity distribution, in the plane (Z-X) perpendicular to the propagation direction, of the qTM modes for a 3D SWG with $\Lambda = 250$ nm, $FF = 0.8$, $H = 260$ nm and with the following width configurations: 250 and 350 nm. The modes' sensitivities are also shown.

The electric field of the structure with $H = 260$ nm and $W = 250$ nm (black-diamond curve) is concentrated on the the vertical side walls, while the field of structure with $H = 260$ nm and $W = 350$ nm (green-asterisk curve) is concentrated on the horizontal side walls. This difference explains why the former has a higher bulk but lower surface sensitivities than the latter. As the region of change in the refractive index considered in the surface sensitivity is mainly on the top surface of the silicon blocks, the contribution of the electric field on the vertical side walls of the block is not greatly affected, hence providing worse surface sensitivity than an electric field concentrated on horizontal surface.

The qTM mode exhibited a maximum bulk sensitivity of 487.4 nm/RIU (black-diamond curve $FF = 0.9$), a bit higher than its 2D counterpart, and maximum surface sensitivity of 28.03 nm/RIU (green-cross curve $FF = 0.7$), almost the same as before (27.41 nm/RIU), indicating a very small overall sensitivity gain over the 2D configuration. Since these values are close to the ones in the best reported SWG waveguides I decided to focus on the 3D qTE modes.

The first thing to notice about the sensitivity of qTE modes is the fact that they exhibit the inversed U-shaped like curve for most of the geometry configurations, differently from the 2D TE case. This effect can be understood by analysing the electric field intensity distributions showed in figure 29. When the $FF = 1$ the electric field intensity distribution on the surface of the waveguide block is most concentrated outside the sensing area (black rectangle). When the $FF = 0.6$, part of the highly concentrated electric field that was previously outside the blocks enters the sensing area, thus increasing the sensitivity.

However, when the FF is further diminished, the electric field on the surface of the block starts leaving the sensing area once again, decreasing, then, the sensitivity. This behaviour is somewhat similar to the one observed of the TM modes, as seen in figure 24.

Figure 29 – Normalised electric field intensity distribution of different qTE modes for various FF . The surface sensitivity of these modes is also displayed. The surface sensing area is shown by the black rectangle.

The qTE modes exhibited a max bulk sensitivity of 476 nm/RIU (green-cross curve $FF = 0.6$) and a surface sensitivity of 24.52 nm/RIU (black-diamond curve $FF = 0.9$). These values are already considerably higher than those found for the TE modes of the 2D periodic waveguides. Unfortunately, this sensitivity was obtained for a FF of 0.9, which indicates that the space between the periodic blocks must be of $250 \cdot (1 - 0.9) = 25nm$. This is a very challenging size feature for fabrication and it would be better if the geometry presented a FF between 0.4 and 0.7.

The qTE modes exhibited increasing surface sensitivity for either higher or lower width values depending on the height value, indicating that there is room for further improvement by changing this parameter. For $H = 260$ nm, the surface sensitivity increased when the W decreased, as reported in previous works²⁰, and for $H = 156$ nm it was the other way around. The optimization of the H for sensitivity, however, will be further explored in the next chapter.

4.3 2D periodic waveguide fabrication feasibility

From the results of the last two sections it became clear that there is a gain from adding one more dimension to the geometry just for the sensitivity of TE-like modes. If TM-like modes are desired, then the 2D SWG provides a very close sensitivity to that of the 3D configuration. However, it is impossible to actually fabricate a 2D SWG, since it possesses an infinite dimension. What can be done, however, is to increase the 3D SWG width until it behaves like its 2D version. In this section I determine this minimum width by increasing the width of the structure and checking the effective index of the propagating mode. This can be seen in figure 30, where the minimum width of the best performing 2D SWG TM mode was determined.

Figure 30 – Dependence of the effective index of the mode of a 3D SWG on the width of the block (W). The parameters are as follows: $\Lambda = 250\text{nm}$, $H = 260\text{ nm}$, $FF = 0.7$. W_∞ denotes the equivalent 2D geometry.

The graph from figure 30 shows that the 3D SWGs supports almost the same modes as their 2D counterparts for widths above 1500 nm for qTM modes and above 3000 nm for qTE modes. The higher saturation length of the width of qTE modes is due to the direction of its electric field: the predominant component of the qTE mode is the x component while for the qTM mode the predominant component is in the Z - Y plane. Thus, qTE modes are more sensible to corrugations in the x direction. Finally, the point of saturation for the 3D structures also provides a first estimate of the spatial resolution of the sensor.

5 BLOCH MODE ENGINEERING IN BAND-FOLDED SWG STRUCTURES

In this chapter, the band-folding strategy to engineer Bloch modes is described and applied to refractive index sensing. In the first section, the relationship between geometric perturbation, Bloch mode amplitudes and the respective Q s are quantified in a band-folded SWG. In the subsequent sections, the characterization of 2D (TE and TM modes) and 3D (qTE only) perturbed SWG structures is shown. The 3D analysis will be made only for qTE modes because, as it was observed in chapter 4, 3D geometries are only beneficial for them. The reflectance spectra were obtained using a RCWA code implemented in our group. All other simulations presented in this chapter were made using COMSOL Multiphysics with the periodic boundary conditions presented in chapter 4.

5.1 Band folding and perturbation of the SWG periodicity

To establish the relationship between geometry and mode properties, it is convenient to define the perturbation parameter as the displacement of the ridge center of the perturbed structure with respect to the unperturbed one, as illustrated in figure 31. Note that this definition applies to both 2D and 3D configurations.

Figure 31 – Definition of the perturbation parameter $Pert$: the distance between the ridge center of the unperturbed SWG to the ridge center of the block of the perturbed structure.

The perturbation parameter affects the relationship between the Bloch mode amplitudes, as defined in equation 3.2, but reproduced below for convenience:

$$A(y, z) = A(z)_{-1}e^{-iGy} + A(z)_0e^{-i0y} + A(z)_1e^{iGy}$$

where $G = \frac{2\pi}{\Lambda_{Pert}}$ is the new periodicity and $A(z)_n$ the Bloch mode amplitudes. From now on, the dependence on z will be omitted for the sake of simplicity. Notice that, for

subwavelength periods, $G > k_0$, which means that the A_1 and A_{-1} components are non-radiating. Therefore, the coupling of the Bloch mode with external radiation is mediated by the A_0 component: the smaller this component is, the more confined (less leaky) is the Bloch mode. The magnitude of A_0 , on the other hand, is dependent on the perturbation parameter ($Pert$): e.g., if $Pert = 0$, then the Bloch mode is fully guided, meaning that $A_0 = 0$. Such feature offers an easy and convenient route to control the resonances Q via the perturbation.

The relationships between perturbation, quality factor, and Bloch mode components of a 2D SWG, illustrated in figure 32a (also used in chapter 4), are quantified in figure 32b. The geometric parameters are as follows: period of 250 nm, height of 260 nm and FF of 60%. The cover is water ($n_c = 1.33$), the waveguide core is silicon ($n_{wg} = 3.5$) and the substrate is SiO_2 ($n_s = 1.45$). The Bloch mode components are extracted by calculating the Fourier series of the Bloch mode obtained using COMSOL, with the same boundary conditions used in figure 22, and considering a TM plane wave excitation at perpendicular incidence. Due to the structure symmetry and perpendicular excitation, the magnitudes of A_1 and A_{-1} are the same. In the limit of $Pert = 0$, the period is halved and so $A_0 = 0$. The Bloch mode is then fully guided, resulting in an infinite Q . The mode radiation losses increase monotonically with the perturbation, thus decreasing the ratio $|A_1/A_0|$ (blue line), and consequently decreasing the Q (black line). When the perturbation is 50 nm, the SWG becomes a conventional (unperturbed) GMR with period $\Lambda_{pert} = 500$ nm, and $Q < 10$ (not shown in the graph). The range of Q s with perturbation between 5 and 10 nm, which are accessible experimentally, quantifies the gain in quality factor that can be obtained with this strategy. From figure 32b, it is seen that the Q -factor can be increased by more than two orders of magnitude as compared to the $Q < 10$ of the GMR structure.

Figure 32 – a) Schematic of the standard unperturbed 2D SWG structure used for the analysis; b) Influence of the perturbation distance ($Pert$) on the Q s and Bloch mode components of TM modes (normal incidence was considered). The Bloch mode components (A_0) and (A_1) were extracted by computing the Fourier components of the main component field (H_y) at the center of the waveguide; c) Examples of the Fourier Series of the main component field (H_y) at the center of the waveguide for different perturbation cases (P1,P2,P3), including the non-perturbed case (P0); d) Reflectance spectra of the highlighted perturbed cases under excitation of a normal plane wave.

