INTERFACE PLASMON POLARITON WAVEGUIDES AND SENSORS

by

Michelle Ye-Chen Xu

A thesis submitted in conformity with the requirements for the degree of Doctor of Philosophy
Graduate Department of Edward S. Rogers Sr. Department of Electrical and Computer Engineering
University of Toronto

Copyright © 2011 by Michelle Ye-Chen Xu
Abstract

Interface Plasmon Polariton waveguides and sensors

Michelle Ye-Chen Xu
Doctor of Philosophy

Graduate Department of Edward S. Rogers Sr. Department of Electrical and Computer Engineering
University of Toronto

2011

This thesis presents a novel micron-sized trapezoidal plasmonic waveguide design, called an Interface Plasmon Polariton waveguide. The guiding mechanism is explained using an effective index method and validated by simulations. The mode cut-off conditions and single-mode guiding properties are both determined using simulation and experimentally demonstrated. The waveguides have a long 1 mm propagation distance at 1550 nm wavelengths.

Using this IPP waveguide, novel dielectric rib, dielectric varying-density hole-array, and metal-groove Bragg grating \textit{in vitro} sensors are designed, fabricated, and characterized. The devices have a 1100 nm/RIU sensitivity and 0.006 RIU sensing resolution obtained from measurements and are validated by theory. The IPP sensors developed in this thesis not only offer competitive plasmonic sensitivity, sensing resolution, signal to noise ratio, result reproducibility, and reusability, they are also easy to fabricate and simple to package. Therefore, these new sensor designs are an enabler for lab-on-a-chip platforms to adapt plasmonic technology.
Acknowledgements

The author would like to thank her research colleagues’ support through out the four years of her study, especially her research advisor Professor Stewart Aitchison and her committee members Professor Gilbert Walker, Professor Mo Mojahedi, and Professor Ofer Levi for the scientific advice, Aaron Zilkie for technical training, Professor Li Qian, Mark Wheeler and Muhammad Zulfiker Alam for the fruitful scientific discussions. Also she would like to thank the Emerging Communications Technology Institute cleanroom staffs and the instrument/software supplier staffs who provided unlimited technical support.

The work done in this thesis would not be completed without the funding support of the NSERC Strategic Network for Bioplasmonic Systems, Ontario Graduate Scholarship in Science and Technology, SPIE Scholarship in Optical Science and Engineering, APSC Graduate Student Endowment, Ewing Rae Graduate Scholarship, Nanotechnology Network Graduate Student Enhancement Award, Doctoral Thesis Completion Grant, Edward S. Rogers Sr. Ontario Graduate Scholarship, University of Toronto Fellowship, BiopSys Great Communicator Poster Prize, Incubic/Milton Chang Optical Society of America Travel Award, Canadian Institute for Photonic Innovations Student Travel Award, Canadian Institute for Photonic Innovations NATO nanotechnology workshop scholarship, and Ontario Center of Excellence Professional Outreach Award.
# Contents

List of Symbols viii

List of Tables xiii

List of Figures xxxii

1 Introduction 1

2 Literature Review 7

2.1 SPP materials ......................................................... 7

2.1.1 Indium Tin Oxide (ITO) ........................................... 8

2.1.2 Noble metals ....................................................... 17

2.2 SPP confinement types ............................................... 18

2.3 SPP dispersive elements and sensors ............................. 23

2.4 IPP sensor evaluation standards .................................. 31

3 Background and Theory 33

3.1 Materials dispersion ................................................ 34
3.2 SPP dispersion
   3.2.1 Dispersion relationship for TM polarization
   3.2.2 Dispersion relationship for TE polarization
3.3 Stripe waveguide dispersion
   3.3.1 EIM calculation of stripe SPP waveguide dispersion
   3.3.2 Material asymmetry in SPP waveguides
   3.3.3 Non-rectangular metal cross-section in stripe SPP waveguides
3.4 IPP waveguide dispersion
   3.4.1 Vertical wall IPP waveguide dispersion
   3.4.2 Trapezoidal waveguide dispersion
3.5 Discrete diffraction in parallel waveguide arrays theory
   3.5.1 Waveguide array theory and modeling
   3.5.2 Discrete diffraction compensation
3.6 Bragg IPP waveguide theory
   3.6.1 Matrix method to calculate periodic stacks
   3.6.2 2D modeling of a 3D Bragg IPP waveguide theory
4 SPP Stripe Waveguide Array Fabrication and Experiments
   4.1 Fabrication of stripe waveguide arrays
      4.1.1 PECVD of SiO₂
      4.1.2 Lift-off technique for stripe SPP waveguide fabrication)
   4.2 End-fire optical characterization setup
   4.3 Discrete diffraction and its compensation in stripe SPP waveguide arrays experiments
5 IPP Waveguide and Bragg IPP Sensors

5.1 Fabrication of IPP waveguides

5.1.1 Wet and dry silicon etching

5.1.2 Metal plating

5.2 Experimental characterization of IPP waveguides

5.3 Fabrication of PMMA-rib Bragg-grating-embedded IPP waveguide sensor

5.4 PMMA-rib Bragg-grating-embedded IPP waveguide sensors

5.5 Fabrication and characterization of PMMA varying-density hole-array Bragg-grating-embedded IPP waveguide sensor

5.6 Design and fabrication of metal groove Bragg-grating-embedded IPP waveguide sensor

5.7 Optical experiment of metal Bragg IPP waveguide sensors

6 Conclusions

A List of Publications

A.1 Patent

A.2 Refereed journal publications

A.3 Work done but not included in this thesis

A.4 Refereed conference publications

A.5 Local meetings

B Fabrication: ITO Etching
C Fabrication: Silver Wet Etch 173

D Fabrication: Lift-off 175

D.1 Metal lift-off using S1818 ............................ 175
D.2 Metal lift-off using S1811 ............................ 176
D.3 2 µm gold layer lift-off on silicon substrate, using S1818 ............................ 177

E Fabrication: $\text{SiO}_2$, Parylene, SU8 Channels 178

E.1 $\text{SiO}_2$ channels (Figure E.1) ......................... 178
E.2 Parylene channels (Figure E.2) ......................... 179
E.3 SU8 channels (Figure E.3) ......................... 180

F Fabrication: Buffered Oxide Etching 182

G Fabrication: Piranha Cleaning Method 184

G.1 Substrate cleaning with Piranha ......................... 184
G.2 Piranha solution preparation ......................... 185

Bibliography 186
## List of Symbols

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Name</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>AFM</td>
<td>Atomic Force Microscopy</td>
<td>54</td>
</tr>
<tr>
<td>BE</td>
<td>Body Ellipsoid (model)</td>
<td>56</td>
</tr>
<tr>
<td>BOE</td>
<td>Buffered Oxide Etch</td>
<td>118</td>
</tr>
<tr>
<td>CPP</td>
<td>Channel Plasmon Polariton</td>
<td>7</td>
</tr>
<tr>
<td>C</td>
<td>Coupling coefficient</td>
<td>83</td>
</tr>
<tr>
<td>c</td>
<td>Speed of light in vacuum</td>
<td>36</td>
</tr>
<tr>
<td>DI</td>
<td>De-Ionized</td>
<td>118</td>
</tr>
<tr>
<td>d\textsubscript{array}</td>
<td>Stripe waveguide center-to-center separation distance</td>
<td>83</td>
</tr>
<tr>
<td>EBL</td>
<td>Electron Beam Lithography</td>
<td>140</td>
</tr>
<tr>
<td>EBPVD</td>
<td>Electron Beam Physical Vapor Deposition</td>
<td>135</td>
</tr>
<tr>
<td>EE</td>
<td>Edge Ellipsoid (model)</td>
<td>58</td>
</tr>
<tr>
<td>EIM</td>
<td>Effective Index Method</td>
<td>44</td>
</tr>
<tr>
<td>ER</td>
<td>Edge Rectangle (model)</td>
<td>58</td>
</tr>
<tr>
<td>e</td>
<td>Electron charge [C]</td>
<td>10</td>
</tr>
<tr>
<td>FBG</td>
<td>Fiber Bragg Grating</td>
<td>27</td>
</tr>
<tr>
<td>FIB</td>
<td>Focused Ion Beam</td>
<td>19</td>
</tr>
<tr>
<td>Abbreviation</td>
<td>Full Form</td>
<td>Page</td>
</tr>
<tr>
<td>--------------</td>
<td>-----------</td>
<td>------</td>
</tr>
<tr>
<td>FRET</td>
<td>Förster Resonance Energy Transfer</td>
<td>8</td>
</tr>
<tr>
<td>FTIR</td>
<td>Fourier Transform Infra-Red</td>
<td>106</td>
</tr>
<tr>
<td>FWHM</td>
<td>Full Width Half Maximum</td>
<td>24</td>
</tr>
<tr>
<td>Fr</td>
<td>Frictional force</td>
<td>34</td>
</tr>
<tr>
<td>Fh</td>
<td>Elastic/restoring force</td>
<td>34</td>
</tr>
<tr>
<td>F_{Coulomb}</td>
<td>Coulomb force</td>
<td>35</td>
</tr>
<tr>
<td>HCl</td>
<td>Hydrochloric acid</td>
<td>10</td>
</tr>
<tr>
<td>IMI</td>
<td>Insulator Metal Insulator</td>
<td>18</td>
</tr>
<tr>
<td>IPP</td>
<td>Interface Plasmon Polariton</td>
<td>6</td>
</tr>
<tr>
<td>IR</td>
<td>Infrared (wavelength between 700 nm to 300 µm)</td>
<td>8</td>
</tr>
<tr>
<td>ITO</td>
<td>Indium Tin Oxide</td>
<td>7</td>
</tr>
<tr>
<td>LHM</td>
<td>Left Handed Materials</td>
<td>43</td>
</tr>
<tr>
<td>LOC</td>
<td>Lab On a Chip</td>
<td>6</td>
</tr>
<tr>
<td>MD</td>
<td>Metal Dielectric</td>
<td>18</td>
</tr>
<tr>
<td>MIM</td>
<td>Metal Insulator Metal</td>
<td>18</td>
</tr>
<tr>
<td>m</td>
<td>Electron mass</td>
<td>10</td>
</tr>
<tr>
<td>NIR</td>
<td>Near Infrared (wavelength between 740 nm to 1.4 µm)</td>
<td>17</td>
</tr>
<tr>
<td>N</td>
<td>Density of electrons $[m^{-3}]$</td>
<td>10</td>
</tr>
<tr>
<td>PECVD</td>
<td>Plasma Enhanced Chemical Vapor Deposition</td>
<td>105</td>
</tr>
<tr>
<td>P</td>
<td>Polarization</td>
<td>36</td>
</tr>
<tr>
<td>RIE</td>
<td>Reactive Ion Etching</td>
<td>116</td>
</tr>
<tr>
<td>RIU</td>
<td>Refractive Index Unit</td>
<td>24</td>
</tr>
<tr>
<td>scmm</td>
<td>Standard Cubic Centimeters per Minute</td>
<td>106</td>
</tr>
<tr>
<td>Acronym</td>
<td>Description</td>
<td>Page</td>
</tr>
<tr>
<td>---------</td>
<td>-------------</td>
<td>------</td>
</tr>
<tr>
<td>SNR</td>
<td>Signal to Noise Ratio</td>
<td>8</td>
</tr>
<tr>
<td>SPP</td>
<td>Surface Plasmon Polariton</td>
<td>1</td>
</tr>
<tr>
<td>SPR</td>
<td>Surface Plasmon Resonance</td>
<td>2</td>
</tr>
<tr>
<td>SR</td>
<td>Sensing Resolution</td>
<td>23</td>
</tr>
<tr>
<td>TE</td>
<td>Transverse Electric</td>
<td>43</td>
</tr>
<tr>
<td>TM</td>
<td>Transverse Magnetic</td>
<td>38</td>
</tr>
<tr>
<td>XPS</td>
<td>X-ray Photoelectron Spectroscopy</td>
<td>10</td>
</tr>
<tr>
<td>( \hat{r} )</td>
<td>Directional vector</td>
<td>34</td>
</tr>
<tr>
<td>( \Im )</td>
<td>Imaginary part of a complex number</td>
<td>66</td>
</tr>
<tr>
<td>( \Lambda_{\text{Bragg}} )</td>
<td>Bragg period</td>
<td>92</td>
</tr>
<tr>
<td>( \lambda )</td>
<td>Wavelength</td>
<td>49</td>
</tr>
<tr>
<td>( \mu_0 )</td>
<td>Vacuum permeability</td>
<td>36</td>
</tr>
<tr>
<td>( \mu )</td>
<td>Permeability</td>
<td>36</td>
</tr>
<tr>
<td>( \omega_p )</td>
<td>Plasma frequency ([\text{rad/s}])</td>
<td>9</td>
</tr>
<tr>
<td>( \omega )</td>
<td>Angular frequency ([\text{rad/s}])</td>
<td>9</td>
</tr>
<tr>
<td>( \Re )</td>
<td>Real part of a complex number</td>
<td>66</td>
</tr>
<tr>
<td>( \tau )</td>
<td>free electron collision time ([\text{s}])</td>
<td>9</td>
</tr>
<tr>
<td>( \varepsilon_c )</td>
<td>Relative permittivity of cladding</td>
<td>45</td>
</tr>
<tr>
<td>( \varepsilon_m )</td>
<td>Relative permittivity of metal</td>
<td>45</td>
</tr>
<tr>
<td>( \varepsilon_o )</td>
<td>Vacuum permittivity ([\text{F/m}])</td>
<td>9</td>
</tr>
<tr>
<td>( \varepsilon_r )</td>
<td>Relative permittivity</td>
<td>9</td>
</tr>
<tr>
<td>( \varepsilon_s )</td>
<td>Relative permittivity of substrate</td>
<td>45</td>
</tr>
</tbody>
</table>
List of Tables

1.1 Comparison of \textit{in vivo} and \textit{in vitro} diagnostic technologies . . . . . . . 3

1.2 Comparison of SPP and fiber diagnostic technologies. ∗ The sample

   volume is that of the IPP waveguide sensor. . . . . . . . . . . . . . . . . 5

2.1 ITO-air radiating mode excited in experiments . . . . . . . . . . . . . . 13

2.2 Comparison of different plasmonic confinement modes. The five deter-

   mining factors are cost, waveguide loss, material compatibility with

   the LOC, dimension compatibility with LOC, and finally, the LOC

   integration readiness. Di. loaded = Dielectric loaded. . . . . . . . . . . 22

2.3 Tabulated planar SPP sensor review. λ is the operating wavelength.

   FWHM: Full Width Half Maximum is the resonance width either in

   wavelength or in angular degree. MIM: Metal-Insulator-Metal. MD:

   Metal-Dielectric interface. IMI: Insulator-Metal-Insulator. ⊥: normal

   incident. ∥ parallel incident. RIU: Refractive Index Unit. ∗: Xu

   calculated. ×/RIU: the sensor measures intensity change. . . . . . . . 24

3.1 Percentile of bound fundamental mode in TE polarization. . . . . . . 71
3.2 Mode indices \( n_{IPP} \) of IPP waveguides having various dielectric mod-
ulations and filled with different index oils. ........................................... 98

5.1 Geometry of RIE silicon for varying RF power for 120 second etch
duration. RIE pressure = 100 mTorr, \( CHF_3 \) flow = 12 sccm, \( SF_6 \) flow
= 30 sccm, and \( O_2 \) flow = 10 sccm. “mask” indicates the shadow mask
width using for photoresist exposure. * and “x” indicates negligible
etching. .......................... ......................................................... 124

5.2 Geometry of RIE silicon for varying pressure for 120 second etch du-
ration. RIE power = 100 Watt, \( CHF_3 \) flow = 12 sccm, \( SF_6 \) flow =
30 sccm, and \( O_2 \) flow = 10 sccm. “mask” indicates the shadow mask
width using for photoresist exposure. * and “x” indicates negligible
etching. .......................... ......................................................... 126

5.3 Geometry of RIE silicon for varying \( CHF_3 \) flow for 120 second etch
duration. RIE power = 100 Watt, pressure = 100 mTorr, \( SF_6 \) flow =
30 sccm, and \( O_2 \) flow = 10 sccm. “mask” indicates the shadow mask
width using for photoresist exposure. * and “x” indicates negligible
etching. .......................... ......................................................... 128

5.4 Geometry of RIE silicon for varying \( SF_6 \) flow for 120 second etch du-
ration. RIE power = 100 Watt, pressure = 100 mTorr, \( CHF_3 \) flow =
12 sccm, and \( O_2 \) flow = 10 sccm. “mask” indicates the shadow mask
width using for photoresist exposure. * and “x” indicates negligible
etching. .......................... ......................................................... 130
5.5 Geometry of RIE silicon for varying $O_2$ flow for 120 second etch duration. RIE power = 100 Watt, pressure = 100 mTorr, $CHF_3$ flow = 12 sccm, and $SF_6$ flow = 30 sccm. “mask” indicates the shadow mask width using for photoresist exposure. * and “x” indicates negligible etching. 132

5.6 IPP Bragg sensor performance summary. The theory spectra, marked as ”The”, in this chapter plot the EIM derived curves and not FDTD simulated. 160
1.1 Illustration of IPP waveguide mode and optical fiber mode. Both structures have similar 10 µm by 10 µm cross-section dimension. IPP has a silver active region. The fiber has a core index of 1.4. The background has unity index. The wavelength of simulation is 1550 nm.

2.1 XPS intensity of ITO samples. 2.1(a) plots the normalized Sn 3d$_{5/2}$ intensity of the native (×), exposed in air for 14 days (solid line), and exposed in air and then HCl washed sample (dotted line). 2.1(b) plots the energy of Sn 3d$_{5/2}$ with the Sn$^{2+}$ and Sn$^{4+}$ fitting curves. 2.1(c) shows the binding energy of indium. In both 2.1(b) and 2.1(c), the red group represents the HCl washed, and the black group represents the native sample.
2.2 Dispersion relationship of the electromagnetic waveguides at the interface of ITO and air. In 2.2(a), the real part of the propagation constant, $\beta$, is represented by the solid line. The imaginary part of the $\beta$ is shown as a dashed line. The two horizontal parallel lines separate the three regions defined by the radiating (RPP), quasi-bound (QBM), and non-radiating (SPP). 2.2(b) is experimental result of the TM-TE ratioed reflection spectrum at internal incident angle $44.7^\circ (\Delta)$, $45.6^\circ (\bigcirc)$, and $46.4^\circ (\times)$, obtained using an Otto configuration.

2.3 Effective indices, $n_{\text{eff}}$, of bound SPP even modes as a function of the ITO thickness at 2500 nm wavelength. Waveguide having 2, 3, 4, 6, and 7 $\mu$m width are illustrated. 2.3(a) plots the real part of the effective index and 2.3(b) plots the propagation distance of the corresponding modes. The inset plots the mode profiles of two different waveguide structures: $7 \mu$m × 100 nm and $7 \mu$m × 50 nm.

2.4 Effective indices of bound SPP even modes as a function of the ITO width at 2500 nm wavelength. Waveguide having 50, 60, and 110 nm thickness are plotted. In the plots, the effective indices of the first four lowest modes are shown and represented by open circle (-○-), open square (-□-), open triangle (-▽-), and cross (-×-). 2.4(a) plots the real part of the effective index and 2.4(b) plots the propagation distance. The inset shows the mode profiles of the first the lowest order modes.
2.5 Simulation of five types of SPP confinement fundamental modes at 1550 nm wavelength. All simulation setups have silver as the metal (material dispersion taken from [1]). 2.5(a) plots the dielectric loaded mode. The dielectric-loaded setup uses a n = 1.4 dielectric stripe. All background indices are 1. 2.5(b) plots the gap mode. 2.5(c) plots the CPP mode. 2.5(d) plots the stripe mode. And, 2.5(e) plots the IPP mode.

3.1 Silver material dispersion as a function of wavelength [1].

3.2 Electromagnetic field penetration depth in silver as a function of frequency. The imaginary part of $\varepsilon_r$ is set to zero for simplicity.

3.3 Illustration of SPPs on metal surface. The undefined x-axis follows the right-hand-rule.

3.4 SPP dispersion at the interface of silver and air. Silver material dispersion is taken from [1].

3.5 SPP penetration depth at the interface of silver and air as a function of wavelength. The dashed blue line represents the penetration depth in air and the solid black line represents the penetration depth in silver. Silver material dispersion is taken from [1].

3.6 Illustration of air-silver-air (IMI) structure. In this figure, $\varepsilon_m$ is the metal permeability, which is sandwiched between the bottom and the top dielectric layers, which have permeability of $\varepsilon_s$ and $\varepsilon_c$, respectively. The metal layer has a thickness of $d$. 

### 3.7 Dispersion of air-silver-air (IMI) arrangement ($\beta_{IMI}$) as a function of metal thickness at 1550 nm. The solid line represents the symmetric mode, and the blue line represents the anti-symmetric mode.

### 3.8 Illustration of EIM. In this figure, the three $z$-extending layers have permittivity $\varepsilon_1$, $\varepsilon_2$, and $\varepsilon_3$. In the finite-width stripe SPP waveguide, $\varepsilon_2 = \varepsilon_{IMI}$ and $\varepsilon_1 = \varepsilon_3 = \varepsilon_{\text{dielectric}}$. The stripe SPP waveguide has a width of $b$.

### 3.9 Mode index of $b = 4 \, \mu\text{m}$-wide stripe SPP waveguide as a function of metal thickness at 1550 nm wavelength. 3.9(a) shows the real part of the effective index; and 3.9(b) shows the imaginary part of the effective index. The black solid lines represent the solution calculated using EIM and the blue dashed lines represent the solutions calculated using the commercial MODE simulation software.

### 3.10 Mode index of $d = 20 \, \text{nm}$-thick stripe SPP waveguide as a function of metal width, at 1550 nm wavelength. 3.10(a) plots the real part of the effective index; and, 3.10(b) plots the imaginary part of the effective index. The black solid lines represent the solution calculated using EIM and the blue dashed lines represent the solutions calculated using the commercial MODE simulation software.
3.11 Mode profile of asymmetric-material stripe SPP waveguides. 3.11(a) illustrates the simulation setup. 3.11(b) is the mode profile (E field intensity) when \(n_c = 1.439\). 3.11(c) is the mode profile (E field intensity) when \(n_c = 1.44\). And, 3.11(d) is the mode profile (E field intensity) when \(n_c = 1.441\).

3.12 Mode indices and sizes of material-asymmetric stripe SPP waveguide as \(n_c\) sweeps between 1.439 and 1.441. 3.12(a) shows the real part of the effective index. 3.12(b) shows the imaginary part of the effective index. And, 3.12(c) shows the \(E_y\) intensity FWHM sampled along the y-axis at \(x = 0\).

3.13 Illustration of cross-section imperfections in silver stripe waveguides. 3.13(a) shows a desirable “under-cut” achieved in lift-off prior to metal deposition. The result of this lift-off is shown in 3.13(b) (AFM scan of the metal stripe surface morphology). 3.13(c) shows an opposite tilt in photoresist results in extruding features on the side walls. Geometric defects of the stripe morphology are shown in 3.13(d) (AFM scan of the metal stripe surface morphology).
3.14 Illustration of the cross-section geometric models used in simulations and the associated mode profiles. The ideal cross-section is a 4 µm × 55 nm rectangle having width \(b\) and thickness \(d\). The body ellipsoid, \(BE\), is a geometry used to model the stripe shown in Figure 3.13(a) and has a semi-major axis \(b/2\) and a semi-minor axis \(d\). The edge ellipsoid, \(EE\), and the edge rectangle, \(ER\), are the two geometries used to model the extruding features on Figure 3.13(d). Both \(EE\) and \(ER\) are additional features on the same base waveguides having dimension 4 µm × 55 nm. The \(EE\) has semi-major axis \(M_{a}\) and semi-minor axis \(M_{i}\). The \(ER\) has width \(w\) and height \(u\).

3.15 Fundamental bound mode effective indices as a function of stripe thickness at a 1550 nm wavelength. The dashed line is the waveguide dispersion of the odd bound mode and the solid line is the dispersion of the even bound mode. -o- represents the effective indices of a 4 µm wide stripe waveguide, shown for comparison. 3.15(a) plots the real part of the effective index and 3.15(b) plots the propagation distance. Note that the propagation distance is defined as the \(1/e^2\) decay length of the field.
3.16 Effective index of a silver waveguide having thickness $d = 55$ nm as a function of stripe width at 1550 nm wavelength. 3.16(a) plots the real part of the effective index and 3.16(b) plots the propagation distance.

-○- represents the ideal rectangle geometry, -×- represents the effective index of the fundamental mode of the BE geometry, and -■- represents the index of the EE geometry with $M_i = 55$ nm and $M_a = 250$ nm.

Solid, dashed, and dot-dashed lines, represent fundamental, second, and third order bound modes, respectively. For a perfect waveguide, the asymptote of the real part approaches 1.449 and the propagation distance approaches 1 mm, and these asymptotes are indicated using red lines in 3.16(a) and 3.16(b) respectively. Note that the propagation distance defined as the $1/e^2$ decay length of the field.

3.17 Effective indices as a function of the cross-section area at 1550 nm wavelength. 3.17(a) plots the real part of the effective index and 3.17(b) plots the propagation distance. -○- represents the ideal rectangle geometry, -×- represents the effective index of the fundamental mode of the BE geometry, and -■- represents the EE geometry with $M_i = 55$ nm and $M_a = 250$ nm. Note that the propagation distance defined as the $1/e^2$ decay length of the field.
3.18 Effective indices as a function of $M_i$ and $u$ at 1550 nm wavelength. Black -○- represents the indices of the EE geometry and red -■- represents that of the ER. For the EE, $M_a = 150, 250, 350, 450, 550,$ and 650 nm are respectively represented by pink, purple, black, dark blue, light blue, and gray. For the ER geometry, the $w = 500, 700, 900,$ and 1100 nm, and are represented by light pink, purple, black, and dark blue, respectively. 3.18(a) plots the real part of the effective index and 3.18(b) plots the propagation distance. Note that the propagation distance is defined as the $1/e^2$ decay length of the field.

3.19 Effective indices as a function of $R$ at 1550 nm wavelength. 3.19(a) plots the real part of the effective index and 3.19(b) plots the propagation distance. Open -○- represents the indices of the EE geometry and solid -■- represents that of the ER geometry. Note that the propagation distance is defined as the $1/e^2$ decay length of the field.

3.20 Effective indices, of a 4 $\mu$m wide 55 nm thick stripe waveguide, as a function of EE semi-minor axis $M_i$ at 633 nm wavelength. 3.20(a) plots the real part of the effective index and 3.20(b) plots the propagation distance. For ellipsoid semi-major $M_a = 300, 400, 500$ nm are respectively represented by black, blue, and red. Note that the propagation distance is defined as the $1/e^2$ decay length of the field.
3.21 Effective indices as a function of $R$ at 633 nm wavelength. 3.21(a) plots the real part of the effective index and 3.21(b) plots the propagation distance. Note that the propagation distance is defined as the $1/e^2$ decay length of the field.

3.22 Schematics of the EIM approach to solve vertical-wall IPP waveguide dispersion. 3.22(a) shows a schematic of the physical waveguide structure. The curved red line represents the SPP evanescent decay and the dashed arrow indicates the SPP resonance in the cavity. 3.22(b) shows an illustration of SPP guiding interfaces. This SPP can be confined by two reflective surfaces constructed on both sides shown in 3.22(c).

3.23 Rectangular waveguide dispersion curves in vacuum. The blue solid line is the light line. The black solid curves (EIM) are the real part of the dispersions of the first three lowest order modes of the 1.5 $\mu$m wide IPP waveguide, where the fundamental mode has the largest propagation constant. The red solid curves (EIM) are the imaginary part of the dispersions of the three modes. In the inset, (a) shows the fundamental mode profile at 3 $\mu$m wavelength, (b) shows the second order mode at a 1.5 $\mu$m wavelength, and (c) shows the third order mode at a 1 $\mu$m wavelength. The curves representing the fundamental, second, and third order modes are marked 1, 2, and 3, respectively.
3.24 The waveguide effective indices of the fundamental, second order, and the third order modes as a function of the waveguide width. The EIM solutions are shown with blue solid curves. The MODE solutions of the 10-µm-deep rectangular waveguide is shown with red dots, the 6-µm-deep rectangular waveguide in black crosses, and the trapezoid structure having \( h = 6 \mu m \) and \( \theta = 18^\circ \) in black dash lines with dots. The trapezoid index is smoothed and the actual data is bound within two percent the curve shown. For the trapezoids, the x-axis plots the \( b \) width. The curves representing fundamental, second, and third order modes are marked 1, 2, and 3, respectively.

3.25 Illustration of a waveguide array structure and the excitation scheme. The silver stripe waveguides are \( b = 5 \mu m \) in width and \( d = 20 \) nm in thickness. The waveguide center-to-center separation is \( d_{\text{array}} = 10 \mu m \). The sample is 1 mm in length. The surrounding material is \( SiO_2 \).

3.26 Illustration of the material indices used in EIM calculation of stripe SPP waveguide arrays.

3.27 Calculated and simulated \( |H_x|^2 \) of parallel waveguide arrays. 3.27(a) plots the field distribution predicted using Equation 3.32. 3.27(b) shows the field distribution predicted using the commercial Beam-Prop software.
3.28 Calculated coupling coefficients as a function of silver stripe thickness. Dashed lines (−−) represent values calculated using the mode interference method, and dotted (⋯) lines represent values calculated using the beam propagation method. Circles (○), triangles (△), and squares (□) represent the coupling coefficients calculated for parallel silver stripes, each having width $d = 4, 5, \text{and } 6 \, \mu\text{m}$ and center-to-center separation of $d_{\text{array}} = 8, 10, \text{and } 12 \, \mu\text{m}$, respectively.

3.29 Intensity pattern detected at output of the waveguide array. The height of the bars indicate the relative power in each waveguide. It shows the spatial distribution of the output intensity pattern for $\theta = 0, 0.9, 1.5, 2.2, \text{and } 2.9$ degrees. Vertical bars show the simulated results, and solid curves show the experimental result. All plots are normalized for visual clarity.

3.30 Illustration of the Bragg-grating embedded IPP waveguide. $n_d$ is the material index of either the air or the oil filler. $n_{PMMA}$ is the material index of PMMA ribs used to modulate the IPP waveguide. $n_{IPP}$ is the mode index of the silver IPP waveguide, either with or without modulation.

3.31 Illustration of a periodic medium. $a_n$ and $c_n$ are the magnitudes of the negative-$z$-traveling waves in the $n^{th}$ layer; and, the $b_n$ and $d_n$ are the magnitudes of the positive-$z$-traveling waves in the $n^{th}$ layer. $n_{st,1}$ and $n_{st,2}$ have thickness $d_{st,1}$ and $d_{st,2}$ respectively.
3.32 Variable and coordinate definition of the periodic stack structure shown in Figure 3.30. In the top illustration, it shows the dielectric (PMMA) modulated silver surface. This is a plot of the y-z plan sliced along the dashed window in Figure 3.30. The corresponding effective medium index for each layer is shown in the bottom illustration. The IPP waveguide mode indices of the native and PMMA-modulated layers are $n_{st,1}$ and $n_{st,2}$ respectively. Each layer has thickness $d_{st,1}$ or $d_{st,2}$.

$a_n$ and $c_n$ are the magnitudes of the negative-z-traveling waves, in the $n^{th}$ layer; the $b_n$ and $d_n$ are the magnitudes of the positive-z-traveling waves, in the $n^{th}$ layer. The E field polarization, as indicated is in the y-direction, as indicated. The layer number is represented by an integer $n$.

3.33 MODE-simulated mode profiles of a native IPP waveguide and a 200-nm-thick PMMA-modulated IPP waveguide. The metal is silver and the background index is one. The simulation wavelength is 1550 nm.

3.34 The reflection spectra of air-filled Bragg waveguides, having periodicities of: $\Lambda_{Bragg} = 765$ nm, 770 nm, and 775 nm.

3.35 The reflection spectra of oil-filled Bragg-grating-embedded IPP waveguides, having fixed $\Lambda_{Bragg} = 567$ nm. The index matching oils have indices $n_d = 1.3442, 1.3538, and 1.3634$, at 1550 nm wavelength.

3.36 The reflection spectra of oil-filled Bragg-grating-embedded IPP waveguides, having fixed $\Lambda_{Bragg} = 570$ nm. The index matching oils have indices $n_d = 1.3346, 1.3442, and 1.3538$, at 1550 nm wavelength.
3.37 IPP mode effective index ($n_{IPP}$) as a function of both waveguide width and background index $n_d$, at 1550 nm wavelength. The waveguide has $\theta = 18^\circ$ and $h = 6 \, \mu m$. .......................... 101

3.38 60-nm PMMA-modulated IPP waveguide mode effective index ($n_{IPP}$) as a function of both waveguide width and background index $n_d$, at a 1550 nm wavelength. The waveguide has $\theta = 18^\circ$ and $h = 6 \, \mu m$. .... 102

4.1 $SiO_2$ deposition rate as a function of temperature. .................. 107

4.2 $SiO_2$ surface roughness as a function of temperature. The inset plots the AFM-scanned surface morphologies of each sample. ............. 107

4.3 $SiO_2$ index as a function of deposition temperature. ............... 108

4.4 Illustration of the lift-off fabrication protocol ......................... 110

4.5 Microscope photograph of the topview of the fabricated stripe waveguide array sample. The waveguides are 5 $\mu m$ in width and 20 nm in thickness. The waveguide center-to-center separation is 10 $\mu m$. Note the yellow tint to the photograph is due to the lighting in the clean-room facility. The brighter colored parts are the silver stripes, which are more reflective under illumination, and the darker parts are the $SiO_2$, which is less reflective under white illumination. ........... 111

xxvi
4.6 Optical excitation experimental setup. The laser is set to have a center emission wavelength at 1550 nm. PBS = Polarization beam splitter λ/2 = half waveplate; Obj.1 is the excitation objective having 40× magnification and NA = 0.65; DUT = device under test; Obj. 2 is the output coupling objective having 20× magnification and NA = 0.4; IR = infrared camera.

