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Resonant optical waveguide biosensor characterization

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RESONANT OPTICAL WAVEGUIDE **BIOSENSOR** **CHARACTERIZATION**

by

Shantanu Pathak

Thesis submitted to the
College of Engineering and Mineral Resources at

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in
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Abstract

Resonant Optical Waveguide Biosensor

Shantanu Pathak

The importance of miniaturized sensors for quick and accurate assessments of a broad spectrum of hazardous biological agents has been highlighted by recent high profile events. Integrated optical devices based on evanescent wave interrogation techniques can register minute refractive index changes enabling detection of bioagents on the sensor surface and providing a potential for compact structure combined with a possibility of detecting several analytes simultaneously by fabricating multiple devices on the same chip. Most commonly integrated optical interrogation techniques suffer from issues of optical alignment and fabrication complexities. In addition the materials used to fabricate integrated optical devices experience drifts in material properties with time in ambient aqueous environmental conditions.

The central topic of this thesis is modeling and experimental evaluation of a new class of sensor design using a vertical stack of resonantly coupled dielectric slab waveguides exploiting evanescent wave interrogation technique. A simple but unique design strives to overcome optical alignment and complex fabrication issues. Also use of state of the art ion-assisted deposition techniques to fabricate the slab waveguide structures overcomes the problem of instabilities in waveguide material in aqueous environments due to porosity in microstructures of thin film materials when grown using conventional physical vapor deposition techniques.

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Chapter-I

Introduction

A biosensor is defined in [8] as *a compact analytical device incorporating a biological or biologically-derived sensing element either integrated within or intimately associated with a physicochemical transducer. The usual aim of a biosensor is to produce either discrete or continuous digital electronic signals which are proportional to a single analyte or a related group of analytes.* The first recorded biosensor was an electrochemical sensor developed for glucose detection by Clark and Lyons [9]. In the past couple of decades, research and development in the sensors area has expanded exponentially in terms of numbers of papers published, financial investments and number of active researchers involved worldwide. There are numerous components to any biosensor configuration and many combinations have been proposed and demonstrated. Only a very few of them have been able to make the transition from research into the commercial market. The field of biosensing is wide and multidisciplinary, spanning biochemistry, bioreactor science, physical chemistry, electrochemistry, electronics and software engineering. Below the basics of biosensing, including the various transduction techniques used, are reviewed.

1.1) Sensors and Transducers

Sensors are devices that incorporate a sensing element either closely connected to, or integrated within, a transducer system. From an instrumentation point of view, a sensor may be defined as a measuring device that converts information from a physical energy domain such as thermal, mechanical, magnetic, chemical, biochemical or biological to a domain that has characteristics of electrical nature such as charge, voltage, current, capacitance, frequency etc. In certain respects a sensor can be regarded as a transducer, because transducers provide electronic signals according to changes in a particular property in its immediate environment. A few examples of transducers most commonly used are in temperature monitoring (thermocouples, thermistors), piezoelectric transducers, flow-meters, humidity sensors, etc.. The transducers described above are usually mass produced with highly predictable behavior and reproducible characteristics.

The data sheets explain a complete behavior of the device under ambient conditions. However this is not the case with the sensors involved in the biological or chemical domain. The technology is not mature relative to transducer technology and has a relatively large batch-to-batch irreproducibility in characteristics. This makes chemical or biosensors difficult to use, with a need for accurate calibration and troubleshooting. A biosensor or a chemical sensor can be distinguished from a normal transducer in that it provides the information about the biological or chemical nature of its surroundings. A physical transducer may be an important part of this sensor; however its overall character is determined by some selective membrane, which has the ability to recognize a single compound among other substances in the samples. A biosensor has three important attributes: [10]

- 1) It must be comprised of a bioactive substance, for example, an enzyme, antibody, membrane or micro-organism.
- 2) This substance must specifically be able to recognize the species of interest.
- 3) It must be in close contact with a suitable transduction system.

Figure 1.1 Principle of the operation of a biosensor [10]

Characteristics of any sensor are a function of application and hence what is acceptable for a particular application may not be tolerable in other circumstances. For instance a very accurate and highly sensitive but bulky sensor may be unacceptable where device

portability is required. Almost all the sensors deviate from ideality because of the inherent nature of the device or an external environmental factor such as temperature, pressure, humidity etc. Hitherto, any sensor should have some desirable characteristics which are listed below [26].

- **Transfer function:** The functional relationship between input and output signal that can be expressed in mathematical terms providing a complete description of the sensor.
- **Sensitivity:** The ability of the device to discern accurately and precisely between small differences in the input signal. It is usually a derivative of the transfer function with respect to the input signal. A sensor is highly sensitive if it produces a large change in output for a small input change.
- **Response time:** Slow response times can be a hindrance in using it as a real time sensor. It can limit the range of possible applications.
- **Hysteresis:** An ideal sensor should have no hysteresis effects when the input stimulus is scaled up or down.
- **Selectivity:** Sensor response should be selective to a particular kind of species concentration so that it generates output signal for that particular agent even in the presence of other chemical or biological agents.
- **Portative:** A sensor should be small enough with minimal paraphernalia to be able to be transported to various locations with ease.

1.2) Transduction Principles

The most important characteristic of a biosensor is its ability to recognize a single compound among other substances in a sample. A biosensor can therefore be described as having two main parts. 1.) A bioreceptor or the biological component that selectively identifies the analyte ensuring molecular recognition transformation of the analyte into a transducer detectable form, and 2.) A transducer which exploits the biochemical transformation by converting the signal into electrical form. To obtain a good electrical output, the bioreceptor and transducer have to be compatible with each other. The biological component can be generally separated into two categories: 1.) biocatalysts (enzymes, intact cells and organelles) where recognition and binding of molecules leads

to a chemical change, and 2.) affinity reactions (antibodies, nucleic acids and cell membrane receptors) where binding is an irreversible change. The transducers used in the recognition of these biological events can be broadly classified into electrochemical, optical, thermal and piezoelectric devices. Many biosensors use transformation or coupling reactions to recognize the analyte. These reactions can also produce variations in electric charge, mass, optical properties etc. which then can be detected directly by the transducer.

1.2.1) Potentiometric biosensors

Potentiometric biosensors, by using a combination of suitable bioreceptors and transducers, monitor the change in the electric potential arising from the binding of an ion to an ionophore. Ionophores are compounds that act as carriers of specific ions across the membranes and hence play a key role in selectivity of ion-selective electrodes [1]. In this detection scheme, the potential across an electrochemical cell containing the biological sensing element is measured to detect any activity in the product or a reactant in the recognition reaction [15]. The most commonly used transducer is the field effect transistor, whose structure is modified using thin film semiconductor techniques. A membrane is attached to the gate and ionic binding to this membrane changes the gate potential which in turn changes the output electrical signal from the FET. The basis of this detection scheme is a thin film transistor, in which the current flowing between source and drain is controlled by the amount of charge on the gate. A chemFET or chemically selective field effect transistor is another FET based potentiometric electrode concept used for biosensing applications. The chemFET is an insulated gate FET where the FET is modified to monitor activity of the presence of ions or other species through charge separation at an interface. The metal gate is replaced by a chemically modified layer capable of extracting or donating charge with respect to an aqueous sample solution. This charge separation is responsible for generating a potential modulating the FET's source to drain current. This current depends on the concentration of analyte. Though the basic working principle is same there are different types of chemFET configurations for biosensing, they are:

- Ion selective FETs or ISFET which respond to ions in the solution

- Enzyme FETS (ENFET) which use immobilized enzymes to measure enzyme species that are coupled to enzymatic reactions.
- Immunological FETs (IMFETs) generate charge separation via antibody-antigen interactions
- Suspended gate FETs use the changes in the work function and dipole orientation generated as a result of interaction of sensing element with gases.

Potentiometric biosensors can be developed into highly reliable and stable devices with considerable advances in the present technology. However the overriding reality is that the cost of manufacture is too high relative to other competing techniques. Microfabrication techniques can be applied to other transducers based on optical or amperometric principles to produce cheaper biosensors. At present Potentiometric sensors based on ion selective FET's are commercialized because of their properties of being small and rigid. They are good in biomedical applications having very fast response times, ideal for dynamic measurements [36].

1.2.2) Amperometric biosensors

The essence of Amperometric biosensors is redox chemistry which measures current that is directly proportional to specific binding. The current changes according to the concentration through an electrochemical electrode coated with biologically active material. There is oxidation or reduction of an electroactive species on an electrode surface [26]. The simplest amperometric biosensors in common usage involve the Clark oxygen electrode. This consists of a platinum cathode at which oxygen is reduced and a silver/silver chloride reference electrode. When a potential of -0.6 V, relative to the Ag/AgCl electrode is applied to the platinum cathode, a current proportional to the oxygen concentration is produced. Normally both electrodes are bathed in a solution of saturated potassium chloride and separated from the bulk solution by an oxygen-permeable plastic membrane [9]. Typical species used in amperometric biosensors are urea, glucose, fructose, sucrose as well as tissue and whole organisms. By using electron-accepting chemicals such as chloranil, fluronil, organic dyes etc, the redox activity of the enzymes can be monitored directly. One of the examples of an amperometric biosensor is a pen-sized glucose meter. This gives glucose read-out 30 seconds after the blood sample

is given [11]. This sensor is based on a ferrocene-mediated enzyme electrode [12]. The principal disadvantage of enzyme electrodes based on consumption of oxygen or production of hydrogen peroxide lies in the dependence of the assay on oxygen. Several configurations were proposed including Enfors [13], showing that oxygen can be generated *in situ* at enzyme electrodes or Clark *et al.* [14] proposing an oxygen reservoir in the form of a silastic drum implanted alongside the enzyme electrodes. The use of a mediator-modified electrode to replace oxygen as an electron acceptor, as in the case of the pen-sized glucose meter, provides a practical solution to the above mentioned problems. Amperometric biosensors can be classified into three generations.

- First generation involves biosensors in which transduction of biological reaction is by redox chemistry i.e. by oxidation or reduction at the electrode surface.
- Second generation uses mediator molecules to transfer electrons from the enzyme after it reduces or oxidizes the specie.
- In the third generation the surface of the electrode is modified by adding molecules allowing direct oxidation or reduction of the enzyme at the electrode. This method does not need a mediator as in the case of second generation amperometric biosensors.

The three common modes of usage in case of amperometric sensors are single use, intermittent use and continuous use. Most fall short of what is desirable from a sensor, however the continuous mode sensor had the best performance with good precision, simple apparatus, and gave a low cost versus data rate [37].

1.2.3) Optical biosensors

Optical detection systems involve measurement of changes in any optical characteristics based on the way the light is modulated. These can be classified into five categories: intensity, wavelength, and polarization, phase and time modulation [1]. Typical examples of intensity or amplitude modulation are absorption, fluorescence, and reflectance measurements. The output signal is directly proportional to the number of transmitted photons because the physical mechanism involves modulation of the number of photons transmitted after absorption or emitted by luminescence, scattering or refractive index changes. Wavelength modulation on the other hand involves

measurement of spectral-dependent variations of absorption and fluorescence and hence provides additional spectral information compared to simple intensity measurements. Fiber-optic absorption spectrometers or Fourier transform infrared spectroscopy can be used to make the spectral variations in the case of absorption measurements. FTIR involves combining spatial specificity with information on the sample's chemical constitution. A chemical species map may be constructed for the whole spatial area by determining IR spectra by measuring the whole spectrum and deconvoluting using a Fourier transform. Phase modulation involves fringe counting or fractional phase-shift detection using interference between separate paths in Mach-Zehnder, Michelson or Fabry-Perot interferometers. The approach is based on the interference of two coherent light beams in different optical fibers or different paths with one beam being modulated by the chemical environment. A phase difference is introduced because of the chemical or biological environment and it is measured by fringe counting (one fringe = 360 degree phase). Also a multimode fiber can be used in which various modes can interfere with one another. A Mach-Zehnder arrangement has been proposed for a hydrogen gas sensor in which an optical fiber is coated with palladium metal film and absorption of gas introduces a strain in the film that is transferred to the fiber. The coated fiber when exposed to hydrogen forms a hydride with an expanded lattice constant. This expands the fiber and changes the optical path length which is measured using a Mach-Zehnder interferometer [16]. In polarization modulated biosensors the physical mechanism used is measurement of changes in rotation of polarization. Changes in polarization occur depending on the chemical interaction and are measured by a polarization analyzer. However this method is prone to errors arising from random polarization changes due to intrinsic polarization variations in the fiber or stress related birefringence. High birefringence monomode fibers can be used to maintain a constant state of polarization, instead of conventional fibers. Most optical biosensors are based on the various light modulation techniques described above. The most commonly used physical parameters that create this modulation are refractive index, path length and to a lesser extent pressure.

Optical fibers and integrated waveguides have made it possible to miniaturize optical sensors and integrate them into a small chip form. The following lists a few

advantages of using an optical mechanism to couple between chemical or biological and electrical domains:

- Electromagnetic interference immunity, which allows the device to be operated in electromagnetically hostile environments.
- Electrical passivity reduces the risk of explosion in chemically explosive environments.
- The use of integrated optics or optical fibers makes it possible to have robust, mechanically stable and compact optical circuitry. This opens up possibilities of having multiple sensors on one chip, or micro sensor arrays.
- There is potential for low-cost mass production.

1.3) Evanescent Wave Biosensor concepts

An evanescent wave is an electromagnetic wave that propagates along the surface but decays exponentially perpendicular to it. They are present in optical as well as acoustic systems but the basic idea remains the same. When a beam directed from a medium of higher refractive index, n_1 to lower refractive index, n_2 , total internal reflection takes place, if the angle of incidence is greater than the critical angle. This generates an evanescent wave that penetrates beyond the reflecting boundary into the rarer medium. Since the energy circulates back and forth across the interface, there is no net flow of energy into the non-absorbing rarer medium. Electric field amplitude of light E , is greatest at the surface and decays exponentially away from the surface [26].

$$E = E_0 \exp(-x / d_p) \quad (1.1)$$

where

$$d_p = \lambda / \left\{ 2\pi n_1 \left[\sin^2 \theta - (n_1 / n_2)^2 \right]^{1/2} \right\}$$

The depth of penetration d_p , is defined as the distance at which electric field falls to $1 / e$ or approximately 36% of its value at surface. The depth of penetration decreases with increasing θ and increases, as the ratio of n_1 / n_2 approaches unity.

Figure-1.2 Exponential decay of the evanescent wave outside the guide [1]

The chemical reaction may be measured on the surface of a waveguide, which can be a dielectric slab waveguide or an optical fiber. The evanescent wave approach offers many advantages in particular applications. They are listed as follows: [26]

- These techniques provide enhanced sensitivity by virtue of a greater number of reflections per unit length as compared to bulk optics attenuated total reflection. This means greater power in the evanescent field and hence a more sensitive device.
- The light to be monitored is always guided with no coupling requirement in the sensor region. This makes having an integrated miniaturized device feasible.
- It is possible to confine the evanescent field to a short distance from guiding interface, thereby avoiding surface and bulk effects.

The most significant problem with evanescent wave sensors is surface contamination. This leads to reduced sensitivity and therefore requires careful design of the biolayer attachment layer to avoid nonspecific binding and/or frequent recalibration of the device. This problem may restrict use of evanescent sensors to disposable situations only, thus accentuating the need for low cost.

1.3.1) Interferometric Sensors

Generally there are two configurations of interferometric sensors. One is a differential interferometer and other is a Mach-Zehnder interferometer. A difference interferometer as a sensitive optical probe was reported by Fattinger et al. [17]. A planar waveguide supports only two fundamental modes of different polarization i.e. transverse

electric (TE) and transverse magnetic (TM). The polarized laser beam is focused on the butt face of the waveguide and both TE and TM modes are excited coherently. The adsorption of molecules to the surface of the waveguide induces a change in effective refractive indices. Since the interaction with the sensing surface is different for the two modes, the induced change in effective refractive indices is also very different. This leads to a relative phase difference between TE and TM polarized light in two guided modes and gives a measure of molecular surface concentration on the sensor surface. The phase difference is given as follows: [1]

$$\Delta\phi = (2\pi L / \lambda)(N_{TE} - N_{TM}) \quad (1.2)$$

In a Mach-Zehnder interferometer the coupled light is split into two channels. One channel acts as a reference and other one is used to measure the molecular surface concentration. The interference patterns generated by recombining the light from the reference channel and sensor channel give a measure of surface adsorption over the sensor channel.