The Fourier series of the Bloch mode at four different perturbations are shown in figure 32c. The x-axis labels the n -component of the Bloch mode. As expected, the $n = 0$ component vanishes when the perturbation is zero (P0), resulting in a fully guided Bloch mode. The contribution of the $n = 0$ component, however, increases monotonically with the perturbation. Such Bloch mode engineering allows an easy access to manipulate the sharpness of the resonances, as shown in figure 32d. Notice that the perturbation also affects the resonance wavelength. This effect is investigated in more detail in section 5.2 of this chapter. Also, the mode is now at $\lambda_0 \sim 1045$ nm instead of 1550 nm, as reported in chapter 4. This happens because the mode at the band edge of the SWG is not located at 1550 nm, but rather at 1045 nm. Although not shown here, the analysis for the TE mode exhibits an analogous behaviour.

The next step is the characterization of these perturbed structures in terms of mode sensitivities and in terms of tolerance to fabrication errors. These are the main subjects of the next section.

5.2 2D Perturbed band folded SWGs - TM and TE modes

To study of the sensitivity of perturbed band-folded SWGs, structures different than those analysed in chapter 4 were used, because their modes were not at the band edge of their band diagrams. Instead, SWGs with band-edge modes around $\lambda_0 = 1300$ nm were investigated, since they have shown one of the highest sensitivities in the simulations. Notice that the materials used for the waveguide core, substrate and cover medium remain the same (as shown in figure 32). Although the analysis is theoretical, fabrication feasibility has been considered in the design of the structures and thus constrained the range of geometric parameters, as discussed in the next paragraphs.

One important fabrication constraint is that the fill-factor (FF) should be neither too high nor too low, which could result in too small feature sizes, such as the distance between each consecutive ridges for high FF values, or high aspect ratios (relation between the ridge height and length), as observed for low FF values. Besides these fabrication constraints, it is also interesting to keep the FF small to increase the range of perturbation values that can be applied to the SWG. Therefore, I opted to use FF values between 40% and 60%. Within these constraints it is safe to assume that the presented structures are amenable to fabrication.

As to the height (H) values, they should not be much higher than the ridge length (L) of the SWG block, so as to maintain feasible aspect ratios. For example, if the core block has a ridge length of $L = 100$ nm, the standard Reactive Ion Etching (RIE) etching process is not capable of fabricating it with a height of $H = 1000$ nm.¹¹⁵ For this reason, I decided to keep the structures limited to an aspect ratio between H and L of 2.5, which has already proven to be feasible in fabricated structures using similar materials [^{115,116}]. As for the period of the structures, it was adjusted for each combination of FF and H to keep the resonance wavelength at $\lambda_0 = 1300$ nm. The comparison between the structures is made in terms of the modal effective index, which is a parameter commonly used for the analysis of photonic waveguides and allows a more qualitative comparison between different structures.

As the first step, a slightly perturbed SWG waveguide is investigated to find the effective index that optimizes its sensitivity, using the height as the tuning parameter. Both TM and TE polarizations are considered, with fill-factors of $FF = 60\%$ (TM), and $FF = 40\%$ (TE and TM), as shown in figure 33. The difference between the FF s is accounted for by fact that TE modes exhibit better sensing performance for lower FF values, while the TM mode showed better sensitivity results for more intermediate FF s, such as 60% (see section 4.1). The additional TM mode study for $FF = 40\%$ will be helpful for a further analysis. The sensitivity dependence on the effective index is shown in left column of figure 33 (a and b), while the right column shows the Q (c and d) variation.

It can be seen from the sensitivity graphs of figures 33a and 33b that both TM and TE modes feature an optimum effective index for the surface sensitivity (black curves), but the TE bulk sensitivity (orange color) increases monotonically with the effective index. Notice that the sensitivities for the TM mode are always higher than for the TE mode, which is accounted for by the strong concentration of electric field in the surface that is characteristic of TM modes. Importantly, the optimum points for bulk and surface sensitivities do not coincide, which highlights the importance of including surface sensitivity in the characterization of these photonic structures.

Figure 33 – Sensitivity (a and b) and Quality Factor (c and d) dependence of slightly perturbed SWG modes on their respective effective indexes. The height varied between 120 and 350 nm for TM modes and 160 and 450 nm for TE modes. The FF of the corresponding structure of each curve is displayed in the legend. The perturbation distance used for the perturbed SWG structures was 5% and 2.5%, respectively for TM and TE modes, of the respective structure's unperturbed period. The highlighted cases of effective indexes, with geometries shown in the drawn table (e), will be useful for further analysis.

The presence of an optimum point (case 0) in the surface sensitivities of both TE and TM modes can be understood in terms of their field confinements: there is a specific field confinement where its evanescent part interacts most strongly with the analyte, as discussed in chapter 4. As the confinement strengthens or weakens beyond its optimum point, i.e., the effective index increases or decreases, the surface sensitivity will be negatively affected since the field will lose “touch” with the analyte by either concentrating towards the waveguide (if confinement is increased) or overpassing the analyte (if confinement is

decreased).

The Q s of the perturbed structures, presented in the graphs from figures 33c and 33d, shows an interesting result: the increase of the effective index does not necessarily leads to a higher Q ; in other words, a stronger confinement does not necessarily result in a higher Q . Although this was observed for the TE modes, as showed in figure 33d, the TM exhibits the opposite effect (see figure 33c). The idea that a higher confinement leads to a better Q is quite common in the literature, but little attention is given to the fact that this is not necessarily always true, especially for TM modes, as showed here.

Now that both the sensitivity and Q of the perturbed SWG modes have been characterised, I move on to the FOM analysis, which is the main parameter to be considered for sensing optimization. Using the data from figures 33a and b, one can observe that TM modes with effective indexes smaller than the one that offer optimum sensitivity (case 0) shows potential for better FOM , since their Q s greatly improve due to the decreasing of the effective index, while TE modes with effective indexes higher than the one that offer optimum sensitivity shows potential for better FOM , due to the increasing Q . Even more, for TM modes, the structure with $FF = 40\%$ offered better Q (figure 33c while barely decreasing the surface sensitivity (figure 33a when compared to the one with $FF = 60\%$, indicating a possible gain in the FOM of the former. As discussed in the previous section, however, the Q is very dependent on the perturbation. For this reason, it is important to analyse the FOM dependence on the perturbation for a few classes of structures for different modal effective indexes. Figures 34 and 35 shows the analysis of three different such classes, which are highlighted in figure 33e as case 0, case 1 and case 2.

Figure 34 – TM mode analysis of different perturbed SWGs. The top-left (a) plot is the surface sensitivity variation with the increase of the perturbation parameter ($Pert$). The bottom-left (b) and top-right (c) plots are, respectively, the Q and FOM values of the modes for different perturbations. Finally, the bottom-right (d) plot shows the dispersion of the modes. The simple line blue curve (TM Case 0) relates to the perturbation of the optimum point found for the surface sensitivity in figure 3, the dashed red curve (TM Case 1) and the circle marked yellow curve (TM Case 2) relate to structures with geometric parameters tuned so the modes have smaller effective indexes.

The first important feature to be observed in figure 34a and figure 35a is that the small perturbations (up to 20 nm) do not significantly impact on sensitivities. In fact, the mode profile itself is essentially unaffected by the perturbation, with the electric field intensity distribution being practically unchanged (please see appendix B). The Q , however, is very dependent on the perturbation, as seen in figure 34b and figure 35b. One feature that is relevant to experimental viability is the Q stability against perturbations. Notice in figure 34b that the Q of the structure case 0 (which is the optimum point for sensitivity) features a sharp drop as the perturbation increase, while the drop for cases 2 and 3 is much smoother. Furthermore, case 1 and case 2 have higher Q s across the perturbation range, thus resulting in a larger FOM , as shown in figure 34c. Therefore, an optimum sensitivity (case 0) does not entail optimum FOM (case 2). A similar behaviour can be observed for TE polarization (figures 35 b and c), albeit less significant.

Figure 35 – TE mode analysis of different perturbed SWGs. The top-left (a) plot is the surface sensitivity variation with the increase of the perturbation parameter ($Pert$). The bottom-left (b) and top-right (c) plots are, respectively, the Q and FOM values of the modes for different perturbations. Finally, the bottom-right (d) plot shows the dispersion of the modes. The simple line blue curve (TE Case 0) relates to the perturbation of the optimum point found for the surface sensitivity in figure 3, the dashed red curve (TE Case 1) and the circle marked yellow curve (TE Case 2) relate to structures with geometric parameters tuned so the modes have higher effective indexes.

The change in perturbation affects the resonance wavelength and effective index, as shown in figure 34d and figure 35d. This fact motivates an investigation of the band diagrams of the perturbed band-folded SWGs. The band diagrams of both TM Case 0 and TE Case 0, which are also representative of the other structures, are shown in figure 36.