4.7 Intensity pattern detected at output of the waveguide array. 4.7(a) compares the TE and TM polarized components of the output intensity patterns, both excited at θ = 0. 4.7(b) shows the spatial distribution of the output intensity pattern for θ = 0, 0.9, 1.5, 2.2, and 2.9 degrees. Vertical bars show the simulated results, and solid curves show the experimental result. All plots are normalized for visual clarity.

5.1 Illustration of silicon wafer crystal orientations. 5.1(a) shows the (100) wafer top surface (top) and cross-section (bottom). And, the 5.1(b) shows the (110) wafer top surface (top) and cross-section (bottom).

5.2 Profilometer scan of wet etched silicon ridge.

5.3 Optical microscope top view of KOH etched silicon being protected underneath an SiO$_2$ hardmask.

5.4 Illustration of the RIE alternative protocol to fabricate IPP waveguides.

5.5 Illustration of etched cross-section dimension definitions.

5.6 RIE anisotropy and etch depth in silicon for varying power for a 120 s etch duration. RIE pressure = 100 mTorr, CHF$_3$ flow = 12 sccm, SF$_6$ flow = 30 sccm, and O$_2$ flow = 10 sccm.
5.7 RIE of silicon at varying pressure for 120 second duration. RIE power = 100 Watt, $CHF_3 = 12$ sccm, $SF_6 = 30$ sccm, and $O_2 = 10$ sccm.

5.8 RIE of silicon at varying $CHF_3$ flow for 120 second duration. RIE power = 100 Watt, pressure = 100 mTorr, $SF_6 = 30$ sccm, and $O_2 = 10$ sccm.

5.9 RIE of silicon at varying $SF_6$ flow for 120 second duration. RIE power = 100 Watt, pressure = 100 mTorr, $CHF_3 = 12$ sccm, and $O_2 = 10$ sccm.

5.10 Illustration of observed cross-section of RIE in silicon for varying $O_2$ flow rates.

5.11 RIE of silicon at varying $O_2$ flow for 120 second duration. RIE power = 100 Watt, pressure = 100 mTorr, $CHF_3 = 12$ sccm, and $SF_6 = 30$ sccm.

5.12 SEM image of RIE (100) silicon having $0^\circ$ side wall angle. RIE power = 100 Watt, pressure = 100 mTorr, $CHF_3$ flow = 12 sccm, $SF_6$ flow = 30 sccm, and $O_2$ flow = 18 sccm. Etching time = 10 min.

5.13 SEM image of RIE (100) silicon having $18^\circ$ side wall angle. RIE power = 120 Watt, pressure = 100 mTorr, $CHF_3$ flow = 12 sccm, $SF_6$ flow = 30 sccm, and $O_2$ flow = 10 sccm. Etching time = 5 min.

5.14 SEM image of a silver plated IPP waveguide.

5.15 Optical excitation experimental setup. The laser is set to have a center emission wavelength at 1550 nm. $\lambda/2 = \text{half waveplate}$; Obj.1 is the excitation objective; DUT = device under test; Obj. 2 is the output coupling objective.
5.16 TM component output intensity profile of a single mode IPP waveguide \((a = \sim 9 \, \mu m, \, b = \sim 5 \, \mu m, \, h = \sim 6 \, \mu m)\). 5.16(a) shows the output for TM polarized light excitation and 5.16(b) shows the output for TE polarized excitation at 1550 nm wavelength.

5.17 MODE simulated and experimentally observed IPP mode profiles. Row “MODE, \(\theta = 0^\circ\)” shows the simulated modes of a rectangular waveguide \((b = 24 \, \mu m, \, h = 6 \, \mu m, \, \theta = 0^\circ)\). Row “MODE, \(\theta = 18^\circ\)” shows the simulated modes of a trapezoid waveguide \((a = 28 \, \mu m, \, b = 24 \, \mu m, \, h = 6 \, \mu m, \, \theta = \sim 18^\circ)\). Row “Exp, \(\theta = 18^\circ\)” shows the experimentally observed mode profile (TM component only) of the fabricated trapezoid waveguide with the dimensions in (b) \((a = \sim 28 \, \mu m, \, b = \sim 24 \, \mu m, \, h = \sim 6 \, \mu m, \, \theta = \sim 18^\circ)\). The “TM” and “TE” markings indicate the excitation polarization. The waveguide boundary is marked with a white dashed line around the fundamental mode in each set.

5.18 Experimentally observed output intensity profile of a flat silver surface with TM 5.18(a) and TE 5.18(b) excitation; and of a 10-\(\mu m\) deep trapezoid waveguide with TM 5.18(c) and TE 5.18(d) excitation. The waveguide boundary is marked with a white dashed line around the mode in 5.18(c).

5.19 SEM image of the completed PMMA-rib Bragg-grating-embedded IPP waveguide. 5.19(a) shows a zoomed in top-view on the PMMA grating ribs. 5.19(b) shows the angled end-view of the waveguide.
5.20 Optical setup to characterize back reflection of Bragg-grating-embedded waveguides. DUT = device under test; Obj. is the output coupling objective. Solid lines represent fiber, dotted lines represent a free space beam.

5.21 The reflection spectra of air-filled Bragg-grating-embedded waveguides, with varying periodicity of $\Lambda_{\text{Bragg}} = 765$ nm, 770 nm, and 775 nm. The black solid lines represent the experimentally observed reflected power spectra, the red dashed lines show the calculated spectra from Section 3.6 Figure 3.34.

5.22 The reflection spectra of oil-filled Bragg-grating-embedded waveguides with $\Lambda_{\text{Bragg}} = 567$ nm. The index matching oils have $n_d = 1.3442, 1.3538$, and 1.3634, at a 1550 nm wavelength. The black solid lines represent the experimentally observed power spectra, and the red dashed lines show the calculated spectra from Section 3.6 Figure 3.35.

5.23 The reflection spectra of oil-filled Bragg-grating-embedded waveguides with $\Lambda_{\text{Bragg}} = 570$ nm. The index matching oils have $n_d = 1.3346, 1.3442$, and 1.3538, at a 1550 nm wavelength. The black solid lines represent the experimentally observed power spectra, and the red dashed lines represent the calculated spectra from Section 3.6 Figure 3.36.

5.24 SEM image (5.24(a)), AFM scan (5.24(b)) and the schematics of cross-section (5.24(c)) of the density hole array.
5.25 The reflection spectrum of air-filled PMMA density-hole array Bragg-grating-embedded IPP waveguides. The black solid line represents the experimentally observed reflected power spectra, and the dashed lines represent the calculated spectra.

5.26 Illustration of metal embedded IPP waveguide used in FDTD simulation.

5.27 FDTD-simulated contour plots of metal-groove-grating FWHM and reflected power versus groove width ($L_{\text{Bragg}}$) and groove height ($H_{\text{Bragg}}$). The FDTD used 100 $\Lambda_{\text{Bragg}} = 775$ nm Bragg gratings, having rectangular grooves in a silver surface.

5.28 Illustration of the second alternative protocol to fabricate metal-groove-grating-embedded IPP waveguides.

5.29 SEM of the metal Bragg IPP waveguide ($\Lambda_{\text{Bragg}} = 564$ nm). 5.29(a) shows the zoomed in top-view of the metal gratings. 5.29(b) shows the SEM of a tilted end-view of the metal Bragg IPP waveguide.

5.30 The reflection spectra of air-filled metal-groove Bragg-grating-embedded waveguides, having varying periodicity: $\Lambda_{\text{Bragg}} = 765$ nm, 770 nm, and 775 nm. The solid lines represent the experimentally observed power spectra, and the dashed lines represent the calculated (FDTD) spectra.

5.31 The reflection spectra of oil-filled metal-groove Bragg-grating-embedded waveguides. The gratings have a fixed $\Lambda_{\text{Bragg}} = 564$ nm. The index matching oils have $n_d = 1.3538, 1.3634, \text{and} 1.3730$ at 1550 nm wavelength. The solid lines represent the experimentally observed power spectra, and the dashed lines represent the calculated (FDTD) spectra.

xxxii
5.32 Comparison of the metal and PMMA grating reflection spectra obtained experimentally. .......................... 159

6.1 Preliminary IPP waveguide sensor packaging proposal. .................. 165

B.1 Optical microscope image of the etched ITO. Each strip is 2 µm in width. ................................................. 172

C.1 Optical microscope image of etched silver film. Each strip is 5 µm in width. ................................................. 174

E.1 $SiO_2$ channel on corrugated silicon substrate. .................. 179

E.2 Parylene channel on corrugated silicon substrate. Note: the cracking in Parylene is unanimous. There may be a recipe to eliminate the cracks. ................................................. 180

E.3 SU8 channel on corrugated silicon substrate. .................. 181
Chapter 1

Introduction

Biotechnology developments in the 21st century have been driven by the enthusiasm to extend our pre-determined biological capabilities. We now can turn water into wine and give “birth” to Dolly. While some of the motives and results are controversial, technology certainly has benefitted and improved our everyday lives. To hear across the mountains, we have invented the satellite radio; to allow the handicapped to walk, we have invented artificial limbs; to mask others’ body odor, we have invented deodorant; and to detect small things, even smaller than what the optical microscope can facilitate, we can use Surface Plasmon Polaritons (SPPs).

SPPs are collective electron oscillations that may be excited by light. An SPP has its energy highly concentrated on the metal surface, such that any surface change (i.e. refractive index change or corrugation in morphology) would cause a change in the SPPs’ properties. Therefore, SPPs can detect a fraction of a molecular density change near a metal surface. They have a wide range of applications, from sub-diffractive
Chapter 1. Introduction

microscopes to sensors. SPP sensors have been used to study drug delivery[2] and to detect protein conformational change[3]. Both of these applications use SPPs to detect a fractional molecular density change accurately, which can not be achieved by applying conventional technologies. Let’s see why.

Most of the common sensors may be categorized into *in vivo* sensors (e.g. sensors which use quantum dots and nanoparticle[1]) and *in vitro* sensors (e.g. SPR, ELISA, and glucose sensors) (Table 1.1). The *in vivo* sensors are usually used to study whole cells. Since the cells are still “alive”, the *in vivo* tests can be used to study pathology and reveal the biological interactions, such as the expression of a protein and the pathway of a biomarker. These *in vivo* tests however suffer from a lack of reproducibility due to the changing pH, temperature, and metabolism of a biological environment; and therefore, often the *in vivo* results must be accompanied by *in vitro* tests, which are conducted under controlled environments[4,5]. *In vitro* tests are more suited for the use in early disease diagnosis, where the known biomarker is already available in the blood stream or sputum, because both may be easily obtained. This method is much less invasive and show clear advantage in offering reliable test results in point-of-care diagnosis. Also, when packaged as a consumer product, *in vitro* sensors may offer at-home diagnosis of some of the most fatal diseases, such as cancer. At-home diagnosis also reduces the manufacturing, hospital labor, physician, and most other time- and resource-related costs. Due to these advantages, according to Kalorama Information, the cancer *in vitro* diagnostic

---

1Both of these particles may be used either *in vivo* or *in vitro* sensors: uptake of particles by high metabolic tissues labels cancer cells in *in vivo* applications; they may also be functionalized to recognize cell surface biomarkers. Then, the labeled cells are detected using *in vitro* flow cytometry.
test market can reach 8 billion dollars by the end of 2012, which is an 11 % growth annually. These market report numbers further reveal the expected impact of \textit{in vitro} sensors in biotechnology research and development.

\textit{In vitro} test methods can be categorized into either passive or active (Table 1.1). The passive tests usually require additional reactions to display results and are observed using the naked-eye – this testing method still relies on human biological visual abilities and therefore has limited milli-molar detection sensitivity \cite{7}. The passive tests are inexpensive however and have sufficient performance for detecting large biological signals, such as diabetes and pregnancy. To detect small biological signals, the detection sensitivity could be drastically reduced by using an active setup (e.g. a light source). In fact, some implementations of the active method are known to have a nano-molar detection limit \cite{6}. With this one-million-fold reduction in the detection limit, it is possible to diagnose diseases at an early stage, where only

<table>
<thead>
<tr>
<th></th>
<th>\textit{In vitro}</th>
<th>\textit{In vivo}</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reproducibility</td>
<td>yes</td>
<td>no</td>
</tr>
<tr>
<td>pH and temp invariant</td>
<td>yes</td>
<td>no</td>
</tr>
<tr>
<td>Non-invasiveness</td>
<td>yes</td>
<td>no</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>Active</th>
<th>Passive</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Sample volume</td>
<td>pico-liter</td>
<td>micro-liter</td>
<td></td>
</tr>
<tr>
<td>Detectable level</td>
<td>nano-molar</td>
<td>milli-molar</td>
<td></td>
</tr>
<tr>
<td>Reusability</td>
<td>yes</td>
<td>no</td>
<td></td>
</tr>
<tr>
<td>Realtime</td>
<td>yes</td>
<td>yes</td>
<td></td>
</tr>
<tr>
<td>Application</td>
<td>most diseases</td>
<td>e.g. diabetics</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>e.g. chemotherapy</td>
<td></td>
</tr>
</tbody>
</table>

Table 1.1: Comparison of \textit{in vivo} and \textit{in vitro} diagnostic technologies
small numbers of biomarkers are available. Labeling these biomarkers for detection however is a time and money consuming process. The only alternative is label-free detection.

A typical label-free active sensor consists of an optically dispersive element, such as a Bragg grating or photonic crystal. This element has a resonant frequency, which changes as the molecular density changes, and can be made of metal, as is in the case of a SPP sensor, or dielectric, as is the case in an optical fiber sensor. Both SPP-based and fiber-based label-free technologies surpass the performance of methods which use un-aid or microscope-aid vision. However, due to optical fiber’s inherent light guiding mechanism, it has most of the electromagnetic field concentrated in the solid core (Figure 1.1(a)), which is not in proximity to the analyte suspended in the cladding, and therefore, the field-analyte contact area is small and the optical power is not efficiently utilized\(^2\). The same problem exists in all other dielectric-waveguide-based sensors. By contrast, an SPP waveguide has most of the power concentrated on the metal surface (Figure 1.1(b)), where the analytes are present; hence, the field-analyte contact area is large, and the optical signal is efficiently utilized to “examine” the analyte. Also, SPP sensors are made with bulk metal or metal-plated substrates, which may be cleaned and reused easily to reduce cost. Therefore, an SPP waveguide has the potential of becoming a superior technology for sensor applications. A summary of the discussion is tabulated in Table 1.2. A more comprehensive review of plasmonic and conventional sensors is available in \(^{10}\).

\(^2\)Fiber technology has the advantage of having low optical power loss to boost the sensor signal and being widely available as commercial products to reduce the sensor device cost.
Chapter 1. Introduction

(a) Optical fiber  (b) IPP technology

Figure 1.1: Illustration of IPP waveguide mode and optical fiber mode. Both structures has similar 10 \( \mu \text{m} \) by 10 \( \mu \text{m} \) cross-section dimension. IPP has a silver active region\[1\]. The fiber has a core index of 1.4. The background has unity index. The wavelength of simulation is 1550 nm.

and a review of prior art on the subject of SPP sensors will be shown in the next chapter.

All of the above comparisons reveal that SPP sensors satisfy the need for result-reproducibility, sensitivity, non-invasiveness, specificity, and continuity/reusability. All of these criteria can not be simultaneously satisfied in one device with any of

<table>
<thead>
<tr>
<th></th>
<th>SPP waveguide(^*) [6, 11]</th>
<th>SPP planar surfaces [11, 7]</th>
<th>Fiber [12]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sample volume</td>
<td>nano-liter</td>
<td>micro-liter</td>
<td>N.A.</td>
</tr>
<tr>
<td>Detectable level</td>
<td>nano-molar</td>
<td>nano-molar</td>
<td>pico-molar</td>
</tr>
<tr>
<td>Ease of functionalization</td>
<td>yes</td>
<td>yes</td>
<td>yes</td>
</tr>
<tr>
<td>Low cost of parts</td>
<td>yes</td>
<td>no</td>
<td>yes</td>
</tr>
<tr>
<td>Inert sensor surface</td>
<td>yes</td>
<td>yes</td>
<td>no</td>
</tr>
</tbody>
</table>

Table 1.2: Comparison of SPP and fiber diagnostic technologies. \(^*\) The sample volume is that of the IPP waveguide sensor.
the conventional methods. The work done and shown in this thesis enables the design and testing of a novel and simple Interface Plasmon Polariton (IPP) waveguide sensor prototype. The demonstrated sensor structure offers guiding of both SPPs and analytes, and also allows the incorporation of plasmonic technology into existing Lab On a Chip (LOC) devices with one simple metal plating process. This design not only presents a superior solution for revealing molecular level interactions, but also validates the SPP phase interactions demonstrated by previous researchers, and therefore contributes to the scientific understanding of SPPs and nano-scale photonics.

This thesis consists of six chapters, seven appended sections, and lastly a bibliography of previous works. Chapter 1 is the introduction, which defines the context. Chapter 2 reviews the prior art and identifies the gaps in the field. Chapter 3 provides the background and theory, showing macroscopic view on SPPs, material dispersion, waveguide dispersion, and then SPP dispersive element design. Chapter 4 focuses on the fabrication of a stripe SPP waveguide and an experimental demonstration of electromagnetic field phase interactions in stripe waveguide arrays. Chapter 5 focuses on IPP sensing devices, first describing IPP waveguide and sensor design and fabrication, and then presenting sensor characterization and device demonstration. Chapter 6 concludes the thesis. The appendices consist of a list of publications (Appendix A) and the fabrication protocols (Appendices B-G) developed while carrying out this project.
Chapter 2

Literature Review

In this chapter, the prior art of SPP sensor design is reviewed. Section 2.1 reviews two SPP materials: Indium Tin Oxide (ITO) and a noble metal, silver. Section 2.2 then reviews five SPP confinement geometries: the dielectric loaded geometry, the gap geometry, the Channel Plasmon Polariton (CPP), the stripe geometry, and the IPP. Section 2.3 reviews the published SPP sensor devices. Finally in Section 2.4, sensor design criterions are determined based on the prior art.

2.1 SPP materials

The focus of this section is to review common materials used to guide SPP, namely ITO and silver. Silver is easily accessible and patterned. Although optically non-transparent in the visible, silver is less lossy (e.g. than gold), and therefore has the
advantage of higher Signal to Noise Ratio (SNR) in a sensor\

ITO is a transparent conducting oxide and is usually presented as a thin film coated on glass substrate. ITO-mediated SPPs are not only an interesting scientific phenomenon, but also may enable a guiding technology that is both visibly transparent and sub-diffractive. For example, ITO could be used as SPP waveguides and electrodes in a LOC device. On such a LOC device, the ITO SPP waveguide could allow SPP-based sensing; the ITO electrodes may be used for electro-wetting and dielectrophoresis; the visible-to-Infrared (IR) transparency of ITO would further allow observations of Förster Resonance Energy Transfer (FRET) and implementations of optical tweezers. Therefore, it is interesting to review the pros and cons of these materials.

2.1.1 Indium Tin Oxide (ITO)

ITO is often used as a 100-300 nm thin-film coated on glass slides. ITO is written as $\text{In}_{2-x}\text{Sn}_x\text{O}_{3+\delta}$, which is formed by doping indium oxide with tin. When the tin doping concentration exceeds the Mott critical level (the doping level is represented by $x$ in the subscripts), ITO becomes conductive. There are two explanations for the free electron formation: an oxygen deficiency (represented by $\delta$ in the subscript) could cause the effective negative charge \cite{13}; or, the doping process is a substitution of $\text{In}^{3+}$ by $\text{Sn}^{4+}$ and results in a net +1 charge per substitution \cite{14}. Despite the different theories on free electron formation, the available ITO material free electron concentration is $\sim 10^{27} \, [m^{-3}]$; and the bandgap is $\sim 4 \, \text{eV}$ ($\text{In}_2\text{O}_3$ has $\sim 2 \, \text{eV}$ bandgap)

\footnote{Silver and gold have similar material dispersions. Most of the discussions on silver also applies to gold in this thesis.}
Therefore, ITO is a conductive and transparent material.

The optical properties of ITO can be represented by the Drude model \([15]\):

\[
\varepsilon_r(\omega) = \varepsilon_\infty - \frac{\omega_p^2}{\omega^2 + i\omega \tau}
\]  

(2.1)

where \(\varepsilon_r\) is the frequency-dependent relative permittivity of ITO, \(\varepsilon_\infty = 3.57\) is the high-frequency relative permittivity, \(\omega_p = 1.89 \times 10^{15} \text{ [rad/s]}\) is the bulk plasma frequency, \(\omega\) [rad/s] is the frequency, and \(\tau = 6.34 \times 10^{-15} \text{ [s]}\) is the free electron collision time \((\omega_p\) and \(\tau\) vary slightly amongst different publications \([16, 17, 18, 19, 20, 21, 15]\)).

Another important prominent optical property of ITO, not shown in the Drude model, is that the film thickness is inversely proportional to the transparency on the hundred-nanometer scale \([22]\).

Though ITO is seemly simple and desirable, it has potential problems if it is to be adapted by SPP sensors. Firstly, the material properties are not well understood. Secondly, ITO is a highly lossy material, which will compromise SNR. These cons will be discussed in more detail below.

The material properties of ITO are difficult to be determined. Taking oxidation as an example, when ITO oxidizes, the \(Sn^{2+}\) losses charges and become \(Sn^{4+}\) \([23]\). This process is significant because it reduces the electron concentration, which is proportional to the plasma frequency:

\[
\omega_p^2 = \frac{Ne^2}{\varepsilon_0 m}
\]  

(2.2)

where \(\omega_p\) is the bulk plasma frequency [rad/s], \(\varepsilon_0\) is the dielectric permittivity of
Chapter 2. Literature Review

vacuum \([Fm^{-1}]\), \(e\) is the electron charge \([C]\), \(m\) is the mass of electrons \([kg]\), and \(N\) is the density of electrons \([m^{-3}]\). Therefore, the surface oxidation that reduces \(N\) will reduce \(\omega_p\), and the original SPP dispersion will be shifted in frequency as well. Hence, oxidation could “kill” SPP, therefore is not desired\(^2\).

Oxidation may be introduced by plasma treatment \[23\] and acid etch \[24, 25\], and is believed to be measurable by examining the binding energies of tin and indium \[23\]. Here, the experiments performed in \[23\] are reproduced using a X-ray Photoelectron Spectroscopy (XPS). This machine is a Laybold MAX 200 and PHI 5500 system, which has an Al Ka photon source energy of 1486.6 eV and the measurement resolution of 0.5 eV, available at Material Science group at University of Toronto. Figure 2.1(a) shows the normalized Sn \(3d_{5/2}\) intensity, which is the combined \(Sn^{2+}\) and \(Sn^{4+}\) emission. The data shown was collected from three samples: a native ITO substrate, a 14-day air-exposed ITO substrate, and an air-exposed and then Hydrogen Chloride (HCl) rinsed ITO substrate. It is clear that the native and the air-exposed samples have similar curves, and that the HCl washed sample curve extends slightly further to the higher energy end of the spectrum. This difference in spectral distribution is due to the increased \(Sn^{4+}\) emission. The \(Sn^{4+}\) emission can be extracted by applying one Lorentzian to represent the \(Sn^{2+}\) and another Lorentzian to represent the \(Sn^{4+}\), as shown in Figure 2.1(b). In the native sample, the \(Sn^{2+}\) to \(Sn^{4+}\) ratio (area-under-the-curve) is 6786 to 3707; and, in the HCl-washed sample, the ratio is 2696 to 2096 – the later sample shows a clear increase in \(Sn^{4+}\). Hence, the

\(^2\)ITO oxidation is a heated discussion in conventional electronic device researches, because it reduces the work function, which surprisingly optimizes the emission efficiency, and is desirable in this case.
HCl-washed sample is more oxidized. This exercise not only validates that oxidation could be created using an acid solution, but also validates XPS as a qualitative method to explore ITO electronic properties.

To estimate the quantitative plasma wavelength shift due to oxidation, one may examine the higher-binding-energy components and the lower-binding-energy components in indium. It is theorized in [26] that the difference between the high- and low-binding energy is directly related to the bulk plasma frequency. Figure 2.1(c) shows a reproduced indium $3d_{5/2}$ energy, its screened Lorentzian fit (i.e. lower-binding energy components), and its unscreened Lorentzian fit (i.e. higher-binding energy components). These measured data agree with previous reports [13] and [15]. The screened Lorentzian peaks at 444.15 eV; and the unscreened Lorentzian peaks at 445.08 eV. The separation between the two peaks is $\sim 0.93$ eV, and this value varies depending on the positioning of the Lorentzians fits. Therefore, the experimental feasibility of this method to estimate the plasma wavelength is questionable, and therefore the material properties of ITO is difficult to be determined.

ITO material properties have been misdefined in papers. For example, [16] suggests a direct relationship between the ITO film thickness and the bulk plasma frequency (Equations (14) and (15) in the paper). The plasma frequency is related to resistivity, which is a material property and is dictated by the doping concentration. The actual variable measured in this paper is called “sheet resistance”, which is a sample property and is inversely proportional to the thickness of the film. Hence applying the correct variable, one will realize the bulk plasma frequency remains the same and does not vary with the film thickness. The bulk plasma frequency dictates
Figure 2.1: XPS intensity of ITO samples. 2.1(a) plots the normalized Sn 3d$_{5/2}$ intensity of the native (×), exposed in air for 14 days (solid line), and exposed in air and then HCl washed sample (dotted line). 2.1(b) plots the energy of Sn 3d$_{5/2}$ with the Sn$^{2+}$ and Sn$^{4+}$ fitting curves. 2.1(c) shows the binding energy of indium. In both 2.1(b) and 2.1(c) the red group represents the HCl washed, and the black group represents the native sample.
Chapter 2. Literature Review

The optical property of ITO is examined here. Figure 2.2(a) shows the ITO SPP dispersion (applying the parameters from [15]). In the figure, the two horizontal parallel lines separate the Radiating Plasmon Polariton (RPP), the quasi-bound modes (QBM), and non-radiating SPP regions. It is clearly seen that ITO-mediated SPPs exist at wavelengths > 2 µm, which overlaps with many natural molecular oscillations and therefore is not desirable. When the wavelength is below 2 µm, one may still obtain an Otto angle-dependent excitation [27], such as the one shown in Figure 2.2(b). The minima in Figure 2.2(b) are tabulated in Table 2.1. These reflection minima are due to the coupling of impinging light with the RPP modes. Therefore, using a prism excitation, it is difficult to determine whether the mode is on the surface or in the bulk. Also, the prism setup is bulky and one may explore the planar ITO SPP waveguide designs.

ITO SPP waveguide properties are studied here. The stripe waveguide type is chosen because it is known to have the lowest loss and therefore may be easily demonstrated experimentally. The cladding region was chosen to be glass because, as mentioned before, ITO is usually coated on glass. The stripe thickness was chosen to be 50-110 nm because these are the typical ITO thin film coating thicknesses. A

<table>
<thead>
<tr>
<th>λ [nm]</th>
<th>ω ×10^{15}[rad/s]</th>
<th>β ×10^6[rad/m]</th>
<th>θ(theoretical) [degrees°]</th>
<th>θ(experimental) [degrees°]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1520</td>
<td>1.24</td>
<td>3.122</td>
<td>49.0536</td>
<td>46.4 (×)</td>
</tr>
<tr>
<td>1570</td>
<td>1.2</td>
<td>2.949</td>
<td>47.4977</td>
<td>45.6 (●)</td>
</tr>
<tr>
<td>1620</td>
<td>1.16</td>
<td>2.763</td>
<td>45.6079</td>
<td>44.7 (∆)</td>
</tr>
</tbody>
</table>

Table 2.1: ITO-air radiating mode excited in experiments
Figure 2.2: Dispersion relationship of the electromagnetic waveguides at the interface of ITO and air. In 2.2(a), the real part of the propagation constant, $\beta$, is represented by the solid line. The imaginary part of the $\beta$ is shown as a dashed line. The two horizontal parallel lines separate the three regions defined by the radiating (RPP), quasi-bound (QBM), and non-radiating (SPP). 2.2(b) is experimental result of the TM-TE ratioed reflection spectrum at internal incident angle $44.7^\circ$($\Delta$), $45.6^\circ$($\bullet$), and $46.4^\circ$($\times$), obtained using an Otto configuration.
Chapter 2. Literature Review

Figure 2.3: Effective indices, $n_{\text{eff}}$, of bound SPP even modes as a function of the ITO thickness at 2500 nm wavelength. Waveguide having 2, 3, 4, 6, and 7 $\mu$m width are illustrated. (a) plots the real part of the effective index and (b) plots the propagation distance of the corresponding modes. The inset plots the mode profiles of two different waveguide structures: 7 $\mu$m×100 nm and 7 $\mu$m×50 nm.

2.5 $\mu$m operating wavelength is chosen because it is larger than the critical SPP-mode wavelength, as shown in Figure 2.2(a). The ITO material dispersion is represented by Equation 2.1. The ITO material dispersion is taken from [15]. And the glass has index of $n_{\text{glass}} = 1.43$.

Figure 2.3 plots the effective indices of the fundamental even modes as a function of ITO thickness. In this plot, the waveguides have widths of 2, 3, 4, 6, and 7 $\mu$m. The propagation distance is defined as the $1/e^2$ electric field decay length.

Figure 2.4 plots the effective indices as a function of the waveguide width. Here the waveguides have three different thicknesses: 50, 60, and 110 nm.

Observing the trend in Figure 2.3 and 2.4, the ITO waveguide loss drastically increases as a function of the film thickness. Bearing in mind that a realistic ITO
Figure 2.4: Effective indices of bound SPP even modes as a function of the ITO width at 2500 nm wavelength. Waveguide having 50, 60, and 110 nm thickness are plotted. In the plots, the effective indices of the first four lowest modes are shown and represented by open circle (○), open square (□), open triangle (▽), and cross (×). Figure 2.4(a) plots the real part of the effective index and Figure 2.4(b) plots the propagation distance. The inset shows the mode profiles of the first the lowest order modes.
coating thickness is 100-300 nm at this film thickness range, the ITO-mediated SPP modes are lossy and not desirable.

In summary, based on prior art and studies conducted in this thesis, ITO may not be the most desirable material for implementing a SPP sensor, neither in a 3D prism setup nor in a 2D waveguide setup, at this time. As this thesis shall provide a foundation for any future work, Appendix B includes an ITO wet etching technique.

\subsection{Noble metals}

Compared to ITO, the dispersion of noble metals are better understood. Many are included in Palik\cite{Palik}. For example, reference\cite{Silver} measures an electrolytically-deposited and chemically-polished silver film characterized at Near Infrared (NIR) wavelengths. Reference\cite{Johnson} uses a thermally heated Mo-boat to deposit metal and then uses a polarimetric method to obtain the material properties. However, the polarimetric method is criticized by Johnson and Christy in\cite{Johnson}, for being dependent on the material surface morphology. Instead in\cite{Johnson}, a three beam method is used, where the normal transmission, reflection and oblique angle transmission data is obtained to generate the material dispersion. By applying the silver parameters from\cite{Johnson}, Section 3.2 will explore the silver-mediated SPP dispersion in more detail.

\footnote{Recall, thicker film has lower resistance. Therefore, a 100-300 nm thick ITO film has a reasonable $\sim 20-100 \, \Omega$ resistance to be used as electrodes.}
2.2 SPP confinement types

The SPP confinement\textsuperscript{4} such as a waveguide mode, may be offered by a primary and a secondary mechanism. The primary mechanism is determined by the physics – as SPPs are the collective electron oscillations, they are confined to the metal surface. The primary mechanism may be SPPs supported by a single metal-dielectric interface, coupled-SPPs supported by a metal thin-film, or coupled-SPPs supported by the gap in between two closely placed bulk metal substrates. Inevitably, tactical arrangements of the metal and dielectric interfaces dictate whether the SPPs are coupled, and if two SPP groups are coupled, to which group they are coupled to. These material arrangements therefore determines the confinement size as well as the dominate polarization. For convenience and consistency, each of the metal-dielectric interface arrangement is named here. The single metal-dielectric interface arrangement will be referred to as Metal-Dielectric (MD). The gap in between two closely placed bulk metal substrates arrangement will be referred to as Metal-Insulator-Metal (MIM). And the metal thin-film arrangement will be referred to as Insulator-Metal-Insulator (IMI).

The secondary mechanism is facilitated by a geometric disruption, and hence a index disruption. This index disruption, similar to the core-cladding boundary in dielectric waveguides, results in confinement. At different degrees of confinement, different mode orders may be observed.

There are five main types of SPP confinements that consist of various combina-
\footnote{The discussion carried out here does not apply to metal nanoparticles.}
tions of the primary and the secondary mechanisms. They are the dielectric loaded confinement \[31, 32\] (Figure 2.5(a)), the gap confinement \[33, 34\] (Figure 2.5(b)), the CPP confinement \[35, 36, 37\] (Figure 2.5(c)), the stripe confinement \[38\] (Figure 2.5(d)), and the IPP confinement \[39\] (Figure 2.5(e)). The mode profile of the above structures are shown in Figure 2.5. They all have different mode dispersions (i.e. the mode index and the mode loss), mode polarizations, and manufacturing costs. Each confinement type is discussed in more details below.