1.3.2) Optical waveguide based biosensors

Biosensors using waveguides as optical transducers work on the same principle as that of fiber optic sensors except that they differ in geometry. A new kind of sensor based on a waveguide called the critical sensor was reported, which is based on the measurement of change of refractive index caused by adsorption of molecules at the sensor surface [18]. The principle of critical sensors is based on Snell's law of refraction. Part of the waveguide is shielded, leaving its effective refractive index constant. The measurement is done by observing the change in the effective refractive index contrast between the unshielded surface and a shielded sensor surface, which in turn changes the deflection angle of light passing the interface between the areas. The sensor is adjusted in such a manner that half of the incoming light striking the interface between the shielded and unshielded region is reflected R and the other half is completely transmitted T . A change in critical angle changes the difference between R and T [18]:

$$\Delta(R - T) = \int_{t_s}^{t_e} \frac{d(R - T)}{d\theta_c} \cdot \frac{d\theta_c}{dN_{eff2}} \cdot \frac{dN_{eff2}}{dt} dt \quad (1.3)$$

The change in intensities can be measured using photodiodes.

The planar configuration uses a glass chip etched with two superimposed uniform diffraction gratings of different periodicities. On the top of this structure there is a high index waveguiding layer of TiO_2 . The light is coupled into the waveguiding layer through one set of the gratings, called the input port, and is coupled out of the waveguiding layer using another set of gratings, called the output port. The detection of the biological agents is done at the surface of the waveguiding layer by an evanescent wave emanating from the waveguide [19]. There are various other configurations using planar waveguides and evanescent waves. The basic mechanism common to all systems is the measurement of changes in effective refractive index caused by the immediate medium in contact with the device surface.

1.3.3) Surface plasmon resonance

The difference between surface plasmon resonance and evanescent spectroscopy is that the waveguide is covered with a thin metal film usually silver or gold. Surface plasmons are transverse magnetic (TM) electromagnetic waves that travel along the interface between a dielectric and a metal and the resonance arises from the interaction of an electron rich surface, such as that of a metal, with a charged particle or with a photon creating an optical-electrical phenomenon. These waves are exponentially attenuated normal to the surface and propagate parallel to the interface. At resonance the photon's energy is transferred to the surface of the metal via clouds of electrons called plasmons. This energy transfer takes place when the quantum energy and momentum of photons exactly matches the quantum energy level and momentum of the plasmons. The light reflected from the metal gives the accurate resonance wavelength. The metal acts as a mirror reflecting all the light except, at a resonance wavelength, when almost all the light is absorbed, exciting the plasmons [19] [1]. Alternatively a single wavelength can be used and the angle can be changed at which the light is incident on the metal surface. The maximum absorption takes place at a fixed angle of incidence. A common configuration used to create surface plasmons is the Kretschmann configuration in which, the light is incident on the film through a prism at an angle greater than the critical angle. The surface plasmon is detected by carefully adjusting the angle of incidence until the reflected intensity is dramatically quenched. This angle is called the critical resonance or

plasmon angle θ_p . Measurement of the shift of angle is directly proportional to the changes in the concentration on the surface layer. Mechanical scanning can be employed to measure the angle; alternatively a cylindrical prism with a CCD array can be used to register the output beam [20].

Figure 1.3 shows a typical instrumentation for the Kretschmann arrangement, where the resonant condition is produced by varying the input angle and the curves show the shift in the resonance angle as a function of film thickness or various monolayers.

Figure1.3-Resonant Dip for films with 1, 2 and 3 monolayers [1]

Figure-1.4 Instrumentation for the Kretschmann arrangement [1]

A typical SPR sensor has a silver film of 40-50 nm thickness evaporated onto the glass plate or prism. The sample to be interrogated is placed on the metal layer and any

change in the sample property shifts the resonance angle, providing a means to measure the changes on the surface. The metal layer is used to enhance the electric field of the evanescent wave within the sample layer.

1.3.4) Resonant optical waveguide biosensors

This biosensor is based on a vertical stack of planar waveguides that forms an optical coupler structure that exploits evanescent wave coupling among the waveguides separated by a buffer. The interaction of evanescent wave with the bioagent is used to detect the changes in the biological medium in contact with the upper, exposed waveguide in the stack. The structure of the device is illustrated in the Figure 1.5.

Figure-1.5 Resonant waveguide biosensor structure [32]

The structure is comprised of two single mode planar waveguides of higher index material separated by spacer layer of lower index on a low index substrate. Optical power enters the top waveguide and under tuned conditions all the optical power is transferred in the lower waveguide from the upper guide after traversing some distance along the length of the device. The periodic exchanges of optical power take place between the two waveguides. The two waveguides act as tuned resonators and hence the name of resonant optical waveguide biosensor. This transfer of power continues over the whole length of

the device. This condition is called phase match or a tuned condition. Properly designed, this tuning is strongly dependent on the effective refractive index of the medium above the top waveguide and any change in the effective index changes the strength of coupling between the two guides. The detection of a bioagent takes place at the top of the waveguide where any change in environment creates a change in the effective index. This changes the phase matched condition and detunes the two waveguides. This is the basis of transduction which detects any changes in the immediate environment at the surface of the upper waveguide.

Most biosensor configurations exploiting integrated optical waveguiding structures and their evanescent fields work effectively under laboratory environments but fail in field applications. This is primarily due to the need for associated support equipment and issues with achieving and maintaining optical alignment. In addition the thin film material used in many integrated optical sensor configurations used to fabricate waveguides is unstable in aqueous environments making the device output drift with time. With correctly chosen materials, the unique design of a resonant biosensor using evanescent wave coupling and a simple vertical stack of thin film waveguide structures strives to overcome the aforementioned deficiencies and seeks to offer a stable, portable and sensitive sensor platform. Initial exploration of the behavior of this sensor configuration is the central topic of this thesis.

1.4) Organization of thesis:

The body of this thesis is organized as follows. Chapter 2 introduces the basic principles of electromagnetics necessary to support this experimental work, including the ray optics and wave optics treatment of dielectric slab waveguides. In addition this chapter briefly touches upon coupled mode theory and the beam propagation method for integrated optics as well as its limitations under certain conditions. Chapter 3 focuses on the simulation of a basic resonant waveguide biosensor configuration using the beam propagation method and compares the results with preliminary experimental work on the actual sensor structure. Chapter 4 deals with the experimental procedure used to evaluate the prototype sensor. The thesis work is summarized and main conclusions drawn in Chapter 5 as well as recommendations for future studies presented.

Chapter-II

Principles of Resonant Waveguide Biosensor Measurements

2.1) Basic Electromagnetics

Light is an electromagnetic wave phenomenon described by the same theoretical principles that govern all forms of electromagnetic radiation. Classical electrodynamics depicts light as having continuous transfer of energy by way of electromagnetic waves. However, the modern view of quantum electrodynamics expresses light as electromagnetic interactions and the transport of energy in terms of elementary particles known as *photons*. In fact light has a dual nature, as it propagates through space in a wavelike fashion and yet displays particle-like behavior during emission and absorption processes. Light may be considered in three different ways; the appropriate viewpoint depends on the nature of the phenomena to be understood [1].

- Light is composed of photons, vectors of energy exchange, which can explain absorption, emission etc
- Light is an electromagnetic wave that can propagate and be diffracted in a non-dispersive medium without energy exchange.
- Light is composed of luminous rays that obey the principles of geometrical optics.

Ray optics, also called geometrical optics, is the simplest theory of light. Historically it was the first optical theory to describe the nature of light. Though it is an approximate theory, it adequately describes most of the daily experiences with light. A more sophisticated approach is wave optics. Actually ray optics is the limit of wave optics when wavelength is infinitely small. It describes many optical phenomena using scalar wave theory in which light is described by a single scalar wave function. Electromagnetic optics provides the most complete treatment of light within the confines of classical optics. The electromagnetic theory of light encompasses wave optics, which, in turn, encompasses ray optics. Electromagnetic radiation propagates in the form of two mutually coupled vector waves, an electric-field wave and a magnetic-field wave [28]. Both are vector functions of position and time. Generally six scalar functions of position

and time are required to describe light in free space, that are related since they must satisfy a set of coupled partial differential equations known as Maxwell's equations [25].

2.1.1) Maxwell's Equations

Maxwell's equations are one of the most elegant and concise ways of expressing the fundamentals of electricity and magnetism. These equations describe the relationship between electric and magnetic fields at any point in space as a function of charge density and electric current at such a point. The wave equation for the propagation of light is derivable from Maxwell's equations, and these are the basic equations of classical electrodynamics. Maxwell's equations expand upon and unify the laws of Ampere, Faraday, and Gauss, and form the foundation of modern electromagnetic theory.

In free space i.e. in the absence of magnetic or polarizable media, their differential form is given below, [24]

$$\begin{aligned}\nabla \times \vec{E} &= -\partial \vec{B} / \partial t \\ \nabla \times \vec{H} &= \partial \vec{D} / \partial t + \vec{J} \\ \nabla \cdot \vec{D} &= \rho \\ \nabla \cdot \vec{B} &= 0.\end{aligned}\tag{2.1}$$

$\vec{E}$ = Electric field intensity (V / m)

$\vec{D}$ = Electric flux density or displacement vector (C / m^2)

$\vec{H}$ = Magnetic field intensity (A / m)

$\vec{B}$ = Magnetic flux density (Wb / m^2)

In addition to Maxwell's field equations, there exists a set of auxiliary equations involving the displacement vector $\vec{D}$, electric field vector $\vec{E}$, magnetic flux density $\vec{B}$, and magnetic field intensity vector $\vec{H}$, which are dependent on the material medium in which the fields being described exist. So for homogenous, linear, isotropic dielectric these equations are: [24]

$$\begin{aligned}\vec{D} &= \epsilon \vec{E} \\ \vec{B} &= \mu \vec{H}\end{aligned}\tag{2.2}$$

where ε and μ are the material permittivity and permeability respectively, both in general being tensors of rank 2. The physical constants ε and μ are the defining constants of the material medium. A medium is said to be homogeneous if ε and μ are not functions of position in material, otherwise the medium is termed as inhomogeneous. An isotropic medium is one in which ε and μ are scalar quantities.

These basic Maxwell's equations are expressed in integral form, as given below,[24]

$$\begin{aligned}
\oint_{loop} \vec{E}.d\vec{l} &= -\frac{\partial}{\partial t} \int_{area} \vec{B}.d\vec{s} \\
\oint_{loop} \vec{H}.d\vec{l} &= \int_{area} \vec{J}.d\vec{s} + \frac{\partial}{\partial t} \int_{area} \vec{D}.d\vec{s} \\
\int_{surface} \vec{D}.d\vec{s} &= Q_{enclosed} \\
\int_{surface} \vec{B}.d\vec{s} &= 0.
\end{aligned} \tag{2.3}$$

2.1.2) Wave Equations

Maxwell's field equations and auxiliary equations can be manipulated so as to result in derived equations describing the relation among two vector fields. The permittivity and permeability in their complex notation are generally expressed as $\varepsilon^* = \varepsilon' - j\varepsilon''$ and $\mu^* = \mu' - j\mu''$ where prime and double prime denote the real and imaginary parts. By taking the curl of Maxwell's field equations the differential wave equations describing both $\vec{E}$ and $\vec{H}$ can be obtained. Assuming the material is homogenous, ohmic and source free then $\rho = 0, J = \sigma \cdot \vec{E}$ and μ^* is a constant, and the reduced wave equation is given by, [25]

$$\begin{aligned}
\nabla^2 \vec{E} &= \mu^* \varepsilon^* \partial^2 \vec{E} / dt^2 + \mu^* \sigma \partial \vec{E} / \partial t \\
\nabla^2 \vec{H} &= \mu^* \varepsilon^* \partial^2 \vec{H} / dt^2 + \mu^* \sigma \partial \vec{H} / \partial t.
\end{aligned} \tag{2.4}$$

Assuming a time variation of the form $\exp(j\omega t)$ yields the differential equation, which is also called the vector wave equation for electric and magnetic fields [25]

$$\nabla^2 (\vec{E} / \vec{H}) = \mu^* \varepsilon^* \partial^2 (\vec{E} / \vec{H}) / \partial t^2 \tag{2.5}$$

The Laplacian ∇^2 operates on all the components of $\vec{E}$ and $\vec{H}$, so this concise vector expression actually represents six scalar equations.

In the above equation inclusion of the dissipative effects in the complex dielectric constant gives $\varepsilon^* = \varepsilon' - j\varepsilon''$ [38]. The necessary condition for $\vec{E}$ and $\vec{H}$ to satisfy Maxwell's equation is that each of the components $(E_x, E_y, E_z, H_x, H_y, H_z)$ satisfies the scalar differential wave equation, [25]

$$\partial^2 \psi / \partial x^2 + \partial^2 \psi / \partial y^2 + \partial^2 \psi / \partial z^2 = 1/v^2 (\partial^2 \psi / \partial t^2)$$

or

$$\nabla^2 \psi = \mu^* \varepsilon^* \partial^2 \psi / \partial t^2.$$

(2.6)

The plane wave solution of the scalar differential wave equation is of the form,

$$\psi = \psi_0 \exp(j\omega t - j\vec{k} \cdot \vec{r}) \quad (2.7)$$

From the vector wave equation for the magnetic field we can find the scalar wave equation for plane waves. Assuming the direction of propagation to be the z axis, the wave vector and position vector reduce to $\vec{k} = k\hat{z}$ and $\vec{r} = z\hat{z}$ respectively. Thus the propagation of phase can be given by $\vec{k} \cdot \vec{r} = kz = nk_0 z$, where n is the refractive index of the propagating medium. If the electric field is x -polarized, then the scalar equation for electric and magnetic fields can be expressed as,

$$\begin{aligned} E_x(z, t) &= A \exp\{j(\omega t - kz)\} \\ H_y(z, t) &= B \exp\{j(\omega t - kz)\}. \end{aligned} \quad (2.8)$$

2.1.3) Boundary conditions

A slab wave-guide is basically a medium of one refractive index imbedded in a medium of lower refractive index such that the medium with the higher refractive index acts as a light trap or guide. To understand the slab wave-guide it is necessary to understand the boundary conditions at the interface. In a homogenous medium, all components of fields $\vec{E}, \vec{H}, \vec{D}$ and $\vec{B}$ are continuous functions of position. At the boundary between two dielectric media and in the absence of free electric charges and currents, the tangential components of the electric and magnetic fields $\vec{E}$ and $\vec{H}$ and the normal

components of electric and magnetic flux densities $\vec{D}$ and $\vec{B}$ must be continuous. Maxwell's equation in integral form can be used to determine the conditions, which must be satisfied by $\vec{E}, \vec{H}, \vec{D}$ and $\vec{B}$ at the boundary between two media with differing ϵ^* and μ^* . The summary of the results is as given below where t denotes the component tangent to the surface separating media 1 and 2 and n denotes the component normal to that surface. The quantities $\vec{J}_s$ and ρ_s represent the surface currents and charge densities respectively.

$\vec{H}_{1t} - \vec{H}_{2t} = \vec{J}_s$
$\vec{E}_{1t} - \vec{E}_{2t} = 0$
$\mu_1 \vec{H}_{1n} - \mu_2 \vec{H}_{2n} = 0$
$\epsilon_1 \vec{E}_{1n} - \epsilon_2 \vec{E}_{2n} = \rho_s$

Figure-2.1 Review of boundary conditions

2.1.4) Reflections at boundaries

Optical structures such as dielectric slab waveguides take advantage of optical characteristics of the material in which the field is propagated. Changes in optical properties at the boundaries between two materials form the basis of many optical

devices. The next few paragraphs discuss basic phenomena such as reflection, refraction and examine the effect on a propagating wave when it is incident on a boundary between two materials.