As is apparent in figure 36 the perturbation does not significantly affect the shape of band-diagram. This feature is evidence of the interpretation that the perturbation does not significantly alter the Bloch mode itself; instead, the perturbation only controls the coupling between the Bloch mode and the radiating modes. One interesting, and unexpected, effect observed in the band diagrams of these structures is the fact that the TE case presented a flat band, as seen in the right column of figure 36, up to an incidence angle of $\pm 6.3^\circ$ (which can be calculated converting the x axis from the graphs of figure 36 from β to oblique incidence angle using equation 2.6). This is an important topic in the literature [117, 118] and these structures could be further explored for this purpose in future works.

Figure 36 – Band diagrams of both TM Case 0 (left) and TE Case 0 (right) modes. The x axis of the graphs is the normalised propagation constant of the modes (β) in relation to the structure's periodicity ($G = 2\pi/\Lambda_{Pert}$). Just the positive x axis and the analysed modes are shown.

In the last step, the tolerance to fabrication imperfections is estimated by altering the geometrical parameters around their optimum point. The parameter most likely to vary is the FF because, although fabrication process based on electron beam lithography are very precise in terms of mask positioning, the etching process largely impacts the length of the blocks and, thus, their FF . This feature motivates the investigation of the sensing parameters to changes in the FF for both TM and TE modes, displayed in figures 37 and 38, respectively. The structures chosen for analyses, this time, were the TM Case 2 and TE Case 2 from previous results, due to the fact that they already show good tolerance to changes in the perturbation.

Figure 37 – Effect of the variation of the FF of the TM Case 2 structure. All geometric parameters, with the exception of the FF , which originally is $FF_0 = 40\%$, remained the same. The perturbation used was of 50 nm.

Figure 38 – Effect of the variation of the FF of the TE Case 2 structure. All geometric parameters, with the exception of the FF , which originally is $FF_0 = 40\%$, remained the same. The perturbation used was of 10 nm.

Although the graphs from figures 37 and 38. shows the results for a single perturbation, they are representative of the effect observed in my simulations considering different ranges of perturbations, either higher or smaller. These results show that the

structures are quite sensible to the variation of the FF of the blocks, especially in terms of the Q , and consequently the FOM , since the sensitivity remains quite similar for both TE and TM modes. The TE mode (figure 38) presented an increase (decrease) of about 50% of the FOM when the FF changed from FF_0 to $FF_0 - (+) 5\%$. Similar performance was observed for the TM mode as well.

The next step was the characterization of a 3D perturbed band folded SWG in order to enhance the performance of the TE modes, which we already know from chapter 4 that could benefit from the more complex 3D structure.

5.3 3D perturbed band-folded SWGs - qTE modes

In this section the performance of a 3D perturbed band-folded SWG for a qTE mode is investigated, since they show potential for better sensing performance according to the results from section 4.2. A 3D perturbed SWG has one more geometric parameter that must be dealt with, which is the side width (W), as illustrated in the schematic of figure 39a. The constraints on all the other parameters, which are the same as for the 2D structure, can be used as a guide to determine the values of W that should be used. For example, given that the FF should be between 40% and 60%, the results from figure 27 indicate that small side widths tend to have lower sensitivities compared to higher ones for a fixed height (H) value. Considering these results, a minimum value of $W = 300$ nm was stipulated for the simulations. As for an upper limit, widths of a few micrometers have already been demonstrated in the literature using gratings of similar materials.¹¹⁹ Finally, the periods of the presented structures were all adjusted so the mode resonance was at $\lambda_0 = 1300$ nm.

The steps of investigation are the same as in the last section. First, the dependences of the sensitivity and the quality factor of slightly perturbed SWG qTE modes on their effective indexes are analysed in order find an optimum sensitivity point. The sensitivities and Q s are shown in figure 39b and figure 39c, respectively. Notice that the bulk sensitivity was omitted due to the high computational demand.

The results from figure 39 already show some interesting effects: the 3D qTE modes behave much more similar to the 2D TM modes than their TE counterparts. First, as seen in the graph from figure 39b, the qTE surface sensitivity curve dependence on the effective index is broadened compared to the TE case and peaks at a more similar effective index (1.97) to the TM mode (1.8). Secondly, and here is the major difference, the Q dependence curve (figure 39c) has the opposite trend than that of the 2D TE case (in the latter, the Q decreases as the effective index gets higher, see figure 33c). These facts can be understood due to the fact that the electric field profile of the qTE mode is not concentrated inside the waveguide, as it is for the TE modes. Instead, they are mainly localized outside the waveguide blocks, mostly on their side walls (as seen in the results from chapter 4, see fig

Figure 39 – Investigation of the sensing parameters of a slightly perturbed 3D SWG (a). Sensitivity (b) and Quality Factor (c) dependence of qTE modes on their respective effective indexes. The height (H) varied between 150-450 nm, the side width (W) between 300-550 nm and the FF was fixed at 60% (as to provide maximum sensitivity, according to results from section 4.2). The perturbation distance used for the perturbed SWG structures 2.5% of the respective structure's period. The highlighted cases of effective indexes will be useful for further analysis.

29). This supports the conclusion that the sensitivities of these structures are intimately connected to whether the electric field profile is concentrated mostly inside or outside the waveguide, and not strictly dependent on the polarization of the mode.

One can also see from the y axis in the graphs of figure 39b and figure 39c that the qTE modes already show better sensitivity and Q than their 2D counterparts, being a strong indicator that these modes have better overall FOM . Similar to the 2D SWG TM modes, the calculations indicate that the 3D SWG qTE modes have potential of FOM improvement for effective index smaller than the one that offers optimum sensitivity (case 0), due to the increase of the Q . Again, because the Q is very dependent on the perturbation, it is important to analyse the FOM dependence on the perturbation for a few classes of structures, namely qTE Case 0, Case 1 and Case 2, highlighted in figure 39d. Figure 40 shows this analysis.

Figure 40 – qTE mode analysis of different perturbed SWGs. The top-left (a) plot is the surface sensitivity variation with the increase of the perturbation parameter ($Pert$). The bottom-left (b) and top-right (c) plots are, respectively, the Q and FOM values of the modes for different perturbations. Finally, the bottom-right (d) plot shows the dispersion of the modes. The simple line blue curve (qTE Case 0) relates to the perturbation of the optimum point found for the surface sensitivity in figure 39, the dashed red curve (qTE Case 1) and the circle marked yellow curve (qTE Case 2) relate to structures with geometric parameters tuned so the modes have smaller effective indexes.

The results from figure 40 show, once again, that the qTE modes share the same properties in terms of the response to the perturbation than that of the TM modes, meaning that all the discussion made in the last section is still valid for these modes as well. However, more importantly, the qTE modes showed a significant gain in sensing performance over their 2D counterparts. Comparing the structure with best surface sensitivity (case 0) of these 2 modes, illustrated in figures 35a and 39a, for example, the qTE presented higher surface sensitivity (about 34% for small perturbations), while maintaining similar Q response, leading to an improvement of the FOM . The improvement is even more evident when the structure with best FOM of these 2 modes, illustrated in figures 35c and 40c, are compared: the TE case 2 presented a FOM of 22 for $Pert = 5$ nm, while the qTE case 2 showed a FOM of 90 for the same perturbation, 4.5 times higher. Besides, the qTE curves presented softer drops of both Q and FOM with the increase of perturbation, as evident by analysing figure 40c and comparing them with figure 35c, indicating that they offer more stability of their sensing performance with the variation of the perturbation.

6 CONCLUSION

This dissertation presented an overview of the current photonic-based systems employed for biosensing, focusing on devices based on silicon waveguides. The theoretical background necessary to understand the phenomena behind these systems was elucidated and the parameters to characterise their sensing performance were defined.

The initial phase of the dissertation sought to understand the sensing behaviour of periodic silicon waveguides, namely SWGs and GMRs, which have great potential as PoC devices, analysing their mode's properties and sensing characteristics for different optimised configurations in terms of their electric field distribution. It was found that their performance is highly dependent on the light polarization.

The TM (2D) and qTM (3D) modes showed similar sensitivities and dependence on the structure's geometry. This is quite interesting, since it leads to simpler structures, though this effect has been ignored in the literature. The fact that the best performing configurations, represented by the taller structures, were associated with a stronger confinement of the electric field is also interesting, since electric field confinement and sensitivity usually have an inverse relation. Both effects can be explained because these modes are highly concentrated on the surface of the waveguide periodic core, meaning that there is not much of a difference for sensing purposes, especially for the surface sensitivity. Notice that a highly confined mode implies a strongly concentrated field on the surface of the waveguide, which might be desired for sensing purposes, even more for the surface sensitivity.

The qTE (3D) modes, however, showed a significant increase of performance compared to their TE (2D) counterparts. This difference is due to the region of highly concentrated electric field presented for these modes. While the modes of the 2D structures presented this field concentration inside the waveguide periodic core, the 3D modes showed an increase of this concentration on the surface of the core for some configurations, thus increasing the mode's sensing capabilities. Differently from the qTM and TM cases and in accordance to previous knowledge, highly confined modes, represented by the taller structures, showed overall worse sensing performance, especially for the surface sensitivity.