The dielectric loaded confinement has a finite-thickness dielectric stripe laying on top of a semi-infinite silver (or gold) piece. This dielectric piece offers material inhomogeneity and guiding of a y-polarized hybrid mode. Because of the constitutive relations, the modal field distribution is “severed” into several parts and can be loosely categorized into the MD arrangement. The hybrid mode is highly lossy. The secondary mechanism is facilitated by the finite width of the dielectric piece. By making the piece wider, higher order modes may be found. Section 3.6 in this thesis shows an implementation of the dielectric-loaded confinement facilitated Bragg waveguide design. One disadvantage of dielectric surface is the complex surface functionalization chemistry.

The gap and CPP confinements consist of slots and grooves cut (e.g. using Focused Ion Beam (FIB)) into bulk silver (or gold). In the gap and CPP confinements (Figure 2.5(b) and 2.5(c)), the primary mechanism is the coupled SPPs bound to the left and right metal walls (MIM). And the secondary mechanism is facilitated by the finite height of the gap. This confinement results in small modes, which are polarized in the x-direction. The center insulator layer is nanometer in width (i.e.
Figure 2.5: Simulation of five types of SPP confinement fundamental modes at 1550 nm wavelength. All simulation setups have silver as the metal (material dispersion taken from [1]). 2.5(a) plots the dielectric loaded mode. The dielectric-loaded setup uses a $n = 1.4$ dielectric stripe. All background indices are 1. 2.5(b) plots the gap mode. 2.5(c) plots the CPP mode. 2.5(d) plots the stripe mode. And, 2.5(e) plots the IPP mode.
tightly bound SPP mode) and therefore results in a highly lossy confinement type. Also due to the small dimensions associated with this confinement type, in order to be implemented as biosensor, there must be pre-processing of the bio-samples to remove cells and large proteins to prevent clogging. In Section 2.3, the performance of the MIM-like sensors are compared to other SPP sensor designs.

The stripe confinement consists of a thin metal stripe, sandwiched in-between two symmetrical dielectric slabs. The primary mechanism is the coupled SPPs bound to the top and the bottom metal-stripe surfaces (IMI). And the secondary mechanism is facilitated by the finite-width of the stripe. This waveguide has large modes, which are polarized in the y-direction. The stripe geometry allows the mode to penetrate deeply into the dielectric region and therefore enables long range surface plasmon mode propagation (i.e. less lossy). In Section 2.3, several IMI sensors are reviewed in terms of the excitation method and sensitivities.

Finally, the IPP confinement primary mechanism is offered by the bottom metal surface (MD), and, the secondary mechanism is facilitated by the two walls on the sides. The mode polarizes in y-direction. The sensors enabled using the IPP confinement will be discussed in Section 2.3.

The different plasmonic confinements are compared and tabulated in Table 2.2. This comparison reveals that the stripe and the IPP structures are the least lossy and have large modes, and therefore will have enhanced sensor sensitivity (as discussed in Section 2.3). In addition to the mode geometry, the “integration readiness” is a quality that estimates the feasibility of the waveguide to be used with LOC. For example, Section 3.3 will later show that the stripe confinement demands highly
Table 2.2: Comparison of different plasmonic confinement modes. The five determining factors are cost, waveguide loss, material compatibility with the LOC, dimension compatibility with LOC, and finally, the LOC integration readiness. Di. loaded = Dielectric loaded.

homogeneous cladding material, which makes this confinement type not ready for LOC integration.

There are of course more complex SPP confinements. For example, the plasmonic nano-wire offers super-high confinement of the mode, and is difficult to excite. Also, the manufacturing facility required to make a nano-wire is not readily available [41, 42].

In summary, these are the SPP confinement types. Recognizing the primary and secondary mechanism in the different SPP confinement types allows one to design dispersive elements, photonic crystals, gratings, and etc. for sensor applications. The coming Section 2.3 compares the existing SPP confinement types in terms of their applicability to sensor platforms.
2.3 SPP dispersive elements and sensors

SPPs have been demonstrated to behave like electromagnetic waves, having both an intensity and phase. Therefore, with the right dispersive element design, SPP waves interfere and exhibit resonant behavior in addition by cutting slits orthogonal to the CPP waveguide propagation direction, Bragg gratings can be realized \[35\]. When periodic holes are drilled in metal films, the phase of SPPs has been demonstrated to interfere like dielectric-mirrors \[43\]. Similar effects may be demonstrated with metal bumps (arranged metal nano-particles on metal films) \[44\], arranged to have bandgaps \[45\] and made into photonic crystal waveguides \[46\]. Photoresist gratings \[47, 48\] and silicon pillars \[49\] can also form SPP bandgap materials. Other optical integrated elements may be made by patterned dielectric stripes (recall the dielectric loaded confinement), such as ring resonators \[50\]. Stripe waveguides can be patterned to have Bragg gratings \[51, 52, 53, 54\] and shaped into Mach–Zehnder interferometers \[55\]. Although some papers such as \[53\] and \[35\] have demonstrated functional SPP dispersive elements\[5\] these elements have not been used to demonstrate changing index sensing.

The following sensor review will first sort the SPP confinement based on the MIM, MD, or IMI arrangement, as these arrangements dictates the factors such as confinement size, polarization, and effective index. Then, to demonstrate the impact of these factors on sensor performance, the same literature is then evaluated based on operating wavelength, band-width, sensitivity, and the Sensing Resolution (SR).

\[5\]Both paper show $\sim 40$ nm FWHM reflected Bragg resonance.
## Chapter 2. Literature Review

Table 2.3: Tabulated planar SPP sensor review. $\lambda$ is the operating wavelength. FWHM: Full Width Half Maximum is the resonance width either in wavelength or in angular degree. MIM: Metal-Insulator-Metal. MD: Metal-Dielectric interface. IMI: Insulator-Metal-Insulator. $\perp$: normal incident. $\parallel$: parallel incident. RIU: Refractive Index Unit. $\ast$: Xu calculated. $\times$/RIU: the sensor measures intensity change.

<table>
<thead>
<tr>
<th>excitation</th>
<th>SPP type</th>
<th>$\lambda$ [nm]</th>
<th>FWHM [nm] or $^\circ$</th>
<th>sensitivity [nm/RIU] or $^\circ$/RIU</th>
<th>SR [RIU]</th>
<th>citation</th>
</tr>
</thead>
<tbody>
<tr>
<td>end-fire</td>
<td>MIM</td>
<td>1000 nm</td>
<td>40 nm$^*$</td>
<td>458.6 nm/RIU</td>
<td>2.2×10$^{-5}$</td>
<td>56</td>
</tr>
<tr>
<td>perforated Au</td>
<td>MIM</td>
<td>720 nm</td>
<td>40 nm$^*$</td>
<td>650 nm/RIU</td>
<td>N.A.</td>
<td>57</td>
</tr>
<tr>
<td>Kretschmann</td>
<td>MD</td>
<td>630 nm</td>
<td>2 $^\circ$</td>
<td>100 $^\circ$/RIU</td>
<td>10$^{-8}$</td>
<td>58</td>
</tr>
<tr>
<td>Kretschmann</td>
<td>MD</td>
<td>800 nm</td>
<td>50 nm$^*$</td>
<td>N.A.</td>
<td>2×10$^{-7}$</td>
<td>59</td>
</tr>
<tr>
<td>Kretschmann</td>
<td>MD</td>
<td>630 nm</td>
<td>2 $^\circ$</td>
<td>79 $^\circ$/RIU</td>
<td>1.85×10$^{-5}$</td>
<td>60</td>
</tr>
<tr>
<td>Kretschmann</td>
<td>MD</td>
<td>800 nm</td>
<td>N.A.</td>
<td>N.A.</td>
<td>2×10$^{-6}$</td>
<td>61</td>
</tr>
<tr>
<td>Kretschmann</td>
<td>MD</td>
<td>670 nm</td>
<td>N.A.</td>
<td>N.A.</td>
<td>9×10$^{-5}$</td>
<td>62</td>
</tr>
<tr>
<td>Kretschmann</td>
<td>MD</td>
<td>630 nm</td>
<td>N.A.</td>
<td>65×/RIU$^*$</td>
<td>35×10$^{-6}$</td>
<td>63</td>
</tr>
<tr>
<td>gratings $\perp$</td>
<td>MD</td>
<td>650 nm</td>
<td>10 nm$^*$</td>
<td>643 nm/RIU$^*$</td>
<td>10$^{-6}$</td>
<td>64</td>
</tr>
<tr>
<td>gratings $\perp$</td>
<td>MD</td>
<td>630 nm</td>
<td>2 $^\circ$</td>
<td>79 $^\circ$/RIU</td>
<td>5×10$^{-6}$</td>
<td>65</td>
</tr>
<tr>
<td>gratings $\parallel$</td>
<td>MD</td>
<td>N.A.</td>
<td>N.A.</td>
<td>1100 nm/RIU</td>
<td>N.A.</td>
<td>66</td>
</tr>
<tr>
<td>Au on slide</td>
<td>MD</td>
<td>600 nm</td>
<td>N.A.</td>
<td>14×/RIU</td>
<td>2.3×10$^{-5}$</td>
<td>67</td>
</tr>
<tr>
<td>Otto</td>
<td>IMI</td>
<td>700 nm</td>
<td>213 nm$^*$</td>
<td>5000 nm/RIU</td>
<td>2.3×10$^{-6}$</td>
<td>68</td>
</tr>
<tr>
<td>gratings</td>
<td>IMI</td>
<td>1550 nm</td>
<td>5 nm$^*$</td>
<td>60000 nm/RIU</td>
<td>N.A.</td>
<td>69</td>
</tr>
<tr>
<td>fiber mode</td>
<td>IMI</td>
<td>800 nm</td>
<td>80 nm$^*$</td>
<td>2500 nm/RIU</td>
<td>5×10$^{-7}$</td>
<td>70</td>
</tr>
<tr>
<td>fiber mode</td>
<td>IMI</td>
<td>1000 nm</td>
<td>100 nm$^*$</td>
<td>1.3×10$^4$ nm/RIU</td>
<td>7×10$^{-7}$</td>
<td>71</td>
</tr>
<tr>
<td>waveguide</td>
<td>IMI</td>
<td>800 nm</td>
<td>40 nm$^*$</td>
<td>5.7×10$^4$ nm/RIU</td>
<td>2.5×10$^{-8}$</td>
<td>72</td>
</tr>
<tr>
<td>waveguide</td>
<td>IMI</td>
<td>600 nm</td>
<td>17 nm$^*$</td>
<td>183 nm/RIU</td>
<td>N.A.</td>
<td>73</td>
</tr>
<tr>
<td>waveguide</td>
<td>IMI</td>
<td>1550 nm</td>
<td>N.A.</td>
<td>120 nm/RIU</td>
<td>10$^{-6}$</td>
<td>74</td>
</tr>
<tr>
<td>fiber</td>
<td>fiber</td>
<td>1550 nm</td>
<td>10 nm</td>
<td>172 nm/RIU</td>
<td>N.A.</td>
<td>75</td>
</tr>
</tbody>
</table>
Chapter 2. Literature Review

Operating wavelength and bandwidth have rather trivial definitions. Sensitivity is defined as wavelength shift per refractive index unit change, \( \frac{d\lambda}{dn} \), and has the unit of \([\text{nm/RIU}]\). SR is defined as, \( SR = \frac{dn}{d\lambda} \times \delta\lambda \), where \( \delta\lambda \) is the resolution of optical spectrometer. In some literatures, the SR is also referred to as the figure of merit of a sensor. At the end of this section, there is a discussion on important sensor design factors, such as sensitivity, SR, SNR, fabrication complications, and packaging dimensions.

The MIM arrangement has the highest SPP confinement, which facilitates strongly localized SPP interaction with the analyte. The inevitable consequence is a high ohmic loss, which will be discussed in Section 3.1. Reference [56] presents a simulation of a dispersive element implemented using MIM waveguide coupled to a short MIM resonant piece. The demonstrated sensitivity is 458.6 nm/RIU at an IR operating wavelength. Reference [57] uses a periodically perforated metal film\(^6\) to demonstrate a 650 nm/RIU sensitivity at a NIR wavelength. Both papers report a similar \( \sim 40 \) nm resonant bandwidth.

The MD arrangement offers guiding of SPPs on a single metal dielectric interface, and has an intermediate SPPs field penetration depth into the sensing medium. It can be excited using a Kretschmann setup, where the prism offers light-SPP momentum matching. When the excitation angle is fixed, this method offers a typical 50 nm bandwidth. When the wavelength is fixed, the resonant dip has \( 2^\circ \) angular width. The sensitivity is 79-100 \( ^\circ /\text{RIU} \), at red and NIR wavelengths [58, 59, 60, 61, 62, 63]. Instead of a prism, gratings can be used to achieve momentum matching with

---
\(^6\)The surrounding wall of each hole can be seen as a MIM arrangement
similar performance \[65, 66\]. Reference \[64\] demonstrates a red-light-excited grating-coupled metal film that provides a 10 nm resonant bandwidth and a $\sim 600$ nm/RIU sensitivity. A single MD may also be excited using a metal-coated glass slide \[67\], where total-internal-reflection offers SPP momentum matching. Using a broad-band source, consists of 500-600 nm wavelength light, the authors observe a 14 times change in detected intensity per RIU.

The IMI arrangement provides the largest field penetration depth into the analytes. Reference \[38\] uses optical fibers to couple into the long range modes. Reference \[68\] uses an Otto setup, implemented using a metal-coated dielectric waveguide core, to excite the long range modes. Their simulation result shows a 213 nm bandwidth and a 3700-5000 nm/RIU sensitivity, at a 700 nm excitation wavelength. Using $\delta \lambda = 0.01$ nm, the SR reported is $2.3 \times 10^{-6}$ RIU. Reference \[69\] reports a grating-coupled long range SPP sensor, operating at 1550 nm wavelength. For a low analyte index, $n = 1.3$, the sensitivity is 1000 nm/RIU, which corresponds to the sensitivity of a MD mode sensor (this value is validated by the experimental results shown in Chapter \[5\]). For a high analyte index, $n = 1.51$, the cladding and analyte form a symmetric plasmonic structure around the thin metal film, and therefore support a long range mode. This large mode size enhances the sensitivity to 60000 nm/RIU. However, the cladding-analyte index mismatch must be maintained below $\sim 0.6$ % to enable this high sensitivity. Reference \[73\] reports a metal coated dielectric waveguide having 183 nm/RIU sensitivity at 600 nm wavelength. This reduced sensitivity, compared to \[68, 69\], is due to the buffer layer, which reduces the mode size and reduces the field-analyte interaction area. To increase the field-analyte interaction
area, [72] deposits metal directly onto a waveguide core, such that the long range mode has a 10 fold increase in mode size and has an enhanced bulk sensitivity of $5.7 \times 10^4$ nm/RIU. Similar performance may be achieved using an optical fiber: references [70] and [71] demonstrate $10^4$ and $10^5$ nm/RIU sensitivity, respectively. Reference [74] shows that the stripe SPP waveguide can also be suspended and surrounded by the analyte fluid. The metal gratings are manufactured on a different layer, and the grating only interacts with the modal “tail”; therefore, the sensitivity is only 120 nm/RIU at 1550 nm wavelength.

The above examples are the existing SPP sensors that fall into the MIM, MD, and IMI arrangements and are tabulated in Table 2.3. There are of course interesting work such as [76] that explores more complicated systems. Lastly, a Fiber Bragg Grating (FBG) sensitivity of 172 nm/RIU [75] is listed as a comparison to the plasmonic sensors.

All prior sensor literatures show concerns for sensor design factors, such as the sensitivity, SR, SNR, testing standards, fabrication issues, and device dimension. In the following section, these design factors are discussed to set the criterions for the project to be carried out in this thesis.

1 Sensitivity

The bulk sensitivity is usually denoted as wavelength shift per change of refractive index unit, nm/RIU. For bulk sensing, a large evanescent field has the advantage of sampling a larger volume, and therefore, offers higher sensitivity. A large evanescent field can also be realized by increasing the operating wavelength, which inherently increases the SPP field penetration depth into the
analyte. A detailed derivation of the field penetration depth is shown in Chapter 3. A large field penetration depth may also be realized by using the IMI layout (recall [72, 77]). However when maintaining the cladding homogeneity poses as a challenge, the MD arrangement is the next best choice.

2 SR (figure of merit)

Recall the existing definition of 

$$SR = \frac{dn}{d\lambda} \times \delta\lambda,$$

where \(\delta\lambda\) is the resolution of optical spectrometer according to conventional definition. Due to the wide range of \(\delta\lambda\) used in the literatures, the SR becomes an unstandardized quantity. For example, while \(\delta\lambda = 0.1\) nm in [71], \(\delta\lambda = 0.01\) nm in [56, 78], and \(\delta\lambda = 0.001\) nm in [74]. Also, to further enhance the SR, [61] uses the pre-binding curve to subtract the post-binding curve, rather than considering the experiment noise. Here, to make the choice of SR more bounded, it may be bettered defined in the following way:

$$SR = \frac{dn}{d\lambda} \times \delta\lambda'.$$  \hspace{1cm} (2.3)

Here, \(\frac{dn}{d\lambda}\) is the same inverse of sensitivity and \(\delta\lambda'\) is the resolving power. The resolving power is the separation between the peak and its first minimum (Rayleigh’s Criterion) and has an unit in wavelength [nm]. Or, the same SR definition may be applied for SPR experiments, by simply replacing \(d\lambda\) and \(\delta\lambda'\) with \(d\theta\) and \(\delta\theta'\), which are defined as the angular resonant width and the angular resolving power, respectively. Also, the minimum SR is dictated by the noise in the system. For example, normal temperature drift in ambient environment is
about 0.01 °C, which corresponds to a variation of water index change of $\delta n = 10^{-6}$ RIU [61]. Thus, typical sensors could not have a minimum detectability smaller than $10^{-6}$ RIU. This minimum detectability is also mentioned in [79], which also proposes a slightly different approach to calculate the SR.

3 SNR

The SNR defined as the SPP signal power versus the noise power in the system. Interestingly, many literatures do not specify SNR. To improve the signal level in a SPP sensor, several methods may be implemented. For example, the SPP signal may be boosted by adding a lock-in amplifier [80]. Or, the sensor can use an IMI configuration, which offers a low loss SPP mode. The noise may be reduced by spatial averaging. A 2D image/spatial averaging technique is used in [60]. Comparing a 24 mm$^2$ beam generated $1.85 \times 10^{-5}$ RIU SR to a 6 mm$^2$ beam generated $2 \times 10^{-6}$ RIU in [61], the former shows higher SR. Also temporal averaging may be applied to reduce the noise power. The noise also comes from the analyte suspension fluid, due to fluctuating ambient temperature, which may not be corrected cheaply. Also, the mechanical connectors also generate noise and may be eliminated by replacing prisms with planar waveguides. However, most SNR boosting techniques have their cons. For instance, a lock-in amplifier demands a beam chopper and a synchronized analyzer, which make the sensor setup bulky and expensive. The IMI structure is difficult to realize in fabrication. And lastly, both area- and time-averaging causes the resonant peak to broaden, which reduces the $\delta \lambda'$ and $\delta \theta'$ and therefore reduces SR.
4 Testing standards

The papers reviewed in this chapter have varying testing standards. For example, various types of fluids are used. Reference [60] and [67] use water-ethanol solutions to characterize the sensor. [72] uses water-salt solutions; [61] uses water-sugar solutions; and, [62] uses water-glycerol solutions. It is important to point out that ethanol is a type of alcohol and has a fast evaporation rate; water also has a high evaporation rate. When these liquids evaporate, the solution index changes; therefore, none of these liquids should be used as a solution base to characterize an index sensor. A stable alternative is an oil based solution, such as the commercially available index matching oil. This oil is less likely to evaporate compared to water and alcohol. And, the material dispersion of index matching oil is well characterized over a wide range of the spectrum.

5 Fabrication issues

Most of the papers reviewed do not address fabrication issues. For instance, the poor metal adhesion on dielectrics has always been a concern [81, 82] and will dictate the reusability and longevity of the SPP sensor; therefore, an adhesion layer such as chromium is always deposited prior to gold or silver deposition. This chromium layer will change the SPP propagation and sometimes may “kill” the SPP. For example, when a chromium layer is added in the Kretschmann setup, the combined metal thickness may not allow the incident

\footnote{However, oil index change may be more susceptible to temperature variations.}
light to penetrate through. As a result, SPPs may not be excited. In the stripe SPP waveguide case, the chromium adhesion layer breaks the symmetry around the metal stripe, and therefore prohibits the long range mode propagation. A discussion on metal plating technique is included in Section 5.1.2.

6 Packaging size

The device size is mainly dictated by the SPP excitation scheme. The prism method is the more bulky excitation method; and the end-fire method (e.g. fiber and waveguide) is the more compact method. Reference [83] presented a device, including excitation source, detector, computer, and the sensor body, that has approximately $60 \text{ cm} \times 60 \text{ cm} \times 60 \text{ cm}$ in dimension. This dimension can be reduced by changing the excitation scheme, the light source, and the display technology. Additionally, recall the comparison in Table 1.2, the SPP planar surfaces requires 1 million times more analyte fluid, comparing to the IPP waveguide sensor; therefore, the larger packaging size could mean a much more invasive diagnostic technique.

2.4 IPP sensor evaluation standards

In summary, to the best of author’s knowledge, the stripe and the IPP waveguide sensors could be the over-all best technologies. Also, the standard parameters laid out in the prior art for a SPP sensor design include: 1. sensitivity, 2. SR, 3. SNR, 4. testing standards, 5. fabrication issues, and 6. packaging size. Following these conclusions and standards, the work done in this thesis will show a novel SPP sensor
design, providing arguably the most optimum design considering all six evaluation
criterions.
Chapter 3

Background and Theory

SPPs may be analyzed on a microscopic level (i.e. particles level) or on a macroscopic level (i.e. with Maxwell’s equations). Both representations are shown in [84]. In this thesis, the macroscopic approach is used to represent the material dispersion, which will then be used to derive the SPP confinement dispersions.

Here, all 3D SPP confinement problems are compacted into 2D, by first computing the confinement dispersion offered by the primary mechanism and then that offered by the secondary mechanism. This compacting method is similar to the effective index method traditionally applied in solving dielectric waveguides, and is first applied to construct the dispersion relationship of the stripe waveguide and the IPP waveguide in this thesis.

Lastly in this chapter, it will also be shown that the effective index technique can be applied to analyze SPP parallel waveguide array interactions as well as IPP Bragg grating resonances. Both of these phenomenons will be verified experimentally
in Chapter 4 and 5 respectively.

### 3.1 Materials dispersion

Recall that in Literature Review, Section 2.1.2 the dispersive nature of silver was measured using a three-beam method, then was modeled with the Drude-Lorentz model to extract the quantities of high-frequency permittivity, plasma frequency, and the electron collision time quantities [1]. This section focuses on the formation of the Drude-Lorentz model.

The Drude-Lorentz model uses an electron-on-a-spring formulation to model free-electron gas behavior. When the electron gas is excited by a harmonic electric field, \( \mathbf{E} = E_0 e^{-i\omega t} \hat{r} \), where the \( \omega \) is the oscillation frequency and \( \hat{r} \) is the directional vector, the individual electron moves as in a damped oscillator. This damped oscillation system consists of the following three forces:

1. the frictional force, \( F_f \), which adds loss and is defined by

\[
F_f = -\frac{m}{\tau} \frac{d\hat{r}}{dt},
\]

where \( m \) is the electron mass, \( dt \) is the time derivative, and \( \tau \) accounts for the electron collision;

2. the elastic/restoring force, \( F_H \), which is represented by Hook’s law,

\[
F_H = -m\omega_o^2 \hat{r},
\]
where $\omega_o$ is the oscillation frequency.

3. the Coulomb force, $F_{\text{Coulomb}}$, is the initial force to displace the electron,

$$F_{\text{Coulomb}} = -eE,$$  \hspace{1cm} (3.3)

where $-e$ is the charge of the electron.

The motion of the electron could be predicted after balancing the forces in this system:

$$F_{\text{total}} = m \frac{d^2 \hat{r}}{dt^2} = F_f + F_H + F_{\text{Coulomb}}$$  \hspace{1cm} (3.4)

In many literatures, the elastic force $F_H$ is omitted due to the common believe that the force used to restore the electron position is negligible \[85\]. After substituting Equation 3.1 and 3.3 into Equation 3.4 and neglecting Equation 3.2, and rearranging, the expression becomes:

$$\frac{d^2 \hat{r}}{dt^2} + \frac{1}{\tau} \frac{d \hat{r}}{dt} = -\frac{e}{m} E_o e^{-i\omega t}$$  \hspace{1cm} (3.5)

The solution to Equation 3.5 is:

$$r(t) = \frac{eE}{m(\omega^2 + i\omega/\tau)}$$  \hspace{1cm} (3.6)

This equation predicts the electron position when it is subject to an oscillating electric field. Equation 3.6 has a complex denominator, and therefore the electron motion is out of phase with respect to excitation.

In bulk material, assuming $N$ non-interacting dipoles per unit volume, the po-
larization $P = -Ne\mathbf{r} = \varepsilon_o(\varepsilon_r - 1)\mathbf{E}$, where $\varepsilon_o$ is the vacuum permittivity, the relative permittivity, $\varepsilon_r$, can be written using Equation 3.6 as:

$$\varepsilon_r = 1 - \frac{\omega_p^2}{\omega^2 + \frac{i}{\tau}}, \quad (3.7)$$

where $\omega_p = \sqrt{\frac{Ne^2}{m\varepsilon_o}}$ is the plasma frequency (recall from Section 2.2). Of course, $i\omega/\tau$ is the damping component, and, in a lossless system, can be removed from the $\varepsilon_r$ expression by setting $\tau = \infty$. This is the Drude-Lorentz model.

In a simple lossless system ($\tau = \infty$), the plasma frequency dictates the spectral boundary between the penetrating and the surface waves. For a plane wave, $\mathbf{E} = E_0 e^{i(k_y y - \omega t)}$, $k_y$ is the propagation constant in the $y$-direction, and is dependent on the material dispersion:

$$k_y = \sqrt{\varepsilon \mu \omega}, \quad (3.8)$$

where $\omega$ is the frequency and the permeability $\mu = \mu_o$ (in a non-magnetic material). Substituting Equation 3.7 into Equation 3.8

$$k_y = \frac{\omega}{c} \sqrt{1 - \frac{\omega_p^2}{\omega^2}}, \quad (3.9)$$

where $c$ is the speed of light in vacuum. It is seen from this equation, $k_y$ may be real or imaginary, depending on $\omega$. When $\omega > \omega_p$, $k_y$ is a real number; and, when $\omega < \omega_p$, $k_y$ becomes imaginary. An imaginary propagation constant indicates a non-propagating wave and results in evanescent decay.

For example, substituting the silver material parameters, published in [1], into
Equation 3.7 Figure 3.1 plots the silver material dispersion $\varepsilon_r$ as a function of wavelength. The plot shows the real part of $\varepsilon_r$ is negative, which indicates a reflective material. Now, by substituting only the real part of $\varepsilon_r$ into Equation 3.9, the non-propagating part of the wave can be treated as an isolated problem. Figure 3.2 plots the $1/e$ electromagnetic field penetration depth into the silver as a function of $\omega/\omega_p$. When $\omega < \omega_p$, the field penetration depth is only tens of nanometers: at 1550 nm wavelength, the penetration depth is $\sim 21.6$ nm; and at 630 nm wavelength, the penetration depth is $\sim 22.1$ nm. Knowing the penetration depth is critical in many applications – in this thesis, the plated metal thickness must exceed the penetration depth to support an IPP mode.

In summary, the plasma frequency determines the boundary between the penetrating and the surface waves (e.g. SPP) on metal surfaces. Now, we are ready to look at how SPP may be represented by wave equations in the $\omega < \omega_p$ regime.
3.2 SPP dispersion

As mentioned in the previous section, when the operating wavelength is longer than the plasma wavelength, or \( \omega < \omega_p \), the electromagnetic wave cannot penetrate into the bulk metal. At the surface, light may couple with the collective electron oscillations, which is called SPP. This section focuses on the wave representation of SPPs on such a metal surface. It will be shown that both negative permittivity and negative permeability materials can support surface waves.

3.2.1 Dispersion relationship for TM polarization

Figure 3.3 illustrates the coordinate definitions for the analysis. For a field propagating in the \( z \)-direction, at the interface between two materials, \( y = 0 \), the transverse magnetic (TM) polarization is defined as having its magnetic field, \( H \), being normal to the plane of incidence and its electric field, \( E \), being parallel to the plane of incidence.
The $H$ field propagating in the positive $z$-direction is expressed by two separate equations to represent decaying waves in the positive and the negative $y$-direction:

$$H_x = \begin{cases} H_0 e^{i(\beta_{SPP} z - \omega t) - k_1 y}, & y > 0 \\ H_0 e^{i(\beta_{SPP} z - \omega t) + k_2 y}, & y < 0 \end{cases}$$

(3.10)

where $H_0$ is the normalization factor and $\beta_{SPP}$ [rad/m] is the propagation constant in the $z$-direction. $k_1$ and $k_2$ [rad/m] are the transverse propagation constants in media 1 and 2, respectively, and are expressed as

$$k_j = \sqrt{\frac{\beta_{SPP}^2}{\varepsilon_j} - k_0^2},$$

(3.11)

where subscript $j = 1, 2$ represents media 1 and 2, and $\varepsilon_j$ is the relative permittivity of the media.

When $\omega < \omega_p$ and both $k_1$ and $k_2$ are positive, the evanescent wave decays in the $|y| > 0$ direction. The $E$ field in the $y$- and $z$-directions are then obtained by substituting Equation 3.10 into Equation 3.12.
Chapter 3. Background and Theory

\[ \nabla \times \vec{H} = i\omega \epsilon \vec{E}. \] (3.12)

\[
E_y = \begin{cases} 
- \frac{H_0}{\omega \varepsilon_1} e^{i(\beta_{SPP} z - \omega t) - k_1 y}, & y > 0 \\
- \frac{H_0}{\omega \varepsilon_2} e^{i(\beta_{SPP} z - \omega t) + k_2 y}, & y < 0 
\end{cases} \] (3.13)

\[
E_z = \begin{cases} 
\frac{H_0 k_1}{\omega \varepsilon_1} e^{i(\beta_{SPP} z - \omega t) - k_1 y}, & y > 0 \\
- \frac{H_0 k_2}{\omega \varepsilon_2} e^{i(\beta_{SPP} z - \omega t) + k_2 y}, & y < 0 
\end{cases} \] (3.14)

The boundary condition, \( y = 0 \), enforces the tangential component of the \( E \) field to be continuous. Thus, the condition \( E_z(y = 0^+) = E_z(y = 0^-) \) must be satisfied for Equation 3.14. Through a simple substitution, one can conclude that the following equality condition, Equation 3.15, must apply for the interface to support a surface wave:

\[ \frac{k_1}{\varepsilon_1} + \frac{k_2}{\varepsilon_2} = 0. \] (3.15)

By studying the above equation, one notices that the SPP wave is only supported at the interface of two materials with permittivities having opposite sign (i.e. one material has positive permittivity and the other has negative permittivity). To find the SPP dispersion relationship, one should substitute the corresponding \( k_j \) from Equation 3.11 into Equation 3.15 and obtain:

\[ \beta_{SPP} = \frac{\omega}{c} \sqrt{\frac{\varepsilon_1 \varepsilon_2}{\varepsilon_1 + \varepsilon_2}}. \] (3.16)

Equation 3.16 is the dispersion relationship of SPPs at a silver-air interface,
Chapter 3. Background and Theory

Figure 3.4: SPP dispersion at the interface of silver and air. Silver material dispersion is taken from [1].

which is the MD material arrangement (recall Section 2.2). Figure 3.4 plots the SPP dispersion at a silver-air interface with the silver material dispersion is taken from [1].

It is also interesting to explore the SPP penetration depth into the dielectric medium. Substituting the silver material dispersion into Equation 3.11 to find $k_y$ in air and silver, one finds a set of penetration depths, as shown in Figure 3.5, which plots the MD SPP penetration depth as a function of wavelength. This plot is shown to support the discussion on increasing sensor sensitivity as a function of increasing wavelength in Literature Review (Chapter 2).

It is important to realize that the SPP penetration depth is different from a plane wave penetration depth discussed at the end of Section 3.1 – a good analogy would be an optical fiber mode: the fiber material by itself is transparent in visible wavelength, and therefore has infinite penetration depth; however, the fiber mode has a finite evanescent tail in glass.
Figure 3.5: SPP penetration depth at the interface of silver and air as a function of wavelength. The dashed blue line represents the penetration depth in air and the solid black line represents the penetration depth in silver. Silver material dispersion is taken from [1].

For completeness, the Poynting vector is also derived here. The Poynting vector is defined as

\[ S = \frac{1}{2} \Re \{ \vec{E} \times \vec{H}^* \}. \]  

(3.17)

By substituting Equations 3.10, 3.13, and 3.14 into 3.17, one gets:

\[ S_y = \begin{cases} \frac{1}{2} \Re \left\{ \frac{\mu_0 k_1}{\omega \epsilon_0} e^{-2k_1 y} \right\}, & y > 0 \\ \frac{1}{2} \Re \left\{ -\frac{\mu_0 k_2}{\omega \epsilon_0} e^{2k_2 y} \right\}, & y < 0 \end{cases} \]  

(3.18)

\[ S_z = \begin{cases} \frac{1}{2} \Re \left\{ \frac{\mu_0^2 \beta_{SPP}}{\omega \epsilon_0} e^{-2k_1 y} \right\}, & y > 0 \\ \frac{1}{2} \Re \left\{ -\frac{\mu_0^2 \beta_{SPP}}{\omega \epsilon_0} e^{2k_2 y} \right\}, & y < 0 \end{cases} \]  

(3.19)
where $k_j^\Re$ is the real part of transverse-propagating vector.