2.1.4.1) Reflection and Refraction

As shown in the Figure 2.2 below let us consider light waves encountering a smooth boundary between two different homogenous media. If the surface is not perfectly reflecting, then a portion of the wave is transmitted from the region of refractive index, n_1 to the refractive index n_2 . The angle of incidence θ_i [radians] is equal to the angle of reflection θ_r [radians] and it is independent of the refractive index values, n_1 and n_2 .

$$\theta_i = \theta_r \quad (2.9)$$

The relation of the angle of the transmitted component, θ_t to the incident angle, θ_i is given by Snell's law, which states that the angle of the transmitted beam is a function of the relative refractive indices.

$$n_1 \sin \theta_i = n_2 \sin \theta_t \quad (2.10)$$

Figure-2.2 Electromagnetic wave incident at the interface of two materials

It can be observed that when a light beam moves from a material of higher refractive index to a region of lower refractive index, i.e. if $n_1 > n_2$ then $\theta_t > \theta_i$. At some particular angle of incidence $\theta_i = 90^\circ$, meaning that none of the beam is transmitted in the medium of lower refractive index and Snell's law simplifies to $\sin \theta_i = n_2 / n_1$. The relation defines the critical angle as $\theta_c = \sin^{-1}(n_2 / n_1)$. For angles of incidence greater than this critical angle, the incident beam experiences total internal reflection – no light is transmitted across the boundary. This is the phenomenon that is the basis of propagation of light in an optical waveguide.

2.1.4.2) Fresnel Equations

Fresnel's equations describe the reflection and transmission of electromagnetic waves at an interface. They give reflection and transmission coefficients for waves polarized parallel and perpendicular to the plane of incidence. Fresnel's coefficients are generally expressed in terms of incident and transmitted angles θ_i and θ_t . It is convenient to decompose any arbitrarily polarized incident wave into two orthogonal components. These components are chosen to be perpendicular and parallel to the plane of incidence [2]. In this section we examine the reflection and refraction of a monochromatic plane wave of arbitrary polarization incident upon a planar boundary between two dielectric media. The media are assumed to be linear, homogenous, isotropic, non-dispersive, and non-magnetic with refractive indices n_1 and n_2 respectively.

TE configuration

Let us consider when the incident wave has electric field polarized in the plane perpendicular or transverse to the plane of incidence as shown in the Figure 2.3 below. The wave has a propagation constant, k_i in a material with a refractive index, n_1 is incident at an angle, θ_i on a region with a refractive index n_2 . A portion of the wave is reflected with a refractive index of n at an angle $\theta_i = \theta_r$. The remainder of the wave is

transmitted with propagation constant k_t at an angle θ_t into the material with refractive index n_2 .

Using the boundary conditions it's evident that the electric field is always parallel and tangential to the interface, so we can say that

$$E_i + E_r = E_t \quad (2.11)$$

The tangential components of the magnetic field are as given below:

$$\begin{aligned} H_{iT} + H_{rT} &= H_{tT} \\ H_i \cos \theta_i - H_r \cos \theta_r &= H_t \cos \theta_t \end{aligned} \quad (2.12)$$

Figure-2.3 TE incidence onto boundary [4]

The above equation can be rewritten using the impedance relation between electric and magnetic field as,

$$\sqrt{(\epsilon_i / \mu_i)} E_i \cos \theta_i - \sqrt{(\epsilon_r / \mu_r)} E_r \cos \theta_r = \sqrt{(\epsilon_t / \mu_t)} E_t \cos \theta_t, \quad (2.13)$$

Since $\theta_i = \theta_r$, $\epsilon_i = \epsilon_r$ and $\mu_i = \mu_r = \mu_t = \mu_m$ being a semiconductor and hence non-magnetic, the above equation can be simplified to give the following equation,

$$n_1 \cos \theta_i (E_i - E_r) = n_2 \cos \theta_t E_t. \quad (2.14)$$

By manipulating the equations above the reflection and transmission coefficients, R_{TE} and T_{TE} can be given as below. The reflection and transmission coefficients define the

relative amounts of fields. The phase shift of a transmitted TE wave is always zero and the reflected TE wave has a phase shift of π radians,

$$\begin{aligned} R_{TE} &= \frac{E_r}{E_i} = \left(\frac{n_1 \cos \theta_i - n_2 \cos \theta_t}{n_1 \cos \theta_i + n_2 \cos \theta_t} \right) \\ T_{TE} &= \frac{E_t}{E_i} = \left(\frac{2n_1 \cos \theta_i}{n_1 \cos \theta_i + n_2 \cos \theta_t} \right). \end{aligned} \quad (2.15)$$

- **External Reflection** ($n_1 < n_2$): Reflection coefficient is always real and negative, corresponding to a phase-shift of π radians. At $\theta_i = 0^\circ$ (normal incidence) $R_{TE} = (n_2 - n_1)/(n_1 + n_2)$ while at $\theta_i = 90^\circ$ (grazing incidence) it increases to unity.
- **Internal Reflection** ($n_1 > n_2$): For small θ_i reflection coefficient is real and positive and its magnitude is $R_{TE} = (n_2 - n_1)/(n_1 + n_2)$ for $\theta_i = 0^\circ$. It increases to unity when $\theta_i = \theta_c$ where $\theta_c = \sin^{-1}(n_2 / n_1)$. For angles greater than critical angle i.e. $\theta_i > \theta_c$ R_{TE} remains unity which corresponds to total internal reflection. Total internal reflection is accompanied by a phase shift which increases from zero at $\theta_i = \theta_c$ to π at $\theta_i = 90^\circ$.

TM configuration

A similar treatment can be applied to the TM case where the magnetic field is always transverse to the plane of incidence as shown in the Figure 2.4. This leads to similar set of equations for reflection and transmission coefficients that are given below,

$$\begin{aligned} R_{TM} &= \frac{E_r}{E_i} = \left(\frac{n_2 \cos \theta_i - n_1 \cos \theta_t}{n_1 \cos \theta_i + n_2 \cos \theta_t} \right) \\ T_{TM} &= \frac{E_t}{E_i} = \left(\frac{2n_1 \cos \theta_i}{n_1 \cos \theta_i + n_2 \cos \theta_t} \right). \end{aligned} \quad (2.16)$$

- **External Reflection** ($n_1 < n_2$): In this case R_{TM} is real and decreases from positive value of $(n_2 - n_1)/(n_2 + n_1)$ at normal incidence until it vanishes at Brewster's angle $\theta_B = \tan^{-1}(n_2 / n_1)$. For an angle of incidence greater than

Brewster's angle R_{TM} reverses sign and the magnitude approaches unity at grazing incidence.

Figure-2.4 TM incidence onto boundary [4]

- **Internal Reflection** ($n_1 > n_2$): For normal incidence R_{TM} is negative and has magnitude $R_{TM} = (n_1 - n_2) / (n_1 + n_2)$. The magnitude of the reflection coefficient decreases with increasing θ_i until it drops at Brewster's angle $\theta_B = \tan^{-1}(n_2 / n_1)$. After Brewster's angle R_{TM} increases and reaches unity at the critical angle. For $\theta_i > \theta_c$ there is total internal reflection and associated phase shift.

2.1.4.3) Total Internal Reflection

There are two types of wave incidence that are of tremendous practical importance. In the case of normal incidence the distinction between TE and TM disappears. However total internal reflection is the condition most relevant to guided wave optical devices. As discussed above in the case of internal reflection, when θ_i was equal to or greater than the critical angle θ_c , R_{TE} and R_{TM} increase with increasing θ_i ,

and therefore T_{TE} and T_{TM} both decrease. This means that no wave is transmitted into the second material, implying total internal reflection. In this case R_{TE} and R_{TM} can be shown to have unit amplitude and that they are complex quantities. Through Snell's law we know that $n_1 \sin \theta_i = n_2 \sin \theta_t$ which can be re-expressed as [3]

$$\cos \theta_t = \sqrt{1 - \left(\frac{n_1 \sin \theta_i}{n_2} \right)^2}, \quad (2.17)$$

and when $\theta_i > \theta_c$ it becomes

$$\cos \theta_t = \sqrt{-\left\{ \left(\frac{n_1 \sin \theta_i}{n_2} \right)^2 - 1 \right\}},$$

which shows that for all incident angles $\theta_i > \theta_c$, $\cos \theta_t$ becomes wholly imaginary. Substituting equation 2.17 into reflection coefficients for TE and TM waves as given in equations 2.15 and 2.16 we get the following results,

$$\begin{aligned} R_{TE} &= \exp \left\{ i2 \tan^{-1} \left[\sqrt{\frac{n_1^2 \sin^2 \theta_i - n_2^2}{n_1^2 (1 - \sin^2 \theta_i)}} \right] \right\} = \exp \{ i\phi_{TE} \} \\ R_{TM} &= \exp \left\{ i2 \tan^{-1} \left[\frac{n_1^2}{n_2^2} \sqrt{\frac{n_1^2 \sin^2 \theta_i - n_2^2}{n_1^2 (1 - \sin^2 \theta_i)}} \right] \right\} = \exp \{ i\phi_{TM} \}. \end{aligned} \quad (2.18)$$

The above equations indicate that while the amplitudes of incident and reflected waves are identical, their phase is altered by ϕ_{TE} and ϕ_{TM} for TE or TM polarized light, respectively because of total internal reflection.

Figure-2.5 Propagation vectors for total internal reflection [3]

This phenomenon can be further understood using the above Figure 2.5 [3]. The critical angle is given by $\sin \theta_c = n_t / n_i$ and for $\theta_i > \theta_c$ both R_{TE} and R_{TM} become complex. In terms of wave functions the transmitted electric field can be given by,

$$\vec{E}_t = \vec{E}_{0t} \exp i(\vec{k}_t \cdot \vec{r} - \omega t) \quad (2.19)$$

where

$$\vec{k}_t \cdot \vec{r} = k_{tx}x + k_{ty}y = k_t \sin \theta_t + k_t \cos \theta_t.$$

From Snell's law we have

$$k_t \cos \theta_t = \pm k_t \left(1 - \frac{\sin^2 \theta_i}{(n_t / n_i)^2} \right)^{1/2}$$

and when

$$\sin \theta_i > n_t / n_i,$$

$$k_{ty} = \pm i k_t \left(\frac{\sin^2 \theta_i}{(n_t / n_i)^2} - 1 \right)^{1/2} \equiv \pm i \beta$$

and

$$k_{tx} = \frac{k_t}{(n_t / n_i)} \sin \theta_i.$$

Hence

$$\vec{E}_t = \vec{E}_{0t} \exp(\mp \beta y) \exp i \left(\frac{k_t x \sin \theta_i}{(n_t / n_i)} - \omega t \right).$$

Neglecting the positive exponential, which is physically not tenable, we have a wave whose amplitude drops off exponentially as it penetrates the less dense medium. The disturbance advances in the x-direction as a surface or **evanescent wave**. Its amplitude decays rapidly in the y-direction, becoming negligible as a distance into the second medium of only a few wavelengths. On an average there is zero net flow through the boundary in the second medium as the energy circulates back and forth across the interface and leads to conservation of energy [3].

2.2) Slab Waveguides

A waveguide is a structure that allows optical confinement by making use of multiple total internal reflections from two or more interfaces. The simplest of all the optical waveguides is the film waveguide which consists of a dielectric film deposited on a substrate. This involves three media: airspace, a film and a substrate with their interfaces parallel to each other unless otherwise specified. The film thickness usually varies from a fraction of a micron to several microns. However, more importantly, the film has an index of refraction larger than the air and the substrate. This makes the waveguide behave as a lens-like medium and the wave in the guide may be considered as continuously passing through and being focused by a sequence of lenses. As shown in the Figure 2.6 below, a plane wave starts from the left of the figure and propagates towards the right. The solid and dashed lines represent the wave fronts and lines of energy respectively. This wave propagates slower in the film compared to the air-space and the substrate due to large refractive index. This causes the wave front to take a concave shape as the wave progresses to the right [6].

Figure-2.6 Waveguide as a lens-like medium [6]

Any structure with the refractive index distribution peaked in the middle will have the same focusing property and can be considered as a lens-like medium. This emphasizes the importance of the refractive index and leads to the important rule in waveguide optics called **the rule of refractive index**. In a multilayer structure with layers parallel to the direction of light wave propagation, light tends to propagate in the region where the refractive index is the largest, or, the wave velocity is the slowest [6].

The key to understanding the phenomenon behind the propagation of light in a slab waveguide is to know what happens to a wave at an interface. There are two distinct models. The ray optic representation is a very simple picture that explains why waveguides have distinct modes and how these behave. The electromagnetic model gives a more complete description and provides expressions for the electric and magnetic fields in the waveguide.

2.2.1) Wave Optics Treatment of Slab Waveguides

The wave optics model is based on the solution of the wave equation. This model leads to field and intensity distributions in the guide and the external media. This is important to determine the interaction of modes with structures outside the waveguide or to understand the behavior of the field, when coupled to another optical structure. Any mode propagating in the slab is actually light energy being guided in the medium or core having finite field amplitudes, decaying into the external media. These propagating waves which are guided by the slab but are not fully confined within it are also called surface waves [7]. This is unlike the waves propagating in rectangular or cylindrical microwave guides, which are totally confined. There are three types of normal modes which are eigensolutions of the wave equation, obtained by solving the boundary conditions of the waveguide. As shown in the Figure 2.7 the waves are bounded (a) in the film in “waveguide” modes, and (b) in the film and substrate in “substrate” modes; (c) in “air” modes also called “radiation” modes the waves fill all three spaces (airspace, film and substrate) [6].

Figure-2.7 Field distribution of TE wave in film [6]

2.2.1.1) Symmetric slab dielectric waveguide

This is a special case of the basic three layer planar waveguide. In this case the waveguiding layer is bounded on both surfaces by identical layers with lesser index. Consider a symmetric slab structure where $\varepsilon_1 = \varepsilon_3 = \varepsilon_0$ and $\varepsilon_2 = \varepsilon$ as shown in Figure 2.8 below with the core of refractive index n_2 and a surrounding medium or the cladding of index n_1 and $n_2 > n_1$.

For a wave traveling in z direction with propagation constant k_z the electromagnetic fields can be expressed in the form

$$\begin{aligned}\vec{E}(x, y, z) &= \vec{E}(x, y) \exp(-jk_z z) \\ \vec{H}(x, y, z) &= \vec{H}(x, y) \exp(-jk_z z).\end{aligned}\tag{2.20}$$

TE Analysis

As shown in the Figure 2.8 the light is propagating in the z direction with its electric field polarized in the y direction. This is the transverse electric, TE case. The light is confined by total internal reflection at the two boundaries but is unconfined in the plane.

