A Highly Sensitive, Integrable, Multimode, Interferometric, Evanescent-Wave Chem/bio Sensor

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A Highly Sensitive, Integrable, Multimode, Interferometric, 
Evanescent-Wave Chem/bio Sensor

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This work is dedicated to my wife, Kazuko. Her encouragement motivated me, her patience and tireless efforts gave me needed time, and her trust empowered me. It is also dedicated to my daughters, Leonora Mizuki and Nanami Karina. Their laughter lifted me and their development always amazed me.
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A fully integrated optical chem/bio sensor complete with integrated source, chemically sensitive waveguide, detector arrays, and associated signal processing electronics on a Si-CMOS chip is a challenging, but highly desirable goal. An evanescent-wave multimode interferometric sensing element is a sensitive method for sensing, which is easily integrated on Si-CMOS. This work is concerned with the design, analysis, and demonstration of a planar multimode interferometric chem/bio sensor that is compatible with the fabrication constraints of Si-CMOS.

A 4000-micron-long interferometric that can be adapted for different agents by a particular sensing layer has been fabricated on silicon using silicon dioxide and silicon oxynitride. Hexafluoro-isopropanol substituted polynorbornene is the sensing layer. This sensor has also been fabricated on a Si-CMOS circuit with embedded photodetectors. A sensor on silicon was demonstrated with a minimum detectable index change of $2.0 \times 10^{-6}$ using an accurate gas delivery system and a custom hermetic waveguide test chamber. A modal pattern analysis strategy has also been developed to extract the optimal SNR from the measured modal patterns. An understanding of the noise processes and spatial bandwidth effects has enabled an experimentally-based prediction of the index sensitivity of a fully integrated multimode chem/bio sensor on Si-CMOS at $9.2 \times 10^{-7}$.

Theoretically, the sensitivity enhancement of high over low index sensing layers and transverse-magnetic over transverse electric modes is described. Also, the sensitivity enhancement of higher-order-transverse modes has been quantified. The wide-angle beam propagation method has been used to simulate the sensor. This simulation showed the relation between the modal pattern repetition period and sensor sensitivity. Further, the modal coupling properties of the multimode y-junction have been described. A second multimode y-junction has been designed to change the modal excitation under the SL, and thus the sensitivity.
The chemo-optic response of the ‘substituted polynorbornene’ polymer, bis-trifluoromethyl
carbinol-substituted polynorbornene to methanol, water, iso-propanol, and benzene has
been measured. Also, its thermo-optic response has been measured. Athermal interfero-
metric chem/bio sensors have then been suggested.

The major findings and demonstrations developed during this investigation have led to
a fundamental understanding of this type of evanescent-wave multimode chem/bio sensing.
Chapter I

INTRODUCTION

An industry research report written in early 2003 [1], states that “…revenues for next-generation biological and chemical sensors will grow from $2.3 billion in 2002 to almost $4 billion in 2007…” This amount of revenue suggests a high and increasing need for chem-bio sensors. From blood glucose testing for diabetes, to replacing slow, complex, labor-intensive material identification methods, more and more optical sensors are being used to detect biological agents. In addition, the military requires small, highly accurate, fast sensors to protect their personnel in the battlefield from both biological and chemical weapons. Industrial companies also need to protect their personnel from accidents arising from the use and manufacture of dangerous chemicals. Further, the aforementioned research report suggests that optical sensors could be used in explosives and narcotics detection.

Regardless of the application, a standard platform which can be adapted by different sensing layers or mechanisms to detect any of these agents with high sensitivity is clearly desirable. Further, this platform must be mass-producible for low unit-cost and ideally should contain all signal processing onboard. For these reasons, a fully integrated optical chemical sensor on a Silicon Complementary Metal Oxide Semiconductor (Si-CMOS) circuit is being developed and tested. This thesis is concerned with the demonstration and investigation of multimode planar waveguide interferometric chem/bio sensors as the optical transducers of fully integrated sensors on Si-CMOS.

1.1 Current Embodiments of Evanescent Wave Sensors

Optical evanescent-wave sensors (EWSs) based on planar waveguides, in particular, are highly sensitive, compact, highly stable devices, which are relatively easily fabricated. These sensors, as the name implies, accomplish detection through an interaction between the evanescent field of a guided mode of light, and the target agent. This interaction may be
direct, or it may be facilitated by a sensitive material, that may absorb or even chemically interact with the agent. This interaction may produce absorption at various wavelengths, fluorescence, or phase changes at one wavelength. In the case of phase change, this phase change can be detected in different ways.

If the change is primarily a phase change, different ‘optodes’ may be used to extract this phase change. These types of sensors to detect chemical or biological agents have been demonstrated in various forms. In integrated optical devices, this phase change can be described by a change in the effective index of one or more guided modes. Highly-resolved sensing of this effective index change has been demonstrated using gratings [2] and [3]; resonant microcavities [4]; and interferometers [5], [6], [7], and [8].

A multimode Mach-Zehnder interferometer (MZI) fabricated on silicon that is fully compatible with silicon CMOS fabrication constraints is described. Multimode MZIs have a large area for sensing and the entire modal pattern output, which responds to the presence of an agent on the sense arm, can be exploited for increased sensitivity.
Chapter II

ORIGIN AND HISTORY OF THE PROBLEM

2.1 Evanescent-wave Sensors

Chemical or biological sensors that detect a direct or indirect interaction between the evanescent field of light guided through a waveguide and a chemical or biological agent are referred to as evanescent-wave sensors (EWS). Planar waveguide EWSs usually have a thin, high-index (1.8-2.0) guiding layer over a relatively lower (1.45) index substrate. This geometry forces a significant fraction of the evanescent field into the region above the waveguide. Changes in the refractive index (RI) of this area (the cover), $n_c$, are felt by the guided light, and alter its propagation through the waveguide. The propagation of the light is governed by its effective index, $n_{eff}$. The effective phase velocity of a guided mode is $c/n_{eff}$. The modal field distribution is also governed by $n_{eff}$ through the transverse wave vector, $\kappa_f$, and the field decay constants, $\gamma_{c/s}$, all of which are functions of $n_{eff}$. The alteration in propagation is represented by the change in effective index, $\Delta n_{eff}$.

A sensitive geometry is one in which changes in some waveguide parameter (layer thicknesses or indices) strongly affect the modal effective index. For specific agents and sensing mechanisms, different geometries may yield good sensitivity. For example, Figure 1a [9], shows a semi-infinite cover layer (C) with index, $n_c$, above a sensing layer (SL) with index $n_l$ and height, $h_l$, and a waveguide film (F) with index $n_f$ and height, $h_f$. If only the SL index, the SL height, and the C index vary during detection, the effective index, $n_{eff}$, of a guided mode of this structure changes with $n_l$, $h_l$, or $n_c$ as per Equation 1.

$$\Delta n_{eff} = \frac{\partial n_{eff}}{\partial n_l} \delta n_l + \frac{\partial n_{eff}}{\partial h_l} \delta h_l + \frac{\partial n_{eff}}{\partial n_c} \delta n_c$$ (1)

The sensitivity of a particular device thus depends on the magnitude of the sensitivity constants, $\frac{\partial n_{eff}}{\partial n_l}$, $\frac{\partial n_{eff}}{\partial h_l}$, and $\frac{\partial n_{eff}}{\partial n_c}$. For example, in Figure 1b, the SL has been removed and thus only changes in the cover index affect the effective index, so $\frac{\partial n_{eff}}{\partial n_c}$ is important. By
Figure 1: Examples of Optical Chemical Sensor Layer Geometries: (a) general, (b) and (c) changing cover index, and (d) small adhesion layer. from Sensors and Actuators B 38-39, pp. 13-28, 1997

comparison, in Figure 1d, the evanescent field passes through a very thin SL. Assuming that \( n_I \) and \( n_c \) stay constant, but \( h_I \) changes, then \( \frac{\partial n_{eff}}{\partial h_I} \) governs the sensor response. In fact, all three effects may be present simultaneously and may act constructively or destructively depending on the materials. Thus, the dimensions, and if possible, the indices of the layers must be chosen carefully to maximize sensitivity.

2.2 Sensitivity of Evanescent Wave Sensors (Vertical)

2.2.1 For TM Modes

A brief investigation into sensitivity optimization by adjustment of guiding layer thickness has been completed. The sensitivity constants of EWSs may be calculated from a zigzag ray model or from a boundary value problem based on Maxwell’s equations [10]. A transverse magnetic (TM) electric field propagating in a semi-infinite 3-slab, step-index, dielectric waveguide is considered. The film, substrate, and cover indices, \( n_f, n_s, \) and \( n_c, \) and film thickness, \( h, \) define the physical structure. All materials are lossless, non-conducting, and have no free charges. Along with the boundary conditions that the tangential electric and magnetic fields be continuous on the boundaries, the field must decay to zero in the cover and substrate regions. It can be shown [10] that the eigenvalue equation for the guided
mode’s effective index, $n_{\text{eff}}$ is Eq. 2. A simple model is shown in Fig. 2.

\[
\tan (h\kappa_f) = \frac{\kappa_f \left[ \frac{n_c^2}{n_{\text{eff}}^2}\gamma_s + \frac{n_f^2}{n_{\text{eff}}^2}\gamma_c \right]}{\kappa_f^2 - \frac{n_c^4\gamma_s\gamma_c}{n_{\text{eff}}^4n_s^2}}
\]  

(2)

The transverse decay constants in the cover and substrate are $\gamma_{c/s} = k_0\sqrt{n_{c/s}^2 - n_{\text{eff}}^2}$, and the film transverse wave vector is given by $\kappa_f = k_0\sqrt{n_f^2 - n_{\text{eff}}^2}$.

In the specific case of a reversible, polymer-based sensor, the preferred sensing mechanism is index change, suggesting a geometry similar to Fig. 1c. Although thickness changes can be used to increase sensitivity, polymeric sensing layers can stretch, creating undesirable uncertainty in sensor response. Thus, in designing this waveguide sensor, all sensitivity coefficients are minimized, except for $\frac{\partial n_{\text{eff}}}{\partial n_c}$, which is maximized. This coefficient may be calculated numerically, or quasi-analytically. The case of a 3-slab waveguide is presented here. When both sides of Eq. 2 are differentiated with respect to $n_c$, the term $\frac{\partial n_{\text{eff}}}{\partial n_c}$ can be isolated, creating an expression for the index sensitivity coefficient. The TM Eigenvalue Equation must be solved numerically to find $n_{\text{eff}}$, but then, the sensitivity coefficient can be found using this expression. The full expression is included in App. E as Eq. 122. However, results using this expression are presented. First, the analytically calculated sensitivity
coefficient has been compared with increasingly accurate numerical estimations (Fig. 3). Convergence between the analytical expression and the numerical estimate is observed for decreasing numerical step sizes.

![Figure 3: Convergence of numerical estimates to the quasi-analytical value of the sensitivity constant, $\frac{\partial n_{\text{eff}}}{\partial n_c}$, for decreasing numerical step sizes in the cover index, $n_c$.](image)

This expression has been used to estimate the sensitivity coefficient, Fig. 4, for two variations of EWSs. Referring to Fig. 2, the structure is defined by the following: $n_f = 1.90$, $\lambda_0 = 0.84 \mu m$, $n_s = 1.45$, and either $n_c = 1.43$ or $n_c = 1.47$. In the first variation, the index of the substrate, $n_s$, is greater than the index of the cover, $n_c$ (1.43), and so more of the evanescent field resides within the substrate than the cover. The thickness for optimal sensitivity is 0.11 $\mu m$. In the second variation, $n_s < n_c$ (1.47), and more of the evanescent field resides within the cover. The highest sensitivity occurs when the waveguide is as thin as possible, just above the cutoff. A sensor with $n_s < n_c$ is more sensitive than a sensor with $n_s > n_c$.

An intuitive explanation for the peak in sensitivity for $n_s > n_c$ is provided. For very thick guiding layers, the evanescent field extending into the cover layer is a relatively small fraction of the total field. For progressively thinner guiding layers, more evanescent field is forced into the upper and lower cladding. When the waveguide layer gets very thin, (ie. approaches cutoff) the field redistributes more and more into the substrate/lower cladding.
Figure 4: Variation in the sensitivity of EWS with waveguide thickness for two cases: for \( n_s > n_c \) and for \( n_s < n_c \). Waveguide Parameters: \( n_s = 1.90, \lambda_0 = 0.84\mu m, n_s = 1.45, \) and \( n_c = 1.43 \) or \( 1.47 \). The EWS layer structure is shown in Fig. 1c.

layer, reducing the cover index change effects. In the case of \( n_c > n_s \), as the waveguide gets very thin, the field redistributes more and more into the cover/upper cladding, increasing sensitivity up to about double that obtained with \( n_s > n_c \).
2.2.2 TE vs TM Modes

Multimode planar waveguide EWS that have a very thin guiding layer are reasonably well-represented as a TE or TM waveguide, following the effective index method [10]. Generally, for a given waveguide, TM modes are more sensitive to index changes than TE modes. Figure 5 shows the index sensitivity of the single TM guided mode compared to that of the single TE guided mode in the same waveguide structure. The structure corresponds to that shown on the left arm of Fig. 5. Importantly, the peak sensitivity of the TM waveguide is about 15% higher than that of the TE waveguide. In addition, the TE mode attains its highest sensitivity at a thinner guiding layer than the TM mode. Thinner layers have more elliptical mode fields and thus it can be more difficult to couple light into them. For these reasons, EWSs are often designed to work with TM modes. For EWSs, it is desired that penetration into the sensing layer is maximized because this enhances the evanescent interaction with the outer layers. However, evanescent penetration does not explain the enhanced sensitivity of TM modes over TE modes. For example, Fig. 6 shows that at peak sensitivity, a TE mode has a larger portion of evanescent field in the sensing layer than a corresponding TM mode at peak sensitivity. Fundamentally, TM modes are more sensitive.

![Figure 5: Comparison of index sensitivity coefficients vs waveguide thickness for transverse-electric (TE) vs transverse-magnetic (TM) waveguides.](image)

\( n_s = 1.465, n_f = 1.920, n_{SL} = 1.430, \lambda_0 = 0.83 \mu m, \) and \( h_{SL} = 0.95 \mu m. \)
Figure 6: Comparison of power fraction in the sensing layer (SL) for maximum sensitivity transverse-magnetic (a) vs transverse-electric (b) modes (same waveguide as in Fig. 5)

due to their different interaction at the layer boundaries. For a set of TM modes, however, increased penetration into the sensing layer does yield higher sensitivity. For example, Fig. 7 shows that the most sensitive TM mode does have the largest fraction of power in the sensing layer (SL).
Figure 7: Comparison of power fraction in the sensing layer (SL) for a transverse-magnetic (TM) mode of a waveguide with the optimal guiding layer thickness (a) vs another slightly thicker waveguide (b).
2.2.3 Sensitivity and Field Fraction

Intuitively, the index sensitivity might be related to either the power fraction or the field fraction in the SL. In fact, the peak in sensitivity is related to the field fraction (magnetic field for TM modes) within the SL. Figure 8 shows the change in magnetic field fraction with guide thickness and the index sensitivity coefficient. It is clear that the functional relationship is the same. Figure 9 compares the power fraction with the same index sensitivity coefficient. It is clear that, while similar, the agreement is not as good, and that the peaks are at different locations.

Figure 8: Comparison between magnetic field fraction within the SL and the index sensitivity coefficient, $\frac{\partial n_{eff}}{\partial n_{SL}}$.

Figure 9: Comparison between power fraction within the SL and the index sensitivity coefficient, $\frac{\partial n_{eff}}{\partial n_{SL}}$. 
2.3 Current Embodiments of Evanescent Wave Sensors

Interaction of a chemical or biological agent with a sensor in one of the geometries above modifies the effective index of the guided modes of the device. Highly-resolved sensing of this effective index change has been demonstrated in gratings [2] and [3], resonant microcavities [4], and interferometers ([5], [6], [7], and [8]).

2.3.1 Multilayer Grating-Based EWS

A highly-sensitive EWS based on a change in resonant angle of a preferentially reflected diffraction order from a reflection grating has been demonstrated by Challener [3]. A 50-nm-deep grating with a period of 0.6 µm is molded into a polycarbonate substrate. Overtop of this substrate, a 15-nm-thick layer of TiO$_2$, a 10-nm-thick layer of SiO$_2$, and another 15-nm-thick layer of TiO$_2$ are deposited forming a multilayer grating (MG) (Figure 10a).

![Figure 10: (a) The layered grating structure used in this sensor. (b) The experimental setup to monitor the change in resonant diffraction order of the grating. from Sensors and Actuators B 71, pp. 42-46, 2000](image)

A helium-neon laser is collimated and focused as shown in Fig. 10(b) by a cylindrical lens before reaching the reflection grating. After reflection off of the grating, the light passes through a slit, and is focused in the plane of the page by a cylindrical lens, where it is detected by a 256-pixel photodetector array. This MG exhibits a peak in reflected intensity at about 31°. In this EWS, the changing index overtop of the layered grating shifts its resonant peak. During the experiment, avidin, a facilitating layer, adsorbs onto the outer TiO$_2$ surface, shifting the resonant angle by 0.080°, (Figure 11a). With the net noise level
at $4 \times 10^{-6}\degree$, and the resonance angle shift per unit of RI at $18.3\degree$, the RI sensitivity is $2.2 \times 10^{-7}$. Note that the index sensitivity specified corresponds to an SNR of one. Using the comparison standard proposed in this work, the index sensitivity would be $6.6 \times 10^{-7}$.

Next, biotin, a protein, is introduced and attaches to the avidin, creating a shift in resonant angle of $0.0005\degree$, a smaller response (Figure 11(b)).

Figure 11: (a) Grating resonant angle shift as Avidin adsorbed onto the TiO$_2$ surface. The SNR is $2 \times 10^4$, which, together with the $18.3\degree$ per RI unit, demonstrates an index sensitivity of $2 \times 10^{-7}$. (b) Grating angle shift as protein attaches to avidin. from Sensors and Actuators B 71, pp. 42-46, 2000

2.3.2 Microcavity EWS

Krioukov has theoretically studied a planar waveguide microcavity (MC) EWS (Figure 12a) because of the potential for high sensitivity [4]. Interferometric EWSs require a long interaction length to accomplish the phase shift required for sensing. In the case of biological sensing, a large amount of biological material may be required to cover that length. In contrast, the MC has a very small surface area, and requires less material, a highly practical advantage. Further, the guided modes of an interferometer pass through the sensing area once, while in an MC, the light in the cavity may pass under the sensing layer multiple times, increasing sensitivity.