By observing the y-component of the Poynting vector in Equation (3.18) $S_y = 0$ if the material is lossless, or $k_j^\Re$ is real. For the z-component, the Poynting vectors have the opposite sign if one of the materials is surface-active and the other material is inactive. The ratio of $S_{z1}$ and $S_{z2}$ at $y = 0$ is:

$$\frac{S_{z1}}{S_{z2}} = \frac{\varepsilon_2}{\varepsilon_1}.$$  \hfill (3.20)

### 3.2.2 Dispersion relationship for TE polarization

In the Transverse Electric (TE) polarization, the $E$ field is normal to the plane of incidence and the magnetic field is parallel to the plane of incidence. By using a similar mathematical analysis as for TM-polarized field in the previous section, one can obtain a similar expression as Equation (3.15).

$$\frac{k_1}{\mu_1} + \frac{k_2}{\mu_2} = 0,$$  \hfill (3.21)

where $\mu_j$ is the relative permeability of the material.

Studying this equation reveals the key to supporting a TE-polarized SPP, which is that one material must possess a positive permeability and the other a negative permeability. Typically, most materials are non-magnetic in the optical spectrum. One exception however is the Left Handed Materials (LHMs), which have been experimentally demonstrated to support TE-polarized SPPs in the microwave wavelength [86]. One of the main advantages of using a LHM is that both TM and TE polarized
Chapter 3. Background and Theory

fields can be used to support SPP. However, the magnetic material is not the focus of this project and the details will not be discussed here.

In summary, the SPP dispersion at a single metal-dielectric interface has been shown in this section. As seen here, the SPP dispersion depends on both material and structure composition. Of course, the SPP propagating at a single metal-dielectric interface would be different from the SPP propagating in a metal thin film or in a metal trench. In the coming two sections, Section 3.3 and 3.4 respectively, the dispersion of the stripe and IPP structures will be derived.

3.3 Stripe waveguide dispersion

The stripe waveguide is a finite-width metal stripe surrounded by a dielectric medium. The metal stripe usually is tens of nanometers in thickness such that the SPP guided on both top and bottom interfaces couple. Many publications have studied the stripe SPP waveguide dispersion, such as [38, 87, 88, 51, 89, 90].

In the first part of this section, a new method is presented to evaluate stripe waveguide dispersion, which is analogous to the Effective Index Method (EIM) used in the dielectric waveguide analysis. In the second part of this section, the change in mode index of the stripe waveguide as a function of material asymmetry is discussed. In the last part, metal stripe cross-section imperfections are shown to alter the mode index as well.
Figure 3.6: Illustration of air-silver-air (IMI) structure. In this figure, $\varepsilon_m$ is the metal permeability, which is sandwiched between the bottom and the top dielectric layers, which have permeability of $\varepsilon_s$ and $\varepsilon_c$, respectively. The metal layer has a thickness of $d$.

### 3.3.1 EIM calculation of stripe SPP waveguide dispersion

This section first shows the dispersion of SPP supported by an IMI material arrangement. And then, the EIM is applied to derive the finite-width stripe waveguide dispersion.

The derivation of the IMI dispersion is similar to the derivation of a MD dispersion. Figure 3.6 illustrates the coordinates and variables to be used in the following derivation.

The H fields in the three layers are defined as:

$$H_x = \begin{cases} 
H_o \left( \cos(k_m y) + \frac{k_s}{k_m} \frac{\varepsilon_m}{\varepsilon_s} \sin(k_m y) \right) e^{i \left( \beta_{IMI} z - \omega t \right)} & , \quad 0 < y < d \\
H_o \left( \cos(k_m d) + \frac{k_s}{k_m} \frac{\varepsilon_m}{\varepsilon_s} \sin(k_m d) \right) e^{i \left( \beta_{IMI} z - \omega t \right)} & , \quad y > d \\
H_o e^{k_s y} e^{i \left( \beta_{IMI} z - \omega t \right)} & , \quad y < 0
\end{cases}$$

(3.22)

where $k_s$ and $k_c$ are the y-momenta in the substrate and the cladding layers, and
$k_m$ is the y-wavevector in the metal layer. They are expressed as:

$$k_c = \sqrt{\beta_{IMI}^2 - \varepsilon_c k_0^2},$$

$$k_m = \sqrt{\varepsilon_m k_0^2 - \beta_{IMI}^2},$$

$$k_s = \sqrt{\beta_{IMI}^2 - \varepsilon_s k_0^2}. \quad (3.23)$$

A point worth mentioning is that the factor $\frac{k_s}{k_m} \frac{\varepsilon_m}{\varepsilon_s}$ is not arbitrarily selected. In an off-axis setup, where the y-center of the metal slab is not at $y = 0$, using a fair share of cosine and sine will not satisfy the boundary conditions.

Using Maxwell’s Equation gives,

$$\nabla \times \vec{E} = i\omega \mu \vec{H}, \quad (3.24)$$

$E_z$ may be found by substituting Equation 3.22 into Equation 3.24:

$$E_z = \begin{cases} 
\frac{H_0}{i\omega \varepsilon_c} \cos(k_m d) + \frac{k_s}{k_m} \frac{\varepsilon_m}{\varepsilon_s} \sin(k_m d) \left([-k_x e^{-k_c (y-d)} e^{i(\beta_{IMI} z - \omega t)}ight], & y > d \\
\frac{H_0}{i\omega \varepsilon_m} \left[ -k_m \sin(k_m y) + \frac{k_s}{k_m} \frac{\varepsilon_m}{\varepsilon_s} k_m \cos(k_m y) \right] e^{i(\beta_{IMI} z - \omega t)}, & 0 < y < d \\
\frac{H_0}{i\omega \varepsilon_s} k_s e^{k_s y} e^{i(\beta_{IMI} z - \omega t)} & y < 0
\end{cases} \quad (3.25)$$

At $y = d$ and $y = 0$, the boundary conditions must be satisfied,

$$\tan(k_m d) = \frac{k_m \left( \frac{\varepsilon_m}{\varepsilon_s} k_s + \frac{\varepsilon_m}{\varepsilon_s} k_c \right)}{k_m^2 - \frac{\varepsilon_m}{\varepsilon_s \varepsilon_c} k_s k_c}, \quad (3.26)$$

which is the SPP dispersion supported by an IMI material arrangement.

In a realistic example, at a 1550 nm wavelength, the silver has a material disper-
sion taken from [1] and the glass has relative permittivity \( \varepsilon_s = \varepsilon_c = 2.0736 \). Figure 3.7 plots the three-layer dispersion, \( \beta_{IM1} \), as a function of the metal layer thickness. In this plot, both symmetric and anti-symmetric modal dispersions are shown. The symmetric mode consists of fields, which point in the same direction in the cladding and substrate; and the anti-symmetric mode consists of fields which point in the opposite directions. According to [91, 92, 38], only the symmetric mode may be excited physically.

Both the symmetric and the anti-symmetric mode merge into a degenerate state, the asymptote. This asymptote corresponds to the MD effective index, \( \beta_{SPP} \) (derived in Equation 3.16) and has an intuitive explanation. When the metal layer becomes infinitely thick, the MD interface at \( y = d \) and the MD interface at \( y = 0 \) separate; and therefore, the SPPs on each interface decouple. As a consequence, the IMI behaves like two independent MD structures.

The above is the IMI material arrangement supported dispersion derivation. It is useful to compare the field expressions in Equation 3.22 with the ones shown in [93]. There is a discrepancy which is due to the different material coordinate definition, which requires different boundary conditions. One may realize, although applied a different material coordinate definition, the IMI dispersion relation shown in Equation 3.26 is the same as the one shown in [93].

To obtain the stripe waveguide dispersion, confinement in the x-direction must be considered. Figure 3.8 illustrates the coordinate and variable definitions to be used for the EIM derivation. The \( E \) field points in the y-direction, therefore, the TE slab equations need to be applied.
(b) Propagation distance ($\sim$ Imaginary)

Figure 3.7: Dispersion of air-silver-air (IMI) arrangement ($\beta_{IMI}$) as a function of metal thickness at 1550 nm. The solid line represents the symmetric mode, and the blue line represents the anti-symmetric mode.

The E fields in the three layers are defined as:

$$E_y = \begin{cases} 
E_o (\cos(k_2 x) + \frac{k_3}{k_2} \sin(k_2 x)) e^{i(k_1 x + b)} e^{i(\beta_{stripe} x - \omega t)}, & x < -b \\
E_o (\cos(k_2 x) - \frac{k_3}{k_2} \sin(k_2 x)) e^{i(\beta_{stripe} x - \omega t)}, & -b \leq x \leq 0 \\
E_o e^{-k_3 x} e^{i(\beta_{stripe} x - \omega t)}, & x > 0 
\end{cases} \quad (3.27)$$

where

$$k_1 = \sqrt{\beta_{stripe}^2 - \varepsilon_1 k_0^2},$$

$$k_2 = \sqrt{\varepsilon_2 k_0^2 - \beta_{stripe}^2},$$

$$k_3 = \sqrt{\beta_{stripe}^2 - \varepsilon_3 k_0^2}. \quad (3.28)$$

Substituting Equation 3.27 into Equation 3.24, $H_z$ is derived:
Figure 3.8: Illustration of EIM. In this figure, the three z-extending layers have permittivity $\varepsilon_1$, $\varepsilon_2$, and $\varepsilon_3$. In the finite-width stripe SPP waveguide, $\varepsilon_2 = \varepsilon_{IMI}$ and $\varepsilon_1 = \varepsilon_3 = \varepsilon_{\text{dielectric}}$. The stripe SPP waveguide has a width of b.

\[ H_z = \begin{cases} 
-\frac{E_o}{i\omega \mu} (\cos(k_2b) + \frac{k_3}{k_2} \sin(k_2b))k_1e^{k_1(x+b)}e^{i(\beta_{\text{stripe}}z-\omega t)}, & x < -b \\
-\frac{E_o}{i\omega \mu} (-k_2 \sin(k_2x) - k_2 \frac{k_3}{k_2} \cos(k_2x))e^{i(\beta_{\text{stripe}}z-\omega t)}, & -b \leq x \leq 0 \\
-\frac{E_o}{i\omega \mu} (-k_3)e^{-k_3x}e^{i(\beta_{\text{stripe}}z-\omega t)}, & x > 0 
\end{cases} \]  

(3.29)

Then, using the continuity of the tangential field at $x = 0$ and $x = -b$,

\[ \tan(k_2b) = \frac{k_1 + k_3}{k_2(1 - \frac{k_3k_3}{k_2})}. \]  

(3.30)

Applying the EIM to calculate the stripe SPP waveguide dispersion, one may set $k_2 = \beta_{IMI}$, and $k_3 = k_1 = \sqrt{\varepsilon_{\text{dielectric}}k_o}$, where $\varepsilon_{\text{dielectric}}$ is the dielectric medium surrounding the metal stripe, $k_o = 2\pi/\lambda$, and $\lambda$ is the operating wavelength. At a 1550 nm wavelength, the silver has a permittivity $\varepsilon_m = \varepsilon_{\text{silver}} = -129 + 3.1573i$ [1].

The dielectric SiO$_2$ has permittivity $\varepsilon_s = \varepsilon_{\text{dielectric}} = 2.0736$. Further discussion on the SiO$_2$ index is available in Section 4.1.1. Figure 3.9 plots the EIM-calculated mode dispersion as a function of the waveguide thickness; and Figure 3.10 plots the EIM-calculated mode dispersion as a function of the waveguide width. The EIM solutions
Figure 3.9: Mode index of $b = 4 \mu m$-wide stripe SPP waveguide as a function of metal thickness at 1550 nm wavelength. 3.9(a) shows the real part of the effective index; and 3.9(b) shows the imaginary part of the effective index. The black solid lines represent the solution calculated using EIM and the blue dashed lines represent the solutions calculated using the commercial MODE simulation software.

are compared to simulation results obtained from the commercial software MODE (by Lumerical Solutions Inc.); and they show reasonable agreement. It should be mentioned that the numerical transcendental equation solver (for solving Equation 3.30) requires $\sim 0.28 \%$ more core-cladding contrast to converge; and therefore, in the computation code, there is a $\sim 0.14 \%$ increase in core index and a $\sim 0.14 \%$ reduction in cladding index to achieve convergence. Further improvements of this code is required.

In summary, the EIM may be used to breakdown a 3D waveguide problem into two 2D problems. Of course, the EIM is not limited to simply the stripe waveguide dispersion derivation. In the following Section 3.4, the EIM is also used to derive the IPP waveguide dispersion.
Figure 3.10: Mode index of $d = 20$ nm-thick stripe SPP waveguide as a function of metal width, at 1550 nm wavelength. 3.10(a) plots the real part of the effective index; and, 3.10(b) plots the imaginary part of the effective index. The black solid lines represent the solution calculated using EIM and the blue dashed lines represent the solutions calculated using the commercial MODE simulation software.

The above shows the ideal strip waveguide dispersion; but, many factors are known to cause changes in the actual waveguide dispersion. For example, metal roughness is known to increase the waveguide loss [94, 95]. There are two additional geometrical factors that alter the stripe waveguide dispersion: an asymmetrical cladding material and a non-rectangular stripe cross-section. In the following two sections, the effects of both will be discussed.

### 3.3.2 Material asymmetry in SPP waveguides

Recall from the discussion on stripe waveguide sensor constraints in Section 2.3 that stripe waveguides require near-perfect material symmetry of the top and the bottom cladding. As mentioned in the “Literature Review” (Chapter 2), [69] showed a loss of
long range mode bulk sensitivity when the fluidic-substrate indices are mismatched by > 0.6 %. However, [69] does not show the change in mode distribution and mode index as a function of material mismatch. Another publication, [96], considered the effect of material asymmetry on the long range modes; however, it does not show the mode profile. Also, [96] demonstrated that a ∼ 4.82 % change in one of the cladding index would completely “kill” the long range mode. All these previous publications show inconsistent material asymmetry tolerance; therefore, it is important to simulate the effect of material asymmetry for this study.

Figure 3.11(a) shows the simulation layout. In the simulations, $n_c$ is the cladding index and is the sweeping variable, and $n_s = 1.44$ is a fixed substrate index. Both the cladding and substrate regions are semi-infinite. The stripe, having width $b = 4 \mu m$ and height $d = 55 \text{ nm}$, is made of silver, whose material dispersion is taken from [1]. The simulation wavelength is 1550 nm.

Figure 3.12(a) shows the real part of the effective index, as $n_c$ varies between 1.439 and 1.441. Figure 3.12(b) shows the associated imaginary part of the effective index. It is seen that the mode index increases as the $n_c$ index increases. This may be explained as an increase in the effective medium index. When $n_c = n_s$, the mode is a long range mode and the loss is at minimum. These plots reveal that a small 0.0694 % change in the $n_c$ index causes a $1.5 \times$ increase in waveguide loss.

Figure 3.11(b), 3.11(c), and 3.11(d) show the the magnitude of E field intensity when $n_c = 1.439$, 1.44, and 1.441 respectively. Observing the three modal profiles, Figure 3.11(c) shows the only long range mode, where the field extends into both cladding and substrate regions. A modal size is plotted in Figure 3.12(c) as $n_c$ sweeps
Figure 3.11: Mode profile of asymmetric-material stripe SPP waveguides. 3.11(a) illustrates the simulation setup. 3.11(b) is the mode profile (E field intensity) when $n_c = 1.439$. 3.11(c) is the mode profile (E field intensity) when $n_c = 1.44$. And, 3.11(d) is the mode profile (E field intensity) when $n_c = 1.441$. 

$\begin{align*}
  n_c &= 1.439 - 1.441 \\
  n_s &= 1.44
\end{align*}$
between 1.439 and 1.441. This plot shows the $E_y$ intensity FWHM sampled along the y-axis at $x = 0$. A small $\sim 0.0694 \%$ change in $n_c$ cause the stripe waveguide mode to “lean” towards either the top or the bottom cladding, and is a contribution to the loss of the sensor sensitivity in [69].

This small index miss-match in the the top and bottom cladding can be easily cultivated by various natural changes in the environmental factors. Recall the $\frac{\delta n}{\delta T}$ for water, discussed in “Literature Review” (Section 2). Reference [61] reported that a $\sim 0.01 \, ^\circ C$ temperature variation of water corresponds to change of $\delta n = 10^{-6}$ in index. Therefore, even a water temperature fluctuation in a sensor device will compromise the long range mode sensitivity.

### 3.3.3 Non-rectangular metal cross-section in stripe SPP waveguides

An imperfect metal stripe cross-section geometry results in a change in stripe waveguide dispersion. Most stripe waveguides are fabricated using lift-off (A detailed description of the lift-off technique is available in Appendix D). When the side-walls of the photoresist are not vertical, the stripe cross-section geometry deviates away from an ideal rectangle. As shown in Figure 3.13(a), two types of imperfections may occur. Firstly, a photoresist “under-cut” can cause the metal to detach from the photoresist side-walls – instead of having a designed ideal 4 $\mu m \times 55$ nm rectangle, the cross-section is a rounded-corner rectangular geometry. The morphology of this type of imperfection is verified using an Atomic Force Microscopy (AFM) and shown in Figure 3.13(b). Secondly, a positive tilt in the photoresist, as shown in Figure
Figure 3.12: Mode indices and sizes of material-asymmetric stripe SPP waveguide as $n_c$ sweeps between 1.439 and 1.441. 3.12(a) shows the real part of the effective index. 3.12(b) shows the imaginary part of the effective index. And, 3.12(c) shows the $E_y$ intensity FWHM sampled along the y-axis at $x = 0$. 
causes the deposited metal to adhere onto the slanted side-walls and form extruding imperfections, as shown in Figure 3.13(d). The extruding silver features in the samples typically have varying width between \(~300-1000\) nm, as well as varying heights between \(~20-50\) nm. Also note that the two “barriers” in Figure 3.13(d) are different in height; this is due to the specimen mount tilt in the metal evaporation chamber typically. The tilt angle, \(\theta\), as defined in Figure 3.13(c), is positive during deposition. It is also important to note that the AFM scan does not display the scale of the horizontal and vertical axis in proportion to each other - instead, the features of the “barriers” are exaggerated so that they are easily observable.

Because of the existence of these two types of geometric imperfections, a comparative study of the ideal and the non-ideal cross-section geometries is conducted to investigate their effect on the mode dispersion and polarization. To isolate the problem of cross-section geometry on the waveguide dispersion, all waveguides used in the study are surrounded by identical dielectric cladding materials and the metal surface is smooth.

To perform the study, Comsol (COMSOLAB) is used to calculate the mode indices of ideal and non-ideal silver stripe waveguides. Figure 3.14(a) shows three geometric models used to mimic the cross-section geometry imperfections. The models have cross-sections parallel to the Cartesian x-y plane and the propagation direction is in the z-direction. In the “ideal” stripe, the width is \(b = 4\ \mu m\) and the thickness is \(d = 55\) nm. To model round-cornered stripe, shown in Figure 3.13(b), a half-ellipsoid is used to approximate the shape of the round corner, which has semi-minor axis, \(d\), and semi-major axis \(b/2\). This geometric model is called the “body ellipsoid” (BE)
Figure 3.13: Illustration of cross-section imperfections in silver stripe waveguides. 

3.13(a) shows a desirable “under-cut” achieved in lift-off prior to metal deposition. The result of this lift-off is shown in 3.13(b) (AFM scan of the metal stripe surface morphology). 3.13(c) shows an opposite tilt in photoresist results in extruding features on the side walls. Geometric defects of the stripe morphology are shown in 3.13(d) (AFM scan of the metal stripe surface morphology).
model. To model the “barriers” in Figure 3.13(d), two additional geometries are used: an “edge ellipsoid” (EE) model having semi-major axis $M_a$ and semi-minor axis $M_i$ and, an ”edge rectangle” (ER) model having width $w$ and height $u$. Note that the main bodies of the waveguides have thickness $d$ and width $b$ in the EE and ER models.

The silver material dispersion has permittivity $\varepsilon_m = -129+3.16i$ at $\lambda = 1550$ nm and $\varepsilon_m = -18.3+0.498i$ at $\lambda = 633$ nm, respectively [1]. The cladding region is assumed to be an uniform, isotropic dielectric glass material having permittivity $\varepsilon_c = 2.0736$ and $\varepsilon_c = 2.1316$ at 1550 nm and 633 nm wavelength, respectively [28]. These values satisfy the boundary condition and allow continuity of the electric field tangential component at the silver-glass interface, so that a bound surface electromagnetic field can be supported. The mode profile of each waveguide geometry is also shown in Figure 3.14(b). The following are the findings.

**Effect of width and thickness of stripe geometry at 1550 nm (ideal case)**

It is known that the waveguide dispersion of a stripe waveguide is a function of the wavelength, width and thickness [38]. To begin the comparative study, the effective index of SPP propagation in a thin metal film is compared to that in a finite, 4 $\mu$m wide metal stripe. Increasing the vertical confinement of the geometry reduces the thickness of the stripe, and forces an increase in the momentum $k_y$ and thus a reduction of the effective index of the mode, as shown in Figure 3.15. In the plot, it is seen that the effective index increases as the metal becomes thicker. Also seen is an asymptote in the symmetric and the anti-symmetric modes indicating a so
Chapter 3. Background and Theory

(a) COMSOL setup

(b) COMSOL modes

Figure 3.14: Illustration of the cross-section geometric models used in simulations and the associated mode profiles. The ideal cross-section is a $4 \mu m \times 55$ nm rectangle having width $b$ and thickness $d$. The body ellipsoid, BE, is a geometry used to model the stripe shown in Figure 3.13(a) and has a semi-major axis $b/2$ and a semi-minor axis $d$. The edge ellipsoid, EE, and the edge rectangle, ER, are the two geometries used to model the extruding features on Figure 3.13(d). Both EE and ER are additional features on the same base waveguides having dimension $4 \mu m \times 55$ nm. The EE has semi-major axis $Ma$ and semi-minor axis $Mi$. The ER has width $w$ and height $u$. 


Figure 3.15: Fundamental bound mode effective indices as a function of stripe thickness at a 1550 nm wavelength. The dashed line is the waveguide dispersion of the odd bound mode and the solid line is the dispersion of the even bound mode. $\approx$ represents the effective indices of a 4 $\mu$m wide stripe waveguide, shown for comparison. 3.15(a) plots the real part of the effective index and 3.15(b) plots the propagation distance. Note that the propagation distance is defined as the $1/e^2$ decay length of the field.

called “degeneracy” [38], which is the effective index of the SPP propagation at a simple MD interface [97] (as discussed earlier in this chapter). It is also observed in Figure 3.15 the infinite-width waveguide has a larger effective index than the finite-width waveguide. Also, one may plot the effective index as a function of width. Figure 3.16 shows the mode solutions of the first three lowest order modes of an ideal rectangular 55 nm thick stripe. The curves show the effective index increases with the stripe width, for all modes, as expected and reported previously in Section 3.3.1 and in [92].
Figure 3.16: Effective index of a silver waveguide having thickness $d = 55$ nm as a function of stripe width at 1550 nm wavelength. Figures 3.16(a) and 3.16(b) plots the real part of the effective index and the propagation distance. -○- represents the ideal rectangle geometry, -×- represents the effective index of the fundamental mode of the BE geometry, and -■- represents the index of the EE geometry with $Mi = 55$ nm and $Ma = 250$ nm. Solid, dashed, and dot-dashed lines, represent fundamental, second, and third order bound modes, respectively. For a perfect waveguide, the asymptote of the real part approaches 1.449 and the propagation distance approaches 1 mm, and these asymptotes are indicated using red lines in 3.16(a) and 3.16(b) respectively. Note that the propagation distance defined as the $1/e^2$ decay length of the field.
Effective index as a function of the stripe width at 1550 nm (non-deal cases)

In this section, the effective indices of the modes guided in the ideal geometry are compared to those guided in the BE, and EE geometries. Figure 3.16 plots the effective indices of the first three lowest order bound symmetric modes for all three geometries as a functions of $b$, for $b$ having values between 2 \( \mu m \) and 20 \( \mu m \). A larger stripe width restricts the momentum in the lateral direction and thus the 2\(^{nd}\) and the 3\(^{rd}\) order modes have higher cut-off widths 6 \( \mu m \) and 20 \( \mu m \) respectively. A similar observation was reported in [98, 99]. A distinct increasing trend in the propagation constants (both the real and imaginary components), as the stripe width increases is also seen for all three geometries. Note that cut-off of the mode is caused by loss of the confinement as the mode index drops below that of the cladding index 1.44; therefore, all orders of modes will have their cut-off at $n_{eff} = 1.44$. Neither the mode solver nor the simulation condition used for this study showed the exact mode cut-off condition. This issue requires further investigation.

The BE geometry has a reduction in both vertical and lateral dimension compared to the ideal rectangular cross-section geometry; therefore, based on the analysis discussed in the previous section, one would anticipate a reduction in the effective indices. This observation agrees with the mode solution result shown in Figure 3.16.

Comparing the propagation distance of the three geometries, in the BE geometry, at 5 \( \mu m \) width, the distance is 1.4 times longer compared to that in the rectangular shape and 1.5 times longer compared to that in the EE geometry. Therefore, there exists a correlation between large cross-section area and high loss. It is also seen,
in Figure 3.16, that the propagation distance approaches an asymptotical value of 1 mm, the propagation distance of an infinitely wide 55-nm-thick silver thin film, found using the analytical expression calculated at 1550 nm wavelength. Additionally, the asymptote of the BE propagation distance is larger than that of the other two geometries, which is due to the smaller metal cross-section.

The effect of cross-sectional area on the effective indices of the modes is revealed in Figure 3.17. In this figure, it can be observed that the propagation distance is inversely proportional to the area. While the real parts of the effective indices of all three geometries nearly overlap, the non-overlapping nature of the three loss curves indicates the loss depends on the shapes of the cross-section. Nevertheless, one can conclude that, during fabrication, the “under-cut” in photoresist, which form the BE cross-section geometry, is beneficial not only for aesthetic purposes but also for reducing the loss of the stripe waveguides.

**Effective index as a function of $M_i$ and $u$ at 1550 nm (non-ideal case)**

Next the effective indices of the modes propagating in the EE and ER geometries are compared. The effective indices of the fundamental symmetric bound mode are plotted in Figure 3.18 as a function of the $M_i$ dimension in the EE geometry, or the $u$ dimension in the ER geometry. The main stripe body has $d = 55$ nm and $b = 4 \, \mu\text{m}$. In the figure, the effective indices are calculated for values of $w$ ranging between 500 nm and 1100 nm, and for different $Ma$ values between 150 nm and 650 nm only. The fundamental mode is present because the waveguide is $4 \, \mu\text{m}$ wide, which is below the cut-off width for the higher order modes, as discussed in the previous section.
Figure 3.17: Effective indices as a function of the cross-section area at 1550 nm wavelength. 3.17(a) plots the real part of the effective index and 3.17(b) plots the propagation distance. -○- represents the ideal rectangle geometry, -×- represents the effective index of the fundamental mode of the BE geometry, and -■- represents the EE geometry with \( M_i = 55 \) nm and \( M_a = 250 \) nm. Note that the propagation distance defined as the \( 1/e^2 \) decay length of the field.
Figure 3.18: Effective indices as a function of \( Mi \) and \( u \) at 1550 nm wavelength. Black \( \circ \)- represents the indices of the EE geometry and red \( \blacksquare \)- represents that of the ER. For the EE, \( Ma = 150, 250, 350, 450, 550, \) and \( 650 \) nm are respectively represented by pink, purple, black, dark blue, light blue, and gray. For the ER geometry, the \( w = 500, 700, 900, \) and \( 1100 \) nm, and are represented by light pink, purple, black, and dark blue, respectively. 3.18(a) plots the real part of the effective index and 3.18(b) plots the propagation distance. Note that the propagation distance is defined as the \( 1/e^2 \) decay length of the field.

At \( Mi = 0 \), the extruding region does not exist for either geometric models, thus, the effective index degenerates to that of an ideal, \( 4 \mu m \times 55 \) nm stripe geometry, as discussed in the previous section.

From the results presented in Figure 3.18 it is clear that even a small deviation in the shape at the edge of the metallic stripe can have a significant effect on the loss dispersion of the SPP mode. Also, the trends of these curves agree with the hypothesis built in the previous parts that an increase in either extruding region dimension raises the propagation constant, and consequently reduces the propagation distance.
**Effective index as a function of $R$ at 1550 nm (non-ideal cases)**

To further compare the modal propagation in the EE and ER geometries, the dependency of the effective index as a function of the geometric areas is explored. A new variable $R$ is defined as the percentage increase in the ideal stripe cross-section, which therefore approximately represents the increase in the mode being guided in the metal. For the EE geometry, $R_{EE} = M_M \times M_i \times \pi / A$, and for the ER geometry, $R_{ER} = w \times u / A$, where $A = 4 \ \mu m \times 55 nm = 0.22 \ pm^2$.

Figure 3.19 plots the effective indices as a function of $R$. It is seen that the real parts of the effective indices increase from 1.4445 to 1.446 as $R$ increases from 0% to 55%. At the same time, the propagation distance reduces from 1.25 mm to 0.7 mm, which is nearly a 50% reduction. Also in the figure, the slopes of both data sets are similar; thus, one may conclude that the ER geometry is a good alternative to the EE geometry, and they both give approximately the same losses in metal-stripe SPP waveguides.

To quantify the propagation loss due to geometrical imperfection, linear fitting is applied to all four curves. For the ER data, \( \Re\{n_{eff}\} = 2.973 \times 10^{-3} R + 1.4446 \). Also \( \Im\{n_{eff}\} = 1.2052 \times 10^{-4} R + 9.8631 \times 10^{-5} \). For the EE data, \( \Re\{n_{eff}\} = 2.6824 \times 10^{-3} R + 1.4445 \), and \( \Im\{n_{eff}\} = 1.306 \times 10^{-4} R + 9.7463 \times 10^{-5} \). \( \Re \) and \( \Im \) indicate the real and the imaginary components of the subsequent variable, respectively.

Next the ER geometry data is extrapolated, in Figure 3.19(b), to locate the effective index at $R = 1$, for the case where $w = 2 \ \mu m$ and $u = 55 \ nm$. The imaginary part of this extrapolated effective index gives a value for the propagation distance of 562.8 $\mu m$ for this case. Taking the confidence bound into consideration, this
propagation distance varies between 591.0 \mu \text{m} and 534.7 \mu \text{m}. These fitted values are reasonably close to 541.6 \mu \text{m}, which is the propagation distance for SPPs bound by a 4 \mu \text{m} \times 110 \text{ nm} ideal metal stripe waveguide, as shown earlier in Figure 3.15(b). The real part of the extrapolated effective index is found to be $\sim 1.448$, which is equivalent to the effective index of the same 4 \mu \text{m} \times 110 \text{ nm} ideal waveguide. This simple calculation demonstrates the validity of the simulation models.

This relationship may also be used to predict the effective index of the waveguide having the cross-section geometry shown in Figure 3.13(d). By substituting in the average area of the two extruding side-walls $1.350 \times 10^{-14} \text{m}^2$, one obtains a 1.1 mm propagation distance for this geometry.

The above extrapolation and comparison with simulated data build confidence to use the linear functions can be used to estimate the waveguide dispersion based on the “extra” area added to the ideal stripe geometry. However, this approximation shall be used cautiously, because, as discussed previously and shown in Figure 3.17, the effective index is not solely dependent on the area but also the geometric shape of the cross-section.

**Effective index as a function of R at 633 nm**

To address the significance of the above linear fitting functions and to examine their applicability to predict effective indices at other wavelengths, the same studies are performed at $\lambda = 633$ nm. Figure 3.20 shows the effective indices as a function of $M_i$ at 633 nm. Three different values of $Ma$, 300 nm, 400 nm, and 500 nm, are used. Observing Figure 3.20, a trend similar to that at 1550 nm is seen: an increase in the
Chapter 3. Background and Theory

68

(a) $\Re\{n_{\text{eff}}\}$

(b) $\Im\{n_{\text{eff}}\}$

Figure 3.19: Effective indices as a function of $R$ at 1550 nm wavelength. 3.19(a) plots the real part of the effective index and 3.19(b) plots the propagation distance. Open $\circ$ represents the indices of the EE geometry and solid $\blacksquare$ - represents that of the ER geometry. Note that the propagation distance is defined as the $1/e^2$ decay length of the field.

effective indices is proportional to the increase in the Mi and Ma dimensions.

The effective indices at 633 nm as a function of $R$ is plotted in Figure 3.21. Fitting them to linear functions, applying the same method used in the previous section, one obtains $\Re\{n_{\text{eff}}\} = 3.5245 \times 10^{-2} R + 1.5212$, and $\Im\{n_{\text{eff}}\} = 1.084 \times 10^{-3} R + 5.0886 \times 10^{-4}$. Also at $R = 1$, $n_{\text{eff}} = 1.556 + 1.6 \times 10^{-3} i$. Comparing this number to the simulated value, $n_{\text{eff}} = 1.549 + 9.522 \times 10^{-4} i$, the propagation distance is under estimated, deviating 40% from the simulated value. The large deviation at 633 nm compared to a small deviation at 1550 nm leads one to argue that the linear approximation of the relationship between the effective index and $R$ is valid only if the mode size is large compared to the stripe cross-sectional area. The size of the mode formed in the stripe waveguide at 633 nm is much smaller than that at 1550 nm, hence, for 633 nm, the relationship between
the effective index and $R$ is of higher order. 633-nm-wavelength applications are not of interest in this thesis, thus it will not be explored further here.