Figure-2.8 Rays propagating in symmetric slab

The scalar wave equation for this case can be given as

$$\partial^2 E_y / \partial x^2 - E_y (k_z^2 - \omega^2 \mu \varepsilon) = 0.\tag{2.21}$$

This is a second order differential equation and has usual solutions, which are broken up into different regions i.e. the core and the cladding. In the core region $|x| \leq t / 2$, the solutions will be [2]

$$\begin{aligned} E_y(x, z) &= A_2 \cos(k_{2x}x) \exp(-jk_z z) \\ E_y(x, z) &= A_2 \sin(k_{2x}x) \exp(-jk_z z), \end{aligned} \quad (2.22)$$

where $k_{2x}^2 = \omega^2 \mu \varepsilon - k_z^2$. The above relations express the standing wave nature of the field distribution because of the superposition of upward and downward propagating waves. They are called even and odd functions because cosine is an even function and sine an odd trigonometric function. In the cladding region [2]

$$\begin{aligned} E_y(x, z) &= A_1 \exp(-\alpha_x x) \exp(-jk_z z) \quad x > t / 2 \\ E_y(x, z) &= \pm A_1 \exp(\alpha_x x) \exp(-jk_z z), \quad x < -t / 2 \end{aligned} \quad (2.23)$$

where $\alpha_x^2 = k_z^2 - \omega^2 \mu \varepsilon_0$. These relations show that the fields are exponentially decaying as x approaches $\pm \infty$. k_{2x} represents the propagation constant in the x direction and α_x is the decay constant in the cladding. From Maxwell's curl equation we obtain the tangential component of H equal to the electric field gradient of the tangential electric field [2]

$$H_z(x, z) = \frac{j}{\omega \mu} \frac{\partial}{\partial x} E_y(x, z). \quad (2.24)$$

Using the above relations we can calculate the magnetic field in the core and cladding. In the core region $|x| \leq t / 2$, the solutions are [2]

$$\begin{aligned} H_z(x, z) &= -\frac{j}{\omega \mu} \{ \pm k_{2x} A_2 \sin(k_{2x}x) \exp(-jk_z z) \} \\ H_z(x, z) &= -\frac{j}{\omega \mu} \{ \pm k_{2x} A_2 \cos(k_{2x}x) \exp(-jk_z z) \} \end{aligned} \quad (2.25)$$

and in the cladding region

$$\begin{aligned} H_z(x, z) &= -\frac{j}{\omega \mu} \alpha_x A_1 \exp(-\alpha_x x) \quad x > t / 2 \\ H_z(x, z) &= -\frac{j}{\omega \mu} \{ \mp \alpha_x A_1 \exp(\alpha_x x) \}. \quad x < -t / 2 \end{aligned} \quad (2.26)$$

Applying the boundary conditions and matching the tangential electric and magnetic fields at the boundaries lead us to even and odd TE mode solutions. The tangential fields are conserved at $x = t / 2$, so applying these conditions for even modes [2]

$$\begin{aligned} E_{\text{tan}} : A_1 \exp(-\alpha_x t / 2) &= A_2 \cos(k_{2x} t / 2) \\ H_{\text{tan}} : A_2 \exp(-\alpha_x t / 2) &= \frac{k_{2x}}{\alpha_x} A_2 \sin(k_{2x} t / 2). \end{aligned} \quad (2.27)$$

Substituting the values of A_1 in equations 2.21 and 2.22 we obtain electric fields for the even modes. In the core region, $|x| \leq t / 2$

$$E_y(x, z) = A_2 \cos(k_{2x} x) \exp(-jk_z z) \quad (2.28)$$

and in the cladding region solutions will be

$$\begin{aligned} E_y(x, z) &= A_2 \cos(k_{2x} t / 2) \exp(-\alpha_x - t / 2) \exp(-jk_z z) & x > t / 2 \\ E_y(x, z) &= A_2 \cos(k_{2x} t / 2) \exp(\alpha_x + t / 2) \exp(-jk_z z). & x < -t / 2 \end{aligned} \quad (2.29)$$

Similarly for odd modes the TE solutions for electric field are as given below

$$\begin{aligned} E_y(x, z) &= A_2 \sin(k_{2x} t / 2) \exp(-\alpha_x - t / 2) \exp(-jk_z z) & x > t / 2 \\ E_y(x, z) &= A_2 \sin(k_{2x} x) \exp(-jk_z z) & |x| \leq t / 2 \\ E_y(x, z) &= -A_2 \sin(k_{2x} t / 2) \exp(\alpha_x + t / 2) \exp(-jk_z z) & x < -t / 2 \end{aligned} \quad (2.30)$$

From the tangential boundary conditions for electric and magnetic fields in equation 2.26 we can obtain the guidance condition for even and odd solutions.

$$\begin{aligned} \tan(k_{2x} t / 2) &= \alpha_x / k_{2x} & (\text{Even Solutions}) \\ \cot(k_{2x} t / 2) &= -\alpha_x / k_{2x} & (\text{Odd Solutions}) \end{aligned} \quad (2.31)$$

Similar analysis produces the eigenvalue equations for TM modes for even and odd modes which are given as below.

$$\begin{aligned} \tan(k_{2x} t / 2) &= \left(\frac{n_2^2}{n_1^2} \right) \alpha_x / k_{2x} & (\text{Even Solutions}) \\ \cot(k_{2x} t / 2) &= -\left(\frac{n_1^2}{n_2^2} \right) \alpha_x / k_{2x} & (\text{Odd Solutions}) \end{aligned} \quad (2.32)$$

Solutions to the Equations 2.31 or 2.32 give the physical solutions which can be plotted graphically as shown in Figure 2.18. The mode profile as shown in Figure 2.10 arises from interference patterns among forward and backward traveling components in the waveguide. Because most optical materials have $\mu \approx \mu_0$ the cut-off frequencies of

the *TE* modes above fundamental are slightly lower, by a factor $\varepsilon_1 / \varepsilon_2$ than the corresponding *TM* modes. The above equations relate to odd and even modes, also called symmetric and anti-symmetric modes respectively. If we now design a waveguide of known thickness, t , and permittivity of core, ε_1 , and cladding, ε_2 , then for a chosen wavelength the Equations 2.31 and 2.32 will have only discrete values, m , of the propagation constant, k_z . These are the modes of the waveguide having single values or ‘eigenvalues’.

Propagation Constant

In any dielectric (core), at any given frequency, the magnitude of the k vector is given by nk_0 where n is the refractive index of the core medium and $k_0 = \omega / c$ is the value of k in free space. Consider the propagation of rays in a wave vector description in a symmetric slab waveguide as shown in Figure 2.9.

Figure-2.9 Wavevectors in a cross section of the waveguide [2]

The z components provide the phase of the wave propagation. The x components create a standing wave pattern by reflection at boundaries and do not propagate. So k_z which is governed by discrete angles of incidence can be expressed as

$$k_z = n_2 \sin \theta_m k_0 = \beta_m, \quad (2.33)$$

where β_m is the m^{th} propagation constant and θ_m is the discrete angle of incidence.

Mode index and incident angle of $m = 0$ mode approach n_2 and 90° , respectively. This

leads to the expression for effective refractive index, $n_{eff} = n_1 \sin \theta_m$ and which gives the propagation constant in terms of effective index as $\beta_m = n_{eff} k_0$.

Cutoff conditions for modes

A mode can be characterized as a condition when the ray travels along a zigzag path in the core using total internal reflection at the interfaces at discrete angles of incidence. Cutoff is the situation when the mode confined to the central layer ceases to be guided. In this condition the modes start to have an oscillatory solution outside the guide, corresponding to radiation or loss of the previously guided wave. For a given thickness and wavelength the index difference can be such that a ray is very close to the critical angle of reflection, in which case the Snell's law reduces to $n_2 \sin \theta_c = n_1$. The propagation constant for the mode at this angle can be given by $\beta_{co} = n_2 k_0$ which leads to $\alpha_x^2 = \beta_{co}^2 - n_2 k_0^2 = 0$. Substituting these values into the odd and even solutions given in equation 2.30 we get the general condition for cut-off of modes in symmetric slab waveguide as

$$k_{2x} t / 2 = m\pi / 2 \quad (m = 0, 1, 2, 3, \dots) \quad (2.34)$$

This shows that the symmetric waveguide will permit a guided mode, at any wavelength, even if the confinement is poor, down to zero thickness.

Also, since $\beta_{co} = n_2 k_0$, then $k_{2x} = k_0 \sqrt{n_2^2 - n_1^2}$ at cut-off. Substituting into equation (2.33) gives the cut-off conditions as:

$$k_0 t_{co} \sqrt{n_2^2 - n_1^2} = m\pi.$$

Figure 2.10 shows a profile of first mode in a symmetric waveguide case with waveguide thickness of $0.5 \mu m$ and an index of 1.6 sandwiched between substrate and clad with index of 1.5.

Figure-2.10 Mode profile for a symmetric waveguide

2.2.1.2) Asymmetric slab dielectric waveguide

The symmetric structures considered earlier relatively easy to analyze analytically. However in practice such structures are very rare in integrated optics. Practically there is a dielectric substrate, used for physical support, a thin dielectric film which acts as the guiding layer, and air as a cladding. The dielectric substrate is considered to be of an infinite thickness, and the guiding layer has a refractive index higher than the substrate. The guiding structure may be produced using sputtering, evaporation, or chemical vapor deposition in the case of a glass substrate, or using thermal diffusion for semiconductor substrates. The asymmetric planar waveguiding structure is shown in the Figure 2.11 below, with three layers with refractive indices such that $n_2 > n_3 > n_1$.

TE analysis

In the asymmetric geometry case there are two different interfaces, one being, core-substrate and the other being, core-clad interface. Matching at the boundaries now involves matching the tangential electric and magnetic fields at each interface. The modes will not be purely 'even' or purely 'odd' as in the case of the symmetric waveguide because of the asymmetry in the waveguide, and hence the field patterns are not symmetric relative to $x = 0$.

Figure-2.11 Rays propagating in an asymmetric slab structure [2]

As in the case of the symmetric guide, the fields will be exponentially decaying in the substrate and cladding and oscillating in the core region. In the core region $|x| \leq t/2$ the fields can be given by [2]

$$E_y(x, z) = A_2 \cos(k_{2x}x + \psi) \exp(-jk_z z). \quad (2.35)$$

where $k_{2x} = \sqrt{\omega^2 \mu_2 \epsilon_2 - k_z^2}$. To take into account the asymmetry, ψ is introduced, which is an extra phase component in the description of the field in the core region. In the substrate and cladding region, i.e. $x > t/2$ and $x < -t/2$ respectively, the fields are given by [2]

$$\begin{aligned} E_y(x, z) &= A_1 \exp(-\alpha_{1x}) \exp(-jk_z z) \\ E_y(x, z) &= A_3 \exp(\alpha_{3x}) \exp(-jk_z z) \end{aligned} \quad (2.36)$$

where $\alpha_{1x} = \sqrt{k_z^2 - \omega^2 \mu_1 \epsilon_1}$ and $\alpha_{3x} = \sqrt{k_z^2 - \omega^2 \mu_3 \epsilon_3}$.

Using first Maxwell's curl equation given in equation 2.1 the tangential component of H in all the three regions can be expressed as, [2]

$$\begin{aligned} H_z(x, z) &= \frac{-j\alpha_{1x}}{\omega\mu_1} A_1 \exp(-\alpha_{1x}x) \exp(-jk_z z) & x > t/2 \\ H_z(x, z) &= \frac{-jk_{2x}}{\omega\mu_2} A_2 \sin(k_{2x}x + \psi) \exp(-jk_z z) & |x| \leq t/2 \\ H_z(x, z) &= \frac{j\alpha_{3x}}{\omega\mu_3} A_3 \exp(-\alpha_{3x}x) \exp(-jk_z z). & x < -t/2 \end{aligned} \quad (2.37)$$

Applying boundary conditions at $x = t / 2$ yields

$$\begin{aligned} E_{\tan} : A_1 \exp(-\alpha_{1x} t / 2) &= A_2 \cos(k_{2x} t / 2 + \psi) \\ H_{\tan} : A_1 \exp(-\alpha_{1x} t / 2) &= \frac{\mu_1 k_{2x}}{\mu_2 \alpha_{1x}} A_2 \cos(k_{2x} t / 2 + \psi) \end{aligned} \quad (2.38)$$

Substituting the values of A_1 in equations 2.34 and 2.35, we obtain electric fields for the even modes. In the core region, $|x| \leq t / 2$ [2]

$$E_y(x, z) = A_2 \cos(k_{2x} x + \psi) \exp(-jk_z z), \quad (2.39)$$

and in the cladding region solutions will be [2]

$$\begin{aligned} E_y(x, z) &= A_2 \cos(k_{2x} t / 2 + \psi) \exp(-\alpha_x - t / 2) \exp(-jk_z z) & x > t / 2 \\ E_y(x, z) &= A_2 \cos(k_{2x} t / 2 - \psi) \exp(\alpha_x + t / 2) \exp(-jk_z z). & x < -t / 2 \end{aligned} \quad (2.40)$$

From the tangential boundary conditions for electric and magnetic fields we obtain the following relations, [2]

$$\begin{aligned} \tan(k_{2x} t / 2 + \psi) &= \frac{\mu_2 \alpha_{1x}}{\mu_1 k_{2x}} \\ \tan(k_{2x} t / 2 - \psi) &= \frac{\mu_2 \alpha_{3x}}{\mu_3 k_{2x}}. \end{aligned} \quad (2.41)$$

To obtain a single equation suitable for numerical solution to calculate the discrete values of k_z , we need to solve the above equations and eliminate ψ . Since they cannot be solved directly they must be combined to eliminate ψ . The tangent function is of the form $\tan(x) = \tan(x \pm m\pi)$. Adding equations 2.40 to eliminate ψ we have the eigenvalue equation for all *TE* modes in the generalized three layer slab waveguide. Integer m indicates the mode number,

$$k_{2x} t = \tan^{-1}\left(\frac{\mu_2 \alpha_{1x}}{\mu_1 k_{2x}}\right) + \tan^{-1}\left(\frac{\mu_2 \alpha_{3x}}{\mu_3 k_{2x}}\right) + m\pi. \quad (m = 0, 1, 2, \dots) \quad (2.42)$$

Similarly for the *TM* analysis a similar process can be used to reach the corresponding eigenvalue equations:

$$\begin{aligned} \tan(k_{2x} t / 2 + \psi) &= \frac{\varepsilon_2 \alpha_{1x}}{\varepsilon_1 k_{2x}} \\ \tan(k_{2x} t / 2 - \psi) &= \frac{\varepsilon_2 \alpha_{3x}}{\varepsilon_3 k_{2x}} \end{aligned} \quad (2.43)$$

Similar to *TE* analysis the equations (2.42) can be summed up to obtain the eigenvalue equation for the *TM* modes in the generalized three layer slab waveguide:

$$k_{2x}t = \tan^{-1}\left(\frac{\varepsilon_2\alpha_{1x}}{\varepsilon_1k_{2x}}\right) + \tan^{-1}\left(\frac{\varepsilon_2\alpha_{3x}}{\varepsilon_3k_{2x}}\right) + m\pi \quad (m = 0,1,2,\dots) \quad (2.44)$$

Figure 2.12 shows a profile of waveguide mode in an asymmetric case where the guide with thickness of $0.5 \mu\text{m}$ and an index of 1.6 is laid on substrate of index 1.4 and cladding is air.

Figure-2.12 Mode profile in an asymmetric case

Dispersion relation for the Asymmetric slab waveguide

In the case of the asymmetric waveguides to the choice of thicknesses and refractive indices to design a waveguide and to optimize design parameters is not straightforward. To simplify the design process, Kogelnik and Ramaswamy [27] provided an analysis from which normalized dispersion curves for the asymmetric waveguide can be formed.

First, a normalized frequency and film thickness is defined [2]

$$V = k_0t\sqrt{n_2^2 - n_1^2}, \quad (2.45)$$

and then a normalized parameter b is defined which is related to effective index,

$$b = (n_{eff}^2 - n_3^2)/(n_2^2 - n_3^2) \quad (2.46)$$

where $n_{eff} = \beta / k_0$.

Finally introducing an asymmetry parameter, a , which for the case of TE modes, ranges from zero, for perfect symmetry, to infinity for highly asymmetric structure,

$$\begin{aligned} a_{TE} &= (n_3^2 - n_1^2) / (n_2^2 - n_1^2) \\ a_{TM} &= \left(\frac{n_2^4}{n_1^2} \right) \left(\frac{n_3^2 - n_1^2}{n_2^2 - n_3^2} \right) \end{aligned} \quad (2.47)$$

These normalized parameters, when substituted into eigenvalue equation (2.41) for TE modes, give a new normalized equation: [2]

$$V\sqrt{1-b} = m\pi + \tan^{-1} \sqrt{b/(1-b)} + \tan^{-1} \sqrt{(b+a)/(1-b)}$$

The plot shown in Figure 2.13 between values of b against v is shown for a series of asymmetry values, a , ranging from 0 to infinity for the fundamental mode [2]. Higher order values of a are obtained by increasing n_2 relative to n_3 , because if n_1 is made equal to n_2 , the guidance condition will be lost. A few observations from the plot are as listed below.

- The effective index b increases as the ratio of guide thickness to wavelength is increased. This causes increased confinement of the field in the higher index region.
- As the effective index tends towards the core layer index, the value of b tends towards unity. This happens for highest ratio of t / λ_0 .

Figure-2.13 Normalized b - v diagram for the fundamental mode [2]

2.2.2) Geometrical optics treatment of slab waveguides

In the previous section we studied basic vector electromagnetics and we considered propagation of light as an electromagnetic field, which mathematically represents a solution of Maxwell's equation, subject to certain boundary conditions at the interfaces between planes of different indices of refraction. In wave-optics, the ray of light represents a plane wave. These plane waves propagate along one of the directions (for example z-direction) and support one or more optical modes with different phase velocity that are characteristic of that mode. There is an alternative approach to this physical optic approach called the geometrical or ray optic approach. Ray optics gives a more intuitive sense of motion though it provides a less complete description. It singles out a particular ray of light from this infinitely wide plane wave and shows how the ray travels through medium. In a slab wave-guide light guidance can be visualized as rays tracing a zigzag path in the film, with total internal reflection occurring at the film-substrate and film-cover interface. The ray optical picture is used to introduce the basic concepts and terminology of dielectric wave-guide theory, including modes of propagation, wave-guide cutoff, propagation constants and effective guide width.