It was also demonstrated, in theory, that 2D periodic waveguides can be indeed designed with parameters that do not impose significant challenges to fabrication, especially for TM modes, by using large 3D periodic waveguides with proper settings. This information also bears on spatial resolution of each mode, with the TE modes being "wider" than TM modes.

The band folding, along with the perturbation, proved to be a successful method

to provide out of plane coupling for SWG modes. This is an important technological requirement, as it greatly simplifies the coupling system. The method works well for both TE/qTE and TM modes, with small perturbations (up to 20nm) barely impacting on their mode's sensitivities, electric field profile and band diagrams, thus maintaining the properties already discussed in the previous paragraphs. The different behaviours between the bulk and surface sensitivities throughout all the structures analysed in this dissertation, including points of maximum value for the perturbed structures, highlights the importance of defining a more specific type of sensitivity for each application.

The main differences between the responses of each polarization of the perturbed band-folded SWGs consisted in the quality factor variation with the perturbation and the impact of the field confinement (modal effective index) on their quality factors, both effects greatly impacting on their mode's figure of merit. Both TM and qTE modes presented a softer drop in their quality factors with the increase of the perturbation of the structure's periodicity when compared to the TE modes. Also, TM and qTE modes with lower effective indexes exhibited greater Qs, while the opposite was observed for the TE modes. This opposite effect between the presented cases is seemingly due to the electric field profile of these structures, with the TM and qTE fields being concentrated on the waveguide's surface and the qTE field being concentrated in the core.

Another useful insight taken from the results of this dissertation is the conclusion, as observed for both qTE and TM modes of the perturbed SWGs, that a more confined mode, therefore with higher effective index, does not necessarily possess a greater Q. Although this is true for some cases, as in the TE modes or as in increasing the FF of the waveguide ridges, it must not be taken for granted.

As to the fabrication feasibility of these perturbed band-folded SWGs, it is possible to increase the tolerance of the mode's FOM to variations of the perturbation distance by sacrificing a little of sensitivity, thus being relatively stable to fabrication errors of this parameter. However, when it comes to the variations of the structure's FF, at least for 2D SWGs, they were not so tolerant, specially for TE modes. The change of this parameter can cause shifts of the resonant wavelength and worsening of the mode's FOM. This effect was less intense on TM modes.

It is also noteworthy that the modes of these perturbed SWGs are accessible using a broadband light source, sparing the use of a fine tuned laser source. They can be excited using a common halogen lamp, for example. This greatly facilitates the experimental measurements of the sensors based on these modes.

Finally, at the end of this dissertation the reader finds a complete characterization of the sensing capabilities of state-of-the-art periodic silicon waveguides, besides a method for accessing these modes in a simple and easy way, which is desired for PoC devices. This method is not dependent on the materials of the waveguide and it comes from the

properties of a periodic waveguide, meaning that it can be straightforwardly adapted for periodic structures of other materials and different periodic configurations, such as a photonic crystal.

BIBLIOGRAPHY

- 1 FRADEN, J. **Handbook of modern sensors**. [S.l.]: Springer, 2010. v. 3.
- 2 JOHNSON, W. Electric tele-thermoscope. **USA Patent**, v. 281884, 1883.
- 3 ATZORI, L.; IERA, A.; MORABITO, G. The internet of things: A survey. **Computer networks**, Elsevier, v. 54, n. 15, p. 2787–2805, 2010.
- 4 KARUNAKARAN, C.; RAJKUMAR, R.; BHARGAVA, K. Introduction to biosensors. In: **Biosensors and bioelectronics**. [S.l.]: Elsevier, 2015. p. 1–68.
- 5 WULFKUHLE, J. D.; LIOTTA, L. A.; PETRICON, E. F. Proteomic applications for the early detection of cancer. **Nature reviews cancer**, Nature Publishing Group, v. 3, n. 4, p. 267–275, 2003.
- 6 MCDERMOTT, U.; DOWNING, J. R.; STRATTON, M. R. Genomics and the continuum of cancer care. **New England Journal of Medicine**, Mass Medical Soc, v. 364, n. 4, p. 340–350, 2011.
- 7 SNYDER, E. L.; STRAMER, S. L.; BENJAMIN, R. J. et al. The safety of the blood supply—time to raise the bar. **N Engl J Med**, v. 372, n. 20, p. 1882–1885, 2015.
- 8 DHAWAN, A. P.; HEETDERKS, W. J.; PAVEL, M.; ACHARYA, S.; AKAY, M.; MAIRAL, A.; WHEELER, B.; DACSO, C. C.; SUNDER, T.; LOVELL, N. et al. Current and future challenges in point-of-care technologies: a paradigm-shift in affordable global healthcare with personalized and preventive medicine. **IEEE journal of translational engineering in health and medicine**, IEEE, v. 3, p. 1–10, 2015.
- 9 LUAN, E.; SHOMAN, H.; RATNER, D. M.; CHEUNG, K. C.; CHROSTOWSKI, L. Silicon photonic biosensors using label-free detection. **Sensors**, Multidisciplinary Digital Publishing Institute, v. 18, n. 10, p. 3519, 2018.
- 10 MASCINI, M.; TOMBELLI, S. Biosensors for biomarkers in medical diagnostics. **Biomarkers**, Taylor & Francis, v. 13, n. 7-8, p. 637–657, 2008.
- 11 BIOSENSORS Market by Type, Product, Technology, Application And Geography - Global Forecast to 2024. [S.l.]: MarketsandMarkets™, 2019.
- 12 JR, L. Q. Monitor and control of blood and tissue oxygen tensions. **ASAIO Journal**, LWW, v. 2, n. 1, p. 41–48, 1956.
- 13 VO-DINH, T. **Biomedical photonics handbook: biomedical diagnostics**. [S.l.]: CRC press, 2014.
- 14 MARTINS, E. **Light management in optoelectronic devices**. 2014. Tese (Doutorado) — University of St Andrews, 2014.
- 15 ORFANIDIS, S. J. Electromagnetic waves and antennas. Rutgers University New Brunswick, NJ, 2002.

- 16 LIEBERG, B.; NYLANDER, C.; LUNSTRÖM, I. Surface plasmon resonance for gas detection and biosensing. **Sensors and actuators**, Elsevier, v. 4, p. 299–304, 1983.
- 17 KUMBHAT, S.; GEHLOT, R.; SHARMA, K.; SINGH, U.; JOSHI, V. Surface plasmon resonance based indirect immunoassay for detection of 17β -estradiol. **Journal of pharmaceutical and biomedical analysis**, Elsevier, v. 163, p. 211–216, 2019.
- 18 LI, X.; SOLER, M.; BELUSHKIN, A.; YESILKÖY, F.; ALTUG, H. Optofluidic nanoplasmonic biosensor for label-free live cell analysis in real time. In: INTERNATIONAL SOCIETY FOR OPTICS AND PHOTONICS. **Plasmonics in Biology and Medicine XV**. [S.l.], 2018. v. 10509, p. 105090E.
- 19 INAN, H.; POYRAZ, M.; INCI, F.; LIFSON, M. A.; BADAY, M.; CUNNINGHAM, B. T.; DEMIRCI, U. Photonic crystals: emerging biosensors and their promise for point-of-care applications. **Chemical Society Reviews**, Royal Society of Chemistry, v. 46, n. 2, p. 366–388, 2017.
- 20 WANGÜEMERT-PÉREZ, J. G.; HADIJ-ELHOUATI, A.; SÁNCHEZ-POSTIGO, A.; LEUERMANN, J.; XU, D.-X.; CHEBEN, P.; ORTEGA-MOÑUX, A.; HALIR, R.; MOLINA-FERNÁNDEZ, Í. Subwavelength structures for silicon photonics biosensing. **Optics & Laser Technology**, Elsevier, v. 109, p. 437–448, 2019.
- 21 TRIGGS, G. J.; WANG, Y.; REARDON, C. P.; FISCHER, M.; EVANS, G. J.; KRAUSS, T. F. Chirped guided-mode resonance biosensor. **Optica**, Optical Society of America, v. 4, n. 2, p. 229–234, 2017.
- 22 WANG, S.; LIU, Y.; ZHAO, D.; YANG, H.; ZHOU, W.; SUN, Y. Optofluidic fano resonance photonic crystal refractometric sensors. **Applied Physics Letters**, AIP Publishing LLC, v. 110, n. 9, p. 091105, 2017.
- 23 MARTINS, E. R.; WANG, Y.; KANIBOLOTSKY, A. L.; SKABARA, P. J.; TURNBULL, G. A.; SAMUEL, I. D. Low-threshold nanoimprinted lasers using substructured gratings for control of distributed feedback. **Advanced Optical Materials**, Wiley Online Library, v. 1, n. 8, p. 563–566, 2013.
- 24 HAUS, H. A. **Waves and fields in optoelectronics**. [S.l.]: Prentice-Hall,, 1984.
- 25 SALEH, B. E.; TEICH, M. C. **Fundamentals of photonics**. [S.l.]: John Wiley & sons, 2019.
- 26 YARIV, A. **Optical electronics**. [S.l.]: Saunders College Publ., 1991.
- 27 GRIFFITHS, D. J. **Introduction to electrodynamics**. [S.l.]: American Association of Physics Teachers, 2005.
- 28 MUKUNDAN, H.; ANDERSON, A. S.; GRACE, W. K.; GRACE, K. M.; HARTMAN, N.; MARTINEZ, J. S.; SWANSON, B. I. Waveguide-based biosensors for pathogen detection. **Sensors**, Molecular Diversity Preservation International, v. 9, n. 7, p. 5783–5809, 2009.
- 29 WANGÜEMERT-PÉREZ, J. G.; CHEBEN, P.; ORTEGA-MOÑUX, A.; ALONSO-RAMOS, C.; PÉREZ-GALACHO, D.; HALIR, R.; MOLINA-FERNÁNDEZ, I.; XU, D.-X.; SCHMID, J. H. Evanescent field waveguide sensing with subwavelength grating