In this implementation, the MC is adjacent to input and output straight ridge waveguides. A small fraction of the light couples evanescently from one ridge waveguide into the
**Figure 12:** (a) Microcavity EWS Schematic. There is coupling between the waveguide modes and the microcavity modes. When the light coupled into the cavity acquires an integer multiple of $2\pi$ radians of phase, the whispering gallery modes are excited and optical power from the input waveguide resonantly builds up. (b) Effect of changing the cover index on the resonance of the microcavity. The point of greatest sensitivity to cover index is at the full width at half max of the resonant peak. *from Optics Letters 27, pp. 512-514, 2002*

MC. After circulating to the other side of the cavity, the same fraction of the MC light couples out into the second ridge waveguide, and after completing the round trip, light similarly couples back into the original waveguide. When the wavelength and effective index of the cavity are such that light passes around with some integer multiple of $2\pi$ radians of phase shift, light resonantly builds up in the cavity as whispering gallery modes (WGM). Simultaneously, less light is coupled out of the cavity back into the first straight waveguide due to destructive interference. The second waveguide, however, still receives power from the MC mode. Thus, at resonance, the MC mode transfers power from the first waveguide to the second. The resonances of the microcavity may be determined by varying the wavelength (using a tunable laser) and measuring the scattered power out of the top of the cavity or the reflection port.

This MC is used as an EWS by fabricating it using one of the layer structures described earlier. Then, as the effective index of the single vertical mode of the cavity changes, the round-trip phase shift in the cavity also changes, shifting the resonant wavelength. In Fig. 7(b), the greatest sensitivity occurs at the wavelength corresponding to the full width at half maximum (FWHM) of the resonance. At this point, a change in resonant frequency results in the largest change in observed power. Further, the author suggests, that in the
shot noise limit, this sensor has a RI sensitivity of $10^{-9}$.

### 2.3.3 Hartman Interferometric EWS

An interferometer has been developed by Hartman et al. ([5], [11], [12], and [13]) for environmental, food-safety, and biomedical sensing. This embodiment of an EWS utilizes a modified Mach-Zehnder-type interferometer as the mechanism to detect the change in effective index created by the sensed agent. A key feature of the Mach-Zehnder structure is the separate sensing and reference waveguides arms. As the light passes under an active sensing region, a change in accumulated phase shift is experienced by the modes of the waveguide. When the light is recombined at the far end of the sensor, these changed accumulated modal phases result in a measurable change in the output pattern. In the single mode case, this corresponds with a sinusoidal variation in intensity. In the case of multiple modes, the change in pattern is very complex, but in general, some points in the pattern will increase in intensity and others will decrease. These changes in intensity indicate chemical detection.

One advantage of this type of interferometric EWS is that the reference and sensing arms are made of almost identical materials. This minimizes some common thermal and other environmental index effects, because the interferometer detects differential phase shifts among modes. Most of the common phase shifts will be cancelled by the interferometric process. In spite of this, an increasing temperature does change the shape and potentially the number of modes present in both guides similarly due to the changing optical size of the waveguides. This possibility must be accounted for in interpreting sensor response.

The key elements of the structure are shown schematically in Fig. 13. An input grating couples 0.670 or 0.780-μm wavelength light from a diode laser into two nearly equal sensing and reference arms. The sensing arm is coated with a chemically or biologically sensitive material. Although not explicitly mentioned, it is inferred that the reference arm either is not covered with this material or the material is rendered insensitive by other means. At the end of the waveguide, there is a beam splitter/combiner that is designed to transfer half of the optical power from one guide to the other and vice versa. Finally, an output grating
couples the light down through the substrate and into a 128-element photodiode array, [14], with pixel dimensions on the order of 60 \( \mu m \). This photodiode array is read to a computer which then completes the signal processing and identification of the agents.

![Diagram of Hartman Interferometric EWS schematic side view and top view.](image)

**Figure 13:** (a) Hartman Interferometric EWS schematic side view. Gratings are used to couple light into and out of the interferometric EWS portion of the device. (b) Hartman Interferometric EWS top view. On the sensing arm only, a chemically or biologically sensitive agent is exposed to the environment. *From SPIE Proceedings 3537, pp. 302-309, 1998*

The response of this sensor to multiple vapor phase agents has been measured (Table 1). Units are given as parts-per-million vapor (ppm\(v\)) or parts-per-billion vapor (ppb\(v\)). The length of the sensing region is estimated at 1-2 cm based on a dimensioned schematic [15].

### 2.3.4 Integrated Interferometric EWS on GaAs

An integrated EWS, with onboard laser, sensing interferometer, and detectors, has been demonstrated by Maisenholder et al. ([8], [16]). Although there is no onboard signal
Table 1: Demonstrated Sensitivities of Hartman Sensor

<table>
<thead>
<tr>
<th>Analyte</th>
<th>Sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Benzene</td>
<td>&lt; 1 ppmv</td>
</tr>
<tr>
<td>Xylene</td>
<td>300 ppbv</td>
</tr>
<tr>
<td>Toluene</td>
<td>&lt; 1 ppmv</td>
</tr>
<tr>
<td>Chloroform</td>
<td>1 ppmv</td>
</tr>
</tbody>
</table>

processing, all optical elements are included on this 5 mm x 0.15 mm integrated chip (Figure 14a). This level of integration ensures a compact device, and that coupling between elements remains constant. The laser is a GaAs, triple quantum well, distributed Bragg reflector (DBR) laser with a measured wavelength of 831.6 nm, and a side-mode-suppression ratio > 30 dB. This laser couples into a single mode, Mach-Zehnder, sensing interferometer which contains a sensing pad. The sensing pad has a 90 nm thick, $\text{Ta}_2\text{O}_5$ (n~2.1) waveguide over top of a 765 nm SiO$_2$ buffer layer. The photodetectors are made from the same materials as the laser.

Figure 14: (a) Fully integrated GaAs-based EWS with DBR triple quantum well laser, single-mode interferometer, sensing pad, and photodetectors. (b) Photodetector current as the liquid over top of the sensing pad changes from deionized water ($n_A = 1.3273$) to 10 vol.% ethanol in water ($n_B = 1.3325$), a change in index of 0.0052. from Electronics Letters 33, pp. 986-988, 1997

The fabrication techniques are key to sensor operation. This integrated sensor is built on Si-doped ($10^{18}/\text{cm}^3$) GaAs substrate. Metal-organic vapor-phase epitaxy (MOVPE), is used to deposit a 1200-nm, n-doped Al$_{0.8}$Ga$_{0.2}$As lower cladding; a 250-nm-thick, higher-index,
lower-energy gap, Al$_{0.3}$Ga$_{0.7}$As core, with 3 quantum wells (830-nm-thick); a 1000-nm p-doped, Al$_{0.8}$Ga$_{0.2}$As upper cladding; and finally a highly p-doped GaAs capping layer. An 8 nm GaInP etch stop is inserted 685 nm below the core within the lower cladding.

Following this deposition, a technique called vacancy enhanced disordering (VED) is used to raise the energy gap within the waveguide region while maintaining it in the laser and photodetector region. In VED, standard photolithography techniques are used to cover some areas with SiO$_2$ and others with SrF$_2$. A high temperature (960°C) anneal is performed for 30s, enabling the holes located under the SiO$_2$ to diffuse into the quantum well, increasing its effective Al content and raising its energy gap. The hole diffusion under the SrF$_2$ is limited. The result is a net increase in the energy gap difference between the SiO$_2$ areas and the areas under the SrF$_2$. This energy gap is equivalent to a difference in absorption wavelength between the two regions of about 35 nm. Thus the SiO$_2$ area becomes non-absorbing to light generated in the SrF$_2$ area and becomes usable as a transparent waveguide.

After this key step, the SiO$_2$ and the SrF$_2$ are removed. Following proton implantation to achieve electrical isolation, the sensor pad is defined. A combination of dry and wet etching down to the GaInP etch stop defines a rectangular sensor area. A 76-nm-thick-SiO$_2$ cladding and a 90-nm-Ta$_2$O$_5$ waveguide layer are then deposited in this area by plasma-enhanced chemical-vapor deposition (PECVD). This step produces a thin, high-index layer structure that is exposed to the environment. Finally the dielectric waveguides are patterned using CHF$_3$ reactive-ion etching (RIE), and the AlGaAs waveguides are patterned using BCl$_3$/Ar electron-cyclotron-resonance etching. This step should produce constant and very good coupling from the laser into the waveguides. In addition, holography is used to define a third order DBR on the waveguide side of the laser.

This sensor is tested by flowing first deionized water (n=1.3273), and then a solution of 10 vol.% methanol-in-water (n=1.3325), over the sensor pad for an index change of 0.00052. As can be seen in Figure 14b, the detector current goes through 2.5 complete cycles or 5.05π radians (rad). As the drift is 39 mrad, the index sensitivity is estimated at $1.3 \times 10^{-5}$.


2.4 Benefits of Multimode Interferometry

2.4.1 Sensitivity Enhancement due to Multimode EWSs

One fundamental hypothesis of this work is that multimode interferometric sensors are better than single-mode interferometric sensors. Because the patterns of multimode sensors are much more complicated, there should be some increased sensitivity to compensate. Of course there are other benefits, which will be described later. Here, we will quantify the improvement in index-sensitivity of multimode EWSs over their single-mode counterparts.

Whether single-mode or multimode, the modal effects of these sensors can be calculated using the effective index method, which will be described in more detail later. Basically, the vertical and horizontal guiding effects can be approximately separated. As we showed earlier, vertically, the TM-like modes are more sensitive than the TE-like modes. Thus we choose to excite primarily TM-like vertical modes in the waveguide. Because of this, the horizontal guiding effects are approximated by TE-like modes.

We have explained in Sec. 2.2.1, an analytical method to estimate the sensitivity of a three-layer TM waveguide. Alternately, we can use multilayer waveguide theory [17] to calculate the effective indices, for small changes in cover index to produce a similar result. Multilayer waveguide theory can also be used to calculate the modal effective indices of the TE-like horizontal waveguides for small changes in cover index. Following the effective index method [10], we use the effective indices of the vertical TM-like modes as the guiding layer indices for the TE-like transverse waveguide. In short, this method can be used to numerically estimate the sensitivity coefficients, $\frac{\partial n_{\text{eff}}}{\partial n_c}$ of all of the transverse modes of structure.

The results are shown here for this calculation. Intuitively, one might guess that the increased sensitivity of the higher-order modes is due to the longer effective path under the sensing layer. This borrows a little from the ray picture of waveguide modes, which is equivalent to the eigenvalue approach. Let’s see if this idea has any merit to explain the trace in Fig. 15.

We hypothesize that the phase (effective path length) accumulated by the two propagating plane waves under the sense layer determines any increase in sensitivity. As the waves
Figure 15: Sensitivities of Transverse Modal Effective Indices to Cover Index Change, calculated from solutions to the waveguide boundary value problem. It is interesting that the peak sensitivity is not the highest-order mode.

As all modes experience the same phase change due to time, it does not contribute to relative phase differences, so it is ignored. However, based on this, the phase angle acquired under the sense layer in one round trip is \( \Delta \phi = 2k_0n_f W/\sin(\varphi) \), where \( \varphi \) is the modal propagation angle (which is given by \( \cos^{-1}(\beta/k_0) \)). The forward distance traveled within one round trip is \( \Delta z = 2W/\tan(\varphi) \). And thus the phase acquired per unit distance is given by

\[
\frac{\Delta \phi}{\Delta z} = \frac{2k_0n_f W/\sin(\varphi)}{2W/\tan(\varphi)} = \frac{k_0n_f}{\cos(\varphi)}. \tag{4}
\]

In this geometry, \( n_f \) is sensitive to the changes in vertical effective index as per Fig. 4. The enhancement in sensitivity is given by the inverse cosine term. Thus we expect that for a mode at angle \( \varphi \), the sensitivity is related to the vertical TM-like sensitivity, \( \partial n_{\text{eff}}^V/\partial n_c \), by

\[
\frac{\partial n_{\text{eff}}(\varphi)}{\partial n_c} = \frac{\partial n_{\text{eff}}^V/\partial n_c}{\cos \varphi}. \tag{5}
\]
Figure 16: Diagram to Estimate Ray Picture Sensitivity of Modes to Cover Layer Index Change. The waveguide has index $n_f$ and is surrounded by a material with index $n_c$. This quantity is plotted for the calculated transverse modes of the waveguide. The agreement is very good except for the highest order modes, which have angles closest to the cutoff for guided modes. At angles close to cutoff, the Goos-Hänchen shift [10] may come into play. The Goos-Hänchen shift can be regarded as an evanescent penetration into the cover layer of a ray that is part of a mode of a waveguide. If we consider that the phase acquired upon reflection is occurring outside the guiding layer and not under the SL, then

Figure 17: Estimate of Sensitivity Coefficient of Transverse Modes by Geometrical Arguments. Solid line is eigenvalue-based prediction and dash-dot is geometrical prediction.
this may explain the less than expected sensitivity of the higher-order modes.

To include the effect of the Goos-Hänchen shift in this way, we consider a new ray picture as follows: We again consider the amount of phase acquired under the film layer within a given amount of forward mode propagation. We consider the same geometrical arguments, and include the effect of the shift. The phase acquired under the SL in one round trip is still \( \Delta \phi = 2k_0 n_f W / \sin(\varphi) \). However, the distance of one round trip is modified by the shift as \( \Delta z = 2W/\tan(\varphi) + 2\cot(\varphi)/(k_0\sqrt{n_f^2\cos^2(\varphi) - n_c^2}) \). And thus the phase acquired per unit distance is given by

\[
\frac{\Delta \phi}{\Delta z} = \frac{2k_0 n_f W / \sin(\varphi)}{2W/\tan(\varphi) + 2\cot(\varphi)/(k_0\sqrt{n_f^2\cos^2(\varphi) - n_c^2})} = \frac{k_0 n_f W / \cos(\varphi)}{W + 1/(k_0\sqrt{n_f^2\cos^2(\varphi) - n_c^2})} = \frac{k_0 n_f / \cos(\varphi)}{1 + 1/(k_0 W \sqrt{n_f^2\cos^2(\varphi) - n_c^2})}.
\]

It is noted that Eq. 6 is essentially the same as Eq. 4, except that it is divided by a factor of \( 1/1 + \Delta \) where \( \Delta \) is very small except in the case when \( n_f \cos(\varphi) \approx n_c \), which occurs

Figure 18: Diagram to Estimate Ray Picture Sensitivity of Modes to Cover Layer Index Change taking the Goos-Hänchen shift into account. The waveguide has index \( n_f \) and is surrounded by a material with index \( n_c \).
only near cutoff. Thus this term becomes significant for only the highest order modes as expected. Let’s see how this modification affects the geometrical predication of sensitivity. This graph is essentially the same as Fig. 17 except that now at the highest-order modes,

![Graph](image)

**Figure 19:** Estimate of Sensitivity Coefficient of Transverse Modes by Geometrical Arguments including Goos-Hänchen shift. Lower line is eigenvalue-based prediction and upper line is geometrical prediction.

we see a drop in sensitivity similar to that initially observed in Fig. 15. This agreement is conclusive. For planar multimode EWSs, like those illustrated, the Goos-Hänchen shift limits sensitivity of the highest-order modes.

Having established the effect of transverse mode angle on sensitivity, the effect of waveguide width on maximum sensitivity can be determined. Similar calculations for waveguides of different widths are shown in Fig. 20. It is clear that there is a fairly steeply increasing sensitivity below 100 $\mu m$, with very slight improvement above that. This corresponds with the slightly increasing propagation angle associated with the highest order modes in wider waveguides. This can only be increased by increasing the transverse index contrast, which enables steeper propagation angles. In addition, the maximum increase in sensitivity over 0.29 (the minimum shown in Fig. 15) is about $1.6 \times$. If we consider the index sensitivity coefficient at the optimal waveguide thickness vertically (0.4), then the sensitivity for the most sensitive transverse mode is about 0.65 regardless of guide thickness. Practically, a 100-$\mu m$ thick waveguide achieves most of this gain without becoming too large. For the materials and geometry specified, the maximum index sensitivity, $\partial n_{eff}/\partial n_c$ is $\simeq 0.46$, which
Figure 20: Improvement in maximum index sensitivity with increasing waveguide width for planar multimode EWSs.

represents a 60% improvement over a comparable single-mode waveguide.

Further, not all of the power or field will be in the highest order modes. It will be divided among various modes. This means that the actual index sensitivity will be a weighted sum of the sensitivities of each of the individual modes. This suggests that coupling methods that induce higher order modes under the SL produce higher sensitivity. The multimode y-junction is key to the excitation of higher order modes, and thus key to device index sensitivity.

2.4.2 Other Benefits of Multimode Interferometry

Besides a sensitivity increase, multimode interferometry has several practical advantages. The waveguides are generally wide, from 50-\(\mu m\) up to 300-\(\mu m\). This allows fabrication alignment tolerances to be somewhat relaxed. That is, if the sensing layer is slightly offset, some small reduction in performance can be expected, but the device will still work well. In addition, the mode field size of wider waveguides facilitates coupling, although the generally sub-\(\mu m\)-sized guiding layer produces a highly elliptical mode shape. Further, the waveguide is less likely to completely stop working if it is scratched. The modal pattern may change, but the device will still function basically the same, unless extensive loss is associated with the scratch. Finally the structure in the entire modal pattern may be used for detection to increase the SNR as will be detailed later.
2.5 The Larger Project

The initial research for this proposal is part of a four-student team-based project to produce a fully integrated, optical EWS (Figure 21). The key physical elements of the sensor are the Si-CMOS chip and detector arrays, the thin-film laser source, and the interferometric waveguide functionalized with a chemically sensitive polymer.

Figure 21: CMOS sensor circuit with embedded laser (conceptual), sensing interferometers, and integrated photodetectors.

The Si-CMOS chip contains laser pads, 8–µm × 8–µm square photodetectors with an 8–µm-pitch, and associated signal processing and readout circuitry. Further, this chip is the substrate upon which the interferometric sensor is deposited. For high sensitivity, the photodetectors need small dimensions to resolve the intensity pattern created by the interferometric sensor. These detectors, the associated circuitry, and the Σ–Δ analog-to-digital converters, also need to detect small changes in intensity, and be extremely low-noise. This low-noise level can partially compensate for reduced sensitivity due to the short interferometer length.