Figure-2.14 Dielectric waveguide [4]

Figure 2.14 above shows a basic dielectric waveguide with a substrate and cladding. The guide is called symmetric if upper and lower claddings have the same index of refraction; otherwise they are called asymmetric waveguides and usually $n_2 > n_1$ and $n_2 > n_3$. In this slab, total internal reflection is required for propagation of a mode

which takes place for angles greater than critical angle θ_c . So for the two interfaces the critical angles are as given as $\theta_{c(\text{Substrate})} = \sin^{-1}(n_3 / n_2)$ and $\theta_{c(\text{Cladding})} = \sin^{-1}(n_1 / n_2)$.

Figure 2.15 below shows three possibilities as angle of incidence is increased gradually. For small angles $\theta < \theta_s, \theta_c$ light incident from the substrate side is refracted according to Snell's law and escapes from the cladding. This is called a radiation mode and there is essentially no confinement of light. For $\theta_s < \theta < \theta_c$, the light is refracted at the film-substrate interface and is totally reflected at the film-clad interface. This light is refracted in to the substrate and the light escapes the structure. This is called a substrate radiation mode and again there is no light confinement. For considerably large incidence angles when $\theta > \theta_s, \theta_c$ there is total internal reflection at both interfaces and the light is trapped inside the guide. This case corresponds to guided mode radiation.

Figure-2.15 Various modes in a slab waveguides [39]

2.2.2.1) Symmetric waveguides

As stated before, a symmetric waveguide has the same index of refraction for the cladding and substrate. Also only discrete modes propagate i.e. not all angles θ are allowed (and sometimes no angles are allowed). Along with the calculation of reflection angles of allowed modes in a waveguide, there is a need to calculate propagation constants also. The amount of zigzag of the optical wave is a function of mode index and so each mode will have a different propagation constant. For a wave traveling in free space the propagation constant is given by $k_0 = 2\pi / \lambda$. The Figure 2.16 below shows the relationships between propagation constants. The effective propagation constant in z direction is k_z and k_y is the component directed normal to reflecting planes.

Figure-2.16 Relationships between propagation constants [4]

Taking into consideration the guide geometry in Figure 2.17 below, $z = \text{constant}$ and in the x direction there will be a phase shift as the wave moves from one boundary ($x = 0$) to the other boundary ($x = t$) and back down again. In one round trip, the twice reflected wave lags behind the original wave by distance $AC - AB = 2t \cos \theta$ as shown in the Figure 2.17 below. There is also a phase shift introduced by each internal reflection at the dielectric boundary. To satisfy the self-consistency condition there needs to be a multiple of 2π radians between equivalent points of phase on the ray's geometrical path. This means the sum of optical path length and two additions of phase advancement given by Equation 2.18 for TE and TM respectively.

$$\frac{2\pi}{\lambda} 2t \cos \theta - 2\phi = 2m\pi \quad m = 0,1,2,\dots \quad (2.48)$$

Figure-2.17 Phase matching condition of wave propagating in slab waveguide [4]

If ϕ_u and ϕ_l [radians] are phase shifts at the upper and lower interfaces respectively and $m = 0, 1, 2, \dots$ then the phase matching condition from the above equation is given by: [4]

$$\frac{4\pi}{\lambda} \cos \theta - \phi_u - \phi_l = 2m\pi \quad (2.49)$$

For symmetric waveguides the substrate and cover index are the same so we have $\phi_u = \phi_l$. Using the transcendental relations given in equation 2.18, we have, [4]

$$\begin{aligned} \tan\left(\frac{\pi}{\lambda} \cos \theta - \frac{m\pi}{2}\right) &= \frac{\sqrt{\sin^2 \theta - \left(\frac{n_3}{n_2}\right)^2}}{\cos \theta} \\ \tan\left(\frac{\pi}{\lambda} \cos \theta - \frac{m\pi}{2}\right) &= \frac{\sqrt{\left(\frac{n_2}{n_3}\right)^2 \sin^2 \theta - 1}}{\left(\frac{n_3}{n_2}\right) \cos \theta}. \end{aligned} \quad (2.50)$$

These transcendental relations are in single variable $\cos \theta$. Plotting both the left hand side and the right hand side against $\cos \theta$ gives intersections which determine the allowed angles θ_m . For example a symmetric waveguide with a width of $2t = 500 \mu m$ and index $n_2 = 1.5$ can support four modes if the wavelength is $\lambda = 300 \mu m$ and the surrounding medium is air. Let $m = 0$ and $m = 1$, since the tangent curve will simply repeat itself for higher integers and as we know cosine function in first quadrant ranges

from 0 to 1, the plot of P and Q against $\cos \theta$ shows that the waveguide will support four modes. If the thickness of the waveguide is decreased then the tangent curves move further apart, however Q remains constant. So the number of intersections and hence the number of propagation modes will decrease. γ / κ

$$P = \tan\left(1.5 \cdot \frac{2\pi}{300} \cdot 250 \cos \theta - \frac{m\pi}{2}\right)$$

$$Q = \sqrt{\frac{1.5^2 - 1 - 1.5^2 \cos^2 \theta}{1.5^2 \cos^2 \theta}}$$

Figure-2.18 Graphical solution of the eigenvalue equation

2.3) Coupled mode analysis

In the slab waveguides described above it was implicitly assumed that the guided modes once formed do not change over the length of the waveguide. However, small perturbations such as those due to permittivity, surface, thickness or introduction of a second waveguide can cause significant energy exchange among various modes of a structure. If the propagation constants of the two modes are different then nondegenerate

coupling theory is used to explain the coupling mechanism. However nondegenerate modes usually display weak coupling. A different approach is used if the propagation constants of the modes being coupled are identical. This is called degenerate mode coupling [24]. Figure 2.19 illustrates various types of perturbations of the original waveguide [2].

Figure-2.19 Various types of perturbations of the original waveguide [2]

Perturbations can be due to permittivity, surface, thickness or presence of another waveguide in the vicinity of the waveguide under consideration. This is depicted in Figures 2.19(a), 2.19(b), 2.19(c) and 2.19(d) respectively. If two waveguides are close enough such that their fields overlap, then light from one waveguide can be coupled into the second waveguide. Various integrated-optic or fiber-optic devices such as couplers and switches are based on the principle that power can transfer between separate waveguides, if brought into close proximity. The formal approach to analyze the excited power going back and forth between two waveguides is to start from Maxwell's equation and to match all the boundary conditions to determine the modes of the overall system. However a simplified approach can be used for weak coupling, in which the field in the

two waveguides can be expressed as a superposition of the guided modes in each of the individual waveguides. Weak coupling is generally observed in the case of nondegenerate modes where two modes with different β 's are coupled whereas strong coupling refers to coupling between two modes with identical β 's. Coupled mode theory assumes that the modes of the decoupled waveguides remain approximately the same and that coupling only affects the amplitudes which vary with position and not the propagation constants. The Figure 2.20 below shows the refractive index distribution and field amplitude of superimposed zeroth order TE modes for two identical symmetric waveguides. Here both the waveguides are $0.5\mu m$ thick, each having refractive index 1.659 and are separated by $1\mu m$. However, introduction of a small asymmetry, for example by changing the refractive index of one of the waveguides, changes the field distribution among the guides. As shown in the Figures 2.20 and 2.21 below the power transfer between the waveguides is not complete and most of the field is concentrated in one of the guides.

Figure-2.20 Phase matched condition ($\Delta\beta = 0$)

In coupled mode theory, the field in a compound slab is expressed as a superposition of guided modes in each of the individual waveguides. Consider two parallel planar slab waveguides with film index n_1 and n_2 of thickness t and separated by a distance $2d$, embedded in a medium of refractive index n . The structure is shown in Figure 2.22 and the wave equation is given by, [24]

Figure-2.21 Non-phase matched condition due to introduction of asymmetry $\Delta\beta \neq 0$

$$\nabla^2 E_y(x, z, t) - \mu_0 \varepsilon \partial^2 E_y(x, z, t) / \partial t^2 = 0.$$

If A_i is the local mode amplitude for which z dependence is to be determined and if $E_{y,i}(x)$ is the functional form of the transverse field amplitude, then the i^{th} waveguide mode can be expressed as,

$$E_{y,i}(x, z) = A_i(z) E_{y,i}(x) \exp(-j\beta_i z).$$

When the separation between the waveguides is large i.e. $d \gg \lambda_0$ the waveguides are decoupled and they carry an optical field whose amplitudes are of the form, [28]

$$\begin{aligned} E_1(x, z) &= A_1(z) u_1(x) \exp(-j\beta_1 z) = A_1(z) e_1(x, z) \\ E_2(x, z) &= A_2(z) u_2(x) \exp(-j\beta_2 z) = A_2(z) e_2(x, z). \end{aligned}$$

Here $u_1(x)$ and $u_2(x)$ are the transverse functions and β_1 and β_2 are the propagation constants which are assumed to be unaltered because of coupling. The amplitude is modified and is considered to be a slowly varying function of distance and this approximation is known as slowly varying amplitude approximation. This approximation

means that $\frac{1}{A_1} \frac{dA_1}{dz} \ll \beta_1$ and $\frac{1}{A_2} \frac{dA_2}{dz} \ll \beta_2$.

Figure-2.22 Two parallel slab waveguides

Due to the presence of waveguide 2 in close proximity there is a perturbation of the medium outside the waveguide 1. In this case waveguide 1 with index n_1 is regarded as being perturbed by a guide of index $n_2 - n$ with a thickness t and separated by a distance of $2d$. In the guided wave structure any change in dielectric constant results in a perturbation in polarization which can be expressed using constitutive relation for electric flux[24] given by

$$\vec{D} = \epsilon \vec{E} + \vec{P}$$

Field E_2 associated with waveguide 2 creates a source of optical radiation into waveguide one.

$$\begin{aligned}\vec{P} &= \epsilon_0(n_2^2 - n^2)\vec{E}_2 \\ \vec{S}_1 &= \mu_0\omega^2\vec{P} = (k_2^2 - k^2)\vec{E}_2\end{aligned}$$

Helmholtz's equation for homogenous and isotropic media is given by

$$\nabla^2 \vec{E} - \mu\epsilon \frac{\partial^2 \vec{E}}{\partial t^2} = \mu \frac{\partial^2 \vec{P}}{\partial t^2}.$$

Helmholtz's equations for waveguide 1 and waveguide 2 in the presence of a source can be written as

$$\begin{aligned}\nabla^2 \vec{E}_1 + k_1^2 \vec{E}_1 &= (\nabla^2 + k_1^2)A_1(z)e_1(x, z) = -\vec{S}_1 = -(k_2^2 - k^2)\vec{E}_2, \\ \nabla^2 \vec{E}_2 + k_2^2 \vec{E}_2 &= (\nabla^2 + k_2^2)A_2(z)e_2(x, z) = -\vec{S}_2 = -(k_1^2 - k^2)\vec{E}_1.\end{aligned}$$

Simplifying both equations gives,

$$\begin{aligned}(\nabla^2 + k_1^2)\vec{E}_1 &= \frac{d^2 A_1}{dz} e_1 + 2 \frac{dA_1}{dz} \frac{de_1}{dz} = -\vec{S}_1 = -(k_2^2 - k^2)A_2 e_2, \\(\nabla^2 + k_2^2)\vec{E}_1 &= \frac{d^2 A_2}{dz} e_2 + 2 \frac{dA_2}{dz} \frac{de_2}{dz} = -\vec{S}_2 = -(k_1^2 - k^2)A_1 e_1.\end{aligned}\tag{2.51}$$

Since the assumption is that A_1 is varying slowly, neglecting the $\frac{d^2 A_1}{dz}$ and $\frac{d^2 A_2}{dz}$ terms in the equations 2.51, we have

$$\begin{aligned}2 \frac{dA_1}{dz} (-i\beta_1) u_1(x) \exp(-i\beta_1 z) &= -(k_2^2 - k^2) A_2 u_2(x) \exp(-j\beta_2 z), \\2 \frac{dA_2}{dz} (-i\beta_2) u_2(x) \exp(-i\beta_2 z) &= -(k_1^2 - k^2) A_1 u_1(x) \exp(-j\beta_1 z).\end{aligned}$$

Further simplifications yields two coupled first order differential equations which are called the coupled mode equations [28]

$$\begin{aligned}\frac{dA_1}{dz} &= -jC_{21} \exp(j\Delta\beta z) A_2(z) \\ \frac{dA_2}{dz} &= -jC_{12} \exp(j\Delta\beta z) A_1(z),\end{aligned}\tag{2.52}$$

where

$$\Delta\beta = \beta_1 - \beta_2$$

and

$$\begin{aligned}C_{21} &= \frac{(n_2^2 - n^2)k_0^2}{2\beta_1} \int_d^{d+t} u_1(x)u_2(x)dx, \\ C_{12} &= \frac{(n_1^2 - n^2)k_0^2}{2\beta_2} \int_{-d-t}^{-d} u_2(x)u_1(x)dx.\end{aligned}\tag{2.53}$$

When the guides are synchronous i.e. they have the same β , the coupled equations are transformed into second order ordinary differential equations with 100% power transfer and they are said to be in a phase matched condition. If $A_1 = 1$ and $A_2 = 0$ the power in the waveguides can be given by [28]

$$\begin{aligned}P_1(z) &= \cos^2(Cz) \\ P_2(z) &= \sin^2(Cz)\end{aligned}\tag{2.54}$$

where $C = C_{21} = C_{12}$ because of power conservation. The half oscillation period of amplitudes is defined as the coupling length given by $L_c = \pi / 2C$. This corresponds to the length at which the wave power transfers and reaches a maximum in the alternate waveguide.

Almost all practical devices are based on asynchronous structures where the guides are not in the phase matched condition. In this case the general solution when β are different and $\delta = \frac{(\beta_1 - \beta_2)}{2}$ the solution for amplitudes is given by [29]

$$\begin{pmatrix} A_1(z) \\ A_2(z) \end{pmatrix} = \begin{pmatrix} \cos(\sqrt{C^2 + \delta^2} z) + j \frac{\delta}{\sqrt{C^2 + \delta^2}} \sin(\sqrt{C^2 + \delta^2} z) & j \frac{C}{\sqrt{C^2 + \delta^2}} \sin(\sqrt{C^2 + \delta^2} z) \\ j \frac{C}{\sqrt{C^2 + \delta^2}} \sin(\sqrt{C^2 + \delta^2} z) & \cos(\sqrt{C^2 + \delta^2} z) - j \frac{\delta}{\sqrt{C^2 + \delta^2}} \sin(\sqrt{C^2 + \delta^2} z) \end{pmatrix} \begin{pmatrix} A_1(0) \\ A_2(0) \end{pmatrix} \quad (2.55)$$

Some important observations can be made from the above unitary matrix in equation 2.55 where the diagonal elements are complex conjugates.

- Total power is conserved even though the power exchange is taking place continuously between two waveguides.
- If $\delta = 0$ there is a phase matched condition and there is complete power transfer from one waveguide to another. This also means that waveguides have identical propagation constants.

2.4) Beam Propagation Method (BPM)

Analytical solutions of wave equations are possible only for simple structures where there is complete analytic knowledge of the modes of the waveguides. However approximate numerical solutions can help determine the mode profiles of complicated structures such as waveguide bends, split Y couples and coupled adjacent waveguides [24]. Various kinds of beam propagation methods (BPMs) have been developed such as fast Fourier transform (FFT-BPM), finite difference (FD-BPM) and finite element (FE-BPM). The FFT-BPM has many disadvantages such as long computational times, inability to use simple transparent boundary conditions at analysis boundaries, and inadequacy in handling large index differences. Incorporating transparent boundary

conditions and use of Padé approximant operators for FD-BPM has made it possible for it to be used for design of optical waveguides made of high-contrast index materials. [30]

The beam propagation method is based on decomposing the spatial mode into superposition of plane waves each traveling in slightly different directions. After traveling through a medium the waves are added back together to get the spatial mode. The main underlying concept in this method is that any optical wave is subject to diffraction and because of the inhomogeneities of the medium there will be a phase shift accumulated by the wave as it propagates which will depend on the index of refraction of the material. Thus, the medium in which the wave is traveling is modeled as a sequence of lenses separated by short sections of homogenous space as shown in Figure 2.23 [31].