- structures in silicon-on-insulator. **Optics letters**, Optical Society of America, v. 39, n. 15, p. 4442–4445, 2014.
- 30 JOANNOPOULOS, J. D.; JOHNSON, S. G.; WINN, J. N.; MEADE, R. D. Molding the flow of light. **Princeton Univ. Press, Princeton, NJ [ua]**, 2008.
- 31 WHITTAKER, D.; CULSHAW, I. Scattering-matrix treatment of patterned multilayer photonic structures. **Physical Review B**, APS, v. 60, n. 4, p. 2610, 1999.
- 32 ČTYROKÝ, J.; WANGÜEMERT-PÉREZ, J. G.; KWIECIEN, P.; RICHTER, I.; LITVIK, J.; SCHMID, J. H.; MOLINA-FERNÁNDEZ, Í.; ORTEGA-MOÑUX, A.; DADO, M.; CHEBEN, P. Design of narrowband bragg spectral filters in subwavelength grating metamaterial waveguides. **Optics express**, Optical Society of America, v. 26, n. 1, p. 179–194, 2018.
- 33 HALIR, R.; CHEBEN, P.; LUQUE-GONZÁLEZ, J. M.; SARMIENTO-MERENGUEL, J. D.; SCHMID, J. H.; WANGÜEMERT-PÉREZ, G.; XU, D.-X.; WANG, S.; ORTEGA-MOÑUX, A.; MOLINA-FERNÁNDEZ, Í. Ultra-broadband nanophotonic beamsplitter using an anisotropic sub-wavelength metamaterial. **Laser & Photonics Reviews**, Wiley Online Library, v. 10, n. 6, p. 1039–1046, 2016.
- 34 GONZÁLEZ-ANDRADE, D.; WANGÜEMERT-PÉREZ, J. G.; VELASCO, A. V.; ORTEGA-MOÑUX, A.; HERRERO-BERMELLO, A.; MOLINA-FERNÁNDEZ, I.; HALIR, R.; CHEBEN, P. Ultra-broadband mode converter and multiplexer based on sub-wavelength structures. **IEEE Photonics Journal**, IEEE, v. 10, n. 2, p. 1–10, 2018.
- 35 XIONG, Y.; WANGÜEMERT-PÉREZ, J. G.; XU, D.-X.; SCHMID, J. H.; CHEBEN, P.; WINNIE, N. Y. Polarization splitter and rotator with subwavelength grating for enhanced fabrication tolerance. **Optics letters**, Optical Society of America, v. 39, n. 24, p. 6931–6934, 2014.
- 36 BENEDIKOVIC, D.; ALONSO-RAMOS, C.; CHEBEN, P.; SCHMID, J. H.; WANG, S.; XU, D.-X.; LAPOINTE, J.; JANZ, S.; HALIR, R.; ORTEGA-MOÑUX, A. et al. High-directionality fiber-chip grating coupler with interleaved trenches and subwavelength index-matching structure. **Optics letters**, Optical Society of America, v. 40, n. 18, p. 4190–4193, 2015.
- 37 SÁNCHEZ-POSTIGO, A.; WANGÜEMERT-PÉREZ, J. G.; LUQUE-GONZÁLEZ, J. M.; MOLINA-FERNÁNDEZ, Í.; CHEBEN, P.; ALONSO-RAMOS, C. A.; HALIR, R.; SCHMID, J. H.; ORTEGA-MOÑUX, A. Broadband fiber-chip zero-order surface grating coupler with 0.4 db efficiency. **Optics letters**, Optical Society of America, v. 41, n. 13, p. 3013–3016, 2016.
- 38 JEONG, S.-H.; SHIMURA, D.; SIMOYAMA, T.; SEKI, M.; YOKOYAMA, N.; OHTSUKA, M.; KOSHINO, K.; HORIKAWA, T.; TANAKA, Y.; MORITO, K. Low-loss, flat-topped and spectrally uniform silicon-nanowire-based 5th-order crow fabricated by arf-immersion lithography process on a 300-mm soi wafer. **Optics express**, Optical Society of America, v. 21, n. 25, p. 30163–30174, 2013.
- 39 WANG, S.; MAGNUSSON, R. Theory and applications of guided-mode resonance filters. **Applied optics**, Optical Society of America, v. 32, n. 14, p. 2606–2613, 1993.

- 40 MAGNUSSON, R.; SHOKOOH-SAREMI, M. Physical basis for wideband resonant reflectors. **Optics express**, Optical Society of America, v. 16, n. 5, p. 3456–3462, 2008.
- 41 RICCIARDI, A.; CAMPOPIANO, S.; CUSANO, A.; KRAUSS, T. F.; O’FAOLAIN, L. Broadband mirrors in the near-infrared based on subwavelength gratings in soi. **IEEE Photonics journal**, IEEE, v. 2, n. 5, p. 696–702, 2010.
- 42 WAWRO, D.; KOULEN, P.; DING, Y.; ZIMMERMAN, S.; MAGNUSSON, R. Guided-mode resonance sensor system for early detection of ovarian cancer. In: INTERNATIONAL SOCIETY FOR OPTICS AND PHOTONICS. **Optical Diagnostics and Sensing X: Toward Point-of-Care Diagnostics**. [S.l.], 2010. v. 7572, p. 75720D.
- 43 MAGNUSSON, R.; WAWRO, D.; ZIMMERMAN, S.; DING, Y.; SHOKOOH-SAREMI, M.; LEE, K. J.; USSERY, D.; KIM, S.; SONG, S. H. Leaky-mode resonance photonics: Technology for biosensors, optical components, mems, and plasmonics. In: INTERNATIONAL SOCIETY FOR OPTICS AND PHOTONICS. **Integrated Optics: Devices, Materials, and Technologies XIV**. [S.l.], 2010. v. 7604, p. 76040M.
- 44 PRIOLO, F.; GREGORKIEWICZ, T.; GALLI, M.; KRAUSS, T. F. Silicon nanostructures for photonics and photovoltaics. **Nature nanotechnology**, Nature Publishing Group, v. 9, n. 1, p. 19, 2014.
- 45 NODA, S.; FUJITA, M. Light-emitting diodes: Photonic crystal efficiency boost. **nature photonics**, Nature Publishing Group, v. 3, n. 3, p. 129, 2009.
- 46 LI, K.; LI, J.; REARDON, C.; SCHUSTER, C. S.; WANG, Y.; TRIGGS, G. J.; DAMNIK, N.; MÜENCHENBERGER, J.; WANG, X.; MARTINS, E. R. et al. High speed e-beam writing for large area photonic nanostructures—a choice of parameters. **Scientific reports**, Nature Publishing Group, v. 6, p. 32945, 2016.
- 47 OTTO, M.; ALGASINGER, M.; BRANZ, H.; GESEMANN, B.; GIMPEL, T.; FÜCHSEL, K.; KÄSEBIER, T.; KONTERMANN, S.; KOYNOV, S.; LI, X. et al. Black silicon photovoltaics. **Advanced optical materials**, Wiley Online Library, v. 3, n. 2, p. 147–164, 2015.
- 48 SCHIFT, H. Nanoimprint lithography: An old story in modern times? a review. **Journal of Vacuum Science & Technology B: Microelectronics and Nanometer Structures Processing, Measurement, and Phenomena**, American Vacuum Society, v. 26, n. 2, p. 458–480, 2008.
- 49 KRAVETS, V. G.; KABASHIN, A. V.; BARNES, W. L.; GRIGORENKO, A. N. Plasmonic surface lattice resonances: a review of properties and applications. **Chemical reviews**, ACS Publications, v. 118, n. 12, p. 5912–5951, 2018.
- 50 FERNÁNDEZ-DOMÍNGUEZ, A. I.; GARCÍA-VIDAL, F. J.; MARTÍN-MORENO, L. Unrelenting plasmons. **Nature Photonics**, Nature Publishing Group, v. 11, n. 1, p. 8, 2017.
- 51 BARNES, W. L. Particle plasmons: Why shape matters. **American Journal of Physics**, American Association of Physics Teachers, v. 84, n. 8, p. 593–601, 2016.
- 52 WANG, F.; SHEN, Y. R. General properties of local plasmons in metal nanostructures. **Physical review letters**, APS, v. 97, n. 20, p. 206806, 2006.