For sensitive operation, a low-noise, coherent laser source is required. A sacrificial layer
permits an epitaxially-grown, lifted-off, thin film, multiple quantum well (MQW) laser, to be transferred onto the Silicon CMOS circuit. One critical issue concerns the coupling between the laser and the waveguide. The active layer of the transferred laser is extremely small (<0.15 µm), and there is uncertainty in the height of the active layer due to deposition uncertainty. The light from the laser is to be coupled into a waveguide layer with a vertical mode field size near 0.26 µm at 632.8 nm. Further, the waveguide layer also has uncertainty in its height. Thus, the accurate deposition of the waveguide material, as well as the physical positioning of the laser are critical to integrated sensor function.

The final element is an interferometric waveguide EWS. This waveguide is a vertically monomode, horizontally highly multimode, Mach-Zehnder interferometer, covered on one arm by a chemically sensitive polymer. The largest possible change in index of this polymer in response to given concentrations of chemical is needed. Further, as much as possible, the response of this polymer should be linearly related to concentration of chemical agent. In addition, the interferometer must extract the maximum sensitivity to chemical-induced index change, in the limited length of the chip. In this EWS, the effective index shift, \( \Delta n_{eff} \), is detected as a shift in the horizontal multimode pattern at the output facet of the sensor. This output pattern is evanescently coupled to the CMOS detectors and read out by circuitry. The detector array captures a slightly integrated, “pixelated” version of the multimode pattern.
MATERIAL CHARACTERIZATION - CHEMICAL AND THERMAL

EWSs often rely on a chemically or biologically sensitive material, a “sensing layer” (SL) to absorb or adsorb the agent, permitting the light to interact with the agent in a concentrated form. In addition, the sensitive material may interact chemically with the agent to provide specificity or amplification of the target agent concentration. Interaction with the agent finally produces a change in the index of refraction, thickness, and/or the absorption of the material. Devices that utilize the absorption are florescence or spectroscopy-based sensors. We are concerned here with devices that utilize changes in the real part of the index of refraction and possibly thickness, to accomplish chemical or biological detection.

While index-based optical chem/bio sensors differ in the method of converting index changes in the material into a change in intensity on a square law detector (grating-based[3], resonant cavity-based [18], or interferometer-based[11]), these devices cannot distinguish index (or thickness) changes induced by the chemical or biological target agent from those induced by other environmental chemicals or temperature change. Therefore it is imperative to compare the relative magnitude of the optical changes induced by these mechanisms with the target-induced changes. As these devices are used in the atmosphere, water vapor is one source of chemical interference for hydrophilic SLs.

EWSs rely on a strong index change caused by the target agent. The polymer sense layer selected for the sensor is bis-trifluoromethyl carbinol substituted polynorbornene, commonly referred to as hexafluoroisopropanol-substituted polynorbornene (HFAPNB). The chemical responses of the polymer HFAPNB to the target agents benzene, isopropanol, and methanol, are measured using ellipsometry, which is enabled by a custom sealed stainless-steel chamber. In addition, the chemical response of HFAPNB to water is also measured as a source of chemical noise.
For polymers that have merits as chemical or biological SLs, the range of thermal index sensitivities is also established. Using a variable-angle spectroscopic ellipsometer and a temperature controlled platform\cite{19}, thermally-induced changes in the polymers, HFAPNB and poly-hydroxystyrene (PHOST), and in the optical materials, SiO$_2$ and SiO$_x$N$_y$ are measured. In addition, the relationship between thermally induced density changes and index changes is examined. The literature is also surveyed to establish the range of temperature responses expected by polymers in general. We compare the thermal or chemical noise to the index sensitivities of several index-based chemical sensors, including the multimode interferometric sensor measured for this work. Finally, mitigation methods, using interferometric techniques and/or active temperature control, are suggested.

These chemical and thermal material sensitivities are compared with the demonstrated index sensitivities of some EWSs. For example, we have previously demonstrated an interferometric EWS\cite{20} with a cover index sensitivity of $2.5 \times 10^{-6}$. We have also measured the thermal sensitivity of the polymer sense layer, HFAPNB, at $-2.4 \times 10^{-4}/^\circ C$. The demonstrated device, which relies on this polymer, requires a thermal stability of better than +/- 0.01 $^\circ C$, for thermal effects not to impact the device index sensitivity.

### 3.1 Chemical

#### 3.1.1 Material Details of Polymer Sense Layer

The polymer, HFAPNB, is used for this work. This polymer has hydroxyl groups. It is expected that like molecules will dissolve suggesting that this may be a good SL for water, methanol, or isopropanol, and other polar molecules. It also has a benzene-like group, suggesting that benzene may also dissolve. The sensing ability of HFAPNB for these materials will be verified in this chapter. HFAPNB in dry monomer form with a molecular weight of 34440 is supplied by Promerus Electronic Materials.

To create polymer films for ellipsometric test, a 20 wt.% solution of HFAPNB in propylene-glycol-methyl-ether-acetate (PGMEA), is created. A bare silicon, wafer is prepared by spinning hexamethyl disilane (HMDS) onto the surface, and then removing the excess by spinning at 5000 rpm for 10s. The HMDS facilitates the adhesion of the polymer
onto the silicon wafer. Following this, the silicon wafer is coated with HFAPNB and the excess polymer is removed by spinning at around 2000 rpm for 30s. Following, this, the polymer is baked at 130 °C to remove the solvent.

Further, this polymer has been proposed as a matrix for next generation photo-resists. As such, it has the capability of becoming photo-definable. A photo-acid generator, 3 wt%, is added to the monomer solution. After spinning and baking, this creates a positive resist polymer sense layer. Exposure with 265-nm-light releases photo-acid which makes the polymer soluble in developer. This photo-definable polymer can be easily used with standard photolithography procedures.

3.1.2 Experimental Setup - Chemical

The apparatus required to characterize changes in the index of refraction, extinction coefficient, and layer thickness of the SL, in response to calibrated concentrations of agent has been developed. Gas delivery and optical characterization systems, Fig. 22, were developed to precisely assess the sensing layer optical response to calibrated concentrations of vapor-phase agents. The gas delivery system delivers vapor phase agent at precise concentrations and flow rates. From there, the agent is delivered to a sealed chamber on a high speed ellipsometer, where changes in the optical properties of materials in response to the agent can be accurately measured.

Figure 22: Gas delivery system and ellipsometric measurement system schematic. N\textsubscript{2} regulated by a 1 standard cubic centimeters per minute (sccm) mass flow controller flows through a bubbler and then into a mixing chamber where it is diluted with a larger flow of N\textsubscript{2}. From there the mixture flows to a QCM before entering the ellipsometric chamber.
The precision gas-mixing system[21] consists of a nitrogen supply, two mass-flow controllers, a chemical bubbler, and a mixing chamber, Fig.22. The mass flow controllers measure the flow rate using the properties of laminar flow. One mass flow controller, with a range of 0-1.2 standard cubic centimeters per minute (sccm) and a flow delivery accuracy of ± 0.01 sccm, is used to control the flow through a chemical bubbler. The chemical bubbler includes a sparger that creates many small bubbles for a high total surface area, shown in Fig. 23. These bubbles pass through the agent of interest in liquid form and agent diffuses from the liquid phase into the nitrogen carrier gas. After this step, the saturated chemical vapor stream is mixed in a glass mixer with a larger flow of N2, controlled by a 0-2500 sccm to create flows with a wide range of chemical vapor concentration. For methanol vapor, this bubbler/mixer system delivers flows between approximately 1 and $7.1 \times 10^4$ ppmv. This chemical vapor flows through a stainless steel piping system first to a sealed chamber that contains a quartz crystal. The flow is monitored by measuring mass uptake in a polymer film, which is determined through the resonant frequency shift in the crystal due to changing mass associated with the gas flow. The QCM can measure frequency changes of 0.12 Hz, which corresponds for a 1-µm-thick film of HFAPNB, to a mass per unit area resolution
of 1.56 ng/cm². This system enables the mass uptake of agent to be accurately linked to chemical concentration.

Figure 24: Ellipsometer and Chemical Vapor Test Chamber. The chamber containing the QCM is to the left of the ellipsometer.

From this chamber, the monitored vapor stream flows to the stainless steel test chamber, Fig. 24, located on a high-speed, spectroscopic ellipsometer [22]. The index and thickness of the same polymer film respond to this gas mixture, and these changes are measured multiple times per minute. The index resolution for this measurement is approximately $1 \times 10^{-4}$. Using this system, methanol vapor can be delivered at concentrations between 0 and $1.4 \times 10^5 \text{ ppmv}$ with a precision of ±1 ppmv. This gas mixture flows to a custom, stainless steel chamber, mounted on a high-speed, spectroscopic ellipsometer [22]. The ellipsometric wavelength-dependent (300 to 1100 nm) data and subsequent data analysis allows accurate assessment of the changes in index and thickness of the sensing material in response to a range of agent concentrations. Data is acquired at a rate of $\sim 0.17 \text{ Hz}$, allowing observation of the transient response of this material. The mass uptake of chemical in the sensing layer, as measured by the QCM, is thus precisely linked to its optical index change. This simultaneous vapor concentration, mass uptake, and optical constant data provide a calibration of the various responses of the sensing layer, and provides accurate physical constants for numerical simulations.

3.1.3 Chemical Response of HFAPNB

The dynamic optical response of the polymer, HFAPNB, to a range of concentrations of common laboratory solvents has been determined using the previously described gas delivery and optical characterization systems. To illustrate the method, we will show the
measurement of methanol vapor in detail. The raw ellipsometric $\psi$ and $\delta$ data, which corresponds to the magnitude ratio and phase angle difference between the reflection coefficients of the TE and TM polarizations, are not shown. The starting point will be the time vs index and time vs thickness data at the wavelength of interest (840 nm).

### 3.1.3.1 Measurements with Methanol

**Nitrogen Saturated with Methanol**  
Figure 25 shows the index and thickness changes over time, of the polymer, in response to air saturated with methanol. The index data shows a sharp peak followed by a gradual fall as the methanol absorbs into the polymer. This suggests that initially, methanol replaces air within the spaces in the polymer, increasing the index. Next, the lower-index methanol stretches the polymer, decreasing the relative amount of polymer to methanol and therefore the index. This hypothesis is further supported by the larger thickness and smaller index after methanol desorption. This deformation of the polymer and the associated non-linear optical constant changes intimately affect sensor response.

![Graph showing index and thickness changes](image)

**Figure 25:** Change in index of refraction and thickness of the polymer, HFAPNB, in response to 71000 ppm methanol-in-air. The vapor stream starts at 15 minutes and ends at 21 minutes. Initial thickness is 1098 nm.

**Nitrogen at One Smaller Methanol Vapor Concentration**  
Figure 26(a) depicts the index response for a change from negligible to 140 ppmm of methanol-in-N$_2$. Figure
Figure 26: (a) Ellipsometric response, $\Delta n_{SL}$, of the chemically sensitive polymer, HFAPNB, to 140 ppmv of methanol vapor. (b) The corresponding QCM response. For low concentrations, $\Delta n_{SL}$ responds linearly with mass uptake and concentration with $\Delta n_{SL} \approx 5.4 \times 10^{-3} [cm^2/g]$ and $\Delta n_{SL} \approx 5.6 \times 10^{-6} [1/ppmv]$. $\Delta n = 0$ corresponds to $n = 1.4301$.

Figure 27: (a) Ellipsometric response, $\Delta h_{SL}$, of the chemically sensitive polymer, HFAPNB, to 140 ppmv of methanol vapor. (b) The corresponding QCM response. For low concentrations, $\Delta h_{SL}$ responds linearly with mass uptake and concentration with $\Delta h_{SL} \sim 1 [nm/cm^2/\mu g]$ and $\Delta h_{SL} \sim 1.4 [pm/ppmv]$. $\Delta h = 0$ corresponds to $h = 925nm$. 
27(a) shows the associated thickness change. The corresponding mass uptake (Fig 26(b)) is measured via QCM frequency shift. Accurate mass flow control devices allow the vapor concentration of agent to be linked to mass uptake and index change in the SL. The test procedure begins with an N\textsubscript{2} purge, continues as a chemical-laden vapor stream is introduced into the chamber, and concludes with another N\textsubscript{2} purge. Figure 26 shows multiple cycles of this procedure. For the sense material, HFAPNB, we observe an index change which scales linearly with concentration change and mass uptake of methanol for concentrations between 0 and 1000 ppmv. Specifically, $\Delta n_{SL} \sim 5.6 \times 10^{-6} \frac{1}{ppmv}$, and $\Delta n_{SL} \sim 5.4 \times 10^{3} \frac{cm^2}{g}$ respectively, where $\Delta (m/A)$ $[g/cm^2]$ is the mass uptake per unit area of the polymer thin film. In addition, the mass uptake per concentration is $[1.32 ng/(cm^2 ppmv)]$. The thickness change is practically insignificant at this concentration change ($\approx 0.2 nm$).

We note a baseline drift in the index response, while the baseline in the mass uptake is essentially constant. These two observations are consistent with the densification of the polymer. Since the mass uptake is constant, the index drift is not a result of chemical remaining within the polymer. Further, the baseline polymer thickness (not shown) also decreases, supporting densification. In fact, Drozdov [23] explains theoretically the experimental observation that compressive and tensile stresses both cause densification of glassy polymers. The cyclic increase and decrease in thickness that we observe in HFAPNB, which is induced by repeated cycling between chemical atmosphere and N\textsubscript{2}, causes tensile stress in the polymer. Thus it is likely that the baseline drift in the index data is caused by polymer densification.

**Nitrogen with Stepped Methanol Vapor Concentrations** Figure 28 shows the changing index and thickness over time as the concentration of methanol vapor is adjusted to 3, 11, 60, 120, 239, 11, and 3 ppmv. The real time fitting routine used has produced some unrealistic discontinuities in the data. An estimate of the corrected optical response is shown as “corrected” data. However, this correction is an estimate only, and thus the overall drift in this measurement may not be indicative of the state of the polymer. However, the changes in concentration that do not occur at discontinuities do provide accurate
indications of changes in optical properties for given changes in concentration. Fig. 29(b)

**Figure 28:** Original and shifted corrected real time fit of time vs \( n_{840\text{nm}} \) (a) and time vs thickness (b) for methanol absorbed into HFAPNB. The concentrations applied are 3, 11, 60, 120, 239, 11, and 3 ppmv. The starting index is 1.4169 and the starting thickness is 1183.5 nm.

**Figure 29:** Original thickness data (a) and corresponding mass uptake data (b) for the same concentration changes as Fig. 28.

shows the corresponding mass uptake as measured by the QCM. The mass uptake given a certain concentration of agent is given by \([1.87\text{ng}/(cm^2\text{ppmv})]\)

The index change and thickness change as a function of concentration is shown in Fig. 30. Based on this data, the index sensitivity to concentration is \(3.4 \times 10^{-6} \text{ [1/ppmv]}\) and the
The index sensitivity to mass uptake is $1.187 \times 10^3 [cm^2/g]$. The thickness sensitivity to concentration is $4.2 \times 10^{-3} [nm/ppmv]$ thickness sensitivity to mass uptake is $2.24 [(nm \, cm^2)/\mu g]$.

**Figure 30:** Index at 840 nm (a) and Thickness (b) Sensitivity of HFAPNB to methanol vapor concentration (corresponds to Fig. 28).

The difference between the index sensitivity to concentration shown in Fig. 30 and Fig. 26, is as yet unexplained. It is noted that the starting thicknesses and indices are also different. The smaller index during the measurement of Fig. 30 suggests that the density of the polymer started out slightly less. However, the starting conditions of these polymers was very similar. Figure 31 shows the relationship between mass uptake and equilibrium chemical vapor concentration. For the sensitivity estimates, the lower sensitivity has been used, as more concentrations were measured.

### 3.1.3.2 Other Solvents

The gas delivery/ellipsometric chamber system can characterize a material's optical response to an agent. This permits quantitative estimation of device response without fabrication. To illustrate this capability, the optical response of the polymer, HFAPNB, to some common chemicals has been measured, Fig. 32. The index response of water is comparable with that of methanol and therefore represents a source of chemical noise in the measurement.

The relationships between concentration and index for methanol, $3.4 \times 10^{-6}/ppmv$; for water, $7.5 \times 10^{-6}/ppmv$; for benzene, $2.8 \times 10^{-5}/ppmv$; and for isopropanol, $8.6 \times 10^{-5}/ppmv$.  

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**Figure 31:** Mass Uptake and Concentration (corresponds to Fig. 30b). $\Delta m/A \simeq 1.87[\text{ng/cm}^2\text{ppmv}].$

**Figure 32:** Index response of the polymer HFAPNB to different concentrations of common lab chemicals.
3.1.3.3 Sensing Layer - Agent-Induced Loss (Absorption)

It is noted that during the ellipsometric measurements of the polymer sense layer, HFAPNB, optical loss, as measured by $k$, the extinction coefficient, or by $\alpha$, the exponential power loss coefficient, can be affected by the detected agent. However, in general, there was minimal observed correlation between loss and chemical concentration, as shown in Fig. 33. Isopropanol as the agent developed an extinction coefficient at $840 \text{ nm}$ of about $1.9 \times 10^{-5}$ with some drift. The loss was, however, observed to be different for different agents. For example, during methanol detection, the loss was not detectable by the ellipsometric apparatus for any concentration. Water and benzene developed approximately the same loss ($k_{840nm} \simeq 3.2 \times 10^{-5}$). This loss can affect the operation of the interferometer. If we estimate that the effective modal loss has the same relation with the cover layer loss as the effective index has with cover layer index, then we can estimate the modal power loss

![Figure 33: Extinction coefficient (at 840 nm) of HFAPNB after absorption of isopropyl alcohol at concentrations of 1, 3.5, 20, and 40 ppmv. Extinction coefficient is \( \simeq 1.9 \times 10^{-5} \).](image-url)
coefficient, $\alpha_{\text{eff}}$, for these agents as follows:

$$\alpha_{\text{eff}} \simeq \frac{4\pi k \partial n_{\text{eff}}/\partial n_c}{\lambda_0}.$$  \hfill (7)

Referring to Fig. 17, the approximate range of modal sensitivity to cover index is 0.3 to 0.45. Thus, not only are higher-order transverse modes more sensitive to agent-induced index changes, they are also more sensitive to agent-induced loss. In fact, when iso-propanol is the agent, $\alpha_{\text{eff}}$ (840 nm), can range from $9 \times 10^{-5}$ to $1.3 \times 10^{-4}$; and when water or benzene is the agent, the range is $1.4 \times 10^{-4}$ to $2.2 \times 10^{-4}$. This can lead to a power reduction under the sense arm (length $\simeq 2000 \mu m$) of 35% for the highest order modes and 25% for the lowest-order modes.