Thus, comparing the results obtained at 633 nm to those at 1550 nm, the effect of the extruding features on the effective indices are distinctly different – the effective index trends are steeper, and are non-linear functions of $R$. Comparing the propagation distance at the two wavelengths also indicates that the mode is less lossy at higher wavelength, which is consistent with previous reports [98]. Note however that the curving fitting performed in this study is based on a general trend in the data, and the fitting parameters are not representative of physical constants.
Polarization dependency on geometry at 1550 nm

Lastly, the polarization dependency of the ideal rectangle, BE, EE, and ER geometries are studied. The fields in all of the geometries were solved to identify the TE polarization component in the guided mode. In the ideal, BE, and EE geometries, the amount of power polarized in the TE direction is calculated to be 0%. Note that for a finite-width SPP thin film waveguide, all six components of the electromagnetic field should be present [38], and a zero percentage only indicates that the TE polarized power is negligible, and therefore, it must be treated cautiously. However, the TE component is significant for the modes guided in the ER geometry. Table 3.1 summarizes the percentage of the power polarized in the TE direction as a function of the $u$ and $w$ dimensions. Observing the data in Table 3.1, a large $u$ value increases the percentage of the TE power. One may speculate that the ER geometry
Table 3.1: Percentile of bound fundamental mode in TE polarization.

<table>
<thead>
<tr>
<th>$u$ [nm]</th>
<th>$w$ [nm]</th>
<th>300</th>
<th>700</th>
<th>1100</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0 %</td>
<td>0 %</td>
<td>1 %</td>
<td></td>
</tr>
<tr>
<td>60</td>
<td>2 %</td>
<td>3 %</td>
<td>3 %</td>
<td></td>
</tr>
</tbody>
</table>

alters the polarization composition more drastically because the sharp corners that support “corner modes” and result in a larger proportion of the power polarized in TE direction. Therefore, despite the previous sections that concluded EE and ER geometries result in similar modal effective indices, the polarization state is altered depending on the chosen geometric model.

In summary, the effect of different stripe-waveguide cross-section geometries on the waveguide dispersion has been explored in this section. Compared to an ideal rectangular cross-section geometry, the BE geometry significantly reduces the loss, by $\sim 40\%$, and the EE and ER geometries increase loss and result in a $\sim 7\%$ reduction in the propagation distance. It is also found that, for the same cross-sectional areas, the BE geometry supports longer propagation distances and thus is a more advantageous structure to support long-range propagation of SPPs. In this case, mode symmetry certainly becomes a concern and shall be studied in the future. Despite the geometric dependence, there is a strong correlation between cross-sectional area and the loss of the stripe waveguide, specifically that increasing the cross-sectional area results in higher loss. Additionally, both the EE and ER geometries are valid geometries to approximate the effective indices of the imperfect waveguides; however, the ER structure alters the polarization state of the bound modes. These findings illustrate
the geometry dependence of SPP waveguide dispersion and polarization.

Based on the analysis performed in this section, the simple IMI stripe waveguide is not the most desirable structure to be used in a SPP waveguide sensor. In contrast, the IPP waveguide offers a simpler-to-implement solution and will be discussed in the coming section.

3.4 IPP waveguide dispersion

The IPP was first introduced in the “Literature Review” (Chapter 2) as a new type of SPP waveguide which has advantageous for sensing in a LOC device. The IPP waveguide has a channel shaped cross-section and enhances the sensitivity by channeling the analyte and the SPPs all in one structure. This section explores the dispersions of both vertical and non-vertical side-walled IPP waveguides.

3.4.1 Vertical wall IPP waveguide dispersion

The EIM was used previously in this chapter to solve stripe SPP waveguide dispersions, having IMI-supported primary guiding mechanism and width-limit supported secondary guiding mechanism. The same EIM concept is used here to derive the dispersion of the vertical-wall IPP waveguide, which has MD primary and metal-wall supported secondary confinement mechanisms.

A schematic of the metallic rectangular IPP channel structure is shown in Figure 3.22(a). The primary mechanism is supported by a MD arrangement and is illustrated in Figure 3.22(b). Here the SPP is confined in the y-axis, and has an E-field
pointing in the y-z plane. This SPP then has a z-direction propagation constant \( \beta_{SPP} \), as defined in Equation 3.16. The secondary confinement mechanism is due to the metal walls (Figure 3.22(c)) – the two reflective walls placed orthogonally to the x-axis creates a cavity, in which standing waves can be supported. The standing waves have estimated x-axis momenta of \( k_x = m_{IPP} \pi/b \), where \( m_{IPP} \) is the mode order and \( b \) is the width of the cavity. To obtain more accurate solutions, each mode, propagating in the z-direction, can be solved by enforcing continuity of the field and its derivative at the boundaries. It is important to realize that the E-field is modeled to be mainly polarized in the y-axis; therefore, the derived dispersion relationship looks exactly the same as the dispersion derived for the stripe waveguide (Equation 3.30). To obtain the correct IPP waveguide dispersion, using Equation 3.30, one must set \( k_{z,2} = \beta_{SPP} \) and \( k_{z,1} = k_{z,3} = \sqrt{\varepsilon_m} k_o \).

The silver relative permittivity \( \varepsilon_m \) has \( \varepsilon_{\infty} = 2 \), \( \omega_p = 0.39 \times 10^{16} \text{ [rad/s]} \), \( \tau = 3.41 \times 10^{-14} \text{ [s]} \), which are the values that best fit the experimental data published in [1]. Air has \( \varepsilon_d = 1 \).

Figure 3.23 shows the \( \omega-\beta_{IPP} \) relationship of the first three lowest order modes guided in a 1.5-\( \mu \)m wide IPP waveguide calculated with the EIM, along with the light line\footnote{Light line is the \( \omega-k \) relationship of the bulk propagating light. For example, light propagating in glass, assuming flat dispersion \( n_{glass} \), has light line \( k_{glass} = n_{glass} \times \omega/c \). Simple dielectric-metal interface supported SPP must have dispersion located to the high of the light line (higher momentum) to be bound at the surface. In dielectric waveguide, the mode is confined when its dispersion falls in between the light lines of the core and the cladding. And, similar concept is called the “light cone” in photonic crystals.}. At high frequencies, the 1.5-\( \mu \)m wide IPP waveguide dispersion curves follow closely to the dispersion of the free-propagating SPPs at a MD interface, and
Figure 3.22: Schematics of the EIM approach to solve vertical-wall IPP waveguide dispersion. 3.22(a) shows a schematic of the physical waveguide structure. The curved red line represents the SPP evanescent decay and the dashed arrow indicates the SPP resonance in the cavity. 3.22(b) shows an illustration of SPP guiding interfaces. This SPP can be confined by two reflective surfaces constructed on both sides shown in 3.22(c).
Figure 3.23: Rectangular waveguide dispersion curves in vacuum. The blue solid line is the light line. The black solid curves (EIM) are the real part of the dispersions of the first three lowest order modes of the 1.5 $\mu$m wide IPP waveguide, where the fundamental mode has the largest propagation constant. The red solid curves (EIM) are the imaginary part of the dispersions of the three modes. In the inset, (a) shows the fundamental mode profile at 3 $\mu$m wavelength, (b) shows the second order mode at a 1.5 $\mu$m wavelength, and (c) shows the third order mode at a 1 $\mu$m wavelength. The curves representing the fundamental, second, and third order modes are marked 1, 2, and 3, respectively.

are located on the right side of the light line. At low frequencies, the IPP waveguide momentum falls to the left side of the light line. Each mode has a cut-off frequency defined by $\beta_{IPP} = 0$. A similar dispersion plot has been shown in [100]. It is important to note that, due to the guiding mechanism of this channel waveguide structure, the cut-off condition is different from what has been established for CPP [35] and stripe waveguides [38].

An important notion of the derived vertical wall IPP waveguide is that the
\[ \tan(k_2 b) = \frac{k_1 + k_3}{k_2 (1 - \frac{1}{k_1 k_3^2})} \] (Equation 3.30) is the dispersion of IPP having infinitely high side-walls, which can never be the case in experimental demonstrations. To verify the validity of the EIM model, MODE (by Lumerical Solutions Inc.) is used to solve the modal properties of finite-height channels, where \( h = 6 \, \mu m \) (as defined in Figure 3.22(a)). The simulation region is surrounded by metal boundary conditions.

The simulated waveguide mode profiles of the first three lowest order modes near their cut-off wavelength is shown in the insets of Figure 3.23 to demonstrate the mode confinement on the left side of the light line. Inset (a) shows the fundamental mode profile at a 3 \( \mu m \) wavelength, (b) shows the second order mode at a 1.5 \( \mu m \) wavelength, and (c) shows the third order mode at a 1 \( \mu m \) wavelength. The three wavelengths picked are the cut-off wavelengths of the modes. And clear mode confinement is revealed by the simulation as well as the EIM method solutions. It is worth mentioning that the field penetration depth in the positive y direction reduces as the wavelength increases, which corresponds to a reduction in the SPP field penetration depth of a MD interface shown in Figure 3.5 in Section 3.2.

The waveguide width dictates the highest allowable order of mode which can be guided. Figure 3.24 plots the mode propagation constant as a function of waveguide width. This figure reveals that the first three lowest order modes can be easily observed experimentally in a 1 mm long waveguide. Both Figure 3.24(a) and Figure 3.24(b) also reveal that the modes share an asymptote, shown by the horizontal lines, with a value of \( \beta_{SPP}/k_0 \), the effective index of a free-propagating SPP at a simple MD interface. This asymptote is also seen in the IMI SPP dispersion plot in Figure 3.7. The values of the asymptotes further validate the correctness of the
Chapter 3. Background and Theory

EIM approach to solving this structure. The EIM results also match well with the MODE-solved results of both 10-µm-deep and 6-µm-deep channels. The similarity between the solutions from the 6-µm-deep and 10-µm-deep channels is expected due to the high confinement of the field at the bottom of the channel; it can therefore be concluded that the two channel depths used in this study have a small effect on the modal dispersion. Note that the propagation distance is defined as the $1/e^2$ decay distance of the field.

3.4.2 Trapezoidal waveguide dispersion

The trapezoidal waveguide is a modified version of the vertical-wall IPP waveguide. A plot of both waveguide structure cross-sections is shown in the Figure 3.24 inset. The trapezoidal waveguide was also simulated using MODE; and the MODE simulation result of the trapezoidal cross-sectioned waveguide is inserted into the effective-index plots of Figure 3.24. Again, the metal boundary condition is used in the simulation. The trapezoids have a height $h = 6 \mu\text{m}$ and wall-angle $\theta = 18^\circ$. The x-axis “waveguide width” represents the bottom width $b$ of the trapezoids. The trapezoid waveguide dispersion curves show an overall trend agreement with those of the rectangular shaped waveguide, and there is an anticipated slight increase in effective index due to the widened $a$ dimension in the geometry.

The main contributions of the trapezoid waveguide shape are an extended mode cut-off width and increased loss. As shown in Figure 3.24, the fundamental mode becomes unbound at $b < 5.08 \mu\text{m}$, the second order mode becomes unbound at $b < 14.08 \mu\text{m}$, and the third order mode becomes unbound at $b < 25.96 \mu\text{m}$ in the trapezoid
waveguide at a wavelength of 1550 nm. The single mode conditions for the rect-
angular waveguides and the trapezoid waveguides are different: The rectangular
waveguide has a second-order-mode cut-off width of approximately one wavelength;
and the trapezoid waveguide has a larger second-order-mode cut-off width of sev-
eral wavelengths. The second effect of the trapezoidal shape is the increased loss,
as shown in Figure 3.24(b). The quantitative relationship between the loss and tilt
angle is under study, and will be shown in a future study. Despite the fact that
the trapezoid shape contributes to the mode loss, the propagation distance of the
plasmon in the trapezoid waveguide is $>1$ mm.

In summary, the design of a large, 5.08-14.08 $\mu$m single-mode silver plasmonic
waveguide at 1550 nm wavelength has been shown here. This waveguide size is com-
parable to the microfluidic channel dimensions, and therefore may be easily adapted
by the LOCs. The experimental demonstration of an IPP waveguide will be shown
in Section 5.2.

This concludes the theoretical descriptions of SPPs. A macroscopic wave equation
approach has been used to represent SPPs propagation in MD, IMI, stripe, and IPP
structures. The wave representation has been validated up by MODE simulations.
In the following sections, this concept will be taken further – the wave equations will
be used to analyze parallel waveguide arrays and SPP grating designs.
Figure 3.24: The waveguide effective indices of the fundamental, second order, and the third order modes as a function of the waveguide width. The EIM solutions are shown with blue solid curves. The MODE solutions of the 10-μm-deep rectangular waveguide is shown with red dots, the 6-μm-deep rectangular waveguide in black crosses, and the trapezoid structure having $h = 6 \text{μm}$ and $\theta = 18^\circ$ in black dash lines with dots. The trapezoid index is smoothed and the actual data is bound within two percent the curve shown. For the trapezoids, the x-axis plots the $b$ width. The curves representing fundamental, second, and third order modes are marked 1, 2, and 3, respectively.
3.5 Discrete diffraction in parallel waveguide arrays theory

The single stripe waveguide guiding mechanism and dispersion were discussed in Section 3.3. In a directional coupler, two waveguides are placed side-by-side in close proximity and a coupled mode is formed, allowing power to transfer back and forth between the two waveguides. This power transfer occurs because in the waveguide a portion of the field overlaps the adjacent waveguide. The same phenomenon may be observed in weakly coupled SPP stripe waveguide couplers. Two core directional couplers based on SPPs have been reported in [101]. In this work, it was initially proposed to pursue directional coupler as an integrated optical components in a LOC, but because of the difficulties in obtaining perfect material symmetry, and the difficulties with cross-section geometry in a stripe waveguide, discussed as discussed in Section 3.3, it has been determined that stripe waveguide may not be practical to be implemented in LOC devices. However, it is still interesting to explore the phase interactions of SPPs, and hence, this section studies the mode coupling in stripe waveguide arrays.

In this section, the coupled mode theory for two waveguides will be developed further to describe waveguide arrays. Then parallel waveguide arrays facilitating discrete diffraction and the EIM used to calculate SPP discrete diffraction in parallel waveguide arrays will be introduced. Finally, simulation results will be shown. The experimental results of SPP discrete diffraction in parallel waveguide arrays is shown in Section 4.3.
Arrays of coupled waveguides provide a system for the study of discrete interactions on an accessible length scale. Figure 3.25 shows a schematic of a waveguide array. Waveguide arrays in various materials systems have been used to observe Bloch oscillations [102, 103], dynamic localization [104, 105], and discrete diffraction [106]. The latter of these is the focus of this study. Discrete diffraction occurs as a result of wave coupling between the waveguides in the array and can thus be engineered by controlling the physical properties of the array and the incident field. For example, the amount of discrete diffraction in a parallel waveguide array can be controlled through linear detuning of nearest-neighbor coupling. In this way, discrete diffraction can be almost eliminated – a “diffraction compensated” system can be made, where instead of having a diverging beam, the wave is confined in only a few waveguides. Also, discrete diffraction has been studied extensively in conventional dielectric waveguide arrays; this study however considers the problem of discrete diffraction and diffraction control in a much newer waveguide array system, SPP stripe waveguide arrays.

Theoretical studies of SPP discrete diffraction in metal gap arrays has been recently performed in [107], and altering the phase angle and the focusing of the excitation source in SPP waveguide arrays has been analyzed in [108]. However, both of these works reported simulations performed in lossy MIM structures which would be complex to demonstrate experimentally. Here, a method to control diffraction of a discrete SPP is demonstrated in a realistic structure that is relatively simple to fabricate. In stripe SPP waveguides, the guided SPPs have an evanescent tail that falls deep into the dielectric material, resulting in a mode size and effective index similar
Figure 3.25: Illustration of a waveguide array structure and the excitation scheme. The silver stripe waveguides are $b = 5 \, \mu\text{m}$ in width and $d = 20 \, \text{nm}$ in thickness. The waveguide center-to-center separation is $d_{\text{array}} = 10 \, \mu\text{m}$. The sample is 1 mm in length. The surrounding material is SiO$_2$.

to the modes guided in a dielectric waveguide. Hence, glass-cladding-surrounded and metal-stripe-guided symmetrical SPP modes can be excited and observed using a readily available end-fire coupling setup [87].

Recent studies have demonstrated SPP diffraction and interference [109, 99], thus revealing the electromagnetic wave properties of SPPs. Diffraction of SPPs, as with diffraction of electromagnetic waves, results in beam expansion in the paraxial region, in a manner which is inversely proportional to the propagation constant, and therefore, cannot be corrected for in the linear regime. Discrete diffraction however, unlike diffraction, is a beam expansion phenomenon observed in artificial periodic waveguide arrays. As mentioned, beam expansion is caused by the neighboring waveguide coupling, which results in a discrete diffraction intensity pattern in the arrays. When only the nearest neighbor coupling is considered, discrete diffraction can be compensated by tilting the angle of the input beam by a phase angle of $\pi/2$.
3.5.1 Waveguide array theory and modeling

For theoretical analysis and simulations, this work applies conventional dielectric waveguide analysis is applied to the SPP waveguides. In an array of identical parallel waveguide arrays that are weakly coupled, the evanescent field in the \( n^{th} \) waveguide experiences nearest neighbor coupling, and is expressed as [93],

\[
\frac{dA_n}{dz} = i\beta_{\text{stripe}} A_n + iC(A_{n-1} + A_{n+1}),
\]  

(3.31)

where \( A \) is the TM field, \( C \) is the coupling coefficient for two identical parallel waveguides, \( \beta_{\text{stripe}} \) is the propagation constant of a stripe waveguide, and \( i = \sqrt{-1} \). When only the \( 0^{th} \) waveguide is excited, \( A_n(z = 0) = 1 \) for \( n = 0 \), and \( A_n(z = 0) = 0 \) for \( n \neq 0 \), as the field propagates along the direction \( z \) the \( n = 0 \) waveguide transfers energy to the adjacent waveguides, and the field in the \( n^{th} \) waveguide can be expressed as

\[
A_n(z) = (i)^n \exp(i\beta_{\text{stripe}} z) J_n(2Cz),
\]  

(3.32)

where \( J_n \) is the Bessel function of order \( n \). The discrete diffraction coefficient \( D_d \) of such a system is defined as [106]

\[
D_d = -2Cd^2 \cos(k_x d_{\text{array}}),
\]  

(3.33)

where \( k_x \) is the propagation constant in the x-direction, \( d_{\text{array}} \) is the center-to-center separation between adjacent waveguides, and \( |k_x d_{\text{array}}| \leq \pi \) defines the first
Figure 3.26: Illustration of the material indices used in EIM calculation of stripe SPP waveguide arrays.

Brillion zone. When the excitation beam is incident on the sample at an oblique angle however, the change in phase angle, $k_x d_{array}$, causes the neighboring waveguides to detune, which can change the sign of $D_d$ and result in anomalous diffraction.

Modeling of the SPP propagation in a waveguide array was performed by adopting the EIM derived in Section 3.3. By applying the EIM, the propagation in a 3D waveguide array can be reduced to a 2D dielectric waveguide problem. Similar to the EIM used to calculate the stripe waveguide dispersion in Section 3.3.1, the thin-film SPP dispersion is first calculated and the $n_{IMI}$ obtained for the $y$-axis. Then, the periodic waveguide array is formed along the $x$-axis, and $n_{IMI}$ is used as the index of the periodic waveguide cores and the $\sqrt{\epsilon_c}$ is used as the index of the cladding. Figure 3.26 is an illustration of stripe SPP waveguide arrays treated as a 2D problem. Propagation in this 2D waveguide array structure was then simulated using the commercial software BeamPROP (by RSoft Design Group, Inc.), using the index values obtained above. In the simulation, the structure was excited using the calculated fundamental mode of a single stripe SPP waveguide.

In this study, the excitation wavelength $\lambda$ is 1550 nm and the stripe thickness is $d = 20$ nm, which provides a long range plasmon mode, as first calculated in
Section 3.3.1. Using the value of silver dispersion at 1550 nm, $\varepsilon_{Ag} = -129 + 3.16i$ [1], and glass cladding dielectric permittivity $\varepsilon_c = \varepsilon_s = 2.07$ [28], one obtains $n_{IMI} = 1.442 + 8.704 \times 10^{-6}i$, which was first calculated in this thesis in Section 3.3.1.

A top view of the calculated intensity profile is shown in Figure 3.27(a). This figure plots the intensity pattern calculated using Equation 3.32 normalized to the intensity of the input, so that $|A(z = 0)|^2 = 1$. The power calculated using the beam propagation method, normalized to the input power, is shown in Figure 3.27(b). The close agreement between the two results confirms that BeamPROP is a fast and less computationally demanding simulation technique, compared to, for example Finite-Difference Time-Domain (FDTD) methods, for examining SPP propagation.

To validate the EIM method, the coupling coefficient of two parallel stripe waveguides generated using BeamProp is compared to the values generated using MODE solutions (by Lumerical Solutions, Inc.). Figure 3.28 plots the coupling coefficient of two parallel silver waveguides for varying stripe thicknesses and widths. To verify the accuracy of the EIM-assisted simulations, the coupling coefficient is calculated using the mode interference method, using the software MODE solutions. Figure 3.28 shows that the two methods agree to within $\sim 6\%$ for thin stripes, however the discrepancies increase to $\sim 20\%$ as the thickness increases. It also reveals that the discrepancies between the two calculation methods are larger for narrower stripes. For example, the discrepancies for the 4-µm-wide stripe are larger than those for the 6-µm-wide stripe. The variations in the discrepancies are the result of the EIM. This method assumes that the y-direction confinement is provided by an infinitely wide thin film, therefore a wider waveguide is closer to the approximation condition.
Figure 3.27: Calculated and simulated $|H_x|^2$ of parallel waveguide arrays. (a) plots the field distribution predicted using Equation 3.32. (b) shows the field distribution predicted using the commercial BeamProp software.
Figure 3.28: Calculated coupling coefficients as a function of silver stripe thickness. Dashed lines (- -) represent values calculated using the mode interference method, and dotted (⋯) lines represent values calculated using the beam propagation method. Circles (○), triangles (▽), and squares (□) represent the coupling coefficients calculated for parallel silver stripes, each having width \( d = 4, 5, \) and 6 \( \mu m \) and center-to-center separation of \( d_{array} = 8, 10, \) and 12 \( \mu m \), respectively.

and leads to a smaller discrepancy between the two calculation methods. Based on observations, the EIM is effective for stripe cross-sections that have a large aspect ratio. For example, for the \( 5 \mu m \times 20 \) nm sample, which has an aspect ratio of 250, it is seen in Figure 3.28 that the two simulation methods show a \(~ 5 \%\) error.

### 3.5.2 Discrete diffraction compensation

Discrete diffraction compensation can be achieved by making \( D_d = 0 \), which corresponds to \( |k_x d_{array}| = \pi/2 \) as mentioned. In a thin metal film, which has a SPP propagation constant \( \beta_{lMT} \), the physical incident angle can be expressed as:

\[
\theta = \sin^{-1}\left(\frac{\pi}{2\beta_{lMT}d_{array}}\right),
\]

(3.34)
Figure 3.29: Intensity pattern detected at output of the waveguide array. The height of the bars indicate the relative power in each waveguide. It shows the spatial distribution of the output intensity pattern for $\theta = 0, 0.9, 1.5, 2.2,$ and $2.9$ degrees. Vertical bars show the simulated results, and solid curves show the experimental result. All plots are normalized for visual clarity.

where $\beta_{IMI} = n_{IMI}k_o$ is the thin metal film SPP dispersion, derived in Section 3.3, and $k_o = 2\pi/\lambda$. Thus $\theta$ is a function of both wavelength and film thickness.

Figure 3.29 plots the EIM-simulated sample output when the incident angles are tuned to 0, 0.9, 1.5, 2.2, and 2.9 degrees. The figure shows the relative peak power of each waveguide and clearly shows a shift in power amongst the waveguides as the excitation angle is rotated away from normal; the initially symmetrical and “diffractive” pattern becomes more asymmetrical and “confined” as the angle is increased. At 2.2 degrees, the intensity in the higher order waveguides is suppressed, compared to the excitation at 0.9, 1.5 and 2.9 degrees. Therefore, it may be determined that 2.2 degrees is the diffraction compensation excitation condition corresponding to $|k_o d_{array}| = \pi/2$. 
It is important to mention that the parallel waveguide mode coupling is not calculated for the IPP structure, because the nearest-neighbor separation in metal side-wall is difficult to realize in practice (A discussion on field penetration depth is available in Section 3.1).

In summary, the wave properties and the guiding of SPPs in stripe waveguide arrays were predicted by conventional electromagnetic wave analysis. Using a modified dielectric waveguide EIM approach, simulation of SPP propagation was carried out using the simple 2D beam propagation technique, and verified with coupled mode theory. It may be concluded that, with appropriate knowledge and adaptation, beam propagation software can be used to simulate SPP propagation in weakly coupled thin-stripe arrays. The experimental results associated with this theoretical study is shown in Section 4.3.

### 3.6 Bragg IPP waveguide theory

In this section, the EIM is applied to model a Bragg stack in a IPP waveguide. If a waveguide is made to have a periodic index modulation along the propagation direction, the mode propagating down the waveguide may experience a resonance effect. Such phenomenon may be observed in Bragg grating embedded dielectric waveguides. For example, Bragg gratings is taught in many fundamental courses and documented in textbooks such as Chapter 12 of Yariv and Yeh [93]; and also, reference [110] proposing a photochemical way to modify optical fiber cladding to achieve this periodic modulation. Only until recently, Bragg gratings have started
Figure 3.30: Illustration of the Bragg-grating embedded IPP waveguide. $n_d$ is the material index of either the air or the oil filler. $n_{PMMA}$ is the material index of PMMA ribs used to modulate the IPP waveguide. $n_{IPP}$ is the mode index of the silver IPP waveguide, either with or without modulation.

to be embedded into plasmonic waveguides. As already mentioned in the Literature Review (Chapter 2), CPP Bragg gratings [35] and stripe waveguide Bragg gratings [51, 52, 53, 54] have been demonstrated in both theory and experiments.

In this section, it will be shown that adding dielectric modulation to the IPP waveguide may also create Bragg resonance – Figure 3.30 shows a schematic of a dielectric-grating-embedded IPP waveguide. The modulated dielectric layer is achieved with ribs of PMMA deposited periodic spacing. When a mode propagating along the waveguide (in the z-direction), the mode index of each PMMA-modulated section is different from the native section; therefore, the Bragg resonance calculation may be mathematically treated as alternating layers of two different mode indices. This will be demonstrated in detail below.

The organization of this section is as follows. First, the layered medium Bragg resonance is calculated using a 2D matrix method [93]. Then, it will be shown how this 2D method may be applied to model the 3D Bragg IPP waveguide problem.
Figure 3.31: Illustration of a periodic medium. \(a_n\) and \(c_n\) are the magnitudes of the negative-z-traveling waves in the \(n\)th layer; and, the \(b_n\) and \(d_n\) are the magnitudes of the positive-z-traveling waves in the \(n\)th layer. \(n_{st,1}\) and \(n_{st,2}\) have thickness \(d_{st,1}\) and \(d_{st,2}\) respectively.

### 3.6.1 Matrix method to calculate periodic stacks

The TE Bloch wave matrix method derived in [93] can be used to derive the Bragg resonance in a layered 2D media, and will serve the purposes of this thesis for two reasons: firstly, it will become more apparent later that the orientation of the x and y-axis would not make a difference in an effective medium method (the x and y-notations will be switched for clarity); and secondly, the main E field polarization of the IPP mode is in the y-direction, as derived in Section 3.4 and therefore, satisfies the TE boundary conditions.

A schematic of the periodic medium and the coordinate definitions are shown in Figure 3.31. The refractive index profile may be written as:

\[
    n_{st} = \begin{cases} 
        n_{st,1}, & n\Lambda - d_{st,1} < z < n\Lambda \\
        n_{st,2}, & (n - 1)\Lambda < z < n\Lambda - d_{st,1}
    \end{cases}
\]  \quad (3.35)
It is clearly observed in Equation 3.35 that \( n_{st}(z) = n_{st}(z + \Lambda) \), where \( \Lambda = d_{st,1} + d_{st,2} \) is the period of the layered media. Each one of these layers has thickness \( d_{st,1} \) or \( d_{st,2} \).

The E field polarized in the y-direction has the following form:

\[
E_{st,y} = \begin{cases} 
(a_n e^{-ik_{st,1}z(z-n\Lambda)} + b_n e^{+ik_{st,1}z(z-n\Lambda)}) e^{i(k_{st,xx}x-\omega t)}, & n\Lambda - d_{st,1} < z < n\Lambda \\
(c_n e^{-ik_{st,2}z(z-n\Lambda+d_{st,1})} + d_n e^{+ik_{st,2}z(z-n\Lambda+d_{st,1})}) e^{i(k_{st,xx}x-\omega t)}, & (n-1)\Lambda < z < n\Lambda - d_{st,1} 
\end{cases}
\]

(3.36)

where \( a_n \) and \( c_n \) are the magnitudes of the negative-z-traveling waves in the \( n^{th} \) layer; and, the \( b_n \) and \( d_n \) are the magnitudes of the positive-z-traveling waves in the \( n^{th} \) layer. And, the \( k_{st,1} \) and \( k_{st,2} \) are the propagation constants and are defined as follows:

\[
k_{st,1} = \sqrt{n_{st,1}^2k_0^2 - k_{st,x}^2},
\]

\[
k_{st,2} = \sqrt{n_{st,2}^2k_0^2 - k_{st,x}^2}.
\]

(3.37)

The magnitude \( E_y \) at the material boundaries, i.e. at \( z = (n-1)\Lambda \) and at \( z = n\Lambda - d_{st,1} \), must be continuous because of the constitutive relations. And therefore, the magnitudes of the \( E_y \) fields have the following relationships at these two boundaries:

\[
a_{n-1} + b_{n-1} = c_n e^{ik_{st,2}d_{st,2}} + d_n e^{-ik_{st,2}d_{st,2}}
\]

(3.38)

For the same reason, the \( H_x \) (\( \propto dE_x/dz \)) magnitude at the material boundaries, i.e. at \( z = (n-1)\Lambda \) and at \( z = n\Lambda - d_{st,1} \), must also be continuous. Therefore, the continuity of the \( H_x \) fields may bring the following relationships:
\[ i k_{st,1z}(a_{n-1} - b_{n-1}) = i k_{st,2z}(c_n e^{ik_{st,2z}d_{st,2}} - d_n e^{-ik_{st,2z}d_{st,2}}) \]
\[ i k_{st,1z}(a_n e^{ik_{st,1z}d_{st,1}} - b_n e^{-ik_{st,1z}d_{st,1}}) = i k_{st,2z}(c_n - d_n) \]

(3.39)

For simplicity, Equation 3.38 and 3.39 are organized into matrices:

\[
\begin{pmatrix}
1 & 1 \\
-i k_{st,1z} & -i k_{st,1z}
\end{pmatrix}
\begin{pmatrix}
a_{n-1} \\
b_{n-1}
\end{pmatrix}
=
\begin{pmatrix}
e^{i k_{st,2z}d_{st,2}} & e^{-i k_{st,2z}d_{st,2}} \\
e^{-i k_{st,2z}d_{st,2}} & -i k_{st,2z}e^{-i k_{st,2z}d_{st,2}}
\end{pmatrix}
\begin{pmatrix}
c_n \\
d_n
\end{pmatrix},
\]

(3.40)

\[
\begin{pmatrix}
1 & 1 \\
-i k_{st,2z} & -i k_{st,2z}
\end{pmatrix}
\begin{pmatrix}
c_n \\
d_n
\end{pmatrix}
=
\begin{pmatrix}
e^{i k_{st,1z}d_{st,1}} & e^{-i k_{st,1z}d_{st,1}} \\
e^{-i k_{st,1z}d_{st,1}} & i k_{st,1z}e^{-i k_{st,1z}d_{st,1}}
\end{pmatrix}
\begin{pmatrix}
a_n \\
b_n
\end{pmatrix}.
\]

(3.41)

From the above two matrices, one may realize the \(c_n\) and \(d_n\) may be eliminated, and \(a_{n-1}\) and \(b_{n-1}\) may be expressed as a function of \(a_n\) and \(b_n\):

\[
\begin{pmatrix}
a_{n-1} \\
b_{n-1}
\end{pmatrix}
=
\begin{pmatrix}
A & B \\
C & D
\end{pmatrix}
\begin{pmatrix}
a_n \\
b_n
\end{pmatrix},
\]

(3.42)

where \(A\ B\ C\ D\) are the matrix elements:

\[
A = e^{i k_{st,1z}d_{st,1}}[\cos k_{st,2z}d_{st,2} + \frac{i}{2}(\frac{k_{st,2z}}{k_{st,1z}} + \frac{k_{st,1z}}{k_{st,2z}})\sin k_{st,2z}d_{st,2}],
\]
\[
B = e^{-i k_{st,1z}d_{st,1}}[\frac{i}{2}(\frac{k_{st,2z}}{k_{st,1z}} - \frac{k_{st,1z}}{k_{st,2z}})\sin k_{st,2z}d_{st,2}],
\]
\[
C = e^{i k_{st,1z}d_{st,1}}[-\frac{i}{2}(\frac{k_{st,2z}}{k_{st,1z}} - \frac{k_{st,1z}}{k_{st,2z}})\sin k_{st,2z}d_{st,2}],
\]
\[
D = e^{-i k_{st,1z}d_{st,1}}[\cos k_{st,2z}d_{st,2} - \frac{i}{2}(\frac{k_{st,2z}}{k_{st,1z}} + \frac{k_{st,1z}}{k_{st,2z}})\sin k_{st,2z}d_{st,2}].
\]

(3.43)
These are the matrix elements for one unit layer in a stacked medium, which consists of one \( n_{st,1} \) section and one \( n_{st,2} \) section. Each section, respectively, has a length of \( d_{st,1} \) and \( d_{st,2} \). Reference [93] refers to this expression as a “unit-cell translation matrix”. When there are \( n \) layers in the periodic medium, ultimately, a \( n \)-layered matrix may have the following expression:

\[
\begin{pmatrix}
a_0 \\
b_0
\end{pmatrix} = \begin{pmatrix} A & B \\ C & D \end{pmatrix}^n \begin{pmatrix} a_n \\
b_n \end{pmatrix}.
\]

(3.44)

In this expression, \( n \) is the layer number, and \( a_0 \) and \( b_0 \) are the magnitudes of the left and right traveling waves at the “input-facet”, and may be used to define the reflection coefficient:

\[
r_n = \frac{a_n}{b_0}.
\]

(3.45)

Also note that the \( a_n \), the left traveling wave from the “output-facet”, is usually zero in an experimental setup; therefore, the expression of the reflection coefficient is merely dependent on the matrix elements \((1,2)\) and \((2,2)\) in \( \begin{pmatrix} A & B \\ C & D \end{pmatrix}^n \). One may notice the definition of the reflection coefficient is the multiplicative inverse of the one derived in [93]. This is due to the phase assignment of the complex numbers for the left and right traveling wave. In [93], \( a_n \) is the positive-\( z \)-propagating wave magnitude and \( b_n \) is the negative-\( z \)-propagating wave magnitude; and, here in Equation 3.36, the definition of the phase is opposite in sign; this results in a different reflection coefficient expression. That being said, the Bragg resonance expression is the same
Chapter 3. Background and Theory

3.6.2 2D modeling of a 3D Bragg IPP waveguide theory

The previous section is the derivation of the reflection coefficient and reflectance for a 2D two-material layered system. Now, in a 3D IPP waveguide (recall Figure 3.30), whose bottom surface is dielectric modulated, e.g. with PMMA, the coated and uncoated sections may be considered to have two different mode indices, $n_{st,1}$ and $n_{st,2}$, and each section has a different length $d_{st,1}$ and $d_{st,2}$ in the $z$ propagation direction, respectively, as shown Figure 3.30. As a result, the PMMA-modulated IPP waveguide will exhibit a resonance effect, which may be approximated using the 2D method derived in the previous section.