-
- 53 COSGROVE, T. **Colloid science: principles, methods and applications**. [S.l.]: John Wiley & Sons, 2010.
- 54 HAYNES, C. L.; DUYNE, R. P. V. **Nanosphere lithography: a versatile nanofabrication tool for studies of size-dependent nanoparticle optics**. [S.l.]: ACS Publications, 2001.
- 55 VESELAGO, V. G. The electrodynamics of substances with simultaneously negative values of ϵ and μ . **Physics-Uspekhi**, Turpion Ltd, v. 10, n. 4, p. 509–514, 1968.
- 56 PENDRY, J. B. Negative refraction makes a perfect lens. **Physical review letters**, APS, v. 85, n. 18, p. 3966, 2000.
- 57 GRIGORENKO, A.; GEIM, A.; GLEESON, H.; ZHANG, Y.; FIRSOV, A.; KHRUSHCHEV, I.; PETROVIC, J. Nanofabricated media with negative permeability at visible frequencies. **Nature**, Nature Publishing Group, v. 438, n. 7066, p. 335–338, 2005.
- 58 SHALAEV, V. M. Optical negative-index metamaterials. **Nature photonics**, Nature Publishing Group, v. 1, n. 1, p. 41–48, 2007.
- 59 YAO, J.; LIU, Z.; LIU, Y.; WANG, Y.; SUN, C.; BARTAL, G.; STACY, A. M.; ZHANG, X. Optical negative refraction in bulk metamaterials of nanowires. **Science**, American Association for the Advancement of Science, v. 321, n. 5891, p. 930–930, 2008.
- 60 MIRKIN, C. A.; LETSINGER, R. L.; MUCIC, R. C.; STORHOFF, J. J. A dna-based method for rationally assembling nanoparticles into macroscopic materials. **Nature**, Nature Publishing Group, v. 382, n. 6592, p. 607–609, 1996.
- 61 KAWATA, S.; INOUE, Y.; VERMA, P. Plasmonics for near-field nano-imaging and superlensing. **Nature photonics**, Nature Publishing Group, v. 3, n. 7, p. 388, 2009.
- 62 BARNES, W. L.; DEREUX, A.; EBBESEN, T. W. Surface plasmon subwavelength optics. **nature**, Nature Publishing Group, v. 424, n. 6950, p. 824–830, 2003.
- 63 LAL, S.; LINK, S.; HALAS, N. J. Nano-optics from sensing to waveguiding. **Nature photonics**, Nature Publishing Group, v. 1, n. 11, p. 641, 2007.
- 64 LU, Y.-J.; KIM, J.; CHEN, H.-Y.; WU, C.; DABIDIAN, N.; SANDERS, C. E.; WANG, C.-Y.; LU, M.-Y.; LI, B.-H.; QIU, X. et al. Plasmonic nanolaser using epitaxially grown silver film. **science**, American Association for the Advancement of Science, v. 337, n. 6093, p. 450–453, 2012.
- 65 SUH, J. Y.; KIM, C. H.; ZHOU, W.; HUNTINGTON, M. D.; CO, D. T.; WASIELEWSKI, M. R.; ODOM, T. W. Plasmonic bowtie nanolaser arrays. **Nano letters**, ACS Publications, v. 12, n. 11, p. 5769–5774, 2012.
- 66 LI, K.; STOCKMAN, M. I.; BERGMAN, D. J. Self-similar chain of metal nanospheres as an efficient nanolens. **Physical review letters**, APS, v. 91, n. 22, p. 227402, 2003.
- 67 GRIGORENKO, A.; ROBERTS, N.; DICKINSON, M.; ZHANG, Y. Nanometric optical tweezers based on nanostructured substrates. **Nature Photonics**, Nature Publishing Group, v. 2, n. 6, p. 365–370, 2008.

- 68 ZHOU, W.; DRIDI, M.; SUH, J. Y.; KIM, C. H.; CO, D. T.; WASIELEWSKI, M. R.; SCHATZ, G. C.; ODOM, T. W. et al. Lasing action in strongly coupled plasmonic nanocavity arrays. **Nature nanotechnology**, Nature Publishing Group, v. 8, n. 7, p. 506, 2013.
- 69 MAIER, S. A. **Plasmonics: fundamentals and applications**. [S.l.]: Springer Science & Business Media, 2007.
- 70 EBBESEN, T. W.; LEZEC, H. J.; GHAEMI, H.; THIO, T.; WOLFF, P. A. Extraordinary optical transmission through sub-wavelength hole arrays. **Nature**, Nature Publishing Group, v. 391, n. 6668, p. 667–669, 1998.
- 71 BARNES, W. L.; MURRAY, W. A.; DINTINGER, J.; DEVAUX, E.; EBBESEN, T. Surface plasmon polaritons and their role in the enhanced transmission of light through periodic arrays of subwavelength holes in a metal film. **Physical review letters**, APS, v. 92, n. 10, p. 107401, 2004.
- 72 CETIN, A. E.; ETEZADI, D.; GALARRETA, B. C.; BUSSON, M. P.; EKSIOGLU, Y.; ALTUG, H. Plasmonic nanohole arrays on a robust hybrid substrate for highly sensitive label-free biosensing. **ACS photonics**, ACS Publications, v. 2, n. 8, p. 1167–1174, 2015.
- 73 KRETSCHMANN, E.; RAETHER, H. Radiative decay of non radiative surface plasmons excited by light. **Zeitschrift für Naturforschung A**, Verlag der Zeitschrift für Naturforschung, v. 23, n. 12, p. 2135–2136, 1968.
- 74 TURBADAR, T. Complete absorption of light by thin metal films. **Proceedings of the Physical Society**, IOP Publishing, v. 73, n. 1, p. 40, 1959.
- 75 SCHASFOORT, R.; TUDOS, A. **Handbook of Surface Plasmon Resonance** Royal Society of Chemistry. [S.l.]: London, 2008.
- 76 HOMOLA, J.; PILIARIK, M. Surface plasmon resonance (spr) sensors. In: **Surface plasmon resonance based sensors**. [S.l.]: Springer, 2006. p. 45–67.
- 77 SINGH, P. Spr biosensors: Historical perspectives and current challenges. **Sensors and actuators B: Chemical**, Elsevier, v. 229, p. 110–130, 2016.
- 78 PRABOWO, B. A.; PURWIDYANTRI, A.; LIU, K.-C. Surface plasmon resonance optical sensor: A review on light source technology. **Biosensors**, Multidisciplinary Digital Publishing Institute, v. 8, n. 3, p. 80, 2018.
- 79 JACKSON, J. D. **Classical electrodynamics**. [S.l.]: John Wiley & Sons, 2007.
- 80 VOLLMER, F.; YANG, L. Review label-free detection with high-q microcavities: a review of biosensing mechanisms for integrated devices. **Nanophotonics**, Science Wise Publishing & De Gruyter, v. 1, n. 3-4, p. 267–291, 2012.
- 81 CONTEDEUCA, D.; BARTH, I.; PITRUZZELLO, G.; REARDON, C.; MARTINS, E.; KRAUSS, T. Dielectric nanohole array metasurface for high-resolution near-field sensing and imaging. 2020.