Figure-2.23 Optical path broken into sequence of lenses [31]

The formulation of FD-BPM involves starting with the wave equation and dividing the principal field into slowly varying envelope function and very fast phase term. The wave equation for the y-directed field $E_y(x, y, z)$ is

$$\frac{\partial^2 E_y}{\partial z^2} + \frac{\partial^2 E_y}{\partial x^2} + k_0^2 \epsilon_r E_y = 0.$$

The principal electric field is divided using the slowly varying envelope approximation to give

$$E_y(x, y, z) = \phi(x, y, z) \exp(-j\beta z).$$

Substitution into the wave equation gives the wide angle formulation [30]

$$2j\beta \frac{\partial \phi}{\partial z} - \frac{\partial^2 \phi}{\partial z^2} = \frac{\partial^2 \phi}{\partial x^2} + k_0^2(\epsilon_r - n_{eff}^2)\phi. \quad (2.56)$$

When it is assumed that $\frac{\partial^2 \phi}{\partial z^2} = 0$, equation 2.56 is reduced to the Fresnel wave equation or paraxial wave equation. In most cases this approximation works well and is the simplest and fastest solver. However wide angle analysis using Padé approximant operators is used when there is large refractive index contrast. A paraxial case is where the field propagation is almost parallel to the direction of propagation and off axial effective index is similar to the axial value. However when the beam is diverging as it propagates, the propagation constant becomes a strong function of off-axial effective index placing an upper limit on how wide a beam may diverge in BPM [30]. Paraxial approximation leads to errors for angles less than 20 degrees whereas the (1, 1) Padé approximant operator is accurate up to 30 degrees. Higher order approximants lead to higher accuracy at large angles but also increase the numerical complexity and hence the computation times [31].

Chapter-III

Optical Modeling and Design of Biosensor

3.1) Simulations Overview

The simulations for the resonant waveguide biosensors were done using Optiwave BPM_CADTM version 4.0 [35]. This tool allows computer aided design of integrated guided wave problems. The software is based on the beam propagation method which allows for a step-by-step method of simulating the passage of light through any waveguiding medium. BPM_CAD considers monochromatic signals and determines their propagation through the structure by solving Helmholtz's equation. The reader is referred to chapter 2 of this thesis for an overview of the theory underlying the beam propagation method. The Fresnel approximation limits the application range of the beam propagation method due mainly to two factors. First, Fourier components of the beams experience phase errors at angles of more than 20 degrees. Second, beams experiencing a change in refractive index by a few percent from the input reference index suffer phase distortions. The BPM simulation tool version used to explore the resonant waveguide biosensor geometry studied in this thesis had the ability to give relatively accurate results because of the use of higher order Padé approximants.

The BPM_CAD tools used for the simulations were *Mode 2D* which is a mode solver and *BPM 2D*. The mode solver program finds the effective refractive indices and the modal fields of any guided mode in the two dimensional structure. The program uses the transfer matrix (TMM) method in 2D for a multilayer planar structure and the alternate direct implicit (ADI) method in 3D [35]. *BPM 2D* simulates light propagation in two dimensional waveguide devices. One of the dimensions is the transverse dimension recognized as the X-direction. The dimension of propagation is recognized as the Z-dimension. The *BPM 2D* simulator is based on the unconditionally stable finite difference method algorithm of Crank-Nicolson. The finite difference method works with discretized values of the field and refractive index. The field and index are discretized in the transverse direction as well as in the direction of propagation.

The resonant waveguide biosensor structure under study is based on coupled mode operation. As a result, this behavior must be simulated. If light from a polarized source is launched into a thin waveguide with a high refractive index, it creates an evanescent field. If there is a similar waveguide in close proximity then this evanescent field interacts with the other waveguide and under certain conditions there is complete power transfer into the other guide. The mode solver utility in the software was used to ascertain the optimum refractive index and thickness of the waveguides for achieving a single mode guidance condition. These waveguides were simulated using *BPM 2D* to observe the variation in the amount of coupling with changes in the various design parameters such as index of the guides, thickness of the guides and their separation.

3.2) Mode Solver

Mode solver was used to determine the thicknesses and indices of the waveguides to be used in the resonant waveguide biosensor. It is necessary that the waveguides used in the biosensor be single mode waveguides. The biosensor uses the variations in the transfer of power between two single mode waveguides as the immediate environment near the top, sensing waveguide is varied.

Initially, in order to confirm its performance, mode solver was used to observe the variations in the modal index with changes in thickness and index of the waveguide or changes due to any variations in the cladding or substrate parameters. Figure 3.1 below shows a symmetric planar dielectric waveguide with thickness $t = 1\mu m$ and index of refraction $n = 1.5$. It is surrounded by substrate and cladding material having an index of refraction of $n = 1.47$.

Figure-3.1 Monomode symmetric slab waveguide

As shown below, simulating this simple structure in mode solver indicated that this waveguide supports only one mode if the input wavelength is 0.633 microns. Figure 3.2 shows the field profile and the modal index of 1.48876015 for this particular waveguide. The angle was found to be $\theta \approx 7^\circ$ which is within the paraxial approximation. Modal index or effective index specifies the ratio of wave velocity in vacuum to that in the waveguide. It can be interpreted as refractive index of an equivalent bulk medium [6]. The center of the waveguide is at $x = 0$.

Figure-3.2 Field profile of monomode slab waveguide shown in Figure 3.1

The number of modes propagating in the waveguide essentially depends on three factors: 1.) namely on the wavelength of the incident light, 2.) thickness of the waveguide, and 3.) the index of refraction of the material used to fabricate the waveguide. Also it is necessary that the waveguide index be higher than the substrate or cladding indices, otherwise there will be no propagation in the waveguide as the input light will escape as substrate radiation modes or airmodes [6]. As explained in the Section 2.1.2 in Chapter 2, there is total internal reflection at both the interfaces and light is trapped inside the waveguide only when $\theta > \theta_s, \theta_c$, where θ is angle of incidence. This corresponds to a guided mode radiation condition. Since this θ depends on the index of refraction of

material, for any waveguide material having index of refraction less than that of the cladding and substrate there will be no guidance and there will only be radiation modes.

3.2.1) Dependence on wavelength of incident light

Taking the previous simulation as a reference point we can simulate the same structure keeping everything else constant and varying the wavelength of the incident light. Referring to the treatment of symmetric slab waveguides using wave optics and geometrical optics treated in Chapter 2, the number of propagating modes in the waveguide is inversely proportional to the wavelength of light. So decreasing wavelength will increase the number of supported modes. This is corroborated by the simulations shown in Figure 3.3 where the wavelength is $\lambda = 0.4\mu m$ keeping everything else constant. Unlike the single mode operation at the previous wavelength, we now have two modes supported by the waveguide. Further decrease in wavelength will increase the number of modes. Also it is important to note that the waveguide is single mode until $\lambda = 0.58\mu m$. Below this wavelength, the waveguide ceases to be single mode. Decreasing wavelength has the same effect as increasing the thickness of the waveguide. This is because for the incoming light the apparent thickness of the waveguide increases.

Figure-3.3 Mode profiles for structure in Figure 3.1 with $\lambda = 0.4\mu m$

3.2.2) Dependence on thickness of the waveguide

As mentioned earlier, decreasing wavelength is the same as increasing thickness of the waveguide and vice versa. So the number of guided modes should increase as the thickness of the waveguide is increased. Also the basic equation of phase match for a symmetrical slab waveguide in Chapter 2 shows that the number of modes is directly proportional to thickness of the guide. For the above symmetric slab waveguide changing thickness from $t = 1\mu m$ to $t = 1.5\mu m$ changes the number of guided modes from one to two. This is shown in the Figure 3.4 below. Also the modal index increases as the thickness increases. These mode indices correspond to the incident angles of the light inside the waveguide. The first mode has the largest incident angle and is closest to 90° . The higher modes approach critical angle after which the waveguide supports only leaky modes. This can be interpreted in a way that large angles of incidence produce modes with modal incidences which try to approach the index of the waveguide itself. Of course the case of modal index equal to the index of the waveguide can be physically seen as light propagating straight down the waveguide without any total internal reflections or a strongly guided mode.

Figure-3.4 Mode profiles for structure in Figure 3.1 with $t = 1.5\mu m$

3.2.3) Dependence on index of the waveguide

Increasing index increases the number of modes propagating through the waveguide. Also a higher index means the wave is confined more within the waveguide as compared to when the index difference between the guide and surrounding media is small. This is because a waveguide can be considered as a lens-like medium which tends to focus a light beam into the guide[6]. The wave propagates slower in the medium with higher index and so its speed is less in the waveguide as compared to substrate or cladding. This distorts the wave front and confines the light within the waveguide. For the present case, if the refractive index of the guide is changed from $n = 1.5$ to $n = 1.6$ the guide becomes a multimode waveguide and supports two modes as shown in Figure 3.5 below. Further Figure 3.6 illustrates how the confinement of the wave is more if the index is increased from $n = 1.6$ to $n = 2.0$ keeping all other parameters constant. The modal index for the guide with $n = 1.6$ is 1.582 and for guide with $n = 2.0$ is 1.980.

Figure-3.5 Mode profiles for structure in Figure 3.1 with $n = 1.6$

3.2.4) Dependence on substrate and cladding parameters

The necessary and essential condition for guidance is that the substrate and cladding should have an index less than that of the waveguide, otherwise there will be no

total internal reflection as light will escape from the waveguide and hence there will be no guided wave propagation. Given that their final boundaries are far from the guide, changes in thickness of cladding or substrate don't affect the modal index of the modes propagating inside the guide. However if the index of the material of cladding or substrate is lowered it effectively increases the Δn between the guide and surrounding media and the waveguide doesn't remain single mode anymore. In the Figure 3.7 shown below the substrate and cladding index are reduced to $n = 1.4$ from $n = 1.47$ in the original structure. This makes the waveguide multimodal as it then supports two modes. Any further decrease in the indices would increase the number of modes supported by the guide.

Figure-3.6 Confinement of wave in the guide and increase in index of the guide

Figure-3.7 Mode profiles for structure in Figure 3.1 with decrease in clad and substrate index.

3.3) Design of coupled waveguides - BPM_CAD

The resonant waveguide device is based on two individually monomode waveguides sufficiently close to each other so that the evanescent wave from one guide interacts with another and there is a power transfer that depends on the coupling coefficients. At the same time, the upper environmentally exposed waveguide must be designed such that its evanescent tail in the biolayer is neither too long (so that it does not detect changes outside the biolayer), nor too short (such that binding events on the biolayer are not detected). When the waveguides are identical, their coupling coefficients are equal and we have a phase matched condition. In this case power transfer among the guides is periodic along the direction of propagation. This can be observed using the BPM simulations and coupling length can be determined. Mode solver on the other hand can be used to determine which pair of these waveguides can be used so that there is a phase matched condition. BPM_CAD was used to experiment with different sets of parallel slab waveguides and observe the variation in their behaviors with variations in the parameters such as index of the guides, thickness of the guides, separation between them and wavelength of the input field. The following simulation shows the behavior of a single waveguide when excited with a certain modal input field.

Figure-3.8 Layout of a linear waveguide with $t = 0.15\mu m$ and $n = 1.6$

The software calculates modal index of the field to be input into the guide by solving for the fundamental mode solution of the guide and taking the substrate and cladding index for the guide as the specified wafer index. All the input modal fields are evaluated considering a symmetric waveguide case. For this case the guide has an index of $n = 1.5$ and is placed on a wafer of index 1.46. The propagation length is 100 microns. The layout in Figure 3.8 shows a 0.15 micron thick waveguide placed on the wafer of index 1.457 and the necessary data for the simulation structure such as length of propagation and the width of the mesh. With input as the TE modal index of the fundamental mode of the selected starting waveguide which is 1.474369 in this case, and wavelength of input field $\lambda = 0.633\mu m$ the optical field propagation in the waveguide is as shown in Figure 3.9.

Since the waveguide simulated above is a linear slab waveguide with neither index variations along the path nor any other perturbations in the vicinity of the guide the light propagates the whole length of the guide without any changes in its characteristics

Figure-3.9 Light propagation in a linear waveguide

except some absorption losses due to the material along the way which are not an important consideration in this case. However an introduction of another waveguide will affect the field in the original waveguide if the other waveguide is close enough to perturb the original waveguide. To show this we take another waveguide 2 exactly similar to waveguide 1 i.e. having the same index and thickness as shown in Figure 3.10. Here the guides have an index of 1.6 and thickness of 0.15 microns each. The wafer index is 1.46 and light is input in the waveguide 1 in the form of the one mode supported by that guide. The simulation region is 100 microns in length and the width is increased to 8 microns as compared to the previous simulation in Figure 3.8.

The presence of waveguide 2 affects or perturbs the field inside waveguide 1. This is shown in Figure 3.11. However, as the separation between the two guides is large and the length of the simulation region is small, consequently the two guides are almost in an uncoupled condition even though they have identical propagation constants. The field from waveguide 1 couples in to waveguide 2 but power transfer is not complete.

Figure-3.10 Two parallel identical slab waveguides separated by 2.4 microns

Figure-3.11 Weak coupling between parallel slab guides with same propagation constants

3.3.1) Coupling between the guides

For the structure shown in Figure 3.10, changing parameters like separation among the guides or increasing the length of simulation region changes the power transfer characteristics among the guides. If the separation is reduced then the evanescent wave from one guide will couple into the other guide. The closer the two waveguides are moved together, the more frequently the power will transfer between the guides. This is because as the separation is decreased the value of C in Equation 2.53 increases because coupling coefficient is directly proportional to the negative exponential of the separation distance and hence the coupling length L_c decreases. As a result, the coupling length is directly proportional to the separation distance. In the case of the two guides in Figure 3.10, since the separation distance among the guides is large the coupling length is also large. If the length of the simulation region is extended then the power transfer between the guides will be visible from the simulation. Conversely the two waveguides can be brought closer so that the coupling length is decreased. Figure 3.12 shows the guides used in Figure 3.10 with the separation distance decreased from 2.4 microns to 1.2 microns and Figure 3.13 shows the corresponding simulation window results

Figure-3.12 Slab waveguides separated by 1.2 microns

Figure 3.13 Strong coupling in parallel slab waveguides

In Figure 3.10, instead of bringing the waveguides closer, the length of the simulation region is increased. Power coupling between the two guides, which was not observable when the simulation region was 100 micron in length, is now in evidence when the simulation length was extended to 1500 microns.

Figure 3.14 Interaction length of 1500 microns for the structure in Figure 3.10

Figure 3.14 shows how the two waveguides behave when the interaction length is increased from 100 micron to 1500 microns. This is the working principle of the resonant optical waveguide biosensor. The coupling coefficients between two parallel waveguides depend on thickness of the guides, index of the guides, separation between them and the wavelength of the input source. However the device property also changes because of changes in the length over which the superstrate is in contact with the top waveguide. So if the top guide and the buried guide are in a detuned condition then a change in interaction length may bring the two guides in tune and result in a complete power transfer between them.

3.3.2) Material Evaluation for Prototype Device

The materials used for fabrication of thin film waveguides were alumina and silicon dioxide. The two most important factors dictating the choice of the materials used were moisture stability of the material and index of refraction. Conventional physical evaporation techniques tend to deposit porous material with lower densities. This causes the properties of the films to degrade and change over a period of time when in contact

with ambient humidity conditions. This is called the “moisture shift” which changes the optical properties of the film. [34]

All the materials used to make the waveguide structures were grown using ion beam assisted deposition (IBAD). Various metal oxides were tested and evaluated including Tantalum Pentoxide (Ta_2O_5) with refractive index of 2.15, Hafnium Oxide (HfO_2) with a refractive index of 1.98 and Aluminum Oxide (Al_2O_3) with refractive index of 1.65. Aluminum Oxide (Al_2O_3) was considered because of its moisture stability and improvement in the optical waveguiding behavior after annealing at 600C in ambient environment. Silicon dioxide is widely studied material with a low index of refraction of 1.46. So this was considered for the spacer layer between the two alumina waveguides. [34]

3.3.3) Simulations of Prototype Resonant Biosensor Structure

The actual structure of the resonant waveguide biosensor designed by Lloyd et al. is shown in Figure 1.5 [32]. While simulating the device a thin waveguide of 0.1 micron was used to act as the superstrate or the biolayer which capped the top guide and acted as an immediate variable index environment for the top guide. Its index was varied from 1.3318 to 1.385 to simulate the loading of the biolayer. The cladding covered the whole biolayer and both the biolayer and the cladding had an index of 1.3318. This was the initial condition of the device where the two parallel slab waveguide were in perfectly tuned condition. The index of the biolayer in simulations was varied from the initial condition of 1.3318 to about 1.4 by changing the index of thin waveguide on top of the upper alumina guide. This changed the propagation constant of the top guide as compared to the buried waveguide and made the two guides go out of tune changing the relative output powers at the end of the guides. Here we see the essence of the transduction nature of the resonant waveguide sensor device. The change in index above the upper guide is transformed into a change in the optical power at the outputs of the waveguide pair which can be quantified to ascertain the change in index.