To model a realistic example, the silver IPP waveguide structure in Figure 3.30 will be considered with width $b = 8 \mu m$, top width $a = 12 \mu m$, and a height $h = 6 \mu m$. At a 1550 nm wavelength, the metal relative permittivity $\varepsilon_m$ has $\varepsilon_\infty = 2$, $\omega_p = 1.39 \times 10^{16}$ [rad/s], and $\tau = 3.41 \times 10^{-14}$ [s], which are the values that best fit the experimental data obtained in [1]. The PMMA ribs has thickness (in the $y$-direction) of 60 nm, and have an index of $n_{PMMA} = 1.4807$ at 1550 nm (measured with an ellipsometer). The PMMA ribs are 100 nm in length (in the $z$-direction). The PMMA ribs form dielectric-modulations that enable the Bragg resonance in an IPP waveguide. Furthermore, the Bragg resonance will shift according to the index of the filling material (e.g. air or oil). If the channel is filled with air, $n_d$ takes on the value of unity; if the channel is filled with oil, $n_d = 1.3346, 1.3442, 1.3538$, and $1.3634$ at 1550 nm.
Figure 3.32: Variable and coordinate definition of the periodic stack structure shown in Figure 3.30. In the top illustration, it shows the dielectric (PMMA) modulated silver surface. This is a plot of the y-z plan sliced along the dashed window in Figure 3.30. The corresponding effective medium index for each layer is shown in the bottom illustration. The IPP waveguide mode indices of the native and PMMA-modulated layers are $n_{st,1}$ and $n_{st,2}$ respectively. Each layer has thickness $d_{st,1}$ or $d_{st,2}$. $a_n$ and $c_n$ are the magnitudes of the negative-z-traveling waves, in the $n^{th}$ layer; the $b_n$ and $d_n$ are the magnitudes of the positive-z-traveling waves, in the $n^{th}$ layer. The E field polarization, as indicated is in the y-direction, as indicated. The layer number is represented by an integer $n$. 
Figure 3.33: MODE-simulated mode profiles of a native IPP waveguide and a 200-nm-thick PMMA-modulated IPP waveguide. The metal is silver and the background index is one. The simulation wavelength is 1550 nm.

To calculate the resonance effect, first, the mode indices \( n_{IPP} \), of PMMA-modulated and native cross-sections, are calculated using the MODE software package (Lumerical Solutions, Inc.). The results are tabulated in Table 3.2. Figure 3.33 shows the simulated mode profile of native and PMMA-modulated IPP waveguides. Note the PMMA thickness used to generate this mode profile is 200 nm, to enlarge the field distribution formed due to the non-homogeneous material compositions. This is a typical field distribution of a hybrid mode. Then, the mode indices and appropriate lengths for each layer are used in the 2D matrix to calculate the reflectance spectrum.

Using an air filled waveguide having \( \Lambda_{Bragg} = 765 \text{ nm} \) as an example, one may set the length of the first air-silver section having \( k_{st,1z}/k_o = n_{IPP,1} = 1.0002 + 9.7743 \times 10^{-5}i \), to be \( d_{st,1} = 665 \text{ nm} \), and the length of the second air-PMMA-silver layer, having \( k_{st,2z}/k_o = n_{IPP,2} = 1.0214 + 2.7765 \times 10^{-4}i \), to be \( d_{st,2} = 100 \text{ nm} \). The total length of this unit cell is \( \Lambda = 765 \text{ nm} \), which is then repeated \( n = 200 \) times. The calculated
Table 3.2: Mode indices \( (n_{IPP}) \) of IPP waveguides having various dielectric modulations and filled with different index oils.

<table>
<thead>
<tr>
<th>( n_d )</th>
<th>without PMMA</th>
<th>with PMMA</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.0002 + 9.7743×10(^{-5})i</td>
<td>1.0214 + 2.7765×10(^{-4})i</td>
</tr>
<tr>
<td>1.3346</td>
<td>1.3405 + 2.7467×10(^{-4})i</td>
<td>1.3527 + 4.9182×10(^{-4})i</td>
</tr>
<tr>
<td>1.3442</td>
<td>1.3503 + 2.6988×10(^{-4})i</td>
<td>1.3615 + 3.9148×10(^{-4})i</td>
</tr>
<tr>
<td>1.3538</td>
<td>1.3601 + 2.6377×10(^{-4})i</td>
<td>1.3707 + 3.8061×10(^{-4})i</td>
</tr>
<tr>
<td>1.3634</td>
<td>1.3700 + 2.6137×10(^{-4})i</td>
<td>1.3798 + 3.7208×10(^{-4})i</td>
</tr>
</tbody>
</table>

reflectance is plotted with a red dotted line in Figure 3.34. Note that \( k_o = 2\pi/\lambda \), where \( \lambda \) is the operating wavelength of 1550 nm.

For an oil filled waveguide, having \( n_d = 1.3346 \) and \( \Lambda_{Bragg} = 567 \) nm, one may set the length of the first air-silver layer, having \( k_{st,1z}/k_o = n_{IPP,1} = 1.3405 + 2.7467 \times 10^{-4}i \), to be \( d_{st,1} = 367 \) nm, and the length of the second air-PMMA-silver layer, having \( k_{st,2z}/k_o = n_{IPP,2} = 1.3527 + 4.9182 \times 10^{-4}i \), to be \( d_{st,2} = 100 \) nm. The total length of this unit cell is \( \Lambda = 567 \) nm, which is repeated \( n = 200 \) times. The calculated reflectance is plotted with a red dotted line in Figure 3.35. Lastly, Figure 3.36 plots another oil-filled Bragg IPP waveguide having a 570 nm Bragg period for comparison. All spectra are normalized to unity peak power.

Figure 3.34, 3.35, and 3.36 show that the Bragg resonance red-shifts proportionally as a function of the increasing Bragg period, \( \Lambda_{Bragg} \), as well as a function of the increasing indices, \( n_{st,1} \) and \( n_{st,2} \). An experimental demonstration of this will be shown in Section 5.4 and 5.5. Both Figure 3.35 and 3.36 show a 1100 nm/RIU sensitivity.

Before concluding, it is important to determine the single mode condition for experimental observation of the Bragg resonance, due to the need for sensor sig-
Chapter 3. Background and Theory

Figure 3.34: The reflection spectra of air-filled Bragg waveguides, having periodicities of: $\Lambda_{\text{Bragg}} = 765$ nm, 770 nm, and 775 nm.

Figure 3.35: The reflection spectra of oil-filled Bragg-grating-embedded IPP waveguides, having fixed $\Lambda_{\text{Bragg}} = 567$ nm. The index matching oils have indices $n_d = 1.3442$, 1.3538, and 1.3634, at 1550 nm wavelength.
Chapter 3. Background and Theory

Figure 3.36: The reflection spectra of oil-filled Bragg-grating-embedded IPP waveguides, having fixed $\Lambda_{\text{Bragg}} = 570$ nm. The index matching oils have indices $n_d = 1.3346$, 1.3442, and 1.3538, at 1550 nm wavelength.

Figure 3.36: The reflection spectra of oil-filled Bragg-grating-embedded IPP waveguides, having fixed $\Lambda_{\text{Bragg}} = 570$ nm. The index matching oils have indices $n_d = 1.3346$, 1.3442, and 1.3538, at 1550 nm wavelength.

Figure 3.36: The reflection spectra of oil-filled Bragg-grating-embedded IPP waveguides, having fixed $\Lambda_{\text{Bragg}} = 570$ nm. The index matching oils have indices $n_d = 1.3346$, 1.3442, and 1.3538, at 1550 nm wavelength.

Figure 3.37 plots the fundamental and second order mode indices of the native trapezoidal waveguide, versus waveguide width and background index. Figure 3.38 plots the fundamental and second order mode indices, of a realistic 60-nm PMMA-modulated trapezoidal waveguide design, having width $b = 8 \, \mu m$, top width $a = 12 \, \mu m$, and height $h = 6 \, \mu m$, versus waveguide width and the background index.

The single mode condition is determined when the fundamental mode exist and the second order mode is cut-off. Figure 3.38 shows that the grating-embedded trapezoidal waveguide having the above dimension is single moded, when the channel is filled with either air or oil having $n_d < 1.37$.

In the following Chapters 4 and 5, parallel waveguide array and Bragg IPP waveg-
Figure 3.37: IPP mode effective index \(n_{IPP}\) as a function of both waveguide width and background index \(n_d\), at 1550 nm wavelength. The waveguide has \(\theta = 18^\circ\) and \(h = 6 \, \mu m\).
Figure 3.38: 60-nm PMMA-modulated IPP waveguide mode effective index \( n_{IPP} \) as a function of both waveguide width and background index \( n_d \), at a 1550 nm wavelength. The waveguide has \( \theta = 18^\circ \) and \( h = 6 \, \mu m \).
uides will be fabricated and characterized to reveal SPP phase interaction and to demonstrate sensing.
Chapter 4

SPP Stripe Waveguide Array

Fabrication and Experiments

As discussed in Chapter 2, the stripe waveguide is the lowest loss type of SPP waveguide. However, also recall the theoretical study on stripe waveguide modes in Section 3.3 found that the material symmetry and the metal stripe cross-section shape play an important role in determining the performance of a sensor based on this design. Therefore, it was determined that the stripe waveguide may not be the simplest option for implementing a SPP waveguide sensor. However nearest-neighbor coupling in the SPP stripe waveguide architecture is of interest for studying SPP discrete diffraction in a waveguide array, and, hence a theoretical analysis of SPP discrete diffraction and its compensation in stripe SPP waveguide arrays were performed in Section 3.5.

This chapter will show the experimental demonstrations of nearest-neighbor cou-
pling and discrete diffraction compensation in SPP stripe waveguide arrays. The organization of this chapter is as follows: first, the fabrication of the stripe waveguide array is outlined, then the optical characterization setup is described. Finally the experimental observations of the nearest-neighbor coupling and discrete diffraction compensation in the stripe SPP parallel waveguide array sample are shown.

4.1 Fabrication of stripe waveguide arrays

Figure 3.25 shows a schematic of a SPP waveguide array. To make such a sample, Plasma Enhanced Chemical Vapor Deposition (PECVD) is used to deposit the dielectric cladding regions and a metal lift-off is used to make the metal stripes. In this section, a systematic procedure is described which can be used to determine the best PECVD deposition condition. Then, the entire stripe SPP waveguide fabrication protocol is described and illustrated.

4.1.1 PECVD of $SiO_2$

PECVD deposits dielectric layers at low temperatures [111] (i.e. $< 400^\circ C$). The deposition system supplies silane ($SiH_4$) and nitrous oxide ($N_2O$), which interact in the deposition chamber to form silicon oxide. The chemical reaction is [112]:

$$3SiH_4 + 6N_2O \rightarrow 3SiO_2 + 4NH_3 + 4N_2. \quad (4.1)$$

Though the chemistry is pre-determined, the quality (i.e. the deposition rate, the surface roughness, and the purity) of the deposited oxide layer varies with tempera-
To study the oxide layer quality, (100) p-type silicon was used as a deposition substrate. Twelve substrate samples were deposited at 250, 300, 350, and 400 °C (three samples for each temperature setting). The PECVD machine used was an Oxford Plasmalab System 100 model. The machine RF power was set to 30 Watts and the chamber pressure was set to 1000 mTorr. The chamber was then supplied with 170 Standard Cubic Centimeters per Minute (sccm) silane (5% in nitrogen) and 710 sccm $N_2O$ flow - a high nitrous-to-silane gas ratio. According to reference [113], a high nitrous-to-silane ratio results in lower oxide roughness. After a 10-minute deposition, the oxide surface roughness was examined by AFM, and, the thickness measured using an ellipsometer (made by Horiba).

Figure 4.1 plots the deposition rate as a function of temperature. Also, Figure 4.2 and 4.3 plot the oxide surface roughness and the index as a function of temperature, respectively. These three plots reveal that all three quality factors reduce in quantity as the deposition temperature increases. This finding agrees with the previously published data [114, 112].

To investigate the oxide purity, reference [112] also discusses the issue of PECVD-deposited oxide composition. Using a Fourier Transform Infra-Red (FTIR) spectroscopy, the study concludes two types of impurities form in the oxide at different temperatures: silanol (Si-OH) incorporation (3450 cm$^{-2}$ - 3650 cm$^{-2}$ FTIR absorption band) happens at substrate temperature of 250-290 °C, and N-H (3400 cm$^{-1}$)

---

1This ellipsometer measures the reflected power in both $p$ and $s$ polarizations and then applies a Fresnel curve fit to obtain the thin film thickness and material dispersion.
Figure 4.1: $SiO_2$ deposition rate as a function of temperature.

Figure 4.2: $SiO_2$ surface roughness as a function of temperature. The inset plots the AFM-scanned surface morphologies of each sample.
incorporation happens at substrate temperature of 350-390 °C. Therefore, to avoid undesirable incorporations, a recommended deposition window is 300 °C.

For the samples made in this thesis, the PECVD deposition conditions are as follows: 30 Watt RF power, 1000 mTorr pressure, 170 sccm silane flow (5 % in nitrogen), and 710 sccm \( \text{N}_2\text{O} \) flow. The deposition temperature was set to 300 °C.

### 4.1.2 Lift-off technique for stripe SPP waveguide fabrication

With the PECVD conditions optimized, stripe waveguide arrays were fabricated. The entire fabrication procedure used is illustrated in Figure 4.4. The substrate material is an intrinsic silicon (100) wafer. On top of the substrate, PECVD is used to deposit a layer of \( \sim 4 \) \( \mu \)m thick \( SiO_2 \). On top of the \( SiO_2 \), photoresist (Shipley-2

---

\[ \text{One may also choose to use wet etch to obtain the silver stripes. A silver wet-etching protocol is documented in Appendix C.} \]
S1811) is spun at 3000 rpm, for 90 s (Figure 4.4(c)). After baking on a hot plate at 105 °C for 2 min, the substrate is exposed on a mask aligner (Karl-Suss MA6) for 5 s (Figure 4.4(d)). The shadow mask used in the exposure procedure contains the negative of the stripe waveguide pattern. The sample is then soaked in Toluene for 5 min. After drying with $N_2$ gas, the sample is developed in MF321 for 60 s, followed by a 60 s deionized water rinse (Figure 4.4(e)). Then, a 20-nm-thick layer of silver is deposited using ebeam evaporation (Figure 4.4(f)). Following a 10-min acetone soak, the photoresist is washed away and the metal stripe waveguides are left behind on the $SiO_2$ (Figure 4.4(g)). Finally, an additional $\sim 4 \mu m$ PECVD $SiO_2$ thick layer is added to achieve material symmetry. Each of the silver stripes in the array has a width $b = 5 \mu m$, and the center-to-center separation of the adjacent waveguides is $d_{array} = 10 \mu m$. An optical microscope image of the completed sample is shown in Figure 4.5. The sample is cleaved to a length of $\sim 1 \text{ mm (z-axis)}$ for optical characterization.

### 4.2 End-fire optical characterization setup

To characterize the waveguide array sample, a free-space end-fire coupling setup was used, shown in Figure 4.6. The excitation and output objectives have $40 \times$ and $20 \times$ magnification, respectively. The polarization is tuned by placing a combination of a polarization beam splitting cube and a half-wave plate in the input beam path. The excitation laser is set to have a center emission wavelength at 1550 nm and a power of 0.5 mW. The sample is placed at the center of a rotation stage having a yaw rotation resolution of 0.2 arc seconds.
Figure 4.4: Illustration of the lift-off fabrication protocol.

1. **Substrate** (a)
2. **PECVD SiO$_2$** (b)
3. **Spin photoresist** (c)
4. **Exposure** (d)
5. **Develop photoresist** (e)
6. **Deposit metal** (f)
7. **Lift-off** (g)
8. **PECVD SiO$_2$** (h)
Chapter 4. SPP Stripe Waveguide Array Fabrication and Experiments

Figure 4.5: Microscope photograph of the topview of the fabricated stripe waveguide array sample. The waveguides are 5 $\mu$m in width and 20 nm in thickness. The waveguide center-to-center separation is 10 $\mu$m. Note the yellow tint to the photograph is due to the lighting in the cleanroom facility. The brighter colored parts are the silver stripes, which are more reflective under illumination, and the darker parts are the $\text{SiO}_2$, which is less reflective under white illumination.

4.3 Discrete diffraction and its compensation in stripe SPP waveguide arrays experiments

Placing the sample (fabricated according to the method described in Section 4.1) onto the optical setup (described in Section 4.2), one may observe discrete diffraction in stripe parallel waveguide arrays as well as the compensation of discrete diffraction.

Figure 4.7 shows the power pattern captured by the near-infrared camera at the output of the array. Recall the guiding mechanism of stripe SPP waveguide prohibits TE modes – In Figure 4.7(a), the TE polarized output is compared to the TM polarized output, both excited at normal incidence, to confirm that the even fundamental mode guided in stripes supports TE-polarized SPPs to a negligible degree. This figure also reveals that the typical discrete diffraction phenomenon is observed in stripe waveguide array samples. Higher order waveguides are not excited due to the limited
Figure 4.6: Optical excitation experimental setup. The laser is set to have a center emission wavelength at 1550 nm. PBS = Polarization beam splitter $\lambda/2 = \text{half waveplate}$; Obj.1 is the excitation objective having $40 \times$ magnification and $\text{NA} = 0.65$; DUT = device under test; Obj. 2 is the output coupling objective having $20 \times$ magnification and $\text{NA} = 0.4$; IR = infrared camera.

1 mm propagation distance through the sample, which is required to obtain a signal level in the higher numbered waveguides that is well distinguished from the noise. Figure 4.7(b) shows the sample output at 0, 0.9, 1.5, 2.2, and 2.9 degrees incident angles. The figure clearly shows a shift in power amongst the waveguides as the excitation angle is rotated away from normal; the initially symmetrical and “diffractive” pattern becomes more asymmetrical and “confined” as the angle is increased. At 2.2 degrees, the output intensity in the higher order waveguides is suppressed, compared to the output at 0.9, 1.5 and 2.9 degree excitation. Therefore, 2.2 degrees is the diffraction compensation excitation condition and corresponds to $|k_x d_{array}| = \pi/2$. In the same plot, the simulated results from Section 3.5 are shown to compare with. Observing the output at normal incidence, the spread of the power into the higher order waveguides is larger compared to the simulated result. This could be due to the uncertainties in the silver dispersion. At larger excitation angles, the comparison plots show reasonable agreement between the theory, simulation, and experimental results for a 1 mm propagation length. This is evidence of discrete diffraction compensation in SPP waveguide arrays. Also, the similarities between the experiment
Figure 4.7: Intensity pattern detected at output of the waveguide array. 4.7(a) compares the TE and TM polarized components of the output intensity patterns, both excited at $\theta = 0$. 4.7(b) shows the spatial distribution of the output intensity pattern for $\theta = 0, 0.9, 1.5, 2.2,$ and $2.9$ degrees. Vertical bars show the simulated results, and solid curves show the experimental result. All plots are normalized for visual clarity.
and simulation supports that the beam propagation method used in Chapter 3.5 is suitable for studying stripe SPP waveguides.
Chapter 5

IPP Waveguide and Bragg IPP Sensors

The concepts of IPP waveguide design were first introduced in Section 3.4 and the Bragg grating calculation was formulated in Section 3.6. In this chapter, the demonstration of IPP waveguides to make LOC sensors will be discussed. Fabrication and experimental characterization of IPP waveguide-based sensors will be presented.

Section 5.1 will discuss IPP waveguide fabrication. Section 5.2 will present an experimental observation of IPP waveguide-supported single and higher order modes. Then dielectric gratings are embedded into the IPP waveguide: Section 5.3 discusses the fabricating PMMA rib gratings; and Section 5.4 presents the optical characterization of PMMA rib grating samples. Then, an alternative dielectric grating implementation, PMMA varying-density hole-array, is designed, fabricated, and characterized in Section 5.5. In the final section, Section 5.6, a new way to embed metal gratings
and a new way to make IPP waveguides are shown. This final design is characterized in Section 5.7.

5.1 Fabrication of IPP waveguides

Due to their large, $\sim 10 \, \mu$m feature size, geometry and simple cross-section (i.e. a channel), IPP waveguide fabrication may be carried out in a standard microfabrication facility. The basic fabrication steps consist of two phases: silicon etching and silver plating.

5.1.1 Wet and dry silicon etching

Both wet and dry anisotropic etching methods have been used to define features in crystalline silicon. The wet etching method utilizes a heated basic KOH solution to attack silicon surfaces; and therefore the etched cross-section relies on the crystal orientation of the wafer. In contrast, the dry etching method uses Reactive Ion Etching (RIE) to attack silicon surface with reactive ions; and therefore, the etched cross-section depends little on the crystal orientation. In this section, both wet and dry methods are used to pattern silicon substrates.

Wet silicon etching

The chemical etching process in wet etching relies on a proper wafer crystal orientation. Figure 5.1 illustrates the two most commonly used silicon crystal orientations (100) and (110). It is well known that silicon (111) surface is more resilient to basic
Figure 5.1: Illustration of silicon wafer crystal orientations. Figure 5.1(a) shows the (100) wafer top surface (top) and cross-section (bottom). And, the Figure 5.1(b) shows the (110) wafer top surface (top) and cross-section (bottom).

solution corrosion, and has the lowest etch rate. As a result, the (100) wafer will have a trapezoid cross-section, and the (110) wafer would have a rectangular cross-section after KOH etching, and the angle is determined by the tilt of the crystal plane.

The wet etching protocol is developed based on the following rationale: the silicon is easily attacked by basic solutions, and therefore, the mask material should be silicon dioxide, which is usually etched by an acidic solution. Typically the thickness of the mask material is not critical in a chemical wet etch process, unlike masks used in the RIE process where physical etching may occur (e.g. at high power). To pattern the oxide hard mask, a patterned photoresist can be used. The photoresist may not directly protect silicon against the etchant because it is also soluble in basic solutions.
The specific wet etching parameters are as follows: On a cleaned (100) p-doped silicon, first, a 6 µm thick SiO$_2$ layer is deposited as a hard mask using PECVD (as discussed in Section 4.1.1). Then, photoresist S1811 (Microposit) is spun on the Si surface at 6000 rpm for 90 s, and dried on hot plate for 2 min. Next the photoresist is exposed by placing the sample under a UV source (emission spectrum peaks at 35 mW/cm$^2$ at 365 nm, and 58 mW/cm$^2$ at 405 nm) for 7 s. The shadow mask used has Cr stripes that are 10 mm long and varying widths, 100, 200, or 500 µm. Finally, the sample is developed in MF321 (Shipley) for 60 s, and rinsed under De-Ionized (DI) water for 1 min. After drying with N$_2$ gas, the samples are ready to be wet etched.

To pattern the oxide hard mask, a hot Buffered Oxide Etch (BOE) is used. The etchant is placed on a 90° C hot plate to be heated to a 57° C solution temperature. Then, the oxide mask is etched for 3.5 min and then rinsed in DI water for 12 min. After drying with N$_2$ gas, the samples are ready to be wet etched.

The 30% KOH solution used for wet etching consists of 70 g of KOH pellets, 190 ml of DI water and 40 ml of isopropyl alcohol. To prepare for etching, the solution is heated to 97° C. The sample is then submerged in the etchant for 25 minutes to achieve a 90 µm etch depth, which translates to a 60 nm/s etch rate. The etched sample then is placed under running DI water for 10 min to remove the solution.

---

1. The selectivity between Si and SiO$_2$ etching is high. However, the procedure about to be demonstrated results in a 90-µm silicon removal. The oxide mask thickness must be increased accordingly.
2. KOH pellets absorb water in the air on second-scale and therefore should be kept in air tight containers at all times.
3. Note that the hot plate setting should be 190° C to achieve a 97° C solution temperature.
4. KOH attacks silicon at a very high rate; therefore, delayed DI water wash will allow localized etching and result in undesirable surface roughness.
Finally, the oxide mask was removed by the BOE solution. To characterize the etched ridge, the sample is scanned by a profilometer, and the output of which is shown in Figure 5.2. The slope of the ridge is \( \sim 55^\circ \), which corresponds to the tilt of the (111) silicon crystal plane. An optical microscope image of the etched sample prior to mask removal is shown in Figure 5.3. In this image, the top oxide hardmask is shown and the silicon underneath can be see through the transparent mask.
Dry silicon etching

In the case of etching amorphous silicon, where anisotropic etching is preferred, RIE offers a more controlled method. For instance, in RIE, there would be no need to pre-define the crystal orientation, and no need to worry about soft-mask adhesion problems (i.e. pealing away from the substrate). Also, RIE could be adapted by non-single-crystalline silicon substrates. An additional advantage, which will be apparent at the end of the section, is the fact that all five input parameters, the power, pressure, $CHF_3$ flow, $SF_6$ flow, and $O_2$ flow, may be used to modify the etched cross-section geometry, independent of the crystal orientation [115].

The RIE process is illustrated in Figure 5.4. All silicon substrates have (100) p-doped substrate. The substrates are 1 cm × 1 cm, which affects the macro-loading [116]. They are acetone washed in an ultrasonic bath for 2 min, and then blow-dried with $N_2$ gas. Then, photoresist S1811 (Microposit) is spun on the Si surface at 6000 rpm for 90 s and dried on a hot plate for 2 min. The exposure is performed under a UV source (35 mW/cm$^2$ at 365 nm, and 58 mW/cm$^2$ at 405 nm) for for 5 s. The shadow mask used has Cr gaps that are 10 mm long and varying in width between 1 and 25 µm, which affects the micro-loading [117]. Finally, the sample is developed in MF 321 (Shipley) for 60 s, and rinsed under DI water for 1 min. The sample then is dehydrated on hot-plate for at least 10 min. Next, the Si substrate having patterned photoresist is placed in the RIE etcher (Minilock-Phantom III RIE/ICP),

---

5The photoresist may peal away during the BOE and KOH etching process. In case of pealing, one may switch to a lower spin speed or a more viscose photoresist.

6This drying process removes water molecules from the sample surface to prevent formation of additional reaction agent in the RIE chamber. Without the drying process, the sample appears very rough.
without contact/cooling oil of any sort. The cathode material used is graphite, and the etching parameters are discussed in more detail below. After etching, the S1811 may be washed away with acetone or a compatible photoresist remover. The final step is metal plating (Figure 5.4(g)), and will be discussed in Section 5.1.2.

The RIE etcher has five parameters that effect the fabrication quality: the power, pressure, $CHF_3$ flow, $SF_6$ flow, and $O_2$ flow. The effect of each parameter is studied and the findings are reported below. The fabrication results and quality are discussed in terms of isotropy, selectivity, etch rate, and roughness. The etched

---

\[\text{[115]}\] reports RIE of silicon using a different etch mask and different chamber chemistry. Therefore, the results shown in this thesis is not expected to reproduce the quantitative data published and rather qualitatively agree with \[\text{[115]}\].

\[\text{[116]}\] These factors may be measured using combined imaging and surface morphological instruments such as SEM and AFM. The samples were diced and stand on their sides to reveal etched cross-
geometry and definitions referred to in the study are illustrated in Figure 5.5.

i). Increasing the RF power increases the F ion concentration, and at the same time, has little effect on the oxygen concentration in the chamber, and therefore, increases the etch rate [118].

Though the chemistry is not changed when tuning the power parameter, the physical and chemical processes of RIE are highly dictated by the power. Etching results from varying the RF power are tabulated in Table 5.1 and plotted Figure 5.6. Based on lab observation, the photoresist color changed drastically as the applied power increases, which is an indication of poor selectivity. This observation is supported by reference [115], in which it was found that the oxide-mask-etching rate is also highly dependent on the power and little on the chemistry. Anisotropic etching is evident at 60 and 180 Watt, the lowest and the highest power applied, sections. The data shown in this thesis was obtained using an optical microscope with a 100 × lens, and a built-in scale bar to determine the isotropy, selectivity, and etch rate. The roughness is examined by observing the clarity of the sample. The selectivity is also confirmed by visually observing the photoresist thin film color change, which is an indication of thin film thickness.
Figure 5.6: RIE anisotropy and etch depth in silicon for varying power for a 120 s etch duration. RIE pressure = 100 mTorr, $CHF_3$ flow = 12 sccm, $SF_6$ flow = 30 sccm, and $O_2$ flow = 10 sccm.

when the side-wall angle, $\theta$, becomes smaller. At high power, the greater anisotropy is due to the increased F ion creation. The reduced anisotropy in between the two extreme cases may be caused by a combined effect of two counter-reacting events: the creation of F ions which increases the anisotropy, and the increasing etch rate of S1811 that resulted in widened features and reduces the quantitative calculation result of anisotropy$^9$. Lastly, higher power increases the silicon etch rate due to the creation of F ions.

ii). Higher pressure forces larger F ion flux on the silicon surface, and therefore contributes to etch rate under specific conditions. Also, a higher pressure helps the oxygen ions to form a passivation layer on the walls, and results in high anisotropy$^{115}$.

$^9 tan(\theta) = (a - b)/(2h)$. This equation does not include the curvature along the walls, such as the one illustrated in Figure 5.10(b). Further investigation is needed to present a comprehensive study.
### RIE Si by varying power

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>2</td>
<td>&lt;1</td>
<td>3</td>
</tr>
<tr>
<td>3</td>
<td>2</td>
<td>2</td>
<td>&lt;1</td>
<td>4</td>
</tr>
<tr>
<td>4</td>
<td>4</td>
<td>4</td>
<td>&lt;1</td>
<td>5</td>
</tr>
<tr>
<td>5</td>
<td>4</td>
<td>4</td>
<td>&lt;1</td>
<td>6</td>
</tr>
<tr>
<td>6</td>
<td>5</td>
<td>5</td>
<td>&lt;1</td>
<td>6</td>
</tr>
<tr>
<td>7</td>
<td>6</td>
<td>6</td>
<td>&lt;1</td>
<td>7</td>
</tr>
<tr>
<td>8</td>
<td>7</td>
<td>7</td>
<td>&lt;1</td>
<td>9</td>
</tr>
<tr>
<td>9</td>
<td>8</td>
<td>8</td>
<td>&lt;1</td>
<td>10</td>
</tr>
<tr>
<td>10</td>
<td>10</td>
<td>10</td>
<td>&lt;1</td>
<td>11</td>
</tr>
<tr>
<td>15</td>
<td>14</td>
<td>14</td>
<td>&lt;1</td>
<td>16</td>
</tr>
<tr>
<td>20</td>
<td>20</td>
<td>20</td>
<td>&lt;1</td>
<td>21</td>
</tr>
<tr>
<td>25</td>
<td>25</td>
<td>25</td>
<td>&lt;1</td>
<td>26</td>
</tr>
</tbody>
</table>

Comment: larger power $\rightarrow$ high anisotropy
larger power $\rightarrow$ low selectivity
large power $\rightarrow$ faster etch rate
power has small effect on roughness

Table 5.1: Geometry of RIE silicon for varying RF power for 120 second etch duration. RIE pressure = 100 mTorr, $CHF_3$ flow = 12 sccm, $SF_6$ flow = 30 sccm, and $O_2$ flow = 10 sccm. “mask” indicates the shadow mask width using for photoresist exposure. $*$ and “x” indicates negligible etching.
Figure 5.7: RIE of silicon at varying pressure for 120 second duration. RIE power = 100 Watt, $CHF_3 = 12$ sccm, $SF_6 = 30$ sccm, and $O_2 = 10$ sccm.