- 82 NARAYANASWAMY, R.; WOLFBEIS, O. S. **Optical sensors: industrial environmental and diagnostic applications**. [S.l.]: Springer Science & Business Media, 2013. v. 1.
- 83 DAMBORSKÝ, P.; ŠVITEL, J.; KATRLÍK, J. Optical biosensors. **Essays in biochemistry**, Portland Press Limited, v. 60, n. 1, p. 91–100, 2016.
- 84 GAVELA, A. F.; GARCÍA, D. G.; RAMIREZ, J. C.; LECHUGA, L. M. Last advances in silicon-based optical biosensors. **sensors**, Multidisciplinary Digital Publishing Institute, v. 16, n. 3, p. 285, 2016.
- 85 SUBRAMANIAN, A. Z.; RYCKEBOER, E.; DHAKAL, A.; PEYSKENS, F.; MALIK, A.; KUYKEN, B.; ZHAO, H.; PATHAK, S.; RUOCCO, A.; GROOTE, A. D. et al. Silicon and silicon nitride photonic circuits for spectroscopic sensing on-a-chip. **Photonics Research**, Optical Society of America, v. 3, n. 5, p. B47–B59, 2015.
- 86 CHEN, Y.; LIU, J.; YANG, Z.; WILKINSON, J. S.; ZHOU, X. Optical biosensors based on refractometric sensing schemes: A review. **Biosensors and Bioelectronics**, Elsevier, p. 111693, 2019.
- 87 STEGLICH, P.; HÜLSEMAN, M.; DIETZEL, B.; MAI, A. Optical biosensors based on silicon-on-insulator ring resonators: A review. **Molecules**, Multidisciplinary Digital Publishing Institute, v. 24, n. 3, p. 519, 2019.
- 88 FAN, X.; WHITE, I. M.; SHOPOVA, S. I.; ZHU, H.; SUTER, J. D.; SUN, Y. Sensitive optical biosensors for unlabeled targets: A review. **analytica chimica acta**, Elsevier, v. 620, n. 1-2, p. 8–26, 2008.
- 89 DENSMORE, A.; VACHON, M.; XU, D.-X.; JANZ, S.; MA, R.; LI, Y.-H.; LOPINSKI, G.; DELÂGE, A.; LAPOINTE, J.; LUEBBERT, C. et al. Silicon photonic wire biosensor array for multiplexed real-time and label-free molecular detection. **Optics letters**, Optical Society of America, v. 34, n. 23, p. 3598–3600, 2009.
- 90 MAURANYAPIN, N.; MADSEN, L.; TAYLOR, M.; WALEED, M.; BOWEN, W. Evanescent single-molecule biosensing with quantum-limited precision. **Nature Photonics**, Nature Publishing Group, v. 11, n. 8, p. 477, 2017.
- 91 TALEBIFARD, S.; SCHMIDT, S.; SHI, W.; WU, W.; JAEGER, N. A.; KWOK, E.; RATNER, D. M.; CHROSTOWSKI, L. Optimized sensitivity of silicon-on-insulator (soi) strip waveguide resonator sensor. **Biomedical optics express**, Optical Society of America, v. 8, n. 2, p. 500–511, 2017.
- 92 GORODKIEWICZ, E.; LUKASZEWSKI, Z. Recent progress in surface plasmon resonance biosensors (2016 to mid-2018). **Biosensors**, Multidisciplinary Digital Publishing Institute, v. 8, n. 4, p. 132, 2018.
- 93 LUAN, E.; AWAN, K. M.; CHEUNG, K. C.; CHROSTOWSKI, L. High-performance sub-wavelength grating-based resonator sensors with substrate overetch. **Optics Letters**, Optical Society of America, v. 44, n. 24, p. 5981–5984, 2019.
- 94 JUGESSUR, A.; DOU, J.; AITCHISON, J.; RUE, R. D. L.; GNAN, M. A photonic nano-bragg grating device integrated with microfluidic channels for bio-sensing applications. **Microelectronic Engineering**, Elsevier, v. 86, n. 4-6, p. 1488–1490, 2009.

- 95 GRIST, S. M.; SCHMIDT, S. A.; FLUECKIGER, J.; DONZELLA, V.; SHI, W.; FARD, S. T.; KIRK, J. T.; RATNER, D. M.; CHEUNG, K. C.; CHROSTOWSKI, L. Silicon photonic micro-disk resonators for label-free biosensing. **Optics express**, Optical Society of America, v. 21, n. 7, p. 7994–8006, 2013.
- 96 CARLBORG, C. F.; GYLFASON, K. B.; KAŹMIERCZAK, A.; DORTU, F.; POLO, M. B.; CATALA, A. M.; KRESBACH, G. M.; SOHLSTRÖM, H.; MOH, T.; VIVIEN, L. et al. A packaged optical slot-waveguide ring resonator sensor array for multiplex label-free assays in labs-on-chips. **Lab on a Chip**, Royal Society of Chemistry, v. 10, n. 3, p. 281–290, 2010.
- 97 WANG, X.; FLUECKIGER, J.; SCHMIDT, S.; GRIST, S.; FARD, S. T.; KIRK, J.; DOERFLER, M.; CHEUNG, K. C.; RATNER, D. M.; CHROSTOWSKI, L. A silicon photonic biosensor using phase-shifted bragg gratings in slot waveguide. **Journal of biophotonics**, Wiley Online Library, v. 6, n. 10, p. 821–828, 2013.
- 98 HU, S.; QIN, K.; KRAVCHENKO, I. I.; RETTERER, S. T.; WEISS, S. M. Suspended micro-ring resonator for enhanced biomolecule detection sensitivity. In: INTERNATIONAL SOCIETY FOR OPTICS AND PHOTONICS. **Frontiers in Biological Detection: From Nanosensors to Systems VI**. [S.l.], 2014. v. 8933, p. 893306.
- 99 FLUECKIGER, J.; SCHMIDT, S.; DONZELLA, V.; SHERWALI, A.; RATNER, D. M.; CHROSTOWSKI, L.; CHEUNG, K. C. Sub-wavelength grating for enhanced ring resonator biosensor. **Optics express**, Optical Society of America, v. 24, n. 14, p. 15672–15686, 2016.
- 100 AMENDOLA, V.; PILOT, R.; FRASCONI, M.; MARAGÒ, O. M.; IATÌ, M. A. Surface plasmon resonance in gold nanoparticles: a review. **Journal of Physics: Condensed Matter**, IOP Publishing, v. 29, n. 20, p. 203002, 2017.
- 101 UNSER, S.; BRUZAS, I.; HE, J.; SAGLE, L. Localized surface plasmon resonance biosensing: current challenges and approaches. **Sensors**, Multidisciplinary Digital Publishing Institute, v. 15, n. 7, p. 15684–15716, 2015.
- 102 MAYER, K. M.; HAFNER, J. H. Localized surface plasmon resonance sensors. **Chemical reviews**, ACS Publications, v. 111, n. 6, p. 3828–3857, 2011.
- 103 LI, X.; SOLER, M.; SZYDZIK, C.; KHOSHMANESH, K.; SCHMIDT, J.; COUKOS, G.; MITCHELL, A.; ALTUG, H. Label-free optofluidic nanobiosensor enables real-time analysis of single-cell cytokine secretion. **Small**, Wiley Online Library, v. 14, n. 26, p. 1800698, 2018.
- 104 SOLER, M.; BELUSHKIN, A.; CAVALLINI, A.; KEBBI-BEGHDADI, C.; GREUB, G.; ALTUG, H. Multiplexed nanoplasmonic biosensor for one-step simultaneous detection of chlamydia trachomatis and neisseria gonorrhoeae in urine. **Biosensors and Bioelectronics**, Elsevier, v. 94, p. 560–567, 2017.
- 105 DANILOV, A.; TSELIKOV, G.; WU, F.; KRAVETS, V. G.; OZEROV, I.; BEDU, F.; GRIGORENKO, A. N.; KABASHIN, A. V. Ultra-narrow surface lattice resonances in plasmonic metamaterial arrays for biosensing applications. **Biosensors and Bioelectronics**, Elsevier, v. 104, p. 102–112, 2018.