3.2 Thermal

3.2.1 Polymers, $\partial n/\partial T$, and CTE

Often the chemically or biologically sensitive material is a polymer. Polymers are easy to process, can have low optical loss, and interact strongly with certain agents of interest. Further, they can potentially be tailored, using additives, to become selective to a small class of agents. Polymers that have been used for EWSs include (refs) HFAPNB[20], polypyrrole [24], Novalac-resin [25], and teflon [26]. These polymers are sensitive to target agents, however, they also have large coefficients of thermal expansion (CTE). In general, the volume CTE, $\alpha$, which has units of volume fraction per degree of temperature change, is proportional to the rate of change of index with temperature $|\partial n/\partial T|$. That is, the index is functionally related to density. For small changes, it is linearly related.

It has been shown that the index of a composite material depends upon the indices of the individual components [27] [28]. The Lorentz-Lorenz index-mixing rule has been tested for various mixtures [29] [30]. This index mixing rule is used to establish a general link between the volume CTE, $\alpha$, of a material and its $\partial n/\partial T$.

When a material expands in response to a temperature increase, the density decrease is equivalent to mixing the original material with vacuum. The Lorentz-Lorenz index mixing rule, Eq. 8, relates the index of a mixture of materials, $n_{12}$, to the volume weighted indices
of the bulk component indices. It is

\[ \frac{n_{12}^2 - 1}{n_{12}^2 + 2} = \phi_1 \frac{n_1^2 - 1}{n_1^2 + 2} + \phi_2 \frac{n_2^2 - 1}{n_2^2 + 2}, \]  

(8)

where \( \phi_1 (\phi_2) \) is the volume fraction and \( n_1 (n_2) \) is the index of substance 1 (substance 2) in the mixture. In the case of expansion due to a temperature change, \( \Delta T \), the second material is vacuum (\( n_2 = 1 \)), and this may be further specified as

\[ \frac{n_{12}^2 - 1}{n_{12}^2 + 2} = \frac{1}{1 + \alpha \Delta T} \frac{n_1^2 - 1}{n_1^2 + 2}. \]  

(9)

For small values of \( \alpha \Delta T \), this produces a linear response,

\[ n_{12}(\Delta T) \simeq n_1 - \frac{n_1^4 + n_1^2 - 2}{6n_1} \alpha \Delta T. \]  

(10)

Under these conditions, \( \partial n/\partial T \) is proportional to \( \alpha \).

This establishes the basic relationship between the volume CTE coefficient, \( \alpha \), and the index of a heated or cooled material. It shows that \( \alpha \), together with index-mixing rules permits an estimation of \( \partial n/\partial T \). Further, \( \alpha \) also describes the thickness change in a film, which can also affect index-based sensors, through expansion induced stress and associated material property changes.

### 3.2.2 Experimental Setup - Thermal

Using spectroscopic ellipsometry and a temperature controlled hotplate, Fig. 34, the index (along with extinction coefficient, \( k \), and thickness, \( t \)) is directly measured at different temperatures. This experimental apparatus has been previously described [19]. In short, thin film polymer samples are held at a constant temperature using a hotplate and a Tempilstik temperature indicator with an Omega thermocouple sensor.

The measured polymers are spin-coated onto a silicon wafer. The process to make HFAPNB has been described in Ch. 3, Sec. 3.1, Subsec. 3.1.1. Poly-hydroxystyrene (PHOST) with a molecular weight of 11 800, was obtained from DuPont Electronic Materials. A 20 wt.% monomer solution of PHOST in PGMEA is created prior to spin coating. The post-spin processing steps are the same as for HFAPNB (except photo-acid generator is not added). The measured inorganic optical materials, SiO\(_2\), and SiO\(_x\)N\(_y\), are deposited
using plasma-enhanced chemical-vapor deposition (PECVD). The recipe used has been previously described [20].

Using the thickness vs temperature data which is obtained ellipsometrically [31], the constrained CTE, $\beta_C$, is found. In all cases the temperature-dependent index of silicon is used to model the layer structure. The $\beta_C$ obtained can be corrected using Poisson’s ratio to the true volumetric CTE, $\alpha$. The details of this correction are described in App. G. In addition, the slope of the index data at different temperatures (for a given wavelength) establishes $\partial n/\partial T$.

### 3.2.3 Thermal Responses

#### 3.2.3.1 Measurements and Interpretation

The ellipsometric measurements of temperature-related changes in the optical constants of HFAPNB, PHOST, SiO$_2$, and SiO$_x$N$_y$, are shown here. Using this data, we directly measure the $\partial n/\partial T$ (at 840 nm), and the constrained CTE, $\beta_C$, of these materials. Figure 35 shows the measurement of these two quantities, for HFAPNB. In EWS sensing, one concern is the glass transition temperature, $T_g$, at which there is a discontinuity in the properties of polymers. The PHOST polymer (Fig. 36) exhibits this discontinuity at about 160°C. Thus, if PHOST is used as a sensing layer, the sensor operating temperature range should exclude this temperature.

Figures 37 and 38 show temperature vs index and thickness data for SiO$_x$N$_y$, and
Figure 35: Ellipsometric data for HFAPNB. The measured $\partial n/\partial T$ is $-1.4 \times 10^{-4}/^\circ C$, and the measured $\beta_C$ is $1.8 \times 10^{-4}/^\circ C$.

Figure 36: Ellipsometric data for PHOST. Of note is the $T_g$ at about 160$^\circ$C. For $T < T_g$, $\partial n/\partial T$ is $-7.9 \times 10^{-5}$, and $\beta_C$ is $1.12 \times 10^{-4}/^\circ C$. For $T > T_g$, $\partial n/\partial T$ is $-2.63 \times 10^{-4}$, and $\beta_C$ is $1.9 \times 10^{-4}/^\circ C$. 
Figure 37: Ellipsometric data for SiO$_x$N$_y$. $\partial n/\partial T$ is $-2.84 \times 10^{-5}/^\circ$C, and $\beta_C$ is $8.9 \times 10^{-6}$.

Figure 38: Ellipsometric data for SiO$_2$. $\partial n/\partial T$ is approximately $-1.84 \times 10^{-5}/^\circ$C, and $\beta_C$ is $2.2 \times 10^{-5}/^\circ$C.
SiO<sub>2</sub>. The constrained CTEs, β<sub>c</sub>, are quite different between the polymers and the organic materials. β<sub>C</sub> for HFAPNB is 20× greater than that for SiO<sub>x</sub>N<sub>y</sub>, and 9× greater than that for SiO<sub>2</sub>. This suggests that temperature changes will cause expansion or contraction related compressive or tensile stresses in layered structures that include both SiO<sub>x</sub>N<sub>y</sub> or SiO<sub>2</sub> and a polymer. There will of course be some stresses even between SiO<sub>x</sub>N<sub>y</sub> and SiO<sub>2</sub> but this effect will be much smaller than that with polymers in the structure.

Figure 39 is a direct comparison between the index temperature sensitivities of SiO<sub>2</sub>, SiO<sub>x</sub>N<sub>y</sub>, and HFAPNB. They show that the ∂n/∂T of SiO<sub>x</sub>N<sub>y</sub> is almost twice that of SiO<sub>2</sub>. However, the ∂n/∂T of SiO<sub>x</sub>N<sub>y</sub> is 8× less than that of HFAPNB. In contrast, the ∂n/∂T of PHOST (T < T<sub>g</sub>) is only 2.8× greater than that of SiO<sub>x</sub>N<sub>y</sub>, presenting a much smaller mismatch. In general, the inorganic materials SiO<sub>2</sub> and SiO<sub>x</sub>N<sub>y</sub> are much less sensitive to temperature changes than the polymers. Further, there is significant variation amongst different polymers. Careful selection of polymers as SLs can reduce the temperature sensitivity of EWSs.

**Figure 39:** Ellipsometrically Measured Index Sensitivity to Temperature Changes for SiO<sub>x</sub>N<sub>y</sub>, SiO<sub>2</sub>, HFAPNB, and PHOST. The slopes, ∂n/∂T, are −2.84 × 10<sup>−5</sup>, −1.8 × 10<sup>−5</sup>, −14 × 10<sup>−5</sup>, and −7.9 × 10<sup>−5</sup> (1/°C).
\[ \frac{\partial n}{\partial T} \text{ via CTE Measurement} \] We wish to determine the volume CTE, \( \alpha \), of the sample, which can be written

\[ \alpha = \frac{\partial (V/V_0)}{\partial T} \text{ (ppm/}^\circ\text{C),} \tag{11} \]

where \( \partial (L/L_0)/\partial T \) represents the rate of fractional volume expansion or contraction for a given change in temperature.

Experimentally, the polymers measured were spin-coated onto a silicon wafer, which confines these thin-films in the xy-plane. This transverse confinement produces additional elongation normal to the wafer surface. Thus, if we measure a fractional increase in film-thickness, we are actually measuring the constrained linear CTE, \( \beta_C \). This property of materials to expand in the longitudinal dimension when compressed in the transverse dimension has been quantified for numerous materials as Poisson’s ratio, \( \nu \). Mathematically, \( \nu = -\epsilon_L/\epsilon_T \), where \( \epsilon_L \) is the fractional increase in length in the longitudinal direction, and \( \epsilon_T \) is the fractional decrease in length in either transverse direction. Accounting for this property, the thermal expansion directly measured ellipsometrically for the constrained thin film must be corrected in order to find the unconstrained linear CTE, \( \beta_U \). Kahle et al. have stated this correction [32], which is Eq. 145. We have also estimated a correction which is slightly different (Eq. 144), however, both provide quite similar results. Further, \( \alpha_U \approx 3\beta_U \).

We have measured the constrained CTE, \( \beta_C \), using spectroscopic ellipsometry for both PHOST (Fig. 36) and HFAPNB (Fig. 35). For HFAPNB, the corresponding unconstrained CTEs for \( \nu = .37 \), are (Eq. 144)

\[ \beta_U \approx 178 \ast \frac{1}{1 + 2(0.37)} = 102 \text{ppm}/K \tag{12} \]

\[ \alpha_U \approx 102(3) = 306 \text{ppm}/K, \tag{13} \]

or (Eq. 145)

\[ \beta_U \approx 178 \ast \frac{1 - .37}{1 + 0.37} = 81 \text{ppm}/K \tag{14} \]

\[ \alpha_U \approx 81(3) = 243 \text{ppm}/K. \tag{15} \]

From this, it seems that this calculation is very sensitive to the value of \( \nu \). and if \( \nu \) is temperature dependent [33], then so is this calculation. Having calculated the volume
coefficient of thermal expansion, $\alpha$, we estimate the change in volume of the thin film due to a temperature change $\Delta T$. We consider the additional volume to be vacuum with an index of refraction $n_2 = 1$.

$$\Delta V(\Delta T) = V_0 \alpha \Delta T.$$ (16)

And referring to Eq. 8, the volume fraction of the original material, at index, $n_1$, is given by

$$\phi_1 = \frac{1}{1 + \alpha \Delta T},$$ (17)

and the volume fraction of the additional vacuum that is added at index, $n_2 = 1$, is given by

$$\phi_2 = \frac{\alpha \Delta T}{1 + \alpha \Delta T}.$$ (18)

We have compared the index change estimated using the Lorentz-Lorenz and three other index mixing rules (Eqs. 128, 131, 133, 135) with that measured directly by spectroscopic ellipsometry for HFAPNB. For this comparison, the Poisson correction factor given by Eq.

![Figure 40: Comparison between measured index change with temperature (at 840 nm) and that predicted by the index mixing rules, for the polymer HFAPNB.](image)

144 has been used. It shows good agreement between experimentally measured $\partial n/\partial T$, and that predicted by the Lorentz-Lorenz index mixing rule. By the same calculation, for PHOST, the unconstrained CTE, $\alpha$, for $T < T_g$ is $1.9 \times 10^{-4}/^\circ C$, and for $T > T_g$ is $3.3 \times 10^{-4}/^\circ C$. For the inorganic material, SiO$_2$, (using $\nu = 0.25$ [34]) $\alpha$, is $4.4 \times 10^{-5}/^\circ C$, and for SiO$_2$N$_y$, (using $\nu = 0.2$ [35]) $\alpha$, is $1.9 \times 10^{-5}/^\circ C$.
For the purposes of this work, the exact values of the volume CTE, \( \alpha \), are not critical, but the concept that they are quantifiably (generally linearly) related to index is. In short, knowledge of either \( \alpha \), (along with the bulk index) or \( \partial n/\partial T \), can be used to establish the temperature sensitivity of these materials.

**Tabular Summary including Published Data** Ultimately, the magnitude of \( |\partial n/\partial T| \) determines a materials index sensitivity to temperature change. For polymers in general, we have tabulated some published values of \( \alpha_U \) (or \( \beta_U \)), and \( \partial n/\partial T \)[36]. They are presented in Table 2. This table shows that based both on CTEs and published values of \( \partial n/\partial T \), there is a wide range of temperature sensitivities. For typical polymers, the \( \partial n/\partial T \) range from from \(-10 \times 10^{-5}/^\circ K\) up to \(-37 \times 10^{-5}/^\circ K\). For the purposes of comparison, we will consider this to bound the performance of standard polymers. The bounds of \( \alpha \) range from \(0.68 \times 10^{-4}/^\circ C\) for polypropylene up to about \(7 \times 10^{-4}/^\circ C\). However, polypropylene is highly resistant to chemical and is unlikely a suitable sensing layer. As such, we consider the reasonable bounds of \( \alpha \) to be between 1 and \(7 \times 10^{-4}/^\circ C\). Both PHOST and HFAPNB fall within this range. There are, in addition, engineered polymers of which ORMOCERs are an example with improved temperature-related properties [37]. The important considerations are that the volume CTE, \( \alpha \), is related to \( \partial n/\partial T \), and that there is a range in the \( \partial n/\partial T \)s and CTEs of different polymer materials.

### 3.2.3.2 Mitigation

We will now examine optical mitigation techniques, accepting that changes in index/thickness of materials in response to temperature change is inevitable. For index-based EWSs, as discussed earlier, the index changes induced thermally cannot be distinguished from those occurring due to the desired chemical or biological change.

Potentially, a separate reference device, identical to the sensing device in every way, except that it is physically isolated from the target agent, could be used to record changes in the sensor occurring due to thermal effects. This isolation could be done using a large mechanical case, that is sealed to the chemical environment. The recorded device output could then be subtracted from the observed changes in the active sensing device digitally.
Table 2: Volume CTE, $\alpha$, Index, $n$, and $\partial n/\partial T$ for polymers in general.

<table>
<thead>
<tr>
<th>Polymer</th>
<th>$\alpha$ ($10^{-4}$/K)</th>
<th>$n$</th>
<th>$\partial n/\partial T$ ($10^{-5}$/K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Poly(butadiene)</td>
<td>7.5</td>
<td>?</td>
<td>?</td>
</tr>
<tr>
<td>Poly(isoprene)</td>
<td>1.9-6.7</td>
<td>1.519-1.6</td>
<td>-37</td>
</tr>
<tr>
<td>Poly(butadiene-co-styrene)</td>
<td>5.3-7</td>
<td>1.534-1.535</td>
<td>-37</td>
</tr>
<tr>
<td>Poly(isobutene-co-isoprene)</td>
<td>4.6-5.6</td>
<td>1.5081</td>
<td>?</td>
</tr>
<tr>
<td>Poly(chloroprene)</td>
<td>6.0-7.2</td>
<td>1.558</td>
<td>-36</td>
</tr>
<tr>
<td>Poly(ethylene)</td>
<td>1.0-1.3</td>
<td>1.426-1.480</td>
<td>?</td>
</tr>
<tr>
<td>Poly(propylene)</td>
<td>0.68</td>
<td>1.49</td>
<td>?</td>
</tr>
<tr>
<td>Poly(tetrafluoroethylene)</td>
<td>0.99</td>
<td>1.376</td>
<td>?</td>
</tr>
<tr>
<td>Poly(acrylonitrile) ($T_g$)</td>
<td>1.0-1.6</td>
<td>1.5-1.524</td>
<td>-9.8</td>
</tr>
<tr>
<td>Poly(acrylonitrile) ($T_g'$)</td>
<td>2.8-3.8</td>
<td>1.5-1.524</td>
<td>-17</td>
</tr>
<tr>
<td>Poly(vinyl chloride) ($T_g$)</td>
<td>0.66-0.73</td>
<td>1.538 (656.3 nm)</td>
<td>-11</td>
</tr>
<tr>
<td>Poly(vinyl chloride) ($T_g'$)</td>
<td>1.7-1.75</td>
<td>1.5-1.524</td>
<td>-11</td>
</tr>
<tr>
<td>Poly(vinyl acetate) ($T_g$)</td>
<td>2.1</td>
<td>1.4669</td>
<td>-29</td>
</tr>
<tr>
<td>Poly(vinyl acetate) ($T_g'$)</td>
<td>6.6-6.7</td>
<td>1.4669</td>
<td>-29</td>
</tr>
<tr>
<td>Poly(methyl methacrylate)</td>
<td>2.25-2.72</td>
<td>1.492 (589 nm)</td>
<td>-11</td>
</tr>
<tr>
<td>Poly(methyl methacrylate) ($T_g$)</td>
<td>5.6-5.8</td>
<td>1.492 (589 nm)</td>
<td>-21</td>
</tr>
<tr>
<td>Poly(styrene) ($T_g$)</td>
<td>1.7-2.1</td>
<td>1.59-1.6 (589 nm)</td>
<td>-14.2</td>
</tr>
<tr>
<td>Poly(styrene) ($T_g'$)</td>
<td>5.1-6.0</td>
<td>1.59-1.6 (589 nm)</td>
<td>-14.2</td>
</tr>
<tr>
<td>Polyamide 6</td>
<td>1.0-1.4</td>
<td>1.519-1.582</td>
<td>-14.2</td>
</tr>
<tr>
<td>Polyamide 66</td>
<td>1.0-1.4</td>
<td>1.519-1.582</td>
<td>-14.2</td>
</tr>
<tr>
<td>ORMOCERs (without fillers)</td>
<td>0.7-1.84</td>
<td>1.42-1.65 (1300 nm)</td>
<td>?</td>
</tr>
<tr>
<td>ORMOCERs (with fillers)</td>
<td>0.18-0.7</td>
<td>1.42-1.65 (1300 nm)</td>
<td>?</td>
</tr>
</tbody>
</table>

(post-detection). However, any difference in the conditions of the two devices will prevent this method from working well. It is fundamentally better to optically remove the thermal effects without resorting to a second device. We will consider here the use of interferometric techniques coupled with knowledge of the relative temperature sensitivity of different materials to partially or completely eliminate temperature dependencies in EWSs.