RIE etching of silicon for varying pressures is tabulated in Table 5.2 and plotted Figure 5.7. The etch depth $h$ increases as the pressure in the chamber is raised. Observing the etch width versus the etch depth, an increasing pressure narrows the trapezoid, thus decreases $\theta$. A nearly vertical side-wall etch, obtained at 180 mTorr pressure, is evidence of anisotropic etching at an increasing pressure. Concerning the surface morphology of the etched surfaces, the 20 mTorr pressure produced little etched depth, and the unprotected Si surface is darkened. Also at 60 mTorr, the exposed Si surface also has reduced optical clarity, which is a sign of surface roughness. Lastly, the surface smoothness rises at higher pressure.

iii). $CHF_3$ is used to enhance the surface smoothness in $SF_6/O_2$ RIE of silicon [115]. The experimental observations from varying the $CHF_3$, summarized in Table 5.3 and plotted Figure 5.8 confirms the paper result. The presence of $CHF_3$ reduces the surface roughness of the sample, which can be visually observed: at 2 sccm flow, the etched surface is dark and the clarity rises as the flow rate is increased to 17
Chapter 5. IPP Waveguide and Bragg IPP Sensors

RIE Si by varying pressure

<table>
<thead>
<tr>
<th></th>
<th>20 mTorr</th>
<th>60 mTorr</th>
<th>140 mTorr</th>
<th>180 mTorr</th>
</tr>
</thead>
<tbody>
<tr>
<td>mask</td>
<td>1</td>
<td>2</td>
<td>3</td>
<td>4</td>
</tr>
<tr>
<td>[µm]</td>
<td>a [µm]</td>
<td>b [µm]</td>
<td>h [µm]</td>
<td>a [µm]</td>
</tr>
<tr>
<td></td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>3</td>
<td>4</td>
<td>5</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>5</td>
<td>6</td>
<td>7</td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>7</td>
<td>8</td>
<td>9</td>
</tr>
<tr>
<td></td>
<td>8</td>
<td>9</td>
<td>10</td>
<td>11</td>
</tr>
<tr>
<td></td>
<td>9</td>
<td>*</td>
<td>10</td>
<td>11</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>*</td>
<td>11</td>
<td>12</td>
</tr>
<tr>
<td></td>
<td>15</td>
<td>*</td>
<td>16</td>
<td>17</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>*</td>
<td>21</td>
<td>22</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>*</td>
<td>26</td>
<td>27</td>
</tr>
</tbody>
</table>

Table 5.2: Geometry of RIE silicon for varying pressure for 120 second etch duration. RIE power = 100 Watt, $CHF_3$ flow = 12 sccm, $SF_6$ flow = 30 sccm, and $O_2$ flow = 10 sccm. “mask” indicates the shadow mask width using for photoresist exposure. * and “x” indicates negligible etching.

comment: larger pressure $\rightarrow$ large anisotropy
large pressure has small effect on selectivity
larger pressure $\rightarrow$ faster etching rate
large pressure $\rightarrow$ smaller roughness
Figure 5.8: RIE of silicon at varying $CHF_3$ flow for 120 second duration. RIE power = 100 Watt, pressure = 100 mTorr, $SF_6$ =30 sccm, and $O_2$ = 10 sccm.

Another contribution of the large $CHF_3$ flow is a reduced selectivity between the photoresist and the silicon surface. As mentioned in [115], at high $CHF_3$ flow rate, the process consists more of physical bombardment and less of chemical etching, and therefore, the etch rate of the photoresist rises. As shown in Table 5.3, at large flow rate, the features are widened at the opening $a$, which usually is a sign of photoresist being etched away in combination with an increased isotropy. There is no significant change in etching rate due to $CHF_3$ flow.

iv). The role of $SF_6$ is to provide the Si surface with F ions, which dictate the etch rate – the more F ions, the higher the etch rate. Table 5.4 and Figure 5.9 summarize the findings from varying the $SF_6$ flow rate. At lower $SF_6$ flow rates of 10 sccm, 20 sccm, and 30 sccm (the 30 sccm etching data is collected from Table 5.1), the etch rate is low and gradually rises, which is consistent with the results published in [115]. Starting at 40 sccm, the etch rate starts to drop due to the convection losses, and, the selectivity is enhanced because of the $SF_6$ flow. Also a low $SF_6$ flow, the
Chapter 5. IPP Waveguide and Bragg IPP Sensors

RIE Si by varying $CHF_3$ flow

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>1</td>
<td>1.5</td>
<td>3</td>
</tr>
<tr>
<td>3</td>
<td>3</td>
<td>2</td>
<td>1.5</td>
<td>4</td>
</tr>
<tr>
<td>4</td>
<td>4</td>
<td>3</td>
<td>1.5</td>
<td>5</td>
</tr>
<tr>
<td>5</td>
<td>5</td>
<td>4</td>
<td>1.5</td>
<td>6</td>
</tr>
<tr>
<td>6</td>
<td>6</td>
<td>5</td>
<td>1.5</td>
<td>7</td>
</tr>
<tr>
<td>7</td>
<td>7</td>
<td>6</td>
<td>1.5</td>
<td>8</td>
</tr>
<tr>
<td>8</td>
<td>8</td>
<td>7</td>
<td>1.5</td>
<td>9</td>
</tr>
<tr>
<td>9</td>
<td>9</td>
<td>8</td>
<td>1.5</td>
<td>10</td>
</tr>
<tr>
<td>10</td>
<td>10</td>
<td>9</td>
<td>1.5</td>
<td>11</td>
</tr>
<tr>
<td>15</td>
<td>15</td>
<td>14</td>
<td>1.5</td>
<td>16</td>
</tr>
<tr>
<td>20</td>
<td>20</td>
<td>19</td>
<td>1.5</td>
<td>20</td>
</tr>
<tr>
<td>25</td>
<td>25</td>
<td>24</td>
<td>1.5</td>
<td>27</td>
</tr>
</tbody>
</table>

Comment: larger $CHF_3$ flow $\rightarrow$ small anisotropy

Heavy $CHF_3$ flow $\rightarrow$ reduced selectivity

$CHF_3$ flow has small effect on etch rate

Heavy $CHF_3$ flow $\rightarrow$ large roughness

Table 5.3: Geometry of RIE silicon for varying $CHF_3$ flow for 120 second etch duration. RIE power = 100 Watt, pressure = 100 mTorr, $SF_6$ flow = 30 sccm, and $O_2$ flow = 10 sccm. “mask” indicates the shadow mask width using for photoresist exposure. * and “x” indicates negligible etching.
Figure 5.9: RIE of silicon at varying $SF_6$ flow for 120 second duration. RIE power = 100 Watt, pressure = 100 mTorr, $CHF_3 = 12$ sccm, and $O_2 = 10$ sccm.

roughness is high, shown as a darkened surface. Also, the feature side-wall angle $\theta$ widens, which is a sign of enhanced isotropy.

v). The role of oxygen is to form a passivation layer on the sidewalls. The passivation layer protects the walls such that they are not physically bombarded by other ion particles [119], and hence enhances the etching anisotropy in silicon RIE. Oxygen ions compete with the F ions during etching, in a process called chemisorption, and therefore inhibits the etch rate [115]. Hence, by deduction, the etch rate of Si is reduced in the presence of a high $O_2$ flow rate, and the selectivity may be reduced. The experimental observation from varying the $O_2$ flow rate are shown in Table 5.5 and plotted in Figure 5.11, which reveal that the oxygen concentration mainly contributes to the anisotropy and the etch rate. The anisotropy increases in direct proportion with oxygen flow. Figure 5.10 shows drawings of the etched cross-sections observed when varying the $O_2$ flow rate: the angle $\theta$ becomes smaller as the $O_2$ concentration in the RIE chamber increases, and at the same time, the
Table 5.4: Geometry of RIE silicon for varying $SF_6$ flow for 120 second etch duration.
RIE power = 100 Watt, pressure = 100 mTorr, $CHF_3$ flow = 12 sccm, and $O_2$ flow = 10 sccm. “mask” indicates the shadow mask width using for photoresist exposure. * and “x” indicates negligible etching.
Chapter 5. IPP Waveguide and Bragg IPP Sensors

(a) $O_2 = 2$ sccm  
(b) $O_2 = 6$ sccm  
(c) $O_2 = 14$ sccm  
(d) $O_2 = 18$ sccm

Figure 5.10: Illustration of observed cross-section of RIE in silicon for varying $O_2$ flow rates.

Figure 5.11: RIE of silicon at varying $O_2$ flow for 120 second duration. RIE power = 100 Watt, pressure = 100 mTorr, $CHF_3$ flow = 12 sccm, and $SF_6$ flow = 30 sccm.

etch rate is reduced. Changes in selectivity were not studied here.

In summary, RIE of silicon with varying $CHF_3$, $SF_6$, and $O_2$ gas mixtures was characterized. It is found that, using the same (100) silicon substrate, varying any of the etch parameters may change the etched cross-section geometries from a rectangle, as shown in Figure 5.12, to a trapezoid, as shown in Figure 5.13. The cross-section geometry is an important factor dictating the IPP waveguide mode dispersion (recall Section 3.4); therefore, adapting a method that allow waveguide dispersion definition via fabrication is critical. It has been shown here that the RIE fabrication process can be used to lithographically define IPP waveguide properties, an important re-
Table 5.5: Geometry of RIE silicon for varying $O_2$ flow for 120 second etch duration.

<table>
<thead>
<tr>
<th>RIE Si by varying $O_2$ flow</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
</tr>
</tbody>
</table>
| ![Table](image)

- RIE power = 100 Watt, pressure = 100 mTorr, $CHF_3$ flow = 12 sccm, and $SF_6$ flow = 30 sccm.
- "mask" indicates the shadow mask width using for photoresist exposure.
- * and "x" indicates negligible etching.

Table 5.5: Geometry of RIE silicon for varying $O_2$ flow for 120 second etch duration.

- RIE Si by varying $O_2$ flow

Table 5.5: Geometry of RIE silicon for varying $O_2$ flow for 120 second etch duration.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3</td>
<td>1</td>
<td>x</td>
<td>3</td>
<td>1</td>
<td>x</td>
<td>1</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
</tr>
<tr>
<td>2</td>
<td>4</td>
<td>2</td>
<td>3</td>
<td>4</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>x</td>
<td>2</td>
<td>2</td>
<td>x</td>
</tr>
<tr>
<td>3</td>
<td>5</td>
<td>3</td>
<td>3</td>
<td>5</td>
<td>3</td>
<td>2</td>
<td>3</td>
<td>3</td>
<td>1</td>
<td>3</td>
<td>3</td>
<td>&lt;1</td>
</tr>
<tr>
<td>4</td>
<td>6</td>
<td>4</td>
<td>3</td>
<td>6</td>
<td>4</td>
<td>2</td>
<td>4</td>
<td>4</td>
<td>1</td>
<td>4</td>
<td>4</td>
<td>&lt;1</td>
</tr>
<tr>
<td>5</td>
<td>7</td>
<td>5</td>
<td>3</td>
<td>7</td>
<td>5</td>
<td>2</td>
<td>5</td>
<td>5</td>
<td>1</td>
<td>5</td>
<td>5</td>
<td>&lt;1</td>
</tr>
<tr>
<td>6</td>
<td>8</td>
<td>6</td>
<td>3</td>
<td>8</td>
<td>6</td>
<td>2</td>
<td>6</td>
<td>6</td>
<td>1</td>
<td>6</td>
<td>6</td>
<td>&lt;1</td>
</tr>
<tr>
<td>7</td>
<td>9</td>
<td>7</td>
<td>3</td>
<td>9</td>
<td>7</td>
<td>2</td>
<td>7</td>
<td>7</td>
<td>1</td>
<td>7</td>
<td>7</td>
<td>&lt;1</td>
</tr>
<tr>
<td>8</td>
<td>10</td>
<td>8</td>
<td>3</td>
<td>10</td>
<td>8</td>
<td>2</td>
<td>8</td>
<td>8</td>
<td>1</td>
<td>8</td>
<td>8</td>
<td>&lt;1</td>
</tr>
<tr>
<td>9</td>
<td>11</td>
<td>9</td>
<td>3</td>
<td>11</td>
<td>9</td>
<td>2</td>
<td>9</td>
<td>9</td>
<td>1</td>
<td>9</td>
<td>9</td>
<td>&lt;1</td>
</tr>
<tr>
<td>10</td>
<td>12</td>
<td>10</td>
<td>3</td>
<td>12</td>
<td>10</td>
<td>2</td>
<td>10</td>
<td>10</td>
<td>1</td>
<td>10</td>
<td>10</td>
<td>&lt;1</td>
</tr>
<tr>
<td>15</td>
<td>18</td>
<td>15</td>
<td>3</td>
<td>18</td>
<td>15</td>
<td>2</td>
<td>15</td>
<td>15</td>
<td>1</td>
<td>15</td>
<td>15</td>
<td>&lt;1</td>
</tr>
<tr>
<td>20</td>
<td>23</td>
<td>20</td>
<td>3</td>
<td>23</td>
<td>20</td>
<td>2</td>
<td>20</td>
<td>20</td>
<td>1</td>
<td>20</td>
<td>20</td>
<td>&lt;1</td>
</tr>
<tr>
<td>25</td>
<td>28</td>
<td>25</td>
<td>3</td>
<td>28</td>
<td>25</td>
<td>2</td>
<td>25</td>
<td>25</td>
<td>1</td>
<td>25</td>
<td>25</td>
<td>&lt;1</td>
</tr>
</tbody>
</table>

- comment: heavy $O_2$ flow $\rightarrow$ more anisotropic
- heavy $O_2$ flow $\rightarrow$ less selectivity
- heavy $O_2$ flow $\rightarrow$ reduced etching rate
- heavy $O_2$ flow $\rightarrow$ reduced roughness

* and "x" indicates negligible etching.
Figure 5.12: SEM image of RIE (100) silicon having 0° side wall angle. RIE power = 100 Watt, pressure = 100 mTorr, $CHF_3$ flow = 12 sccm, $SF_6$ flow = 30 sccm, and $O_2$ flow = 18 sccm. Etching time = 10 min.

requirement for making practical devices, as is the case for conventional waveguide devices. Therefore, the above results demonstrate the advantages of RIE over KOH etching of silicon for making IPP waveguides.

Based on the results of the RIE parameter study, the optimum parameters are chosen to make the 18°-side-wall-angle trapezoid IPP waveguide structure required for the remainder of the thesis. These optimum parameters are: RIE RF power = 100 Watt, pressure = 120 mTorr, $CHF_3$ flow = 12 sccm, $SF_6$ flow = 30 sccm, and $O_2$ flow = 10 sccm. A backside supply of Helium gas with 2 sccm flow rate is also used for sample cooling, which may reduce the etching rate. The etching time is 5 minutes to achieve an $h = \sim 6 \mu m$ depth and $\theta = \sim 18^\circ$ side wall angle. Or, using a 10 min etching time, an etch depth of $h = \sim 10 \mu m$ can be achieved with the side wall tilt angle remaining the same.
Figure 5.13: SEM image of RIE (100) silicon having 18° side wall angle. RIE power = 120 Watt, pressure = 100 mTorr, $CHF_3$ flow = 12 sccm, $SF_6$ flow = 30 sccm, and $O_2$ flow = 10 sccm. Etching time = 5 min.

5.1.2 Metal plating

The previous section developed an optimized method for making trenches in silicon with $h = \sim 6 \mu m$ and $\theta = \sim 18^\circ$. The final step in fabricating the IPP waveguide is the metal plating process, as illustrated earlier in Figure 5.4(g). In this section, metal plating will be applied to the patterned silicon template from Section 5.1.1 to complete the IPP waveguide fabrication.

Metal plating is a general technique to coat metal on a template substrate. IPP waveguide surface plating is slightly more complicated than the metal deposition process used in the making of stripe SPP waveguides (e.g. see Section 4.1), because the metal is exposed in the IPP geometry and the metal adhesion to the template material must not be compromised. The discussion in this section includes the choice of the adhesion material and the silver deposition condition.
It is known that silicon and noble metal have poor adhesion. Previous works suggest scribing the silicon surface for improved adhesion [120]. However, this method only creates a rough surface morphology and cannot be applied to the channel bottom, and therefore cannot be used for IPP waveguides. Another solution to improve adhesion while still maintaining the smoothness of the substrate is to pre-plate chromium to the substrate as an adhesion layer. Improved adhesion can be quantified using an AFM mechanical scribing method [121].

Metal plating of the trench waveguide from Section 5.1.1 was performed using Electron Beam Physical Vapor Deposition (EBPVD) (made by Edwards Auto 306, Wilmington, MA). First the chamber is pumped down to $< 3 \times 10^{-6}$ mbar. Then, a crucible containing chromium pellets is “warmed” up at $\sim 10$ mA for $\sim 10$ minutes. Then the current is turned to $\sim 15$ mA for deposition at $\sim 0.1$ nm/s rate. The chromium adhesion layer deposited by this process is usually 50 nm in thickness. After the chromium deposition is finished, the current is returned to zero, and the pellet-holder is rotated to the crucible containing silver. The silver pellets also require warming up at 15 mA for $\sim 20$ min, and the deposition current is set to 30 mA for depositing at $\sim 0.1$ nm/s rate. The totally deposited thickness of silver must be thicker than the electromagnetic wave penetration depth at the designed wavelength$^{10}$. The surface roughness of silver deposited with this method was measured using an AFM to be $< 1$ nm. A SEM of the IPP waveguide final product is shown in Figure 5.14.

Metal plating is the final step to make an IPP waveguide. As the metal plating

---

$^{10}$The penetration depth or the skin depth is calculated in Section 3.1
thickness is larger than the field penetration depth, the top surface of the silver layer can guide the IPP modes. In the coming Section 5.2, IPP waveguide sample will be optically excited and characterized.

5.2 Experimental characterization of IPP waveguides

This section discusses the optical setup used to characterize the IPP waveguides as well as the mode profile observed at the output of the IPP waveguides. The IPP waveguides are excited using the end-fire coupling scheme, which is shown in Figure 5.15 and is similar to the scheme used to excite the waveguide arrays in Section 4.2. Here, to excite the IPP waveguide, the input light is 5 mW of 1550-nm-wavelength TE-polarized collimated laser light with a 2 mm beam diameter ($1/e^2$ below peak intensity). The TE and TM polarization states are defined as the input
Chapter 5. IPP Waveguide and Bragg IPP Sensors

Figure 5.15: Optical excitation experimental setup. The laser is set to have a center emission wavelength at 1550 nm. $\lambda/2 =$ half waveplate; Obj.1 is the excitation objective; DUT= device under test; Obj. 2 is the output coupling objective.

The laser electric field oscillating in the x- and the y-direction in Figure 5.15, respectively. The laser light was coupled into the waveguide using an objective lens to best match the waveguide mode. To manipulate the excitation polarization, a half-wave-plate was placed prior to the input objective lens. At the output facet of the waveguide, an objective lens, followed by a polarization beam splitter, was used to project the image on to an IR camera or a detector.

Figure 5.16 shows an experimental demonstration of SPP propagation in the IPP trapezoidal waveguide sample similar to the one shown in Figure 5.14 with $a = \sim 9 \mu m$, $b = \sim 5 \mu m$, $h = \sim 6 \mu m$ and a 1 mm length. As illustrated in the dispersion plot in Figure 3.24, a trapezoid channel with these dimensions is single moded at 1550 nm. The observed TM-polarized mode profile is shown in Figure 5.16(a). Single mode operation is confirmed by moving the transverse position of the sample and noting that the shape of the output mode remained unchanged. Also TE excitation does not excite a mode, as observed in Figure 5.16(b). From this set of images, it is confirmed that the mode guided on the bottom of the waveguide is TM polarized and can be excited efficiently with incoming TM polarized light.

Higher order modes can be observed in wider waveguides. Figure 5.17 shows
Chapter 5. IPP Waveguide and Bragg IPP Sensors

Figure 5.16: TM component output intensity profile of a single mode IPP waveguide (a $\sim 9 \, \mu m$, b $\sim 5 \, \mu m$, h $\sim 6 \, \mu m$). Figure 5.16(a) shows the output for TM polarized light excitation and Figure 5.16(b) shows the output for TE polarized excitation at 1550 nm wavelength.

the three lowest-order mode profiles measured from a 1 mm long waveguide having $a = 28 \, \mu m$, $b = 24 \, \mu m$, $h = 6 \, \mu m$, compared with the MODE-simulated rectangular and trapezoid waveguide mode profiles. The rectangular waveguide modes (Row "MODE, $\theta = 0^\circ$") and trapezoid waveguide modes (Row "MODE, $\theta = 18^\circ$") show similar intensity profiles due to the fact the mode is tightly confined at the bottom of the channel. Because the modes are far from the cutoff condition, their profiles are merely modified by the tilt of the side walls. Comparing row "MODE, $\theta = 18^\circ$" with row "Exp, $\theta = 18^\circ$", a close similarity is seen between the simulation and the experimental observation. Row "Exp, $\theta = 18^\circ$" also shows observation of no TE excitation verifying that the modes are excited only by TM polarized light.

Lastly, to verify that the modes observed are due to the presence of the channels, the results are compared to a single silver interface. Figure 5.18 shows the output intensity profiles for both TM and TE input excitations of a silver surface. In the case of the flat silver surface we observe no confinement of power in the transverse direction. This observation is similar to that in Figure 3.(c) in [122], and supports the
Figure 5.17: MODE simulated and experimentally observed IPP mode profiles. Row “MODE, $\theta = 0^\circ$” shows the simulated modes of a rectangular waveguide ($b = 24 \, \mu m$, $h = 6 \, \mu m$, $\theta = 0^\circ$). Row “MODE, $\theta = 18^\circ$” shows the simulated modes of a trapezoid waveguide ($a = 28 \, \mu m$, $b = 24 \, \mu m$, $h = 6 \, \mu m$, $\theta = \sim 18^\circ$). Row “Exp, $\theta = 18^\circ$” shows the experimentally observed mode profile (TM component only) of the fabricated trapezoid waveguide with the dimensions in (b) ($a = \sim 28 \, \mu m$, $b = \sim 24 \, \mu m$, $h = \sim 6 \, \mu m$, $\theta = \sim 18^\circ$). The “TM” and “TE” markings indicate the excitation polarization. The waveguide boundary is marked with a white dashed line around the fundamental mode in each set.
fact that the channel sidewalls indeed offer confinement to TM polarized propagation. Figure 5.18(c) shows the experimentally recorded mode profiles for a 1 mm long, 6 µm wide, 10 µm deep channel excited with TM-polarized light, and Figure 5.18(d) the profile for TE-polarized light. For the TE excitation we cannot observe the mode, which confirms the predicted guiding mechanism. Also the high intensity spot in Figure 5.18(c) falls deeper below the sample surface, indicating that the mode is guided along the bottom of the channel and that the plasmon waveguide is operating as expected.

5.3 Fabrication of PMMA-rib Bragg-grating-embedded IPP waveguide sensor

In Section 5.1, the IPP waveguide fabrication was shown. This bare IPP waveguide, such as the one shown in Figure 5.14, may be further embedded with gratings as discussed in Section 3.6 to make a sensor device.

Taking the bare IPP waveguide that has an inverted trapezoid shape having a bottom width $b = \sim 8 \text{ µm}$, top width $a = \sim 12 \text{ µm}$, and a height $h = \sim 6 \text{ µm}$, the procedure to embed a PMMA-rib is as follows: first, PMMA (950 A2 MicroChem Corp.) is spin-coated at 6000 rpm for 90 s. The sample is then baked at 180 °C to evaporate the solvent. The film thickness is measured to be $\sim 60 \text{ nm}$ (AFM scan). The Electron Beam Lithography (EBL) is used to direct-write the grating pattern into the PMMA (500 µC/cm² dose, 2 nA current, and 5 nm step size). Then, the exposed sample is developed in MIBK-IPA solution with a 1:3 ratio for 60 s. The final product has 100
Figure 5.18: Experimentally observed output intensity profile of a flat silver surface with TM \(5.18(a)\) and TE \(5.18(b)\) excitation; and of a 10-\(\mu\)m deep trapezoid waveguide with TM \(5.18(c)\) and TE \(5.18(d)\) excitation. The waveguide boundary is marked with a white dashed line around the mode in \(5.18(c)\).
Figure 5.19: SEM image of the completed PMMA-rib Bragg-grating-embedded IPP waveguide. 5.19(a) shows a zoomed in top-view on the PMMA grating ribs. 5.19(b) shows the angled end-view of the waveguide.

nm (in z-direction) PMMA-rib Bragg gratings adhering at the bottom of the IPP waveguide. An SEM image of the angled end-view (in the propagation z-direction) of the completed sample is shown in Figure 5.19. The gratings are 100 nm in width (z-direction) and 60 nm in height (y-direction). Five different waveguide samples were made, each embedded with a different grating periodicity: $\Lambda_{\text{Bragg}} = 567$ nm, 570 nm, 765 nm, 770 nm, and 775 nm. These are the same specifications used in the theoretical analysis of dielectric modulated IPP waveguides in Section 3.6. Each Bragg-grating period is repeated 200 times.
Figure 5.20: Optical setup to characterize back reflection of Bragg-grating-embedded waveguides. DUT = device under test; Obj. is the output coupling objective. Solid lines represent fiber, dotted lines represent a free space beam.

### 5.4 PMMA-rib Bragg-grating-embedded IPP waveguide sensors

To characterize the Bragg resonances of the dielectric modulated waveguides shown in Figure 5.19, the optical setup illustrated in Figure 5.20 is used. A tunable laser (JDS Uniphase SWS15101) is set to emit 3 dBm power, which scans over the 1525 nm to 1565 nm wavelength range. A 3.3 $\mu$m focusing lens fiber is used to excite the waveguides. To capture the back-reflected signal, a fiber circulator is place at the input facet. The mode excitation is confirmed by observing the output mode using an IR camera.

In the experiment, the open channels of the $\Lambda_{\text{Bragg}} = 765$ nm, 770 nm, and 775 nm waveguides are filled with air (assumed to have an index of unity), and the open channels of the $\Lambda_{\text{Bragg}} = 567$ nm and 570 nm waveguides are filled with index oil. The index oils (Series AAA by Cargille Labs) have dielectric indices of $n_d = 1.3346$, 1.3442, 1.3538, and 1.3634, at a 1550 nm wavelength.
A Bragg resonance shift can be demonstrated by changing the grating period, $\Lambda_{\text{Bragg}}$. The Bragg resonance shifts due to changing grating periodicity is shown in Figure 5.21 together with the theoretical spectra calculated in Section 3.6. The figure reveals a distinct $\sim 10$ nm wavelength shift for each 5 nm change in grating period in agreement with the shifts in the spectra calculated from theory in Section 3.6. The experimentally obtained resonant width is $\sim 15$ nm FWHM in wavelength.

A Bragg resonance shift can also be demonstrated by changing the dielectric filler index, $n_d$. Figure 5.22 and 5.23 show the measured reflection spectra for different dielectric fillers for the $\Lambda_{\text{Bragg}} = 567$ nm and 570 nm samples respectively and reveals a distinct $\sim 11$ nm wavelength shift for each 0.01 change in RIU, which converts to a $\sim 1100$ nm/RIU sensitivity. All spectra are normalized to unity peak. These experimental results again are in agreement with the theoretical predictions in Section 3.6.

It is also important to determine the SR of the sensors according to the definition given in Section 2.3 $SR = dn/d\lambda \times \delta \lambda'$. Recall that $dn/d\lambda$ is the inverse of sensitivity, therefore for the sensors above, $dn/d\lambda = 1/1100\text{nm/RIU} = 10^6 \text{RIU/m}$. Also recall $\delta \lambda'$ is the resolving power, therefore for the sensor above, $\delta \lambda' = 8 \times 10^{-9}$ m. Therefore, $SR = dn/d\lambda \times \delta \lambda' = 0.008 \text{RIU}$. 
Figure 5.21: The reflection spectra of air-filled Bragg-grating-embedded waveguides, with varying periodicity of $\Lambda_{\text{Bragg}} = 765 \text{ nm}, 770 \text{ nm},$ and $775 \text{ nm}$. The black solid lines represent the experimentally observed reflected power spectra, the red dashed lines show the calculated spectra from Section 3.6 Figure 3.34.

Figure 5.22: The reflection spectra of oil-filled Bragg-grating-embedded waveguides with $\Lambda_{\text{Bragg}} = 567 \text{ nm}$. The index matching oils have $n_d = 1.3442, 1.3538,$ and $1.3634,$ at a $1550 \text{ nm}$ wavelength. The black solid lines represent the experimentally observed power spectra, and the red dashed lines show the calculated spectra from Section 3.6 Figure 3.35.
Figure 5.23: The reflection spectra of oil-filled Bragg-grating-embedded waveguides with $\Lambda_{\text{Bragg}} = 570$ nm. The index matching oils have $n_d = 1.3346, 1.3442,$ and $1.3538,$ at a $1550$ nm wavelength. The black solid lines represent the experimentally observed power spectra, and the red dashed lines represent the calculated spectra from Section 3.6 Figure 3.36

5.5 Fabrication and characterization of PMMA varying-density hole-array Bragg-grating-embedded IPP waveguide sensor

Using the same IPP waveguide fabrication protocol, described earlier in Section 5.1, the Bragg gratings may also be implemented using PMMA varying-density hole-arrays rather than PMMA ribs. One advantage of using a varying-density hole-array is that the resonant spectral width can be narrower, due to the reduced index contrast leading to a smaller SR. Also, fabricating the varying-density hole-array costs $20$ times less EBL machine time. In this section, varying-density hole-array Bragg grating embedded trapezoidal IPP waveguides are fabricated and characterized.

The fabrication of varying-density hole-array gratings is conducted inside the
same IPP waveguides in a similar fashion as the PMMA rib Bragg gratings, except a different EBL writing mechanism is used to generate the holes.

Starting with a trapezoidal waveguide that has an inverted trapezoid shape with bottom width \( b \approx 8 \ \mu m \), top width \( a \approx 12 \ \mu m \), and a height \( h \approx 6 \ \mu m \), PMMA (950 A2 MicroChem Corp.) is spin-coated at 6000 rpm, for 90 s. The sample is then baked at 180 °C to evaporate the solvent. The hole array can then be exposed using EBL. The EBL is a direct-write method, therefore, the final pattern may be determined by the beam step size. For example, applying a fixed dosage at a fixed pulse repetition rate, a 25 nm-diameter beam moving with a 1 nm step size gives approximately twice the exposure comparing to a beam that moves with a 2 nm step size (i.e. change in number of overlapping exposures). However if the same beam is instructed to move at 100 nm step size, each exposure sites would be distinct and non-continuous, creating an array of holes.

Applying this technique, Figure 5.24(a) is the result. Arrays of holes are formed inside the PMMA after development, and the hole-to-hole separation corresponds to the beam step size, \( d_{\text{step}} \). Figure 5.24(b) shows an AFM scan of the surface morphology in a small region of the sample marked by the box in Figure 5.24(a). A higher density of holes results in lower medium effective index, and the Bragg period is determined by the separations of the regions having the same density. A cross-section schematic of the density-hole array is shown in Figure 5.24(c). Four samples are made for characterization and sensing demonstration, having Bragg periods of \( \Lambda_{\text{Bragg}} = 760 \text{ nm}, 765 \text{ nm}, 770 \text{ nm}, \) and 775 nm. Each Bragg-grating period is repeated 200 times. It is important to note that the AFM images do not show unanimously
uniform Bragg periods. This could be caused by stitching error, machine instability, and/or AFM scanning errors.

The same end-fire coupling setup from Section 5.4 (Figure 5.20) is used to characterize the samples.

To theoretically predict the effect of the density-hole arrays, an effective medium method is used, illustrated in Figure 5.24(c). The portion containing more holes can be approximated as a 25-nm thick PMMA layer ($n_{PMMA} = 1.4807$), which has a waveguide mode index of $n_{st,1} = 1.0058 + 1.6892 \times 10^{-4}i$, and the region containing no holes is measured to be a $\sim 50$ nm thick PMMA layer, which has a waveguide mode index of $n_{st,2} = 1.0161 + 2.4817 \times 10^{-4}i$. The 25-nm thick layer has a total length of $d_{st,1} = 600$ nm (corresponding to 7 exposures). And, the length of the 50-nm thick section is $d_{st,2} = \Lambda_{Bragg} - d_{st,1}$. Applying these values, the Bragg resonance is calculated using the matrix method presented in Section 3.6.

Both the experimentally and the theoretically obtained spectra are shown in Figure 5.25. The resonant wavelength shift of 11 nm due to a 5 nm change in grating period is observed. The experimentally measured resonant curve shape matches the calculated results, and the actual peak is shifted by 11 nm with respect to the calculated curves. The cause of this discrepancy could be due to the fabrication errors mentioned earlier. A detailed investigation of the resonant wavelength difference is needed and will be performed in a future work.

One advantage of the density-hole array grating is that it uses a 100 nm EBL step size, rather than the 5 nm step size required for the rib gratings discussed in Section 5.3. This means the EBL machine time is reduced by a factor of 20. Also, the Bragg
Figure 5.24: SEM image (5.24(a)), AFM scan (5.24(b)) and the schematics of cross-section (5.24(c)) of the density hole array.
Figure 5.25: The reflection spectrum of air-filled PMMA density-hole array Bragg-grating-embedded IPP waveguides. The black solid line represents the experimentally observed reflected power spectra, and the dashed lines represent the calculated spectra.

resonance has a near-halved resonance width (10 nm FWHM in wavelength compared to 16 nm), due to the reduced contrast in the density-hole layout in the $n_{st,1}$ and $n_{st,2}$ layer, which usually translate into a desirable lower SR. One main disadvantage of the density-hole array grating however is that the large coverage of PMMA on the silver surface may cause complications in the surface functionalization of a sensor. Therefore, this grating layout may not be desirable for use in a sensor.