- 106 WANG, B.; DÜNDAR, M. A.; NÖTZEL, R.; KAROUTA, F.; HE, S.; HEIJDEN, R. W. van der. Photonic crystal slot nanobeam slow light waveguides for refractive index sensing. **Applied Physics Letters**, American Institute of Physics, v. 97, n. 15, p. 151105, 2010.
- 107 HUANG, M.; YANIK, A. A.; CHANG, T.-Y.; ALTUG, H. Sub-wavelength nanofluidics in photonic crystal sensors. **Optics express**, Optical Society of America, v. 17, n. 26, p. 24224–24233, 2009.
- 108 LEE, M.; FAUCHET, P. M. Two-dimensional silicon photonic crystal based biosensing platform for protein detection. **Optics express**, Optical Society of America, v. 15, n. 8, p. 4530–4535, 2007.
- 109 TOCCAFONDO, V.; GARCÍA-RUPÉREZ, J.; BAÑULS, M.; GRIOL, A.; CASTELLÓ, J.; PERANSI-LLOPIS, S.; MAQUIEIRA, A. Single-strand dna detection using a planar photonic-crystal-waveguide-based sensor. **Optics letters**, Optical Society of America, v. 35, n. 21, p. 3673–3675, 2010.
- 110 NUNES, P.; MORTENSEN, N. A.; KUTTER, J. P.; MOGENSEN, K. B. Photonic crystal resonator integrated in a microfluidic system. **Optics letters**, Optical Society of America, v. 33, n. 14, p. 1623–1625, 2008.
- 111 PITRUZZELLO, G.; KRAUSS, T. F. Photonic crystal resonances for sensing and imaging. **Journal of Optics**, IOP Publishing, v. 20, n. 7, p. 073004, 2018.
- 112 ZHANG, W.; GANESH, N.; BLOCK, I. D.; CUNNINGHAM, B. T. High sensitivity photonic crystal biosensor incorporating nanorod structures for enhanced surface area. **Sensors and Actuators B: Chemical**, Elsevier, v. 131, n. 1, p. 279–284, 2008.
- 113 NEHL, C. L.; LIAO, H.; HAFNER, J. H. Optical properties of star-shaped gold nanoparticles. **Nano letters**, ACS Publications, v. 6, n. 4, p. 683–688, 2006.
- 114 SHEN, Y.; LIU, T.; ZHU, Q.; WANG, J.; JIN, C. Dislocated double-layered metal gratings: Refractive index sensors with high figure of merit. **Plasmonics**, Springer, v. 10, n. 6, p. 1489–1497, 2015.
- 115 ARRUDA, G. S. de. Análise da transmissividade de luz para aplicações em células solares.
- 116 MARTINS, A.; LI, K.; LI, J.; LIANG, H.; CONTEDEUCA, D.; BORGES, B.-H. V.; KRAUSS, T. F.; MARTINS, E. R. On metalenses with arbitrarily wide field of view. **ACS Photonics**, ACS Publications, v. 7, n. 8, p. 2073–2079, 2020.
- 117 LALANNE, P.; COUDERT, S.; DUCHATEAU, G.; DILHAIRE, S.; VYNCK, K. Structural slow waves: parallels between photonic crystals and plasmonic waveguides. **ACS photonics**, ACS Publications, v. 6, n. 1, p. 4–17, 2018.
- 118 JEAN, P.; GERVAIS, A.; LAROCHELLE, S.; SHI, W. Slow light in subwavelength grating waveguides. **IEEE Journal of Selected Topics in Quantum Electronics**, IEEE, v. 26, n. 2, p. 1–8, 2019.
- 119 TRIGGS, G.; FISCHER, M.; STELLINGA, D.; SCULLION, M.; EVANS, G.; KRAUSS, T. Spatial resolution and refractive index contrast of resonant photonic crystal surfaces for biosensing. **IEEE photonics journal**, IEEE, v. 7, n. 3, p. 1–10, 2015.

120 HARPER, K. R. Theory, design, and fabrication of diffractive grating coupler for slab waveguide. Brigham Young University-Provo, 2003.

Appendix

APPENDIX A – BRIEF EXPLANATION OF COMSOL AND RCWA SIMULATIONS OF PERIODIC STRUCTURES

This section contains a brief overview of the overall process of finding the modes of periodic structures using both Rigorous Coupled Wave Analysis (RCWA) and COMSOL Multiphysics, with an emphasis on the latter. The RCWA is a semi-analytical method developed by researchers of the Georgia Institute of Technology, Atlanta, EUA, to the determination of the electromagnetic behaviour of periodic structures. It is based on the Fourier Series expansion of the electromagnetic field (Bloch modes) and it was implemented in MATLAB by one of the PhD students of our research group (Augusto Rezende Martins). A good didactic implementation of this method can be found in¹²⁰. COMSOL is a commercial finite element solver and a multiphysics simulation software, with in-built application modules, including wave optics. The next paragraphs contains the main steps taken in order to find the waveguides' modes.

To exemplify the process of finding a waveguide's mode, let's use the waveguide of figure 41a, consisted of an uniform slab of glass ($n = 1.5$) with a periodic perturbation above it (height = 100 nm) surrounded by air. The period used was of 500 nm, large enough to allow diffraction inside the waveguide core for the visible spectrum, thus meaning this structure supports QGMs. One easy way of finding the wavelength (or frequency) of these modes is by just plotting the spectral reflectance of this waveguide assuming a external plane wave incidence, as seen in figure 41b, where this spectrum was calculated using both RCWA and COMSOL (in the latter, using excitation ports).

Figure 41 – a) Schematic of a periodic waveguide upon excitation of a TE plane wave with a 10° angle of incidence. b) Reflectance spectrum. The blue continuous curve was obtained using COMSOL and the red dashed one using RCWA.

First of all, it can be observed that both COMSOL and RCWA gave us very similar results, what it expected from a simple 2D simulation like this one. Each reflectance peak corresponds to an excited quasi guided mode that ends up coupling light backwards. From the reflectance spectrum of figure 41b one can obtain the modes wavelengths from the local peaks.

Until now, just the response of a periodic structure to an external plane wave excitation was simulated, however, the SWG can not be excited in this way, since it operates in the deep-subwavelength regime (if the same reflectance spectrum was to be calculated, not a single resonance peak would appear). One must, therefore, use another method to calculate the modes. COMSOL does provide three tools to directly finding waveguide modes, being the first two: *Boundary Mode Analysis* and *Mode Analysis*. The former requires the user to include numeric ports as boundary conditions in order to indicate the direction of propagation of the waveguide, thus not allowing the use of periodic conditions. The latter exists just for 2D simulations and assumes the direction of propagation outside the simulation plane.

Just the third one, called *Eigenfrequency*, is suitable for our problem, since it exists for both 2D and 3D simulations and the direction of propagation is taken directly from the periodic boundary conditions. In order to use the *Eigenfrequency* solver one must pay

close attention to three parameters. The first one is the periodic boundary condition. After choosing the desired boundaries to be periodic, one must specify what COMSOL calls *Floquet k-vector* $\mathbf{k}_F$. This is nothing more than the $\mathbf{k}_{||}$ of equation 2.6, while the adding periodicity term G comes from the geometry of the simulation window (which can be seen in figures 22 and 26).

To clarify this, figure 42a shows the propagation constant of TE modes of a uniform glass waveguide for different wavelengths, calculated using the semi-analytical solution of the slab waveguide¹⁵ (the code was implemented in MATLAB by the author). The green line β_c represents the $\mathbf{k}_{||}$ (propagation constant) of a mode found in the COMSOL *Eigenfrequency* simulation, which itself depends on both the geometry of the structure simulated (in this case, the window of simulation), and $\mathbf{k}_F$ used as input. The result of the COMSOL simulation will be exactly the frequencies in which the green line intercepts the propagation curves. This means the only way of obtaining the modes for other wavelengths is by either changing the simulation window, which can not be done for the SWG (due to, consequently, changing the structure's period), or by changing the value of $\mathbf{k}_F$.

Figure 42 – Propagation constant (a) of 4 different TE modes of a uniform glass ($n = 1.5$) waveguide (b) of 600nm thickness surrounded by air. The *Eigenfrequency* solver will find modes for a fixed propagation constant value β_c , specified by the problem's geometry and boundary condition. The propagation constants for different wavelengths were calculated using MATLAB (code written by the student).

The second important parameter is the frequency region that COMSOL should look for when finding the modes. The reflectance spectrum of figure 41b already gives us these regions, so it is pretty straightforward for this case. However, if the modes are completely unknown, it can take a very long time until finding the right region.

The last thing to be careful of is COMSOL multiple results possibilities. Even for a simple case like the waveguide of figure 41a, COMSOL will respond with frequencies that have no physical meaning. In fact, most values indicated by COMSOL will be wrong.

Figure 43 shows us a list of frequencies COMSOL has found when looking for modes of the structure of figure 41a, along with some typical mode profiles distributions. Since a quasi guided mode is expected, one can discard incompatible mode profiles.

Figure 43 – List of mode frequencies output and typical TE mode profiles with (green mark) and without (red cross mark) physical meaning.

Having all this in mind, one is able to easily find the TE mode frequencies of the waveguide of figure 41a using COMSOL's *Eigenfrequency*. With that done, the next step was a comparison between the modes obtained using *Eigenfrequency* with the ones found using the RCWA/COMSOL external wave excitation method. This comparison can be seen in figure 44.

Figure 44 – Comparison between the mode wavelengths obtained using *Eigenfrequency* and External Excitation methods. The table shows us the exact wavelength values obtained from each method. The TE electric field distribution of each mode obtained with both methods is also shown.

Apart from some minor phase changes of the electric field distribution inside the waveguide between two methods, one can clearly see that both of them gave us the

same mode. It is also important to note that the fields outside the waveguide show more differences because the *Eigenfrequency* method has no interference with any incoming light.

APPENDIX B – ELECTRIC FIELD INTENSITY DISTRIBUTION OF PERTURBED BAND-FOLDED A 2D SWG

In figure 45 the electric field intensity distribution of a TM mode of a perturbed band-folded SWG for different perturbations is shown. The structure used for analysis is the TM Case 0 of figure 33e). Its field distribution was calculated using COMSOL in the same way as the fields from chapter 4.

Figure 45 – : Electric field intensity distribution of the TM Case 0 (see figure 33e) for geometric details) for different perturbations are shown.

It is clear from the above results that the electric field intensity distribution of these structures barely changes for small perturbations. The fields observed for the other TM modes as well as the TE modes are also very stable for small perturbations.

Annex

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