For interferometric devices, in order to establish a thermally insensitive device that is still chemically or biologically sensitive, two criteria must be satisfied. First, \textit{one arm must be sensitive to the agent in question and the other must not}. Second, \textit{the phase shift between the arms occurring due to temperature must be held to zero}. As interferometric EWSs are generally guided wave devices, we can further specify this. For simplicity, a single-mode device is considered. Many of these ideas can also be extended to multimode devices. First, we select materials so that only the material covering the guiding layer on one arm is chemically sensitive. The net modal phase difference, $\Delta \phi$, between the modes traveling through the separate interferometer arms developed due to temperature change, $\Delta T$, can

48
be written as

\[ \Delta \phi = \phi_1 - \phi_2 \]

\[ = \frac{2\pi}{\lambda_0} \left\{ \left[ n_{\text{eff}1} + \left( \frac{\partial n_{\text{eff}}}{\partial n_c} \right)_1 \frac{\partial n_{c1}}{\partial T} \right] L_1 - \left[ n_{\text{eff}2} + \left( \frac{\partial n_{\text{eff}}}{\partial n_c} \right)_2 \frac{\partial n_{c2}}{\partial T} \right] L_2 \right\}. \]  

(19)

Of interest in the change in this phase difference with temperature. In the limit of small \( \Delta T \), this may be expressed as

\[ \frac{\partial \Delta \phi}{\partial T} = \frac{2\pi}{\lambda_0} \left\{ \left( \frac{\partial n_{\text{eff}}}{\partial n_c} \right)_1 \frac{\partial n_{c1}}{\partial T} L_1 - \left( \frac{\partial n_{\text{eff}}}{\partial n_c} \right)_2 \frac{\partial n_{c2}}{\partial T} L_2 \right\}. \]  

(20)

where \( \left( \frac{\partial n_{\text{eff}}}{\partial n_c} \right)_1 \) \( \left( \frac{\partial n_{\text{eff}}}{\partial n_c} \right)_2 \) is the index sensitivity coefficient of a mode of arm 1 (arm 2) to index change in the cover layer and \( \frac{\partial n_{c1}}{\partial T} \) \( \frac{\partial n_{c1}}{\partial T} \) \( \frac{\partial n_{c2}}{\partial T} \) is the rate of change of index with temperature on the material on arm 1 (arm 2). \( L_1 \) \( L_2 \) is the path length under the sense layer on arm 1 (arm 2). The intensity output of any interferometric waveguide device for which this difference is 0 will be temperature insensitive. We will explore some alternate methods to create this condition.

3.2.3.3 Mitigation using the Identical Materials

The simplest way to keep \( \Delta \phi = 0 \) is to use exactly the same materials with the same thicknesses on both arms. In this case, \( \frac{\partial n_{c1}}{\partial T} = \frac{\partial n_{c2}}{\partial T} \) and \( \left( \frac{\partial n_{\text{eff}}}{\partial n_c} \right)_1 = \left( \frac{\partial n_{\text{eff}}}{\partial n_c} \right)_2 \).

Therefore if we choose \( L_1 = L_2 \), temperature changes will not affect the phase difference between the arms. We desire to maintain this temperature stability while at the same time allowing only one of the two arms to be exposed to a chemical or biological agent. An obvious solution is to isolate one arm with a chemical or biological barrier material.

One simple solution is to spin-coat glass to completely cover one of the arms. This glass could be patterned by common microelectronics fabrication methods (lithography, reactive-ion-etching etc.) to coat only arm making it chemically insensitive. The issue is that this coating has an associated CTE. Thus any mismatch between the CTE of the covering material, and that of the underlying waveguide stack (SiO\(_2\)/SiO\(_x\)N\(_y\)/polymer) leads to tension or compression and associated deviations from the original \( \frac{\partial n}{\partial T} \). These deviations create temperature-related phase differences between the two arms, an undesirable effect. If, however, a chemically impervious material has a CTE that closely matches that of the stack,
this problem will not occur. This method is conceptually identified by Fig. 41. This figure shows one possible interferometric layer structure, with one arm covered by a chemically-impervious glass. This is the layer structure in the two adjacent waveguides between the y-junctions. There is a 1-2 $\mu$m-thick layer of SiO$_2$, and then an approximately 0.2 $\mu$m-thick layer of SiO$_{x}N_y$ (for 840 nm operation). For single-mode operation, these waveguides are about 0.2 $\mu$m-thick. Above the high-index ($n \simeq 1.9$) SiO$_{x}N_y$, an approximately 1-$\mu$m-thick layer of some sensing polymer is spin-coated and defined lithographically. We will investigate candidate materials to determine if any have the desired properties.

For a more quantitative assessment, the combined CTE of the SiO$_{x}N_y$/HFAPNB stack is considered. Referring to Fig. 41, let $t_a(\Delta T)$ be the temperature dependent thickness of the SiO$_{x}N_y$ layer, and $t_b(\Delta T)$ be the temperature dependent thickness of the HFAPNB layer. $(\beta_c)_a$ and $(\beta_c)_b$ are the corresponding constrained CTEs, and $t_{a0}$ and $t_{b0}$ are the
thicknesses at $0 \Delta T$. The net constrained CTE of the stack is calculated as follows:

$$t_a(\Delta T) = t_{a0}(1 + (\beta_c)_a \Delta T)$$

$$t_b(\Delta T) = t_{b0}(1 + (\beta_c)_b \Delta T)$$

$$t_a(\Delta T) + t_b(\Delta T) = t_{a0} + t_{b0}(1 + \frac{t_{a0}(\beta_c)_a + t_{b0}(\beta_c)_b}{t_{a0} + t_{b0}} \Delta T)$$

$$(\beta_c)_{a+b} = \frac{t_{a0}(\beta_c)_a + t_{b0}(\beta_c)_b}{t_{a0} + t_{b0}}.$$  \hspace{1cm} (21)

That is the combined constrained CTE is simply a thickness weighted average of the individual layer constrained CTEs. Thus the combined CTE of the stack is

$$(\beta_c)_{a+b} = \frac{0.2\mu m(8.9 \times 10^{-6}/\degree C) + 1(1.8 \times 10^{-4}/\degree C)}{1.2\mu m}$$

$$\simeq 1.5 \times 10^{-4}/\degree C.$$ \hspace{1cm} (22)

Thus the combined constrained CTE of this stack is just slightly less than that of the polymer itself. Via Eq. 144, the true volumetric CTE, $\alpha$, can be estimated (with $\nu \simeq 0.37$) at $2.6 \times 10^{-4}/\degree C$. This is indicative of a polymer. Thus this method is feasible if a chemically impervious polymer can be found, that has a similar CTE. In short, this method will work if the constrained CTE of the sensing layer is nearly equal to that of the capping layer, and the capping layer is chemically resistant. For polymer SLs, this suggests a polymer capping layer.

Alternately, if such a material cannot be found, then very good temperature control could be used to largely eliminate the stress and potential index variation associated with mismatched CTEs between the waveguide layer stack and the covering material. Thus it is logical to ask, “what are the capabilities of active temperature control devices for integrated optical devices?”

**Mitigation by Temperature Control** In this section, the ability of cooling methods that can be used with integrated optical devices is investigated. With adequate cooling, at a reasonable power, any impermeable material could be used to cover the reference arm and maintain essentially equal path lengths for a range of temperatures. In addition, in a fully integrated device, these coolers could be used to reduce thermal effects in lasers and detectors. Active cooling methods fall into 2 categories: solid state coolers (Peltier coolers)
and liquid-based coolers. At this time, liquid coolers are not considered because they add another agent to the system that could act as chemical noise. Thus we consider Peltier coolers here.

Peltier coolers can be fabricated using junctions of n and p semiconductor materials. They use the Peltier effect \cite{38} to transport heat parallel to the junction. Typically, these devices are fabricated using $Bi_2Te_3$ because of superior thermal properties, however, fabrication constraints limit the use of $Bi_2Te_3$ in integrated devices. Winjngarrrds et al. \cite{39} show that Peltier coolers can be fabricated at a slightly lower performance in polySi and polySiGe. These materials are compatible with many planar waveguide optical device material systems and in addition with Si-CMOS, presenting the possibility of fully-integrated, cooled chem-bio sensor systems.

The key performance metric is the achievable temperature stability. It is desired, not only to have the capability to remove (or add) heat, but to keep the fluctuation in temperature below some value. The thermally-induced index fluctuation must be minimized. Sloman et al. \cite{40} have performed a review of these stabilizing systems. For sensors within temperature controlled environments, temperature stabilities as small as $+/−3.5\mu K$ have been demonstrated by Priel\cite{41}. However in sensors exposed to the environment, the demonstrated sensitivities are near $+/−1\text{ mK}$. For example Bradley et al. \cite{42} describe using a thermistor bridge to control a Peltier junction to stabilize the temperature of a laser diode to better than $+/−300\mu K$. Sloman et. al \cite{40} demonstrated a $+/−1\text{ mK}$ temperature stability using a digitized thermal output to a computer software implemented control loop. However, this degree of temperature control was achieved using the $Bi_2Te_3$ material system \cite{41} on an aluminum block, which was clearly not an integrated device. Thus, we assert that a temperature control of $+/−1\text{ mK}$ has already been achieved in non-integrated devices and is potentially achievable in integrated devices.

Because polySi and polySiGe are the materials of choice for temperature control of integrated devices, and not $Bi_2Te_3$, there are some further limitations to their performance. First, the thermal conductivity of polySi($n \sim 24\text{ W/m/K}$) is about $12\times$ greater than that of $Bi_2Te_3(n \sim 2\text{ W/m/K})$, and about $4\times$ greater than that of polySiGe($n \sim 4.5\text{ W/m/K}$).
Thus for integrated devices, polySiGe is the material of choice. Other issues also influence the performance of integrated coolers. Wijngarrrds et al. suggest that both the contact resistance between the metal and the semiconductor and the parasitic thermal conductivity of a support membrane on which the device sits, can limit the maximum attainable temperature difference. In fact, they [42] estimate that an integrated Peltier cooler can cool up to 2.1 K below ambient temperature. This is more than sufficient for an integrated device, which simply must maintain a constant temperature. Further, it is the control loop as well as the response time of the cooler that ultimately determines temperature stability. A control loop for an integrated device could be the same and therefore have comparable performance with a non-integrated cooler. Thus, by comparison with a non-integrated device, $+/−1\text{mK}$ is estimated as the attainable resolution of temperature control for an integrated chem/bio sensor cooled by an integrated Peltier cooler. For one polymer, HFAPNB($\partial n/\partial T$ = $2.4 \times 10^{-4}/°C$), this limits the index resolution of the sensor to to $4.8 \times 10^{-7}$. Polymers with smaller $\partial n/\partial T$($\simeq -7.9 \times 10^{-5}$) permit a smaller index sensitivity ($1.6 \times 10^{-7}$) for the same temperature stability.

A slight variation on this method could involve capping both arms. If a material could be found that could be made chemically sensitive or insensitive, but maintain the same CTE, then any mismatch in CTE would be the same on both arms, maintaining equal temperature induced phase differences.

Assuming that temperature control can be implemented, but not perfectly, it is still desired to cover one arm, while not inducing expansion related index differences in the sensing polymer film. A cap with space between it and the sense polymer would work. This cap would permit the SL layer stack to expand unobstructed. Fabrication is the issue. It could be designed and constructed separately from the waveguide and then applied after the interferometer was created. However, it must be sealed to a tiny waveguide. Alternately, some sacrificial material could be deposited over the sense polymer, which could be covered by a permanent glass cap. Following that, the sacrificial material would be removed. This method, while also simple in concept, may be difficult to achieve in practice. This method is shown conceptually in Fig. 42.
**Figure 42:** Endcap concept. The cap is designed to have some gap between it and the underlying waveguide material, preventing compression-induced index variation with the non-confined arm.

### 3.2.3.4 Mitigation using Different Materials

Capping or covering the same materials requires material properties that are difficult to find and fabrication methods that are difficult to achieve. An alternate method uses a different, chemically insensitive material on the reference arm. By its nature, it satisfies the requirement of chemical insensitivity. In this implementation, \( \frac{\partial n_{c1}}{\partial T} \neq \frac{\partial n_{c2}}{\partial T} \). In general, the polymer SL will have a 2 or 3 times greater index sensitivity to temperature than chemically insensitive materials (like SiO\(_2\)). Further, we assume that we do not cross the glass transition temperature, \( T_g \), of either material as this significantly changes \( \frac{\partial n_{c}}{\partial T} \).

However, to equalize the acquired phase due to temperature changes, some changes in the interferometer must be implemented. Considering Eq. 20, for the temperature sensitivity in the phase difference to be zero,

\[
(\frac{\partial n_{eff}}{\partial n_c})_1 L_1 = \frac{\partial n_{c2}/\partial T}{\partial n_{c1}/\partial T}(\frac{\partial n_{eff}}{\partial n_c})_2 L_2.
\]  

(23)

Both \( \frac{\partial n_{eff}}{\partial n_c} \), and \( L \) are adjustable parameters in the optical design of the waveguide layer structure. Let us consider the benefits and limitations of adjusting either or both.
Equalization By Adjusting Modal Index Sensitivity. We have previously shown, Fig. 4, that for planar waveguides, for layer stacks like those shown in Fig. 41, the guiding layer thickness can be used to adjust the index sensitivity coefficients, $\partial n_{\text{eff}} / \partial n_c$, of guided modes. This corresponds approximately to adjusting the mode field power distribution within each layer. We have also previously shown that optimal sensitivity for EWSs occurs at specific guiding layer thicknesses. Because the chemically sensitive polymer typically has a temperature index sensitivity 2 to 3 times greater than that of appropriate insensitive materials, it would require a reduction in sensitivity on the sensing arm to achieve temperature insensitivity. That is, the power in the chemically sensitive polymer would be reduced to reduce the index sensitivity to temperature. However, that would correspondingly reduce chemical sensitivity. Thus, this method would be undesirable unless the difference in CTE between the two different materials were very small. This method is not considered further.

Equalization By Adjustment of Optical Path Length. Considering Eq. 23, the waveguide layers are designed to keep $(\partial n_{\text{eff}} / \partial n_c)_1 = (\partial n_{\text{eff}} / \partial n_c)_2$. Then, to maintain a zero net phase shift in response to temperature change, we must adjust the lengths of the two interferometer arms so that

$$\frac{L_2}{L_1} = \frac{\partial n_{c1} / \partial T}{\partial n_{c2} / \partial T}.$$ (24)

The most easily implemented method to equalize the temperature sensitivity by adjusting lengths is to simply to increase the actual physical length of one arm compared with another. As the sensing arm typically has a higher temperature sensitivity, this means lengthening the reference arm. This requires some optical design to ensure that loss to radiation modes is minimized or at least equal for both arms. However, this design is not difficult in practise. This increase in reference arm length can be accomplished in a variety of ways, the simplest of which involves some form of s-bend on the reference arm. Although the initial phase difference will be different, the phase change as a result of temperature will be the same. One key to this method, practically, is that the optical source must have a coherence time greater than the greatest possible net time difference between the two arms. The main drawback for a fully integrated devices is that additional space is required.
for the reference arm. In addition, this would produce a non-symmetric interferometer. However, this is not really a problem, as it is the increased phase difference that is critical to interferometric EWS sensing. Further, although there would be some asymmetry in the interferometer, a 50/50 y-junction could still be designed.

### 3.3 Conclusion

In conclusion, this chapter has investigated the sensitivity of the optical constants of optical materials, mainly polymers, that have merits as SLs to chemical and thermal changes. The relative sensitivity of the polymer HFAPNB to different chemicals has been quantified. In addition, the thermal index sensitivity of optical materials, and mainly polymers, has been investigated. It has been shown that temperature related index changes in polymers are related to expansion. It has also been shown that polymers are much more sensitive to temperature changes than inorganic optical materials like SiO$_2$ and SiO$_x$N$_y$. This information can be used to create temperature insensitive devices by using a combination of temperature control and interferometric optical design.
4.1 Introduction

Simulation of the device requires modeling of a variety of elements. The key elements to be simulated include the source, the detectors, and the chemically-sensitive waveguide. As this project has involved different personnel, the source modeling is to be done by M. Thomas. The detector modeling has been done by D. Kim. However, the spatial bandwidth effects and noise properties of the detectors are considered in Ch. 7. This chapter concerns the simulation of the chemically sensitive multimode interferometric waveguide.

Experimental inputs include an illumination profile, the interferometric waveguide geometry, and indices of refraction. In these simulations, the effect of illumination profile is considered. The source is considered to be a ideal single wavelength source. The interferometric waveguide has a given surface-relief pattern, and a layer structure composed of different materials with different indices of refraction. Ellipsometry provides index and thickness measurements of the sensing layer as they change with absorbed chemical, the data required to simulate the changing sensor response. This device has primarily been simulated using the beam propagation method (BPM).

4.2 Chemically Sensitive Waveguide Simulations

4.2.1 Effective Index Method

For all simulations, the effective index method [10] is used. This is a method used to approximate the modal properties of a two-dimensional waveguide cross-section using two one-dimensional calculations.

The effective index-based waveguide simulations are performed in stages. First, the propagation constants and field profiles of the single transverse-magnetic-like (TM) guided
modes for each vertical waveguide are calculated. These propagation constants are calculated based on the approach of Chilwell and Hodgekinson [17]. The associated transcendental eigenvalue equation is solved with a quasi-graphical numerical method of finding the zeros. The layer sets (dielectric multilayer stacks) consist of the reference layer set and the sensing layer set. The reference layer set is located over the entire interferometer except where the sensing occurs and does not change with applied chemical. Referring to Fig. 21, the sensing occurs within the black rectangle. Everywhere else contains the reference layer set. The sensing layer set, located on one interferometer arm, changes with chemical as the index and to a small degree, the thickness of the sensing layer changes. Thus, the propagation constants and mode profiles of the guided modes must be found for each chemical concentration measured. The required indices and thicknesses have been measured ellipsometrically, accurately indicating the chemical absorption.