## 5.6 Design and fabrication of metal groove Bragg-grating-embedded IPP waveguide sensor

The previous two sections showed methods to make IPP waveguide sensors by embedding dielectric gratings into the IPP waveguides. Here in this section, a second
alternative making a grating-embedded IPP waveguide sensor will be shown involving a metal groove grating. First, the metal groove grating layout will be designed, then a metal groove grating embedded IPP waveguide will be fabricated and its Bragg resonance characterized.

To design the metal-groove grating, a series of FDTD simulations (Lumerical Solutions, Inc.) are run on the silver grating structure depicted in Figure 5.26 for $\Lambda_{\text{Bragg}} = 775$ nm and air as filler. The $L_{\text{Bragg}}$ and the $H_{\text{Bragg}}$ values (defined in Figure 5.26) are varied in the simulations to reveal two parameters: the FWHM of the reflected Bragg wavelength, and the reflected intensity. A Bragg resonance FWHM versus $L_{\text{Bragg}}$ and $H_{\text{Bragg}}$ contour plot is shown in Figure 5.27(a). Recall that the FWHM is proportional to $\delta \lambda'$, the resolving power; therefore, a smaller FWHM would reduce the SR of a sensor, and is therefore more desirable.

The reflected power at resonance as a function $L_{\text{Bragg}}$ and $H_{\text{Bragg}}$, is plotted in Figure 5.27(b). The reflected power of the gratings is calculated using a software built-in power meter, and has the following expression:

$$R(f) = \frac{1}{2} \int \Re(S(f)) \cdot dS, \quad (5.1)$$
Figure 5.27: FDTD-simulated contour plots of metal-groove-grating FWHM and reflected power versus groove width ($L_{Bragg}$) and groove height ($H_{Bragg}$). The FDTD used 100 $\Lambda_{Bragg} = 775$ nm Bragg gratings, having rectangular grooves in a silver surface.

where $R(f)$ is the normalized transmission as a function of frequency; $S(f)$ is the Poynting vector; and $dS$ is the surface normal. A higher reflected power offers higher SNR in a sensor, and is therefore more desirable.

Observing the two contour plots in Figure 5.27, a larger grating pitch leads to a narrower resonance, however, reduces the strength of the grating and lowers the reflected power. Therefore, there is a trade-off between FWHM and SNR.

The fabrication of the metal-groove Bragg IPP sensors introduced in this section is completely different from the dielectric Bragg IPP waveguides discussed previously. The process is illustrated in Figure 5.28. The gratings are made first on the silicon substrate (Figure 5.28(a) - 5.28(e)). Then, the channels are added on top (Figure 5.28(f) - 5.28(k)). Lastly, a final metal plating step forms the metal-groove grating and also mediates IPP mode propagation (Figure 5.28(l)).
Chapter 5. IPP Waveguide and Bragg IPP Sensors

The details of the fabrication are as follows: the process starts with a clean silicon wafer (Figure 5.28(a)), on which EBL-resist ZEP 520A is spin coated at 6000 rpm, for 60 s (Figure 5.28(b)). Then the sample is placed on a hot plate at 180°C for 2 min. After the ZEP is dried, EBL is used to expose the ZEP (2 nA current, 200 µC/cm², 5 nm beam step size). The sample is then developed in ZED-N50 (made by Zeon Chemicals L.P.). The developing time is dependent on the width of the slit opening in the ZEP: for a 50 nm wide slit opening, the development time is typically 5 minutes; and for a 100 nm slit opening, the development time is typically 1 minute. Then the developed sample is rinsed in MIBK:IPA at 9:1 ratio for 60 s (Figure 5.28(c)). The ZEP openings are 50 nm and 100 nm in width, on two different samples respectively, and 1 inch in length. After the sample is dried with N₂ gas for 60 s, it is ready to be etched.

The same silicon RIE method, described in Section 5.1.1, may also be used for etching gratings. The RIE parameters are: RIE power = 100 Watt, pressure = 100 mTorr, CHF₃ flow = 12 sccm, SF₆ flow = 30 sccm, and O₂ flow = 20 sccm. Backside cooling with Helium is applied at 10 sccm. The etching time is 20 seconds to achieve a ~ 120 nm etch depth and nearly vertical side-walls, with θ = 0°. This is the fabrication step illustrated in Figure 5.28(d).[11]

---

[11]Notes for silicon RIE: 1. The etch rate is closely related to the feature size. All of the etch data is tabulated in Section 5.1.1 for large features. The etch rate for micron-sized features are 20 nm/sec. Also, RIE lag is observed 1 µm wide lines (These features are not characterized and indicated as “x” in the tables). The lag is severe while etching 50 nm and 100 nm wide features, which reduce the etch rate to ~ 6 nm/sec. 2. The total etched depth is also dictated by the sample cleanliness. Since none of the samples are chemically cleaned (i.e. ashing) prior to RIE, the etch rate of a 2-minute job, 12.5 nm/sec, is lower than of a 5-minute job, 20 nm/sec. Therefore, the “true” etch rate of silicon should be greater than 20 nm/sec. A detailed investigation will be carried out in a future study.
Figure 5.28: Illustration of the second alternative protocol to fabricate metal-groove-grating-embedded IPP waveguides.
After RIE, the EBL-resist may be removed by ZDMAC solution (Zeon Chemicals L.P.) for 60 s; then, the gratings are ready to be incorporated with the channels (Figure 5.28(e)). On top of the gratings, \( \sim 6 \, \mu\text{m} \) of \( \text{SiO}_2 \) is deposited using PECVD (set at 1000 sccm silane/nitrogen flow, 1000 sccm \( \text{N}_2\text{O} \) flow, 1500 mTorr pressure, 150W power, and \( 300^\circ\text{C} \) plate temperature, for 20 min). Then, 100 nm of chromium is deposited using an e-beam evaporator (Edwards Auto 306, Wilmington, MA). On top of chromium, photoresist (Microposit S1818) is spun at 3000 rpm, for 90 s, and then baked at 100\(^\circ\text{C}\), for 2 min. The photoresist is then exposed (35 \( mW/cm^2 \) at 365 nm, and 58 \( mW/cm^2 \) at 405 nm) for 20 s, and developed (in Shipley MF321) for 1 min. The sample is rinsed in DI water and dried using \( \text{N}_2 \) gas. Then, the exposed chromium is removed by CR-4 (Sigma-Aldrich) for 30 s (Figure 5.28(i)) and BOE is used to remove the exposed \( \text{SiO}_2 \) at 60 \( ^\circ\text{C} \) for 2.5 min, as shown in Figure 5.28(j).

Now the photoresist and the Cr protection can be cleaned off by an acetone rinse for 1 min followed by a CR-4 rinse for 60 s, as shown in Figure 5.28(k).

To complete the metal Bragg IPP waveguide fabrication, the sample is deposited first with a 100 nm Cr adhesion layer and then a 300 nm silver using e-beam evaporator (Edwards Auto 306, Wilmington, MA), as shown in Figure 5.28(l).\(^\text{12}\)

An SEM image of the fabricated device is shown in Figure 5.29. The channel walls are \( h = \sim 6 \, \mu\text{m} \) in height and have a bottom and top widths of \( b = \sim 8 \, \mu\text{m} \) and \( a = \sim 14 \, \mu\text{m} \), respectively. This is a slightly larger channel opening and does not allow second order mode propagation. Two sets of samples are made for optical

\(^{12}\)Note that the channel material is not limited to \( \text{SiO}_2 \); it could be made of Parylene and SU8. The fabrication protocols for Parylene and SU8 are presented in Appendix E.
characterization: the first set has grating periods $\Lambda_{\text{Bragg}} = 765 \text{ nm}, 770 \text{ nm}, \text{ and } 775 \text{ nm}$ groove dimensions of $L_{\text{Bragg}} = \sim 50 \text{ nm}$ and $H_{\text{Bragg}} = 50 \text{ nm}$, and filled with air ($n_d = 1$). The second sample has Bragg grating $\Lambda_{\text{Bragg}} = 564 \text{ nm}$, groove dimensions of $L_{\text{Bragg}} = 30 \text{ nm}$ and $H_{\text{Bragg}} = 30 \text{ nm}$, and filled with varying index oil fillers (Series AAA by Cargille Labs) having index $n_d = 1.3538, 1.3634, \text{ and } 1.3730$ at a 1550 nm wavelength. On both samples, the grating period is repeated 100 times.

5.7 Optical experiment of metal Bragg IPP waveguide sensors

The same end-fire coupling setup from Section 5.4 (Figure 5.20) is used to characterize the samples.
A Bragg resonance shift can again be demonstrated by changing the grating period, $\Lambda_{\text{Bragg}}$. The Bragg resonance shifts in the reflection spectra due to changing grating periodicity is shown in Figure 5.30. The figure reveals a distinct $\sim 11$ nm wavelength shift for each 5 nm change in grating period. The experiment resonant width (FWHM) is $\sim 18$ nm in wavelength.

A Bragg resonance shift can also again be demonstrated by changing the dielectric filler index, $n_d$. Figure 5.31 plots the reflection spectra of the $\Lambda_{\text{Bragg}} = 564$ nm sample versus filler oil indices and reveals a distinct $\sim 11$ nm wavelength shift for each 0.01 change in RIU, which converts to a $\sim 1100$ nm/RIU sensitivity. All spectra are normalized to unity peak power. The experiment shows agreement with the design shown in Section 5.6. The experimentally observed resonance clearly has a narrower resonance. This could be caused by the fact that the gratings are smoothed.

To calculate the SR (recall in Section 2.3) of the theoretically simulated metal
Figure 5.31: The reflection spectra of oil-filled metal-groove Bragg-grating-embedded waveguides. The gratings have a fixed $\Lambda_{\text{Bragg}} = 564$ nm. The index matching oils have $n_d = 1.3538, 1.3634,$ and $1.3730$ at 1550 nm wavelength. The solid lines represent the experimentally observed power spectra, and the dashed lines represent the calculated (FDTD) spectra.

Bragg IPP sensor, $dn/d\lambda = 10^6$ RIU/m and $\delta \lambda' = 12 \times 10^{-9}$ m; therefore, $SR = 0.012$ RIU. From the experimental data, $dn/d\lambda = 10^6$ RIU/m and $\delta \lambda' = 6 \times 10^{-9}$ m; therefore, $SR = 0.006$ RIU.

Recall from Literature Review (Chapter 2) that the SNR is also an important sensor design criterion. From the tabulated IPP mode indices in Table 3.2, the hybrid modes in the PMMA-modulated IPP waveguides have twice the loss comparing to the SPP modes in the waveguide without PMMA modulation – the SNR in metal grating therefore is much more improved comparing to the PMMA rib Bragg IPP sensors. Figure 5.32 compares the experimentally obtained metal grating output spectrum at resonance with PMMA rib grating at resonance. The comparison reveals a $\sim 6$ times higher signal power from the metal grating waveguides. Under optimized conditions, the simulation of the same devices reveals a $> 10$ times improvement using metal
gratings. This plot shows a 0.6% reflected power for the metal gratings, which needs to be improved in a future work.

In conclusion, by using metal gratings rather than dielectric gratings, without introducing other changes, the SR is maintained and the SNR is improved by at least 6 times. Metal grating embedded IPP waveguides are also the best of the three methods to be implemented in a sensor.

All of the characterized Bragg IPP waveguide sensor performance factors (i.e. three sensors presented in Chapter 5) are tabulated in Table 5.6. Clearly, the simulated results show much higher powers compared to the experimentally obtained data. This discrepancy could due to a collected effect of mode-coupling loss, sample surface roughness, non-optimized signal collection and excitation scheme, and optical system loss. These factors shall be explored in a future project.
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>PMMA rib in air Exp.</td>
<td>N.A.</td>
<td>8</td>
<td>N.A.</td>
<td>A*</td>
<td></td>
</tr>
<tr>
<td>PMMA rib in air FDTD</td>
<td>N.A.</td>
<td>8</td>
<td>N.A.</td>
<td>B*</td>
<td></td>
</tr>
<tr>
<td>metal in air Exp.</td>
<td>N.A.</td>
<td>17</td>
<td>N.A.</td>
<td>7×A</td>
<td></td>
</tr>
<tr>
<td>metal in air FDTD</td>
<td>N.A.</td>
<td>17</td>
<td>N.A.</td>
<td>10×B</td>
<td></td>
</tr>
<tr>
<td>PMMA hole in air Exp.</td>
<td>N.A.</td>
<td>6</td>
<td>N.A.</td>
<td>10×A</td>
<td></td>
</tr>
<tr>
<td>PMMA hole in air FDTD</td>
<td>N.A.</td>
<td>6</td>
<td>N.A.</td>
<td>B</td>
<td></td>
</tr>
<tr>
<td>PMMA rib in oil Exp.</td>
<td>1100</td>
<td>10</td>
<td>0.008</td>
<td>C**</td>
<td></td>
</tr>
<tr>
<td>PMMA rib in oil FDTD</td>
<td>1100</td>
<td>10</td>
<td>0.008</td>
<td>D**</td>
<td></td>
</tr>
<tr>
<td>metal in oil Exp.</td>
<td>1100</td>
<td>9</td>
<td>0.006</td>
<td>6×C</td>
<td></td>
</tr>
<tr>
<td>metal in oil FDTD</td>
<td>1100</td>
<td>16</td>
<td>0.012</td>
<td>10×D</td>
<td></td>
</tr>
</tbody>
</table>

Comments: the experimental data could be improved. At this phase of the project, \(*B \simeq 100 \times A\), \(**D \simeq 100 \times C\).

Table 5.6: IPP Bragg sensor performance summary. The theory spectra, marked as "The", in this chapter plot the EIM derived curves and not FDTD simulated.
Chapter 6

Conclusions

This thesis has presented the design, fabrication, and characterization of novel IPP waveguides and Bragg-grating-embedded IPP waveguide sensors, demonstrating non-invasive in vitro sensor designs with competitive performance. The large IPP waveguide geometry offers easy fabrication, simple packaging, and integration into LOC devices. Despite the device losses discussed in Chapter 5, all sensor signal levels are more than sufficient to provide competitive detection.

From the discussion in Chapter 2, competitive sensors are evaluated according to sensitivity, SR, SNR, testing standards, fabrication issues, and device dimension. These criteria are applied here to summarize the IPP Bragg sensor performance with respect to other sensor architectures. The values of these performance factors for the three sensors presented in Chapter 5 are tabulated in Table 5.6.

1 Sensitivity

Both the PMMA-rib Bragg-grating-embedded IPP sensor and the metal-groove
Chapter 6. Conclusions

Bragg-grating-embedded IPP sensor demonstrate a 1100 nm/RIU sensitivity, which is competitive with the other sensor architectures in the prior art.

2 SR (figure of merit)

A new definition of SR, $SR = \frac{dn}{d\lambda} \times \delta\lambda'$, was proposed in Section 2.3, different from the definitions used in the published literatures, in hopes to unify the sensor testing standards. Applying the new SR definition, the IPP sensors were evaluated. All the Bragg IPP-based sensors presented in the thesis have a $\frac{dn}{d\lambda} = 10^6$ [RIU/m]. The PMMA-rib Bragg-grating-embedded IPP sensor resonance offers a resolving power of $\delta\lambda' = 8 \times 10^{-9}$ [m]; therefore, the SR of the PMMA-rib IPP sensor is 0.008 RIU. The metal-groove Bragg-grating-embedded IPP sensor resonance offers a resolving power of $\delta\lambda' = 6 \times 10^{-9}$ [m]; therefore, the SR of the metal-grating IPP sensor is 0.006 RIU. Both of these SRs are well above the ambient-noise-dictated detection limit of $10^{-6}$ RIU (also discussed in Section 2.3); therefore they are practical SRs. Lastly, the IPP sensors presented can “see” a $< 0.01$ index change and hence can “see” a micro-molar molecular density change, therefore exceeds the performance of an optical microscope (recall Chapter 1).

3 SNR

Unlike in the published literatures, the experimental setup in this thesis excludes signal-boosting techniques such as a lock-in amplifier, signal spatial averaging, and signal temporal averaging. The SPP signal is boosted only by utilizing a less lossy IPP mode. From experiments, the fabricated metal groove
Bragg-grating-embedded IPP sensor improves the SNR by 7 times, compared to the PMMA-rib Bragg IPP sensor, as shown in Section 5.7. The simulated results show a 10 times improvement. Most of the existing SPP sensor literature does not discuss the absolute power detected, therefore further comparisons with other sensors can not be made.

4 Testing standards

Unlike in the published literatures, where alcohol and water solutions are used to characterize the sensors, all sensors characterization performed in this thesis (Section 5.4 and 5.7) use a stable index oil based solution. The oil is less likely to evaporate and has a well-known calibrated material dispersion. Also, as mentioned in Item 2 above, a new definition of SR is proposed to encourage standardization of the characterization variables.

5 Fabrication issues

In this thesis, all three types of IPP sensors (Section 5.4, 5.5, and 5.7) have a dielectric material substrate coated first with a chromium adhesion layer and then a silver layer. The chromium layer helps to extend the longevity of the sensor (Section 5.1.2). Also, the IPP waveguide mode is resilient to environmental and material changes, and therefore helps to relax many normally stringent fabrication conditions. Lastly, the IPP waveguides have > 1 micron feature sizes, therefore their fabrication can be carried out in most existing microfabrication facilities.

\footnote{All experimental data are averaged to remove noise. All original data has SNR > 10.}
Chapter 6. Conclusions

6 Packaging size

Because a 2D planar excitation scheme can be used, the IPP sensor devices in this thesis are much more compact than any prism-excited device, and at the same time has fewer mechanical connections.\(^2\)

Also it follows from the above evaluations that the IPP sensors may be readily adapted by a LOC integrated system. Figure 6.1 shows a preliminary design of the LOC packaging. The pump, the light source, and the detector all have approximately 1 cm × 0.5 cm × 0.5 cm dimensions. The final device would have a packaging dimension of approximately 10 cm × 10 cm × 10 cm. This is a much reduced size comparing to the conventional LOC designs. The life-time of each component is also projected in the figure: the short life-span of the sensor body is dictated by the surface chemistry shelf-life and must be replaced every 10 month\(^3\); and, the long life-time of the light source, detector, and the fiber circulator offer reusability and therefore reduce material consumption and cost. Both compactness and cost-effectiveness makes this sensor design more practical than other sensor architectures.

In conclusion, plasmonic in vitro sensors built using the novel Bragg-grating-embedded IPP sensor design offers competitive performance in a superior sensor architecture, simultaneously satisfying the need for non-invasiveness, result-reproducibility, good sensitivity, and continuity/reusability in one device. Therefore, because of its

\(^2\)Mechanical connections are believed to be bulky and introduce noise. They also cause packaging alignment complications and are labor intensive in the manufacturing process.

\(^3\)The 10-month shelf-life is a chemical property shared amongst all functionalized surfaces. Comparing this technology to the one-time-use nanoparticles, which offer 14 day particle aggregation period, the 10-month reusable IPP sensor offers a much longer sensor body lifetime and shelf-life.

\(^4\)Compared to the performance of the MD SPP sensors.
improvements over the existing plasmonic devices, the Bragg-grating-embedded IPP waveguide sensors presented in this thesis provide an enabler for LOC devices to adapt plasmonic technology. In addition to contributing to the existing scientific knowledge set, with incorporation of biological and/or chemical materials for specific binding detection the sensor designs presented here can provide a foundation for solving real-life problems such as treating disease and illness at early stages.
Appendix A

List of Publications

A.1 Patent

1. James Stewart Aitchison (50%), Yechen Xu (50%), confidential subject, Invention disclosure submitted to the university on August 17, 2010.


A.2 Refereed journal publications


### A.3 Work done but not included in this thesis


### A.4 Refereed conference publications


A.5 Local meetings


Appendix B

Fabrication: ITO Etching

All fabrication protocol provided in this thesis was developed in the University of Toronto cleanroom. The purpose to document these protocols is to provide a foundation for any related work. The exact condition may not apply elsewhere and when carried out by a different personnel.

First, the ITO sample is cleaned according to the following recipe:

1. 6 min in acetone
2. 6 min in methanol
3. rinse with DI
4. $N_2$ dry the sample
5. 30 min dehydration @ 120° C

***The following ITO wet etching recipe was communicated from Dr. Lu’s group at Material Science.

1. spin primer, Hexamethyl-disilizane (HMDS), 30 s, 3000 rpm
Appendix B. Fabrication: ITO Etching

2. bake at 200\(^\circ\) C, 2 min
3. spin S1813, 9 s @ 500 rpm; then 60 s @ 2000 rpm
4. bake 110\(^\circ\) C on hotplate (small pieces), 2 min
5. soft-baking, 90\(^\circ\) C, 3 min
6. exposure 50 s
7. develop MF 319, 30 s, (or TMAH. MA-D331)
8. hard baking 100\(^\circ\) C, 30 min

***The following is the modified version of the above recipe. By using the following recipe, one may easily obtain 2 \(\mu\)m wide ITO strips, as shown in Figure B.1.

1. clean the sample following the same method
2. spin primer: p-20. cover the top surface with primer, and let it sit for 3-5 min. then, spin 90 sec @ 3000 rpm
3. bake the primer at 95\(^\circ\) C for \(\sim\) 1 min
4. spin photoresist: S1818. cover the top of the sample surface with S1818, spin immediately, 90 sec @ 3000 rpm
5. bake the sample 115\(^\circ\) C, 2 min
6. exposure: 8 s, soft contact, sample-mask distance 100 \(\mu\)m.
7. develop: MF321. \(\sim\) 1 min @ room temperature.
9. after the ITO is all washed off, dip the sample in acetone - the photoresist should come off immediately.
Appendix B. Fabrication: ITO Etching

Figure B.1: Optical microscope image of the etched ITO. Each strip is 2 µm in width.
Appendix C

Fabrication: Silver Wet Etch

All fabrication protocol provided in this thesis was developed in the University of Toronto cleanroom. The purpose to document these protocols is to provide a foundation for any related work. The exact condition may not apply elsewhere and when carried out by a different personnel.

By using the following recipe, one may easily obtain 5 µm wide ITO strips, as shown in Figure [C.1].

The etching solution consists of the following chemicals (0.36 µm/min etch rate):

- 120 ml DI water
- 40 ml methanol (CH₃OH)
- 10 ml hydrogen peroxide (H₂O₂)
- 10 ml ammonium hydroxide (NH₄OH)

Comments:

1. this solution does not etch SiO₂.
Figure C.1: Optical microscope image of etched silver film. Each strip is 5 µm in width.

2. for smoother etching: dip the sample in for 1 s, take it out, dip it back in for another second, repeat.

3. related publication: "In order to achieve different etching rates, the concentration of $H_2O_2$ was varied in the solution from 1.2% to 4%, the resulting values for etch rate were about 3 nm/s for the 1.2% solution and about 100 nm/s for the 4% solution" Hauder et al. Microelectronic Engineering, Volume 60, Issues 1-2, January 2002, Pages 51-57. The same paper also talks about ferric nitrate etching.
Appendix D

Fabrication: Lift-off

All fabrication protocol provided in this thesis was developed in the University of Toronto cleanroom. The purpose to document these protocols is to provide a foundation for any related work. The exact condition may not apply elsewhere and when carried out by a different personnel.

D.1 Metal lift-off using S1818

NOTE: the original protocol was communicated by Dr. Liang from McMaster. Dr. Liang’s Toluene protocol was developed based on S1813 which is a less viscous photoresist. Because S1818 is much thicker than S1813 (at the same spin speed), the toluene soaking time used in this protocol is much longer.

1. clean wafers or glass slices using piranha (see the piranha protocol in Appendix G)

2. spin P-20. (leave P-20 on the sample for 10 s prior to spinning 1818. After spinning, let it dry for ~ 1 min)
Appendix D. Fabrication: Lift-off

3. spin S1818, 3000 rpm, 30 s (note: spin immediately)

4. soft-bake on hotplate, 95° C for 90 s

   (a) for lift-off, bake a bit longer than the usual photoresist protocol (e.g. ~ 2 min) and increase the temperature to 115° C.
   
   (b) 115° C is temperature set on the hot plate – the thermometer measured temperature is only 100° C at the hot spot on the hot plate.

5. expose, 5 s, soft mode, mask distance:100 µm (note: for lift-off EXPOSE a bit longer than usual (e.g. 8 s))

6. submerge in Toluene for 6 min (note: may need to extend the soaking time to 10 min. Then, Blow dry and drybake, 90° C on hotplate for 15 sec)

7. develop, around 60 s (note: very thin sample will take a longer time to be developed, ~ 1:30 min. Now, you can verify the undercut by changing the focal plan of the microscope objective.)

8. bake on hotplate or oven at 60° C for 30 min (this one is optional for lift-off protocols as long as the metal deposition is not too fast.)

9. mount the samples into E-beam evaporator, evaporate 50 nm Cr first, and then evaporate Au. (note: less than 0.3 nm/s rate is good.)

10. immerse in acetone

   (a) acetone may be replaced by AZ300
   
   (b) when all procedures are done properly, the lift-off occurs within few minutes. if the photoresist is overheated during metal deposition, lift-off may require whipping the surface with a cloth to physically take off the photoresist
   
   (c) one may leave the substrate in solution overnight, and then use ultrasonic

D.2 Metal lift-off using S1811

1. drop P-20 on the substrate, and leave for 1 min (note: make sure that P-20 covers the entire surface of the sample)

2. spin P-20, 6000 rpm, 60 sec (after spinning, let it dry for ~ 1 min)
3. drop excessive amount of S1811 on to the sample and spin immediately, 6000 rpm, 60 sec (note: spin immediately)

4. soft-bake on hotplate, 115° C (reading on the hotplate meter), 90 sec

5. expose using mask aligner, 5 sec, soft contact, mask distance: 33 μm

6. submerge in Toluene, 6 min

7. blow dry and bake dry on hotplate, 90° C, 15 sec

8. develop, around 1-1.5 min (note: very small sample will take longer time to be developed, ~ 1:30 min. Now, you may verify the undercut by changing the focal plan of the microscope objective.)

9. 20 nm of silver (note: less than 0.3 nm/sec is good.)

10. immerse in AZ300T, the photoresist should come off in a few minutes.

**D.3 2 μm gold layer lift-off on silicon substrate, using S1818**

1. drop spin P-20, wait for 10 sec. and then spin @ 6000 rpm for 60 sec. let it dry for 60 s

2. drop S1818, spin immediately @ 2000 rpm for 60 sec

3. soft-bake on hotplate @ 115° C for 90 sec

4. exposure, 8 sec (thick resist), soft contact, 33 μm distance

5. submerge in Toluene for 6 min (may extend to 10 min)

6. blow dry using air gun and then bake dry

7. develop, around 1-1.5 min (note: because it has been soaked in Toluene, development should be on the longer side.)

8. evaporation, 50 nm of Cr first, then 2 μm of gold (note: Cr must be deposited under 0.15 nm/sec; or, it may flake off.)

9. immerse in AZ300T.
Appendix E

Fabrication: $SiO_2$, Parylene, SU8 Channels

Note: this is an original protocol developed for this thesis. All fabrication protocol provided in this thesis was developed in the University of Toronto cleanroom. The purpose to document these protocols is to provide a foundation for any related work. The exact condition may not apply elsewhere and when carried out by a different personnel.

E.1 $SiO_2$ channels (Figure E.1)

1. clean silicon substrate (note, the substrate is not limited to silicon.)

2. PECVD: silane/nitrogen 1000 sccm, $N_2O$ 1000 sccm, pressure 1500 mTorr, power 150 Watt (for 300 nm/min deposition) @ 300° C for 20 min

3. Electron beam metal coating: 100 nm chromium @ 0.1 nm/s

4. spin coat S1818 @ 3000 rpm, 90 s
Appendix E. Fabrication: $SiO_2$, Parylene, SU8 Channels

Figure E.1: $SiO_2$ channel on corrugated silicon substrate.

5. hot plate 105°C, 2 min
6. UV exposure, 20 s
7. develop in MF 321, 60 s
8. rinse in DI water, 60 s
9. chromium etch in CR-4, 30 s
10. $SiO_2$ etch in Buffered Oxide Etch, for 2 min in solution temperature 60°C
11. acetone rinse, CR-4, and $N_2$ gas dry
12. metal coating (optional)

E.2 Parylene channels (Figure E.2)

Note: Parylene has poor adhesion with silicon surfaces; therefore, for any process involves heating, temperature must be ramped up gradually.

1. clean silicon substrate
2. parylene coating: (13 grams of Parylene C powder yield 6 µm thick film)
3. electron beam metal coating: 100 nm chromium @ 0.1 nm/s
4. spin coat S1818 @ 3000 rpm, 90 s
Appendix E. Fabrication: $\text{SiO}_2$, Parylene, SU8 Channels

Figure E.2: Parylene channel on corrugated silicon substrate. Note: the cracking in Parylene is unanimous. There may be a recipe to eliminate the cracks.

5. hot plate 105°C, 2 min (place the sample on the hotplate when it is still in room temperature, and then turn on the hot plate.)

6. UV exposure, 20 s

7. develop in MF 321, 60 s

8. rinse in DI water, 60 s

9. chromium etch in CR-4 (if Cr is 100 nm, etch for 30 s If Cr is 200 nm, etch for 60 s at room temperature)

10. RIE Parylene: 150 W RIE power, 98 sccm $\mathrm{O}_2$, Pressure 200 mTorr, 15 min

11. chromium removal in CR-4 (if Cr is 100 nm, etch for 30 sec. If Cr is 200 nm, etch for 60 s at room temperature)

12. DI water rinse

13. $\mathrm{N}_2$ gas dry

E.3 SU8 channels (Figure E.3)

1. clean silicon substrate

2. spin coat SU8-50 @ 1000 rpm, 60 s
Appendix E. Fabrication: $SiO_2$, Parylene, SU8 Channels

Figure E.3: SU8 channel on corrugated silicon substrate.

3. prebake: $65^\circ C$, 10 min
4. softbake: $95^\circ C$, 30 min
5. UV exposure, 30 s
6. postbake: $65^\circ C$, 1 min, and then, $95^\circ C$, 10 min
7. develop in SU8 Developer, 5 min
8. rinse in IPA
9. $N_2$ gas dry
10. hardbake @ $170^\circ C$
Appendix F

Fabrication: Buffered Oxide Etching

All fabrication protocol provided in this thesis was developed in the University of Toronto cleanroom. The purpose to document these protocols is to provide a foundation for any related work. The exact condition may not apply elsewhere and when carried out by a different personnel.

1. PECVD $SiO_2$ @ 40 nm/min for 5 min @ 300° C
2. spin S1811 onto sample
3. soft-bake @ 115° C, 90 s
4. exposure soft contact, 5 s, 33 $\mu$m distance
5. develop 1-1.5 min
6. Put on the Trionic acid resistant gloves.
7. follow the BOE safety procedure
Comments:

1. Recall Section 5.6 uses a hot BOE solution. Here a BOE solution at room temperature is used.

2. The etch rate is usually an exponential curve as a function of the solution temperature. Also, it is important to know that the solution temperature is different from the hot plate setting.

3. The average etch rate of thermally grown oxide in the 10:1 BOE solution is 600 Å/min; and 900 Å/min for sputtered oxide. Thus, for 200 nm thick SiO$_2$, use \( \sim 4 \) min to etch away the glass.

4. The solution deteriorates with use and the etch rate may become lower over-time.

5. When etching is finished, carefully remove the wafer holder from the solution and immerse it into a bucket of DI water.

6. Leave the wafer holder in DI water for a few minutes. Shake gently.

7. Remove the wafers from the wafer holder using a pair of tweezers. Place the wafer, one at a time.
Appendix G

Fabrication: Piranha Cleaning

Method

All fabrication protocol provided in this thesis was developed in the University of Toronto cleanroom. The purpose to document these protocols is to provide a foundation for any related work. The exact condition may not apply elsewhere and when carried out by a different personnel. Also, this may not be an original protocol developed for this thesis. The documentation of this protocol is for completeness; and there is no intention to plagiarize.

G.1 Substrate cleaning with Piranha

1. sonication in Tri-chlor ethylene, 5 min (note: optional)
2. sonication in acetone, 5 min
3. sonication in ethanol, 5 min
4. sonication in DI water, 5 min (note: can be replaced by DI water)
5. piranha etch, 10-20 min (note: piranha solution should be prepared fresh)
6. rinse in DI, 1 min (note: the samples may be soaked in DI water to prevent contamination.)
7. dehydration bake, 135°C, 20 min (note: the temperature setting depends on the material. 135°C is good for most samples)

**G.2 Piranha solution preparation**

1. prepare a large beaker, leave room for overflowing Piranha
2. prepare 3 portion (in volume) of sulfuric acid ($H_2SO_4$) and 1 portion (in volume) of 30% hydrogen peroxide ($H_2O_2$)
3. pour the sulfuric acid in a beaker
4. pour the hydrogen peroxide in the same beaker
5. the solution is ready in 10 min (note: the solution bubbles)

Comments:

1. The reaction is HIGHLY EXOTHERMIC.
2. As soon as the samples are out of the Piranha solution, they should never be in air. Otherwise, the samples could be contaminated again.
3. the cleanliness of glass substrates could be confirmed by contact angle measurement (hydrophilic).
Bibliography


son, and H. Irth, “Development of surface plasmon resonance biosensor assays 
for primary and secondary screening of acetylcholine binding protein ligands,” 

[3] D. Dell’Orco, M. Miller, and K.-W. Koch, “Quantitative detection of conforma- 
tional transitions in a calcium sensor protein by surface plasmon resonance,” 


tion testing of glucose-detecting biosensors: Current methods and recommenda- 