The thicknesses for the alumina top guide and alumina buried guide used for the device were 194nm and 144 nm respectively with refractive indices of 1.659. They were separated by a buffer of silicon dioxide of thickness 1110nm with an index of 1.457 [32].

Figure 3.15 shows the layout of the structure in BPM_CAD for simulation. The waveguides are placed on a substrate of index 1.457 which is approximate index of silicon dioxide. Instead of inserting a separate waveguide for silicon dioxide the substrate itself acts as a buffer with a separation distance of 1110nm and index of 1.457. The modal field is input in the top guide with a wavelength of 633nm.

Figure-3.15 Resonant waveguide biosensor as laid in BPM_CAD

Figure 3.16 shows the simulation of the structure in Figure 3.15. The simulation shows the layout of guides is in the tuned condition i.e. the waveguides have the same propagation constants and hence evanescent field from one can penetrate into the other guide leading to a complete power transfer. Also, Figure 3.17 shows globally normalized overlap integral with distance. The first complete power transfer is at approximately 200 microns which is the coupling length for the device. The power overlap integral is an integral of two fields one being the propagating field and second being the reference field. To calculate power overlap integral with the fundamental mode, an integral is calculated using the actual waveguide field and modal field of the specified waveguide. The power overlap integral can be either globally or locally normalized. Global normalization takes into account the power loss due to radiation outside the mesh whereas local normalization does not take this into account [5].

Figure-3.16 Perfectly tuned case with biolayer index of 1.3318

Figure-3.17 Globally normalized overlap integral vs. distance

If the two waveguides are solved separately in mode solver, modal indices can be found for the two waveguides. If they are the same there will be coupling between the two guides. Referring to Figure 3.15 the top guide is solved using a substrate of silicon dioxide with an index of 1.457 and cladding of 1.3318. For the buried guide the substrate will be Borofloat with index of 1.4701 and cladding will be silicon dioxide which acts as a buffer layer in the actual structure.

Figure 3.18 shows the mode profile and modal index when solved for the top guide using the parameters mentioned above. Figure 3.19 shows the modal profile for the buried guide with its modal index. Since they are both close in value the guides are in a coupled or resonant condition and any change in this value due to thickness or index variation will make Δn_{eff} become large and decrease the coupling among the guides.

Figure-3.18 Mode solution for the top guide

Figure-3.19 Mode solution for the buried guide

3.3.4) Simulating loading of the biolayer

In real world applications the top guide is capped with a thin layer of biomatrix which is exposed to the bioagent to be detected. Depending on the surface loading of this biomatrix which occurs upon binding of the desired target to the biolayer, there will be a corresponding change of index which eventually detunes the waveguides. In the simulations this is reproduced by inserting a thin waveguide of 0.1 micron with an index of 1.3318. This is the index of water at 633nm and this was the case when the two waveguides were phase matched. To simulate the surface loading of the biomatrix the index of this thin waveguide is changed so that the modal index of the top guide changes. The changes in the index of the thin waveguide were made in the range of 1.3318 to 1.4 at 633nm. The proposed design of a real device will be a stack of films on the Borofloat substrate. Given the way BPM_CAD handles waveguide geometry layouts, these layers had to be drawn sideways on a wafer as shown in Figure 3.15. Since the device to be simulated had its orientation transformed by 90^0 because of the rotation involved, all simulations performed using TE polarization of input light would be TM polarization in the real device.

Initially the structure was simulated for refractive indices of 1.3318, 1.3411, 1.3495, 1.3637 and 1.385 of the biolayer at 633nm. Figures 3.20 to 3.23 show how progressive increments in the index of the biolayer changes the amount of coupling among the guides and how increasingly most of the power is concentrated in the top guide with very little power penetrating into the buried guide.

Figure-3.20 Biolayer index 1.3411

Figure-3.21 Biolayer index 1.3495

Figure-3.22 Biolayer index 1.3637

Figure-3.23 Biolayer index 1.385

Figure 3.24 shows a plot of globally normalized output power versus change in index of the biolayer for the simulations shown above. The plot in Figure 3.25 shows the behavior when evaluated over a larger number of index values. This plot of simulation data shows that the power exchange among the guides follows an oscillatory behavior as the index of the biolayer is varied for an interaction length of 600 microns.

Figure-3.24 Index vs. output power (600 microns interaction length)

Figure-3.25 Index vs. output power (600 microns interaction length)

If the interaction length is increased from 600 microns to 2400 microns the plot for index vs. power in output waveguides is shown in Figure 3.26.

Figure-3.26 Index vs. output power (2400 microns interaction length)

A few observations can be made from the behavior of the power exchange among the two waveguides for interaction lengths of 600 microns and 2400 microns. These are summarized below.

- Change in interaction length affect the way the power varies in the top guide with index of the biolayer. When the interaction length is 600 microns, the power in the top guide is increasing while in the case of 2400 micron interaction length the power in the top guide is decreasing as index is increased to detune the waveguides. This is due to number of times the power transfer takes place among the two waveguides.
- In the case of 600 microns interaction length, a change of index from 1.3318 to 1.3478 causes the power in the top guide to reaches a maximum value. The $(\Delta P / \Delta n)_{600} = 5.659$. This can be viewed as the usable region in the device which can give important information about the any variation in the immediate

environment of the top guide. However in case of 2400 micron interaction length the $(\Delta P / \Delta n)_{2400} = 106.48$. This shows a significant increase in the sensitivity of the device as the interaction length is increased.

- For interaction length of 600 microns considering 10% and 90% of normalized power, the contrast ratio is 0.8212. However the contrast ratio for 2400 microns interaction length considering 10% and 90% of normalized power is 0.6779. This shows that even though increasing interaction length increases the sensitivity of the device, it reduces the power contrast ratio making it more susceptible to noise. Also it needs more real estate on the chip to have larger interaction length. A compromise is needed to have optimum sensitivity with high signal to noise ratio and least real estate.

Chapter-IV

Experimental Results

4.1) Experimental Overview

In order to experimentally validate the design by Lloyd et al. [34] and experimentally corroborate the above simulations, a resonant optical waveguide stack of the biosensor structure was fabricated on a borofloat substrate. The resonant waveguide stacks on borofloat substrates were fabricated by Denton Vacuum [41]. The fabrication involved serial deposition of alumina and silicon dioxide waveguides on a polished borofloat substrate using ion beam assisted deposition [34]. The first step in the process was deposition of the lower most alumina layer which is be the buried guide with a thickness of $1454 \text{ \AA}$. Post anneal thickness of this layer was expected to be $1440 \text{ \AA}$. which is the thickness used in all the simulations. This was followed by deposition of the silicon dioxide buffer layer of $11200 \text{ \AA}$. A stainless steel shadow mask was used to deposit the 1959A thick top alumina layer for the upper, sensing waveguide. Use of the shadow mask provided the ability to discern among the two waveguides carrying the optical power as the top guide and the buried guide terminated at different lateral positions on the wafer. Post-anneal thicknesses for the spacer and topmost alumina layer were expected to be $11100 \text{ \AA}$ and $1940 \text{ \AA}$ respectively. Post anneal index for alumina and silicon dioxide were expected to be 1.659 and 1.457, respectively. The annealing of the Denton samples was completed at WVU and was done at 600°C using a Thermolyne F6000 box furnace in ambient air. Thermal annealing was found to be required in order for the alumina films to guide with reasonably low loss. It is believed this anneal assisted in crystalline form transformation of the alumina which reduces the variations in the refractive index of the film thus reducing the scattering of light propagating within it [34]. To evaluate the affects of annealing on the waveguiding properties of the film, a 633nm He-Ne laser was coupled into the waveguide using a prism coupler. Figure 4.1 and 4.2 shows pre anneal and post anneal behavior of light propagation in the alumina waveguide.

Figure-4.1 Pre anneal Propagation
of light

Figure-4.2 Post anneal Propagation
of light

It is obvious from the pictures in the Figures 4.1 and 4.2 above that annealing improves the waveguiding behavior of the alumina guides. Thermal annealing of the waveguide stack was followed by spin coating of a layer of polymethyl methacrylate (PMMA) and its patterning using photolithography process. As evident from the simulations, changes in the interaction length of the top guide with the immediate environment, i.e. biolayer, changes the results significantly. The PMMA photolithography process was necessary to pattern the channels of different lengths on the top guide. The PMMA patterned sample was mounted on the prism coupler to couple light into the top guide and a flow cell was attached to the sample covering the channels. Sucrose solution with different concentrations was flowed through the flow cell and used as an experimental index-change environment for the top guide. A prism coupler was used to couple a 633 nm HeNe laser into different length PMMA wells resulting in different interaction lengths of the top guide with the sucrose solution. The waveguide output was captured after the well interaction using a CCD camera for evaluation.

4.1.1) Experimental setup

Figure 4.3 shows the experimental setup used to investigate the behavior of the device with various concentrations of sucrose solution interacting with the top guide. A Metricon Model 2010 prism coupler was used to couple light into the top waveguide. The waveguide stack sample with patterned PMMA flow cell chambers was clamped against the prism using an air pressure operated plunger. A 633nm He-Ne laser source was used to couple light into the top guide. The two waveguides are detuned when the light is

guiding in the waveguide with PMMA layer on the top guide. However when the light comes across the region that is free of PMMA i.e. the interaction region, the amount of light exchange and periodicity is dependent on the index of the material in the immediate environment of the top guide. The plunger helps to hold the sample closely against the prism producing a coupling spot of about 1mm in diameter. A coupling spot represents the area of intimate contact between the prism and the sample. Once the coupling spot is observed and the laser source aligned with the coupling spot, the whole assembly is rotated using a servo motor. This changes the angle of the laser incident on the face of the prism which in turn changes the angle of incidence at the interface between prism and sample. At certain discrete angles the light is guided into the waveguide and it interacts with the sample contact region to be evaluated using the CCD camera. Also the Figure 4.3 shows how the top guide terminates at a different position from the bottom guide due to the masking during layer deposition at Denton Vacuum. Figure 4.4 shows a picture of the experimental setup.

Figure 4.3 Schematic layout of the experimental setup

Figure 4.4 Picture of the experimental setup

4.1.1.1) Verification of modal index-Prism Coupler

Prism coupling is one of the ways to excite slab waveguides with an external free space beam. Apart from coupling light into the waveguide it is also used as a non-intrusive way of characterizing thin film waveguides on substrates. Figure 4.5 shows the geometry of the prism coupler. To enable coupling of a beam into the waveguide, the index of prism should be higher than that of a substrate. The substrate with a film on it is then clamped against the prism and the dust particles or surface roughness provides the required air gap.

At the prism/air interface with $n_p > n_1$ the beam is totally internally reflected and this creates a standing wave pattern in the prism. The mode in the prism with a propagation constant of $\beta_p = n_p k_0 \cos \theta_m$ is stationary in the x direction but propagates in the z direction. If the air-gap between prism and the film is very small then the transverse field distribution extends out of the prism decaying exponentially and coupling to a mode of a waveguide with phase matching propagation constant of β_m [7]. This is also called optical tunneling as it's similar to tunneling of particle through energy barrier.

Figure 4.5 Diagram of prism coupler [7]

In all the experimental evaluation of the prototype sensor a Metricon Prism Coupler Model 2010 was used to couple light into the top alumina waveguide. Prism coupler also enables the calculation of propagation constant and hence was used to measure the propagation constant of the alumina waveguide and the values were compared with the modal index given by the mode solver.

Mode solver was used to calculate the modal index of a waveguide with $t = 194\text{nm}$ and $n = 1.659$ at 633nm wavelength. The modal index was found to be 1.4911 and the angle of propagation was found to be $\theta = 25.99^\circ$. This is well within the limits for (1, 1) Padé approximant operator which can be accurate up to 30° [30]. The alumina waveguide with same parameters was found to have propagation constant of 1.4938 which is fairly close to the simulated value.

4.1.2) PMMA patterning process

Poly methyl methacrylate, PMMA is a member of family of polymers called acrylics. It is a vinyl polymer that is polymerized by free radical vinyl polymerization from a monomer vinyl methacrylate as shown in Figure 4.6. During free radical polymerization, one of the two bonds between the two carbons ruptures, leaving one unshared electron on each carbon atom. An atom with an unpaired electron is very reactive which is called a free radical [21].

Figure-4.6 Free radical vinyl polymerization [21]

PMMA is ultra-high resolution, high contrast; positive tone resist used for imaging and non imaging microelectronics applications. It is a used for direct write e-beam as well as x-ray and deep UV lithography. Standard PMMA is formulated with 495,000 and 950,000 molecular weight (MW) resins in both chlorobenzene and anisole. PMMA has two primary drawbacks. It has low sensitivity which requires exposure doses in the range of 500mJ/cm² at a wavelength of 248 nm and 1-2mJ/cm² at 8.3A [23]. Various sensitizers can be added to PMMA to reduce the exposure doses. A disadvantage of PMMA is very low plasma etch resistance. This necessitates a thick film of PMMA to protect a very thin film that is to be etched, so that the patterned PMMA survives the whole etch process.

In the resonant waveguide biosensor experiment, PMMA was used to make the patterns over the top guide of the structure to define well regions of different interaction lengths. This pattern also gave a region to attach the flow cell through which the analyte solution was channeled. Nano PMMA A6 495K with 6% in anisole from MicroChem Corp. was used to lithographically pattern the wells over the top waveguide. The plots in Figure 4.7 and 4.8 below show the optical properties and spin speed curves for the PMMA used [22].

Figure-4.7 Optical property of 495 PMMA resists [22]

Figure-4.8 Spin speed curves for 495 PMMA resist 6% in anisole [22]

The processing guidelines for PMMA lithography were followed from the datasheets available from MicroChem. Initially all the tests for patterning PMMA were done on 3" silicon wafers before migrating to actual borofloat samples. The initial procedure followed for PMMA photolithography is given below,

- **Substrate Cleaning:** The samples were cleaned using acetone and methanol rinse and were blow dried using nitrogen.
- **Coating PMMA:** Based on the spin speed curves shown in Figure 4.7 above, initially the 3" silicon samples were spun at 4000 rpm which gave a thickness in the range of 0.3 microns. Static dispense was employed to pour PMMA on the

sample and 5-8ml of PMMA was used for every spin. The samples were spun at the specified speeds for 30 seconds.

- **Pre Bake:** After the coating of PMMA the samples were baked on hot plate to dry the PMMA at 170⁰C for 90 seconds.
- **Exposure:** A Research devices model M-1 infrared mask aligner system was used to expose the PMMA. The mask was in contact with the coated sample during the exposure. Exposure time was 30 seconds and the wavelength used for exposure was 365nm.
- **Develop:** MIBK: IPA in the ratio of 1:1 was used to develop the exposed PMMA by immersing the samples in the developer. De-ionized water of resistivity greater than 18 meg-ohm-cm was used as an agent to stop the development process. Immersion of sample in MIBK: IPA and DI water were performed for 30 seconds each. The sample was then blow dried with nitrogen to remove all water droplets from the patterned surface.

The above explained process did not give satisfactory results. The PMMA was not exposed properly and developing did not remove PMMA completely from the exposed areas. The thickness of PMMA left on the sample after exposure was measured using a mechanical step measurement technique and it was decided that increasing exposure times might take off the residual PMMA left on the wafer after development. The most obvious reason for residual PMMA was the exposure wavelengths associated with the M-1 aligner. In PMMA both cross linking and fragmenting of polymeric chains occur because of exposure to appropriate wavelengths [23]. However the wavelength source used was not sufficient to initiate this process as PMMA is a deep UV resist. Our initial assumption was to increase the time of exposure which would compensate for deficiencies in the used light source. Based on this assumption the time of exposure was increased from 30 seconds up to 90 seconds. The maximum exposure limit on M-1 aligner is 99 seconds after which the shutter automatically shuts off and the exposure is stopped, however the lamp inside the assembly is not shut down. To increase the exposure time PMMA was exposed repeatedly with each exposure time being 99 seconds. When this procedure was found ineffective the shutter was disabled and was kept open all the time making it possible to have a continuous exposure for periods longer than 99

seconds. The exposure time was gradually increased in the increments of 10 minutes and the results were analyzed. Repeated increments in times up to 2 hours did not provide better results. The bulb in a system like M-1 aligner gives out a wide range of wavelengths but the optical filters used in the optical path between the lamp and sample filters most of the wavelengths and emits only 365nm.