The effective indices produced are used as input to a ‘horizontal’ beam propagation method (BPM) [43] or to a coupled-mode simulation that produces output modal patterns comparable to those measured from the actual device.

4.2.2 Beam Propagation for Device Simulation - Strategy 1

The beam propagation method (BPM) [43] is a finite-difference based method for simulating integrated optical components which, by applying certain approximations, becomes computationally less intensive than the full finite-difference method. Being a finite-difference method, it is a numerical implementation of the scalar or vector electromagnetic wave equation derived from Maxwell’s Equations. A brief summary of the theoretical origin of the method is presented here with a goal of specifying the key approximations used in the simulation of the multimode sensor.

To illustrate the method, some key elements of the scalar version of the method are summarized here. The derivation begins with the two-dimensional scalar wave equation:

\[
\frac{\partial^2 \phi(x, z)}{\partial x^2} + \frac{\partial^2 \phi(x, z)}{\partial z^2} + n^2(x, z)k_0^2 \phi(x, z) = 0.
\]  

(25)

The key efficiency of the BPM is

\[
\phi(x, z) = u(x, y, z)e^{ik_z z}.
\]

(26)
This exact modification separates most of the fast changing phase in the propagation direction from the slower changing envelope function, $u$. Applied to the scalar wave equation, this results in

$$\frac{\partial^2 u(x, z)}{\partial z^2} + 2ik\frac{\partial u(x, z)}{\partial z} + \frac{\partial^2 u(x, z)}{\partial x^2} + (k_0^2n^2(x, z) - k^2)u(x, z) = 0. \quad (27)$$

At this point, the standard approximation of the BPM is to simply remove the first term in Eq. 27. Removal of this term is justified if the field, $u$, is slowly varying in $z$ and at least its magnitude is less than the third term. As the field varies in $x$ (the field profile) this is valid for many fields. However, for wide-angles and wide waveguides, this approximation is not valid. An alternate approach treats the second derivative in the propagation direction as an operator ($D \equiv \frac{\partial}{\partial z}$), and solves for this operator. This provides an analytically correct solution, Eq. 28, which is restricted to propagation in one direction (through selection of either the positive or negative square root). This equation develops as follows:

$$Du(x, z) = i\kappa \left\{ \pm \sqrt{1 + \frac{1}{k^2} \left( \frac{\partial^2}{\partial x^2} + k_0^2n^2(x, z) - k^2 \right)} - 1 \right\} u(x, z) \quad (28)$$

This equation can only be solved if the square root term is approximated. It has been shown that the Pade approximation of this term [44] is more accurate for a similar number of terms than a comparable Taylor series expansion. The Pade approximations are polynomials, with increasing numbers of terms for more accuracy. A high order Pade approximation (4,4) is used to simulate the multimode waveguide. A convergence study has suggested that this approximation is more than adequate for the simulation of this multimode interferometric sensor.

Using this numerical method, two different elements will be investigated:

1. the sensor response to index changes on the sensing arm. This will include an estimate of the modal pattern repetition period; and

2. the modal coupling that occurs in the multimode $y$-junction. This will include creating a matrix which can estimate the output field for any input field.
Both of these simulations, when taken together, will offer insight as to how the illuminating modal field affects the device sensitivity. It may suggest that an input coupler/splitter which excites higher-order modes in the sensing portion of the waveguide creates a more sensitive multimode interferometric sensor.

4.2.2.1 Sensor Response to Index Changes on the Sensing Arm

The BPM as described is first used to simulate the sensor. A multimode electric field pattern, consisting of an equal weighting of the 0\textsuperscript{th}, 5\textsuperscript{th}, 10\textsuperscript{th}, ..., and 45\textsuperscript{th} modes illuminates the sensor. This illumination is expected to excite a number of high-order modes in the two interferometer arms. If so, it should produce high sensitivity to index change, based on the arguments in Ch. 2. Fig. 43 shows the raw numerical output of the simulation after propagation through the input waveguide and initial y-junction. The field pattern generated is then used to illuminate the remaining portion of the sensor. For this remaining portion, a separate simulation was performed for each of 100 stepped index changes on the sensing arm, for a total index change of $1 \times 10^{-3}$. Figure 44 shows the sensing portion of the waveguide and the recombining y-junction for one such simulation. The final result of the simulation is an electric field for each of the index changes, which is shown in Fig. 45. The sensing ability of these patterns is explored in Ch. 6.

![Figure 43: First half of sensor simulation showing the input multimode y-junction after illumination by a multimode pattern.](image)
Figure 44: Second half of simulation showing the sensor and output y-junction. Corresponds with Fig. 43.

Figure 45: Beam prop simulation of sensor over a range of cover index of $1 \times 10^{-3}$. 
4.2.2.2 Modal Coupling Properties of the Multimode Y-junction

The modal coupling properties of the multimode y-junction are also investigated using the BPM. The boundaries of the y-junction are shown in Fig. 46. Mode fields in any waveguide structure, are orthogonal to each other [45]. In the BPM simulation undertaken here, the composite fields developed by the BPM can be described as follows:

$$\phi(x, z) = \sum_{m=1}^{M} a_m \phi_m(x) e^{j\beta_m z},$$

(29)

where \(\phi(x, z)\) represents any composite electric field, and \(\phi_m(x)\) represents the \(m^{th}\) mode-field of the waveguide. The BPM can also be used to calculate the mode field of each of the eigenfunctions (mode-fields) of the waveguide in question. Then, by applying mode orthogonality, any field calculated by the BPM can be broken down into its component mode fields as follows:

$$\int_X \overrightarrow{\phi}(x, z) \overrightarrow{\phi^*}_m(x) \, dx = a_m e^{j\beta_m z}. $$

(30)

It is noted that the mode power is given by \(|a_m|^2\).

For the multimode y-junction, it is desired to know for a given input mode, what fraction of the power couples into a given mode of each interferometer arm. Also of interest is the input-mode dependent loss if present. Both of these quantities are determined for the

Figure 46: The multimode y-junction. The centerline is a line of symmetry. The reference layer set exists within the y-junction. A uniform index exists outside.
100–µm y-junction. It is noted that the index contrast used was slightly higher in this simulation, than in the sensitivity study in Ch. 2, as the index inputs were taken from an earlier ellipsometry study. However, the results are to be considered applicable as a countable number of additional high-order modes are allowed, and as will be shown, they minimally affect sensor index sensitivity.

To determine the mode coupling properties of the y-junction, each input mode is simulated in turn. The 9th order mode is shown for example. Figure 47 shows the y-junction under illumination by a 9th-order mode. It is evident from this contour plot that some mode coupling is occurring in the y-junction. For this mode, the power coupled into each mode of the right arm of the y-junction is shown in Fig. 48. It is noted that the majority of the power is coupled into the 9th order mode of the right (and left) waveguide. However, there is also significant coupling to the modes nearest to the 9th in propagation constant and mode number. Coupling is minimal to modes of order less than 4 or greater than 25. Figure 49 shows the original(a) BPM field and the field after modal decomposition and then recomposition (b). There is no discernable difference, demonstrating the robustness of the method. This robustness was observed for each of the modes of the structure.

![Figure 47: Input multimode waveguide illuminated by the 9th order mode. The output of this simulation is used to quantify the modal coupling into the two interferometer arms.](image)

The mode coupling observed in Fig. 48 directly affects sensor sensitivity. Recalling
**Figure 48:** Relative power coupled into the modes of the right arm of the multimode y-junction after illumination of the input waveguide by a $9^{th}$-order mode. The best coupling is to the $9^{th}$-order mode of the right arm waveguide.

**Figure 49:** Original mode intensity profile and the ‘recombined’ mode intensity created using the mode weightings obtained by modal decomposition. The very good agreement demonstrates the robustness of the decomposition.
that the multimode sensor has basically a higher sensitivity for higher-order modes, the
distribution of modes affects the mean path length under the sense layer. First, the mode
couplings for some more input mode fields are shown in Fig. 50. For modes of order \( \leq 50 \),
the multimode y-junction creates coupling with the modes closest to the input mode in
mode number or propagation constant. For intermediate order modes (between 60 and
209), the y-junction couples power into a wide range of modes, but the order is less than
that of the input waveguide. For the highest order input modes, power is coupled into
modes of order approximately half that of the input mode. Essentially half of the peaks go
to one arm and half to the other. Regardless of the reason, even with a very high order
excitation of the input waveguide, the maximum order excited in the interferometer arms
are close to half of the maximum possible order. This means that regardless of the input
field, maximum sensitivity using this y-junction cannot be attained.

In fact, using the sensitivities shown in Fig. 15, a mean index sensitivity can be cal-
culated by creating a weighted average of mode power and mode sensitivity. Figure 51
illustrates the relationship between input mode number and relative sensitivity. Specifi-
cally,

\[
\frac{\partial n_{\text{eff}}}{\partial n_{\text{SL tot}}} = \frac{1}{\sum_{i=1}^{N} P_i} \sum_{i=1}^{N} \frac{\partial n_{\text{eff}}^i}{\partial n_{\text{SL}}} P_i,
\]

(31)

where \( P_i \) represents the power in the \( i^{th} \) mode when entering the SL waveguide. It is noted
that modes of order less than half that of the maximum develop only a slightly increased
index sensitivity. This explains the result of Fig. 51, which essentially shows that for any
input mode, high or low, the average improvement in index sensitivity is at most 14%.

The mode dependent loss is shown in Fig. 52. It is in general small, but does increases
slightly for higher-order modes. It is not significant to the sensor sensitivity. This loss is
considered to represent coupling to radiation modes of the waveguide. Further, though it
has not been shown, the BPM simulations confirm that the y-junction is symmetric and
that the power is equally split regardless of the mode excitation as long as the illumination
field is centered on the input waveguide.
Figure 50: Mode power coupled from a range of input modes into either arm of the interferometer. This response is characteristic of this multimode y-junction design.

Figure 51: Mean index sensitivity calculated via power fraction. The potential improvement due to exciting higher-order modes in the SL is not observed for any input mode.
Figure 52: Input mode dependent loss. Shows small increase in loss for increasing mode number.
Chapter V

EXPERIMENTAL DETAILS OF MEASUREMENT

5.1 Device Details/Design

A sensor-on-a-chip is created by first fabricating the necessary CMOS circuitry, which includes detector arrays, analog-to-digital converters, and readout circuitry. This is followed by the deposition and definition of the planar waveguide structures. The waveguide process developed and materials used must not impair the functionality of the existing CMOS circuits. The base structure (Fig. 53(a)) includes a 1-\(\mu\)m SiO\(_2\) \((n_{840nm} \sim 1.465)\) lower cladding layer that isolates the waveguide from the circuit. It also includes a 0.20-\(\mu\)m high-index \((n_{840nm} \sim 1.920)\), low-loss, SiO\(_x\)N\(_y\) guiding layer, and a 1-\(\mu\)m SiO\(_2\) upper cladding deposited on a silicon wafer. These materials are deposited using a plasma enhanced chemical vapor deposition (PECVD) system [46]. For both materials, the deposition temperature is 200\(^\circ\)C, which does not damage the CMOS circuit. The low frequency plasma regime is used \((\sim 380 kHz)\) with an RF power density of \(\sim 110\) \(mW/cm^2\). Following this, standard lithography methods and reactive ion etching (RIE) are used to define the surface profile of the waveguides (Fig. 53(b)). Next, on the sensing arm, a 2000-\(\mu\)m\(\times\)100-\(\mu\)m channel is etched down to the SiO\(_x\)N\(_y\) guiding layer, and 1-\(\mu\)m-thick layer of the chemically sensitive polymer, HFAPNB \((n_{840nm} \sim 1.430)\), is spin-coated to create the sensing layer. Figure 54 shows the waveguide cross-section during the various processing steps. The initial SiO\(_2\) and SiO\(_x\)N\(_y\) deposition (a) is followed by the definition of the interferometer using protective photo-resist and RIE (b) and (c). A channel is defined over the sensing arm only using similar methods (d) and (d). Finally, the polymer SL, HFAPNB, is spin-coated over the entire interferometer. Figure 55 shows the vertical mode distribution within the sensing arm (approximated by the effective index method), and Fig. 56 shows the corresponding profile in the reference arm. The key difference between the sensing arm and the reference arm is the amount of mode field within the HFAPNB SL. On the sensing arm, 27\% of the
magnetic field lies within the SL versus 0.19% on the reference arm. A slightly thicker (by 0.05-0.1 \( \mu m \)) SiO\(_2\) buffer layer, however, would prevent any evanescent field from entering the HFAPNB layer on the reference arm, slightly increasing overall sensitivity.

**Figure 53:** (a) Cross-section of interferometric sensor. From bottom-to-top, the waveguide structure includes a 1-to-2-\( \mu m \)-thick SiO\(_2\) layer and a 0.20 to 0.25-\( \mu m \)-thick SiO\(_x\)N\(_y\) guiding layer \((n_{840nm} \sim 1.920)\). On the “sensing” arm (left-side), there is a 0.95-\( \mu m \)-thick layer of the ‘substituted polynorbornene’ polymer, HFAPNB, \((n_{840nm} \sim 1.430)\) above the guiding layer. On the reference arm, there is a 1-\( \mu m \)-thick SiO\(_2\) layer between the guiding layer and the 0.95-\( \mu m \) HFAPNB layer. (b) Surface relief of interferometric sensor.

Multimode MZI EWSs have been fabricated using these materials on silicon and on a CMOS-chip, Fig. 57, that includes embedded detectors and associated signal processing circuitry [47]. The efficiencies of a large yield Si-CMOS process is best maintained when the die size remains a few mm, and therefore, the devices reported here are designed to fit within a nominal size of 4.6\( mm \times 4.7mm\), consistent with a standard size of the MOSIS foundry [48]. The MZIs are 4500-\( \mu m \) long and have 100-\( \mu m \)-wide waveguides separated by a maximum of 20 \( \mu m \)(Fig. 53(b)). The interferometer arms are 2000 \( \mu m \) in length. These wide waveguides support nominally 300 modes. The mode field of the lowest order transverse mode is shown in Fig. 58. The input side of the interferometer is split at a y-junction, which has a \( \sim 3.3^\circ \) branching angle and a length of 750 \( \mu m \). An active sensing arm and a passive reference arm are both located immediately after the y-junction. On the passive reference arm, an SiO\(_2\) buffer layer is used to prevent any interaction between the
Figure 54: Processing steps to create the waveguide: (a) PECVD is used to deposit SiO$_2$ and SiO$_x$N$_y$; (b) and (c) Photo-lithography and reactive-ion-etching (RIE) are used to define the waveguides; (d) and (e) Photo-lithography and RIE are again used to open a channel on the sensing arm; (f) Polymer SL is spin-coated over the entire structure.

Figure 55: The vertical magnetic field distribution within the sensing layer set. About 27% of the field lies within the sensing layer.
Figure 56: The vertical magnetic field distribution within the reference layer set. Only 0.19% of the field lies within the sensing layer.

The large vertical evanescent field and the sensing material. On the active arm, the large vertical evanescent field extends into the chemically sensitive layer. Upon interaction with an agent, which alters the index of the sensing layer, the carrier phase acquired by each guided mode is uniquely changed. The resulting modal phase differences induce changes in the composite modal pattern at the interferometer output. In addition, the index variations in the sense arm can result in inter-modal coupling to other guided or radiative modes, which affects the final modal pattern and total received power.

Recently, a photo-definable SL has been used to facilitate device processing. The addition of photo-acid generator to the monomer suspended in PGMEA (propylene glycol methyl ether acetate) has created a positive exposure polymer sensing layer. This has permitted a simpler process to create sensing interferometers (Fig. 59). Again PECVD is used to deposit the lower cladding and guiding layers, (a) SiO$_2$ and SiO$_x$N$_y$. This is followed by the definition of the interferometer using protective photo-resist and RIE (b) and (c). The polymer SL is then spin-coated over the entire structure, exposed, and developed away leaving SL only on the reference arm. It has also produced an increased index contrast for the waveguides due to the easy removal of the polymer everywhere except over the sensing arm. In this case, the reference arm shown in Fig. 53(a) (right side) does not have the SiO$_2$ buffer layer. The mode field, Fig. 60, is shifted further into the substrate in this structure,
**Figure 57:** Waveguides deposited on a Si-CMOS circuit that includes photo-detectors and associated signal processing electronics.

**Figure 58:** The lowest order transverse mode electric field on the reference side.
and there is a small portion of the field within the air. Thus, this structure is used when the agent is highly dispersed in air and so must be absorbed and concentrated in the polymer sense layer to affect the propagating modes.

Figure 59: Processing details using a photo-definable polymer. (a) PECVD is used to deposit SiO$_2$ and SiO$_x$N$_y$. (b) and (c) Standard photolithography is used to define the interferometer structure (e) and (f) Photo-definable polymer is spin-coated, exposed, and developed to produce SL only over the sensing arm.

Figure 60: The vertical magnetic field distribution within the reference layer set when a photodefinable SL is used. It is assumed that the chemical is dispersed in air, and so does not affect the mode field.
5.2 Sensor Measurement Setup

The interferometric sensor is evaluated using the previously described gas delivery system and a separate, sealed, stainless steel chamber that contains the interferometric sensor, represented schematically in Figure 61. Light from an 830–$nm$ Fabry-Perot semiconductor laser is coupled into the TM modes of the interferometer. The excitation spot is $\simeq 10\mu m$ in diameter, and is positioned by visually monitoring the scattered light, ensuring that both arms of the interferometer receive approximately half of the coupled power. The output modal pattern is imaged via a long working distance objective onto a CCD array that captures images at 30 frames per second. These frames are then digitally averaged for an effective optical integration time of $\sim 1\, s$. The long working distance of the objective enables the waveguide facet to be imaged from within the 1.5-inch-wide steel chamber, but the numerical aperture (0.4) does not capture approximately two-thirds of the modes, which exit the waveguide at the steepest angle. Care is taken to ensure stable coupling at the MZI input to minimize coupling-induced modal pattern fluctuations. In the absence of agent, the total power is stable to $\pm 0.3\%$ over a measurement interval of 80 minutes. Power variation, however, are correlated with agent concentration. However, we have found that the modal image structure is a more reliable indicator of chemical concentration than total power, and therefore all images are normalized to constant power. The accurate gas delivery of the chemical agents permits this sensor response to be linked to chemical concentration and through the ellipsometric measurements, to index change within the sensing layer. Simultaneously with modal image acquisition, the QCM records the mass uptake of the target agent. These QCM readings provide additional confirmation of the concentration and hence index changes.

5.2.1 Waveguide Test Chamber

A custom-built waveguide test chamber, Fig. 63 has been fabricated to permit testing of the sensor in both non-integrated and integrated forms. It uses long-working distance objectives to couple light into the waveguide and to image the waveguide output facet inside the chamber.
**Figure 61:** Integrable sensor and material test schematic. A controlled flow rate and concentration of vapor phase agent is delivered to the waveguide test chamber.

**Figure 62:** The experimental setup showing gas delivery system, 660 nm laser beam, and stainless steel waveguide test chamber.
To test the integrated circuit using this stainless steel chamber, a custom apparatus has been designed and built. The Si-CMOS chip is mounted on a silicon board. It is then wire bonded to contacts on the silicon board. The silicon board is then set on a platform within the chamber, Fig. 64. The approximately 100-µm-diameter gold contacts connect with flexible “pogo pins” that are held by a custom designed stainless steel bridge, Fig. 65. This bridge not only holds the pogo pings, but also secures the silicon board onto a stainless platform within the chamber. The tops of these pogo pins connect to a hermetic, ceramic electrical feedthrough mounted in the lid of the chamber, Fig. 66. The tops of this feedthrough then connect to appropriate test devices to monitor and record the chip output. Through this apparatus, the Si-CMOS chip was tested using a controlled concentration of chemical vapor produced by the gas delivery system.
Figure 64: Multimode interferometric chem/bio sensor on a Si-CMOS chip mounted on and wire-bonded to a silicon board with 100-µm gold contacts

Figure 65: Stainless steel bridge fabricated to connect the Si-CMOS chip to test devices, by connecting to a gold plated silicon board.

Figure 66: Sealed waveguide test chamber with electrical connection to chip made through bridge and through ceramic electrical feedthrough mounted in the lid of the chamber.
5.3 Sample Outputs

Depending on the device under test, there are two possible outputs from this measurement setup. To test interferometric waveguides on silicon, the CCD camera captures images of the output multimode pattern. One such pattern is shown in Fig. 67. These images are captured regularly over time. The peak row of each pattern is selected for further processing. Some pixels from this peak row are shown in Fig. 68. The scale is 0-255, but because 30 images are averaged per recorded frame, the resolution is actually 0.033, on a scale from 0 to 255. Some differing pixel responses, which are shown in Fig. 68, correspond to a methanol vapor concentration change of 75 ppmv. In fact, there is a clear change in most of the pixels at 125 minutes, which marks the change in concentration. However, the pixels may respond with a large or small change, and may respond positively or negatively for the same chemical change.

**Figure 67:** Image of an output multimode pattern from the multimode sensor (100-µm wide).

**Figure 68:** Representative pixels from corresponding to the maximum row in Fig. 67. The pixels have widely varying responses to the methanol vapor.

The integrated sensor on Si-CMOS has a set of evanescently coupled photodetectors arranged in a linear array below the end of the waveguide. These detectors are directly
connected to analog-to-digital converters, which produce a digital output proportional to the captured optical power. Figure 69 shows the output of the integrated sensor under a change of vapor from pure N\textsubscript{2} to N\textsubscript{2} saturated with methanol vapor. It is noted that there is a strong drift to the signal. This is most likely due to changes in the coupling of the external laser to the waveguide. However, there is a clear change in sensor output at 150 (minutes). (\(\approx 1.4 \times 10^5 \text{ppmv}\)). Both of these detection schemes produce output from a

![Figure 69: Pixel response of Si-CMOS multimode sensor externally illuminated by a 840 nm semiconductor laser. A saturated methanol vapor stream is delivered to the sensor at 90s and replaced with a N\textsubscript{2} purge at about 300s.](image)

number of pixels, each of which responds differently to index changes on the sensing arm of the interferometer. How can these disparate responses be combined to increase the SNR and ultimately improve the sensor performance?
Chapter VI

MODAL PATTERN ANALYSIS AND RESULTS

6.1 Problem Introduction

How can changes in the multimode pattern be exploited for the best sensitivity (and SNR) given an existing source, waveguide, and detector combination? Multimode patterns, sources, detectors, and waveguides each have characteristics that affect the measured modal patterns. Sources and detectors have noise. Detection systems have specified resolutions and numerical apertures. Different waveguides may have different sensitivity to chemical. In spite of the physical characteristics of the different detection system, all produce noisy multimode patterns that respond to agent. A representative captured multimode image is shown in Fig. 70(a). Figure 70(b) shows the corresponding one-dimensional (integrated vertically) intensity. The difference between intensity patterns at 0 ppmv and 37 ppmv methanol-in-N₂ is shown in Fig. 70(c). In contrast, the variation or noise corresponding to a steady, near-zero concentration is shown in Fig. 70(d). The goal is to accurately identify significant modal pattern changes such as those shown in Fig. 70(c) in the presence of the modal pattern noise shown in Fig. 70(d). The difference between the signal in Fig. 70(c) and the noise in Fig. 70(d) illustrates that the sensing of tens of parts-per-million of methanol in vapor is readily achievable. Optimal pattern interpretation, i.e. signal processing to optimize the signal-to-noise ratio (SNR) allows significant improvement in sensitivity.

The interpretation of the output patterns from a Mach-Zehnder type multimode interferometric chem/bio sensor for optimal agent sensitivity (and SNR) is considered. Figures-of-merit (FOM) are methods or recipes for processing the modal output data to accurately relate changes in multimode patterns to index changes in the sense layer (SL) on one interferometer arm. An ideal FOM:

1. is a reliable and quantifiable relationship to the index change and thus the equilibrium
concentration of agent. The simplest relation is one in which the figure-of-merit is directly proportional to the index change.

2. produces the highest possible SNR in the presence of noise,

3. produces the same result for the same change in concentration regardless of the particular starting multimode pattern. Each measurement varies due to subtle changes in coupling, which results in a variation in the relative powers coupled into different modes of the input waveguide. This cannot affect the sensor response.

4. produces meaningful output for a wide range of spatial resolutions in the patterns. This means that the FOM can be applied equally to measured patterns from a CCD or a linear Si-CMOS array, and to simulated modal patterns. The sensitivity may, however, change for different spatial resolutions.

5. utilizes information from as many points on the multimode pattern (pixels) as possible. We assert that the multimode pattern contains information over its entire length.

6. reflects the underlying cyclic nature of the multimode pattern with index change in the SL.
6.1.1 Sample Measured and Simulated Multimode Patterns

6.1.1.1 Latest Measured Patterns(1) and Corresponding Simulation

Figure 71 shows the best experimental data attained at this time. The peak row of the captured CCD images is displayed over time. During this test, the methanol vapor concentration changed between 24, 54, 75, 149, 59, 30, 15, and 8 ppmv. Clearly defined shifts in the modal patterns are evident within these images. For comparison, the chemical mass uptake as measured by an inline QCM, is shown in Fig. 72.

Figure 71: Peak row over time of data as methanol vapor concentration changed between 24, 54, 75, 149, 59, 30, 15, and 8 ppmv.

149 ppmv corresponds to a SL index change of between $5.0 \times 10^{-4}$ and $8.3 \times 10^{-4}$. Figure 73 shows simulated data over a change in SL index from 0 to $1 \times 10^{-3}$, which includes the experimental data range. It is noted that a noise level representative of that observed experimentally has been added to the simulated data for comparison purposes. We wish to develop a high SNR in response to index change in the SL for each data set.
Figure 72: Methanol mass uptake in HFAPNB polymer SL for an $\sim 0.95$-$\mu$m-thick HFAPNB film.

Figure 73: Peak row over time of beam prop simulation of sensor over a range of cover index of $1 \times 10^{-3}$. The resolution of the simulated multimode patterns are much finer, primarily due to the inclusion of higher order modes. A repetition in the pattern is visible in this image.
This measurement was done on interferometers with a 0.25 \( \mu m \) core, for a reduced sensitivity compared with the previous measurement. It’s sensitivity is not expected to be as good. Further, the stability of the experimental setup was not as good during this measurement. The concentration was changed to 3 and then to 5.7 \( ppmv \) of methanol vapor, which corresponds to a SL index change of between 2 and \( 3 \times 10^{-5} \). After equilibrium the concentration was returned to 0 and then this was repeated. The 3 \( ppmv \) change did not appear to reach equilibrium at all. The mass uptake, measured by an inline QCM, is shown in Fig. 74.

**Figure 74:** A second measurement at small concentrations. The black lines indicate methanol vapor concentration changes of +3, +2.7, -5.7, +3 +2.7, and -5.7 \( ppmv \) respectively.

in Fig.75. Cycle 1 begins at about 80 minutes and cycle 2 begins at about 270 minutes.
Figure 75: Mass of Uptake in Polymer Sense Layer for 0.95 \( \mu m \)-thick HFAPNB film. The methanol vapor concentration was changed to 3, 5.7, and then 0, twice.
6.2 Candidate Figures-of-Merit (FOM)

Three FOMs will be considered to interpret these modal patterns. They are mean absolute error, column-center of power, and maximal ratio combining. To describe these candidate FOMs, some definitions are required:

- each pixel produces a value proportional to the incident intensity times the pixel area times the integration time, optical energy. It may also be considered as an average optical power, i.e. the optical energy divided by the integration time. For standardization, we will use the term “pixel power” (P) to represent this average power of one pixel measurement;

- for a stream of K modal pattern images, each having I rows and J columns, the power in a pixel of the image is represented by $P(i, j, k)$;

- for a stream of K linear modal patterns, each having J columns, the pixel power is represented by $P(j, k)$;

- a power difference pattern between a modal pattern at time index, $M$, and another at later time index, $N$, is defined in one of the following ways:

$$\Delta P_{MN}(i, j) = |P(i, j, M) - P(i, j, N)|, \forall i \& j \quad (32)$$

$$\Delta P_{MN}(j) = |P(j, M) - P(j, N)|, \forall j \quad (33)$$

- the standard deviation, $\sigma$, in the time varying power of a digitally captured pixel, $P(I, J, k)$, over a time period, T (which corresponds to K images) is:

$$\sigma_T(I, J) = \left\{ \frac{1}{K} \sum_{k=1}^{K} [P(I, J, k) - \mu_{IJK}]^2 \right\}^{0.5}, \quad (34)$$

where $\mu_{IJK}$ is the corresponding mean of the same pixel over the time period, T;

6.2.1 Mean Absolute Error

The mean absolute error can be used as an aggregate measure of modal pattern change by comparing an image with an earlier reference image. Essentially, it shows how all points in
the multimode pattern are changing relative to the same points in the reference pattern. The mean absolute error (MAE) with first frame, $MAE_{1k}$, measures between the aggregate error between one modal pattern at time index, 1 (a reference), and another at time index, $k$. It is defined as follows:

$$MAE_{1k} = \frac{1}{IJ} \sum_{i=1}^{I} \sum_{j=1}^{J} \Delta P_{1k}(i,j), (\forall k)$$

(35)

In practice we choose the reference pattern to be a mean of a set of patterns over an initial reference minute of the measurement ($P(i, j, N) \simeq < P(i, j, k) >_{1\text{min}}$) during which time we assume there is no chemical. This simply reduces the noise in the reference.

This FOM averages the large changes of highly sensitive pixels with the smaller changes of lower sensitivity pixels, thus reducing sensitivity. These lower sensitivity pixels may include some dark surrounding pixels. However, the $MAE_{1k}$, is useful for discerning trends in the complicated multimode pattern. Further, it is a very simple and thus easily implemented FOM, which is useful for a Si-CMOS implementation.

### 6.2.2 Column Center of Power

Changes in the column (transverse) center-of-power (CCOP) of the multimode pattern can also be used to indicate index changes in the SL. The CCOP is simply the first moment of pixel power in the transverse direction. The CCOP FOM is calculated as follows:

$$CCOP(k) = \frac{\sum_{i=1}^{N} \sum_{j=1}^{M} j P(i, j, k)}{\sum_{i=1}^{N} \sum_{j=1}^{M} P(i, j, k)},$$

(36)

and the change in this measure, $\Delta CCOP_{1k}$ between time index, 1 (a reference), and time index, $k$, is given by

$$\Delta CCOP_{1k} = CCOP(k) - CCOP(1).$$

(37)

In addition, by definition, the CCOP method exploits the entire pattern, and does not require the prior selection of specific pixels. Also, because the output of $CCOP$ is a position, it is largely insensitive to intensity fluctuations in the source, and suppresses this noise to increase sensitivity. Pattern normalization by total power can be used to make other figures-of-merit power-insensitive; however, the inherent power normalization of this
FOM is advantageous. It has the potential disadvantage that it is possible for changes in the pattern to offset each other resulting in no change observable FOM change when index change occurs. This is likely to be observed for large SL index changes. Considering its reduced sensitivity to fluctuations in source intensity, and that it does not require prior selection of pixels, this FOM is considered as a measure of modal pattern change for small SL index changes.

6.2.3 Optimal Ratio Combining

Optimal combinations of the observations of a set of sensors, each observing an event with a different SNR, has been studied extensively [49]. For this sensor, there are many pixels, each recording a slightly different version of the sense event with a different SNR. The optimal combination of pixels should maximize the SNR and maintain a quantifiable relationship with the sensing layer index, and hence chemical concentration. We assume that the noise of each pixel is uncorrelated and has Gaussian statistics. Experimentally, we find limited correlation among pixels due primarily to the modal structure of the image. We look for the optimal weights \( w_j \), to assign to the changes occurring in each pixel in response to chemical.

By maximizing the joint SNR, we find that the optimal combination is The derivation of the FOM associated with maximal ratio combining is outlined here. \( \Delta P_{1k}(j) \) is the observed difference of the \( j^{th} \) pixel between time index \( k \) and the reference time (time index 1, which is an average over one minute). \( \alpha_{1k}(j) \) is the associated signal value. The noise is assumed to be additive white Gaussian with mean \( \mu_j \) and variance \( \sigma_j^2 \). Since the noise parameters are estimated at the beginning of the measurement, we assume that the mean \( \mu_p \) has been subtracted out from the observed change in the pixel. Therefore, the noise, denoted by \( \nu(j, k) \), is zero mean. Thus each pixel’s value can be mathematically expressed as :

\[
\Delta P_{1k}(j) = \alpha_{1k}(j) + \nu(j, k) \quad \text{where } \nu(j, k) \sim N(0, \sigma_j^2) \tag{38}
\]

At any given time instant \( n \), we linearly combine the data from different pixels as follows :

\[
\Delta P_{1k} = \sum_{j=1}^{N} w_j \Delta P_{1k}(j) \tag{39}
\]
where \( w_j \) are the weights and \( N \) is the number of pixels. This equation simplifies to:

\[
\Delta P_{1k} = \sum_{j=1}^{N} w_j \alpha_{1k}(j) + \sum_{j=0}^{N} w_j \nu(j, k) \quad \text{where } \nu(k) \text{ is } N(0, \sigma^2) \quad \text{and} \quad (40)
\]

\[
\sigma^2 = \sum_{j=1}^{N} w_j^2 \sigma_j^2, \quad (41)
\]

We have used the fact that the noise from different pixels is uncorrelated. The weights \( w_j \) are chosen to maximize the signal-to-noise ratio (SNR). The SNR at time \( k \), denoted by \( \rho_k \), is defined so that:

\[
\rho_k^2 = \frac{\alpha_{1k}^2(j)}{\sigma^2} \quad (42)
\]

The optimum weights are chosen as follows:

\[
\rho_k^2 = \frac{\left( \sum_{j=1}^{N} w_j \alpha_{1k}(j) \right)^2}{\sum_{j=1}^{N} w_j^2 \sigma_j^2} = \frac{\left( \sum_{j=0}^{N} (w_j \sigma_j) \left( \frac{\alpha_{1k}(j)}{\sigma_j} \right) \right)^2}{\sum_{j=1}^{N} w_j^2 \sigma_j^2} \quad (43)
\]

\[
\leq \frac{\sum_{j=1}^{N} (w_j \sigma_j)^2 \left( \sum_{j=1}^{N} \left( \frac{\alpha_{1k}(j)}{\sigma_j} \right)^2 \right)}{\sum_{j=1}^{N} w_j^2 \sigma_j^2} \quad \text{via Cauchy-Schwartz inequality} \quad (44)
\]

\[
\Rightarrow \rho_k^2 \leq \sum_{j=1}^{N} \frac{\alpha_{1k}^2(j)}{\sigma_j^2} \quad (45)
\]

The equality is satisfied iff:

\[
w_j \sigma_j = \frac{\alpha_{1k}(j)}{\sigma_j} \quad (46)
\]

\[
\Rightarrow w_j = \frac{\alpha_{1k}(j)}{\sigma_j^2} \quad (47)
\]

And so the optimum combined value is given by:

\[
\Delta P_{1k} = \sum_{j=1}^{N} \frac{\alpha_{1k}(j)}{\sigma_j^2 \Delta P_{1k}(j)} \quad (48)
\]

The only estimate of \( \alpha_{1k}(j) \) available is \( \Delta P_{1k}(j) \) itself. And so the best estimate of the combined value is:

\[
\Delta P_{1k} = \sum_{j=1}^{N} \frac{\Delta P_{1k}^2(j)}{\sigma_j^2} \quad (49)
\]

We note that Brennan [49] suggests these same weights when evaluating maximal-ratio diversity for fading multi-path detection of radio transmissions. To maintain linearity in
\( \Delta P \), which is proportional to index change, we take the square root of this quantity. We therefore define our FOM of modal pattern change, \( S \), as follows:

\[
S(k) \equiv \left\{ \sum_{j=1}^{N} \frac{\Delta P_{jk}(j)}{\sigma_j^2} \right\}^{1/2}.
\]  

(50)

This quantity is simply the root-mean-square SNR of all pixels. It is reiterated that for this to be the optimal estimator, the noise patterns in the different pixels must be uncorrelated. We have noted correlation in the signals of different pixels. However, separation of signal and noise is difficult as it requires knowledge of the maximum frequency of the signal (which is related to the material response time). Any noise below this frequency cannot be separated from the signal in practice. This practically simple measure can easily be implemented using standard CMOS technology, allowing an integrated device that processes measured modal patterns in real time. Furthermore, the reference image, \( < P(0,j) >_{1\text{min}} \) and \( \sigma_j^2 \), can be reassessed at any time allowing \( S \) to represent the change in concentration from the reference time. This reassessment also allows elimination of long term drift or pattern cycling, which can occur with optical phase-based sensor systems.