Based on the above results it was decided to use a bare 250W super high pressure mercury lamp from a Canon PLA-501F mask aligner that would emit power and range of wavelengths sufficient to break the bonds in the PMMA resist. The usable wavelengths emitted by this lamp were a combination of g-line (436nm), h-line (405nm) and i-line (365nm). Keeping the rest of the procedure same as mentioned above, coated PMMA was exposed using the bare lamp. After trying out various exposure times, 6 minutes exposure gave the best and most repeatable results. Furthermore, MIBK: IPA in the ratio of 1:3 was found to give better resolution and features when used to stop the development process in comparison to DI water. For all further PMMA processes, MIBK: IPA in the ratio of 1:1 was used to develop the resist and MIBK: IPA in the ratio of 1:3 was used to stop the development. The Figure 4.9 below shows a typical borofloat sample with PMMA patterned on alumina waveguides.

Figure-4.9 PMMA pattern on borofloat sample with alumina waveguides

4.1.3) Experiments

As shown in Figure 4.3 and 4.9 the input 633nm He-Ne laser light was coupled in the top alumina layer using the prism coupler. The four wells formed a region where the top guide interacts with the immediate environment, in this case the immediate environment being sucrose solution of different concentrations. The numbered wells as shown in Figure 4.9 had lengths of $600\mu\text{m}$, $1200\mu\text{m}$, $1800\mu\text{m}$ and $2400\mu\text{m}$, respectively. The concentrations of the sucrose solution used as the test/analyte environment were 5%, 11%, 20% and 33% corresponding to indices of refraction of 1.3411, 1.3495, 1.3637 and 1.385, respectively. A flow cell designed by LAI was clamped to the sample covering the whole well structure and the sucrose solution was flowed through it. Sensor response was measured using Quantum Imaging Retiga 1300 cooled, digital CCD camera provided by LAI equipped with a 50mm lens and placed at a distance of about 18 inches from the wafer surface. Initially to test the idea, a cover slip was placed on the wells and light was coupled into the top guide. The cover slip was first fully wet with water and then in sucrose solution. The intensity of light in the top guide showed a significant increase when the cover slip dipped in sucrose was introduced on the wells. This is illustrated in the Figures 4.10 and 4.11 respectively.

Figure-4.10 Cover slip dipped in water

Figure-4.11 Cover slip dipped in sucrose solution

In all the experiments, the light was coupled into the top guide with a TM polarization and observations were taken for four different interaction lengths with various sucrose solution concentrations flowing in the immediate test environment of the top guide in the flow cell chamber. Pictures were captured for various cases for further analysis. Figure 4.12 and Figure 4.13 show the images for 0% and 33% sucrose solution concentration respectively when the interaction length was $2400\ \mu m$.

Figure-4.12 Image with 0% sucrose concentration with $2400\ \mu m$ interaction length

Figure-4.13 Image with 33% sucrose concentration with 2400 μm interaction length

4.1.4) Image and statistical analysis

The images acquired during experiments required a quantitative analysis to determine the sensor response to various sucrose concentrations. Due to the fact the images were acquired using CCD camera at very low exposure times, to enhance the features in the image; Adobe Photoshop 7.0 was used to adjust the highlights and shadows uniformly across the image. In addition the brightness and contrast levels were changed in the image. All these adjustments were uniform for all the images analyzed for measurement purposes. After applying these changes to the whole image, a small rectangular portion between the patterned PMMA layer termination and the top guide termination was selected for further analysis because this was representative of any variations in the sensor response to different sucrose analyte indices in its immediate environment. This is shown in Figure 4.14. All the pictures were taken without changing the camera position and the rectangular area used in all images to select the area of interest had fixed dimensions; thus guaranteeing that same area at same lateral positions was grabbed for all the images.

Figure-4.14 Rectangular area used for analysis

This rectangular area under consideration was input into a three dimensional array using MATLAB command “imread”. The command “rgb2gray” was used to convert this three dimensional array into grayscale intensity image. The resultant matrix was displayed as an image using the “image” function in MATLAB. Each element of the matrix specifies the color of the rectangular segment in the image. This is shown in Figure 4.15.

Figure-4.15 Image graphics object of grayscale intensity image

The above image is actually 35x15 matrix array and each element of that array represents pixel intensity value. The column average of the pixel values over the length will give the loss in the top waveguide arising due to scattering out of the guide over that region. The plot of average pixel intensity values for each column over the number of pixel columns down the guide is as shown in graphs below. These plots of scattered power as a foundation of guide length represent the optical loss of the top guide in this region far from the PMMA analyte well, which should be the same independent of the analyte. Figure 4.16 shows the loss in the waveguide for well length of 600 μm and Figure 4.17 is loss in waveguide when well length is 2400 μm . The error bars are obtained from adding the pixels in a particular column and calculating the standard deviation value.

Figure-4.16 Distance vs. average pixel values 600um well (Loss in the waveguide)

Figure-4.17 Distance vs. average pixel values 2400um (Loss in the waveguide)

Every linear polynomial fit for different sucrose concentration percentages has a slope along with an error in the estimate of that slope which is the standard error associated with the calculated coefficients in a linear polynomial fit. Standard error by definition is the estimate of uncertainty in the calculation of the regression coefficients like slope and intercept in case of linear regression. Figures 4.18 and 4.19 illustrate the slopes for various sucrose concentration percentages and a linear polynomial fit with a zero slope forced through it. The y-axis intercept value of that zero slope linear

polynomial fit is then used to re-plot the loss in the waveguide over distance for various sucrose concentrations. This is based on the assumption that the loss in the waveguide which is represented by the slope will remain the same irrespective of the analyte.

Figure-4.18 Slopes of linear polynomial fits for different sucrose concentrations in $600\ \mu\text{m}$ well

Figure-4.19 Slopes of linear polynomial fits for different sucrose concentrations in 2400 μm well

Using the value of zero slopes linear fit as shown in Figures 4.18 and 4.19 for 600 μm and 2400 μm well, the loss in the waveguide can be re-plotted with this new value of constant slope, which is shown in Figures 4.20 and 4.21.

Figure-4.20 Re-plotting loss in the waveguide for 600 μm well

Figure-4.21 Re-plotting loss in the waveguide for 2400 μm well

4.1.5) Comparison – Experimental and Simulated Results

Finally the simulated results from the BPM 4.0 were compared with the experimental results obtained from image analysis. The software tool outputs power in

the waveguide at the end of propagation. The power can be specified in two ways depending on the requirement. It can either be a power overlap integral with the fundamental mode or intensity integral within the waveguide boundaries. In this case the output power at the end of propagation for the top guide is considered calculated using the intensity integral at the boundaries of the waveguide [5].

Image analysis on the other hand gave average pixel intensity values at the end of the top guide. The two results were plotted as a function of refractive index of sucrose. Figure 4.22 and 4.23 show the plots comparing the two results for first and fourth well respectively.

Figure 4.22 Simulated and Experimental Results for 600 μm Well

Figure 4.23 Simulated and Experimental Results for 2400 μm Well

Figure 4.23 shows a gradual variation in the experimental results for the top guide intensity as compared to the modeling results. This can be attributed to accumulation of residual sucrose on the surface.

Chapter-V

Conclusions and Future Work

This work presented the results of initial experimentation evaluating the use of a Resonant Optical Waveguide structure as the refractive index change transduction element in a biosensor device. Experiments establish the proof of concept of this biosensor architecture. Experimental results indicate a gradual change in the output intensity in the top guide with changes in the concentration of sucrose solution flown through the flow cell in contact with the resonant optical waveguide structure in case of 2400 μm well length. Important results are summarized below:

- For a well length of 600 μm , the ratio of change in power in the top guide to the change in solution index is $\left(\frac{\Delta P}{\Delta n}\right)_{600} = 5.659$ whereas for a well length of 2400 μm it is $\left(\frac{\Delta P}{\Delta n}\right)_{2400} = 106.48$.
- Contrast ratio of normalized power in the 600 μm well is 0.8212 whereas for the 2400 μm well it is 0.6779.
- Increased sensitivity in case of longer interaction length device must be weighed against decrease in contrast, device real estate, and signal to noise considerations.

The results of this work demonstrate a potential for the resonant optical waveguide transducer to serve as a simple, stable and sensitive sensor platform for a wide range of applications.

A remaining issue to be resolved in this work is that despite encouraging experimental results, the simulated and experimental results do not correspond indicating an inability to predict sensor behavior. This can be attributed to various factors. Extremely tight control over thickness and index of the waveguides is required for the device. The device is very sensitive to even small changes in these parameters causing such that even a small change results in a significant change in the coupling coefficients among the guiding layers. As with most evanescent interrogation schemes it may be

possible that improper surface cleaning before and during testing can cause shifts in the output signal.

Future work may entail an effort to establish a better control over film thickness and optical behavior of the films through better growth techniques. Also during the study of coupling behavior among the waveguide structures it was found that the coupling lengths obtained from the BPM simulator varied from the coupling lengths obtained using coupled mode theory. This is shown in as table in Figure 5.1.

Index of Superstrate	Coupling length in μm (CMT)	Coupling length in μm (BPM 2D Simulator)
1.3318	189.60	194.75
1.3411	158.57	168.30
1.3495	120.80	137.88
1.3637	78.42	97.54
1.385	47.80	62.49

Figure 5.1 Comparison of coupling lengths using BPM simulator and CMT

Understanding of assumptions used in BPM and their affect on the simulations of sensor structure is required to exploit the full potential of the simulation tool. Also exploration of the sensor structure using Finite Difference Time Domain (FDTD) method will be useful. Unlike FDTD, BPM is done entirely in frequency domain and hence fails in case of strong non-linearities. Also FDTD does not use the slowly varying envelope approximation in the paraxial direction as done in the case of the beam propagation method [5]. In addition, more experiments are needed to verify modeling results and to obtain the optimum evanescent tail design along with experiments with different biolayer in order to test new structure design based on the modeling results. These future efforts should help to further establish the role of resonant optical waveguide structure as a high performance transducer for biosensor applications.

Appendix A: Steps to use Prism Coupler

This describes basic measurement procedure to be used in the lab for making prism coupling measurements of thickness and index of thin films on a substrate. Appendix B describes additional steps incase of any mal-functioning during the measurement procedure.

1. Turn on the laser and the interface box followed by the software Metricon 2010 Version 1.61.30 DIO. If the table is not referenced the dialog box will prompt by asking the user to do a reference scan before making any measurements. User can choose to perform a manual or auto referencing procedure although for most cases auto referencing should suffice.
2. Figure below shows the initial screen that opens as the software is turned on. The buttons below shows the various options that can be invoked. Clicking the parameters button will open up a window where initial measurement parameters can be specified such as substrate index, prism index, scan parameters etc.

Metricon 2010 New Measurement Parameters

Current Recipe: None Add Delete Save ? Disable Recipe OK Start New Measurement

User Name:

Meas. Type: single film (prism coupling)

Wavelength: 632.8 TE TM

Prism Code: 6615.0

Prism Index: 2.1677 TE 2.1677 TM

Scan Start: 0 (1.6882)

Scan Stop: -.3210 (1.1179)

Step Size: Full Half

Substrate Index: 3.49 <not preset>

Auto Skip Modes: ☐ Mode offset

Repetitions: 1

Print format: on command

Save format: on command

ID prompt: no extra prompt

Filename: C:\Program Files\Metricon\2520nwards.met Browse Recipe notes...

Cal File: N/A

- The screen below shows the actual measurement screen that can be invoked by clicking on Manual measurements on the home screen. Either auto scan can be performed or a manual scan can be done using the control pod. Also polarization can be changed depending on the measurement type desired. After all the parameters are specified the sample should be clamped against the prism using the plunger and the laser should be aligned with the coupling spot. If there is difficulty viewing the coupling spot, refer to Appendix B.

4. After performing the measurements the software automatically picks up modes and calculates the thickness and index of the film along with the standard deviation in the measurements provided more than two modes are found. An example is shown in the picture below. Also using recalculate button on the home screen the values can be recalculated by adding or deleting the modes if the software is unable to pick up modes correctly. Also other advanced feature such as mode offset and auto skip can be invoked using this screen. For more on this refer to Appendix B.

Appendix B: Issues with Prism Coupler

- **Viewing the coupling spot**

If the coupling spot is not visible, cleaning the prism and the sample surface with lens paper helps for a coupling spot on contact. In case of films on a transparent substrate it is more difficult to view the coupling spot. In this case increase the pressure of the plunger in the increments of 2-3 psi. Do not increase the pressure over 55 psi.

- **Anti-reflection coating on the detector**

The detector is covered with an anti-reflection coating and should not be cleaned with any organic solvents such as acetone and methanol as it would take that anti-reflection coating off the surface and cause an extra mode to appear while taking measurements. Also during referencing there is an appearance of a third peak instead of a second peak which may affect measurements. The detector currently used in the system has its anti-reflection coating taken off due to ageing and so a common masking tape is used to avoid any spurious reflections.

- **Overcoupling**

Due to decreased air gap between the film and prism, overcoupling can occur and may affect the accuracy of the readings by shifting the mode positions slightly in case of films on high index substrate. Overcoupling degrades measurement accuracy in thickness measurement more than index measurements. The best way to detect overcoupling visually is when the coupling spot looks significantly larger than usual size. If this is the case the pressure of the plunger can be reduced in increments of 2-3 psi till first mode depth is 30% or less of baseline value. Also laser can be misaligned with respect to the coupling spot to reduce the overcoupling affects. Figure A-1 below shows way to quantify overcoupling in thickness measurements for silicon dioxide films on silicon. There is very little affect of overcoupling on index measurements.

Figure A-1: Overcoupling in thickness measurements of SiO₂ films

- **Standard Deviation Exceeds normal level**

There is an occasional message saying standard deviation exceeds normal levels. This usually is in the thickness measurements rather than index measurement. This can happen because software picks up noise as one of the modes degrading the measurement. It can also happen if it fails to take the first mode into consideration while doing calculations. This can be rectified by using the mode offset feature. If none of the above reasons reduce the standard deviation then chances are that the film under consideration has a graded index.

- **Other System Issues**

There may be occasional instances when the system freezes and the rotating table does not respond to the control pod. In this case check all connections with the interface box followed by rebooting the system, and then doing a reference scan before proceeding with measurements. In addition it is a good practice to keep the gain settings low as there

are chances of picking up spurious noise as one of the modes degrading the measurement accuracy.

Appendix C: PMMA

- **HANDLING NANO PMMA & COPOLYMER SERIES RESISTS**

Use precautions in handling flammable PMMA solutions. Avoid contact with eyes, skin, and clothing. Use with adequate ventilation. Avoid breathing fumes. Wear chemical-resistant eye protection, chemical gloves (PVA for chlorobenzene solutions) and protective clothing when handling NANO PMMA & Copolymer Series Resist products. NANO PMMA & Copolymer Series Resists cause irritation in case of contact with eyes, skin, and mucous membranes. In case of eye contact, flush with water for 15 minutes and call a physician immediately. Review the current MSDS (Material Safety Data Sheet) before using.

- **MATERIAL AND EQUIPMENT COMPATIBILITY**

NANO PMMA & Copolymer Resists are compatible with glass, ceramic, unfilled polyethylene, high-density polyethylene, polytetrafluoroethylene, stainless steel, and equivalent materials. Chlorobenzene is a powerful solvent and will attack various elastomers such as BUNA N, EPDM, HYPALON, and NEOPRENE. It will also attack PVC, CPVC and polyester. VITON A is recommended for both O-rings and tubing.

PROCESSING ENVIRONMENT For optimum results, use NANO PMMA & Copolymer Series Resists in a controlled environment. 20 - 25o ±1oC (68 - 77oF) is suggested.

- **STORAGE**

Store upright in original containers in a dry area above 50F. Do not refrigerate. Keep away from sources of ignition, light, heat, oxidants, acids, and reducers. Shelf life is 13 months from date of manufacture.

- **DISPOSAL**

Each locality, state, and county has unique regulations regarding the disposal of organic solvents such as NANO PMMA Series Resists. It is the responsibility of the customer to dispose of NANO PMMA Series Resists in compliance with all applicable codes and regulations. See MSDS for additional information.

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