### 6.3 Comparison of Candidate FOMs

In order to determine the strengths and weaknesses quantitatively of the individual figures-of-merit, an objective test methodology is required. The preferred traits of the figures-of-merit must be identified, and then quantified upon a set of test modal patterns. For the initial tests, we will measure the FOMs performance as far as comparability and sensitivity. In this case, two performance measures will be used:

1. concentration sensitivity over a concentration range, and
2. linearity over a concentration range.

### 6.3.1 Latest Measured Patterns(1) and Corresponding Simulation

The most recent sensor measurement used an experimental setup that has been continually tuned for stability and as such demonstrates the performance of the sensor most accurately. During this test, concentrations of methanol vapor of 24, 54, 75, 149, 59, 30, 15, and 8...
ppmv were applied. The corresponding modal patterns have been interpreted using the candidate figures of merit. The results for optimal ratio combining (S), column center-of-power (ΔCCOP₁), and mean absolute error (MAE₁) are shown in Figs. 76, 77, and 78 respectively.

Figure 76: Modal Pattern Interpretation using the optimal ratio combining FOM, S. The noise at the highest concentration is \( \sigma = 0.11 \).

Figure 77: Modal Pattern Interpretation using MAE. The noise at the highest concentration is \( \sigma = 0.030 \).

First, we compare the sensitivity and linearity of these FOMs. It is clear from Fig. 78, that the CCOP FOM results in the largest relative noise level or the smallest SNR. It also
Figure 78: Modal Pattern Interpretation using CCOP. The noise at the highest concentration is $\sigma = 0.096$.

does not have a large signal in response to agent concentration. The MAE and optimal-ratio-combining figures-of-merit both develop low noise. For this measurement, the noise is appropriately measured at the highest concentration of agent, at which the noise in the mass flow controller is the lowest. Figure 79 shows the mean level at a given concentration for each FOM. A line fit through the concentration points up to $75 \text{ ppmv}$ combined with the measured noise level determines the sensitivity. It is noted that at concentrations greater than $75 \text{ ppmv}$, the modal pattern response is no longer linear in index as will be shown later through simulation. Based on the slope and noise level, the MAE does have a slightly higher sensitivity. However, when put on a comparable scale, the S FOM, is more linear with concentration (and thereby index change in the SL). Further, the CCOP FOM clearly has the largest deviation from linearity. This is partly due to its increased noise level, and partly due to the FOMs properties. This comparison is summarized in Fig. 3.

Table 3: Comparison of Figures of Merit.

<table>
<thead>
<tr>
<th></th>
<th>S</th>
<th>MAE</th>
<th>$\Delta$CCOP</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sensitivity</td>
<td>480 ppbv</td>
<td>310 ppbv</td>
<td>9400 ppbv</td>
</tr>
<tr>
<td>Linearity Deviation</td>
<td>10</td>
<td>18</td>
<td>23</td>
</tr>
</tbody>
</table>
Figure 79: Comparison of Slope and Linearity of candidate figures-of-merit. The rms deviation from linearity is shown in the top left of each plot.
The simulated data shown in Fig. 73 has also been processed using the three candidate FOMs. Figure 80 shows the results after processing with the CCOP and optimal-ratio FOMs. The CCOP FOM is simply noisier, and therefore not preferred. This apparent noisiness is actually a result of the much smaller signal. For the highly resolved modal pattern, the center-of-power is moving only slightly.

Figure 80: Simulated modal patterns processed by the ‘S’ and $\Delta CCOP$ FOMs.

Figure 81 shows the simulated data as processed by the optimal-ratio and the MAE FOMs. The MAE FOM is more sinusoidal in index change. It has a higher slope and therefore sensitivity closer to zero index change. However, the optimal-ratio FOM is more
linear with index over a larger range. This ‘elongation’ in the response for the optimal-ratio FOM is due to the weighting process which highly weights pixels with large power changes. Comparatively, the MAE FOM equally weights all pixels regardless of amount of power change. The sinusoidal nature of the modal pattern response to index change was not accounted for in the derivation of the optimal-ratio FOM.

It is also noted that both the MAE and optimal ratio FOMs are most sensitive for modal patterns closest to the reference pattern. This, then, is another benefit of multimode sensing. It requires no bias to set the interferometer at the most sensitive point. It is automatically there. Further, if the reference image is reset, the sensitivity again returns to most sensitive. Practically, this requires accounting of the index change (so it can be added to the response after the reference frame has been reset).
Another sensor measurement will also be evaluated using these FOMs. The modal patterns shown in Fig. 74 have been interpreted using the candidate figures of merit. The maximum concentration change applied was 5.7 $ppmv$, which corresponds to a SL index change between 2 and $3 \times 10^{-5}$. The results for optimal ratio combining ($S$), column center-of-power ($\Delta CCOP_{1k}$), and mean absolute error ($MAE_{1k}$) are shown in Figs. 82, 83, and 84 respectively. Fig. 75 shows the corresponding QCM data. During this test, the concentration changed by a very small amount. Therefore, the index change on the sensing arm is very small $\simeq 3.2 \times 10^{-5}$. It is clear from Fig. 4, that the CCOP FOM is better in this case. The MAE and optimal-ratio-combining figures-of-merit both develop similar SNRs, although the MAE FOM is slightly better.

Now, we wish to compare the sensitivity of these FOMs. The sensitivity is compared by measuring the concentration change that develops an SNR of 3.

**Table 4:** Comparison of Figures of Merit.

<table>
<thead>
<tr>
<th>Sensitivity</th>
<th>$S$</th>
<th>$MAE$</th>
<th>$\Delta CCOP$</th>
</tr>
</thead>
<tbody>
<tr>
<td>4900 $ppbv$</td>
<td>4100 $ppbv$</td>
<td>2350 $ppbv$</td>
<td></td>
</tr>
</tbody>
</table>

**Figure 82:** Modal Pattern Interpretation using the optimal ratio combining FOM, $S$. The noise is $\sigma \simeq 0.23$. 

96
Figure 83: Modal Pattern Interpretation using MAE. The noise is $\sigma \approx 0.12$.

Figure 84: Modal Pattern Interpretation using CCOP. The noise is $\sigma \approx 0.10$. 
6.3.2 Tabulated Comparison and FOM Selection

The candidate modal patterns have been compared using two measured, and one simulated set of modal pattern data. The tabulated results are summarized in Table 5. For the best dataset (1), it is clear that the S and \( MAE_{1k} \) FOMs are much more sensitive that the CCOP FOM. However, for the other dataset (2), the CCOP is more sensitive. However, because the CCOP is far noisier for the best dataset, it is not selected. The MAE and S FOMs are considered further. For the simulated data Fig. 81, because the \( MAE_{1k} \) has an absolute sinusoid relationship to index, its slope and sensitivity is greater near 0 index change. However, the slope reduces faster over a smaller index range. The S FOM has a slightly reduced sensitivity near the origin, but maintains a close to linear relationship with index change for a larger index range. Thus both FOMs are appropriate depending on the application. Both FOMs will be used to estimate device sensitivity.

<table>
<thead>
<tr>
<th></th>
<th>S</th>
<th>MAE</th>
<th>( \Delta CCOP )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sensitivity (1)</td>
<td>480 ppbv</td>
<td>310 ppbv</td>
<td>9400 ppbv</td>
</tr>
<tr>
<td>Linearity Deviation (1)</td>
<td>10</td>
<td>18</td>
<td>23</td>
</tr>
<tr>
<td>Sensitivity (2)</td>
<td>4900 ppbv</td>
<td>4100 ppbv</td>
<td>2350 ppbv</td>
</tr>
</tbody>
</table>

6.4 Comparison of Simulated and Experimental Data

Having selected the FOMs to implement, the simulated and experimental sensitivities of the sensor may be compared. Figure 85 shows the results of interpretation by the ‘S’ FOM. The functional relationship between the S FOM and index change is \((\sin^2)^5 \) (with a period of \(5.7 \times 10^{-3}\)). Figure 86 shows the results of interpretation by the MAE FOM. Both the simulated and experimental data show a sinusoidal relationship with \( \Delta n_{SL} \). This is expected due to the underlying sinusoidal phase response of each mode. The pattern should repeat when each mode coupled into the sensing arm simultaneously acquires \( 2\pi \) radians of phase. For the simulated data, this occurs about \( \Delta n_{SL} = 5.7 \times 10^{-4} \). For the experimental data (dots) this occurs at a much larger \( \Delta n_c \). Figure 86 also shows a fit of the experimental
data (dashed) to an absolute value sinusoid and reveals a measured SL period of $9 \times 10^{-4}$. This suggests that the input coupling demonstrated experimentally has excited more modes than in the simulation. Because the input coupling is difficult to estimate in practice, this difference is acceptable and understandable.

![Graph](image)

**Figure 85:** Simulated and experimental results interpreted by the ‘S’ FOM. The solid line is simulated data (left axis). Dots show experimental results (right axis). Crosses show these results corrected by the ratio of sensitivity of the highest to lowest order modes.

These FOMs offer an overall view of the repetition period (in SL index) of the multimode patterns. As such, they are demonstrated as useful tools in the study of multimode interferometers, and perhaps waveguides in general. For the multimode interferometric sensors, the repetition period ultimately determines the sensitivity. A short repetition period in $\Delta n_c$ (like the simulated data) provides a higher initial sensitivity (as well as a faster turnaround). A longer repetition period provides a lower initial sensitivity, but with saturation at a much larger SL index change. This period is likely determined by the weighting of power in each mode that travels under the SL. This weighting is determined by the input coupling and the mode coupling effects of the initial multimode y-junction.
Figure 86: Simulated and experimental results interpreted by $MAE_{1k}$. The solid line is simulated data (left axis). Dots show experimental results (right axis). Crosses show these results corrected by the ratio of sensitivity of the highest to lowest order modes.

6.5 Device Sensitivity

In this chapter, the measured multimode patterns have been processed by three separate strategies, or FOMs. Through two measured, and one simulated set of multimode patterns, it has been shown that the $MAE_{1k}$ and S FOMs are appropriate for modal pattern interpretation, and may be selected depending on measurement requirements.

In addition, the FOMs have been used to reveal the repetition period of modal patterns in $\Delta n_{SL}$. They also show the relationship between the repetition period and the sensitivity. That is a smaller repetition period creates a higher sensitivity. This then, brings up a new question: “What determines the pattern repetition period in $\Delta n_{SL}$? The hypothesis is that the modal power distribution in the interferometer arms ultimately determines this.

Finally, using these FOMs, the device sensitivity (on Silicon) may be estimated. The minimum detectable change is here defined as that change which develops a SNR of 3. Both the index sensitivity and the methanol vapor concentration sensitivity are estimated using both the MAE and S FOMs based on the best measured data set (1). In addition, using the ellipsometric data, Ch. 3.1, we can extend the device concentration sensitivity to other agents. The device sensitivities are presented in Tab. 6. For comparison with other devices, the demonstrated index sensitivity is less than $2 \times 10^{-6}$. In addition, the < 60ppbv
demonstrated benzene vapor sensitivity compares favorably with that of the Hartman sensor (Tab. 1) at < 1ppmv. Note that the index sensitivities displayed in Fig. 32 are used to calculate these sensitivities.

**Table 6: Measured Sensitivity of Sensors on Silicon.**

<table>
<thead>
<tr>
<th>Sensitivity</th>
<th>S</th>
<th>MAE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methanol</td>
<td>480 ppbv</td>
<td>310 ppbv</td>
</tr>
<tr>
<td>$\Delta n_{SL}$</td>
<td>$1.6 \times 10^{-6}$</td>
<td>$1.1 \times 10^{-6}$</td>
</tr>
<tr>
<td>Isopropanol</td>
<td>19 ppbv</td>
<td>13 ppbv</td>
</tr>
<tr>
<td>Benzene</td>
<td>57 ppbv</td>
<td>39 ppbv</td>
</tr>
<tr>
<td>Water</td>
<td>210 ppbv</td>
<td>150 ppbv</td>
</tr>
</tbody>
</table>

### 6.6 A New Y-junction to Modify the Modal Excitation and the Sensitivity

The modal pattern repetition period of the interferometric sensor is determined by the index profile of the tapered y-junction (Fig. 53 (b) left and right sides). This y-junction has a characteristic mode transfer function. That is, for a given amount of power in the modes of the input waveguide, a different amount of power is coupled into the modes of the output waveguide. The y-junction mode coupling properties along with the modes excited in the input waveguide determine the modal excitation in the sensing and reference arms. It is the modes excited in the interferometer arms, and principally the sensing arm, that determine the modal pattern repetition period in SL index. By changing the y-junction index profile, the sensor designer can modify the modal pattern index period by changing the modes excited under the sensing arm allows the sensor designer to modify the index period of the sensor, directly impacting device sensitivity.

An new y-junction, Fig. 87, has been designed for this interferometric sensor which consists of two angled portions on each side of the y. The angles are selected in order to excite a range of higher-order modes within the SL. The modal excitation of this structure is shown in Fig. 88. The incident field consists of the lowest order mode of the input waveguide. The modes coupled into the sensing arm waveguide are shown in the Fig. . They consist of higher-order modes (order $\hat{\lambda}$ 260), which are more sensitive to SL index change. The modal
pattern repetition period, when this y-junction replaces the y-junctions in Fig. 53 (b) and when the modal excitation is the lowest order mode of the input waveguide, is shown in Fig. 89. The change in y-junction/excitation combination is clearly modifying the modal pattern repetition period. (In this case it actually makes it longer in SL index.) However, the key point is that the modal excitation is adjustable and therefore, so is the sensor sensitivity.

**Figure 87:** New two-angle y-junction, with angles of 65.5 and 68°, that can excite a range of higher-order modes in the sensing arm of the interferometer. The single input and two output waveguides are 100-µm-wide and the wavelength is 840 nm.

**Figure 88:** Modes coupled into the right and left arms of the interferometer for the same conditions as in Fig. 87.
Figure 89: Comparison between modal pattern repetition period of y-junction in Fig. 46 with one illumination pattern and that of the new two-angle y-junction (Fig. 87) with a zero-th order modal illumination. The modal pattern repetition rate has been modified by this new junction. Fig. 87.
The resolution or sensitivity of a sensor is indicated by the minimum detectable amount of an agent. This amount is determined by the signal-to-noise (SNR). Although mentioned in the literature, there is not a fixed comparison standard for sensor sensitivity. A method for establishing the sensitivity or minimum detectable change of sensors based on the bit-error-rate (BER), the standard performance measure of communication channels, is outlined here. Further, the elements that affect the SNR are investigated. The sensing device creates a (preferably) large signal in response to an agent. The hardware, as well as the sensor environment, determine the noise level. Sources of noise in the experimentally measured (i.e. external source) sensor will be compared with those in a fully-integrated sensor that is limited by fundamental noise sources. These noise sources may include in fluctuations in position due to thermal or mechanical instability. The may also include optical or electrical fluctuations in the laser source, or the detector. This comparison of noise levels allows an estimate of the device sensitivity of a fully integrated Si-CMOS sensor.

7.1 Assessing Sensitivity

7.1.1 Current Practice

We wish to estimate the minimum detectable concentration change (MDCC) or index change (MDIC) of the sensor, after the modal pattern has been interpreted by an appropriate FOM. The criteria used to compare the sensing ability or minimum detectable change (MDC) vary considerably in the literature. Schneider et al. [50] use a detection limit based on a 10% change in signal intensity. Specifically,

\[ A \text{ detection limit of } 2 \, \mu g/L \text{ has already been demonstrated, whether measured in terms of the initial rate } (\text{< 5 min}) \text{ or at quasi-equilibrium (30-60 min), a phase response of } 0.05 \, \pi \text{ rad (a 10% change in signal intensity)} \text{ being used as the} \]
...a signal change of three times the standard deviation of the baseline signal (the signal obtained when the buffer solution is being pumped over the sample)....

Brandenburg et al. [6] also report a detection limit corresponding to a concentration change resulting in a signal greater than three times the standard deviation. Although specific to biological agent detection, Blair and Chen [52] specify a detection limit based on twice the standard deviation. Recognizing that environmental noise may ultimately limit sensitivity, it is useful to specify the sensitivity in terms of the inherent sensor system noise.
7.1.2 Method for Sensitivity Estimation

Here, we discuss the basis for these sensitivity estimates and suggest a common comparison standard. We use a methodology similar to the binary bit-error rate (BER) formalism, the standard performance measure for communication channels. Simply, the sensitivity is represented by a minimum detectable change (MDC) in sensor output. The MDC is the smallest possible change in sensor output that bounds the total probability of measurement error, $p_E$, at some specified value ($p_E \leq X$). This total error is given by

$$p_E = p(NC)p(C\mid NC) + p(C)p(NC\mid C),$$  \hspace{1cm} (51)

where $p(NC)$ is the probability of no chemical being present, $p(C\mid NC)$ is the probability of indicating chemical when none is present, $p(C)$ is the probability of having chemical present, and $p(NC\mid C)$ is the probability of not indicating when chemical is present. Referring to Fig. 90 (a), $P(C\mid NC)$ is the area under the solid curve to the right of the black line, the detection threshold. The detection threshold, $T$, is the sensor output level against which all instantaneous sensor measurements are compared. Output below $T$ is considered not detection and vice versa. $P(NC\mid C)$ is the area under the dash-dot curve to the left of the detection threshold. This figure shows a Gaussian probability distribution, but any appropriate distribution can be used to find $p_E$. For communication channels, the systems are usually designed, so that $p(NC) = p(C) = 1/2$ (also depicted in Fig. 90).

For sensors, the vast majority of the time, chemical is not present. That is, $p(C) << p(NC)$, resulting in $p_E \sim p(C\mid NC)$. In other words, it is mainly the noise distribution when chemical is not present that determines the total probability of error. This condition, for Gaussian distributions, will be examined. The black lines in the following figures represent the detection threshold, $T$. The standard deviation of both the chemical (C) and no-chemical (NC) distributions are $\sigma_C = \sigma_{NC} = 1$. The solid line is for $p(NC)$ and the dash-dot is for $p(C)$. Also, the total error, $p_E$, bound is chosen to be $X = 0.0014$. By incrementally increasing $p(NC)$, the case of $p(C) << p(NC)$ is approached.

Figure 90(b) shows that for $p_E \leq X$, the mean levels in the C and NC states, $\mu_C$ and $\mu_{NC}$, are separated by a signal increase of 6. This, then is the minimum detectable change.
(MDC). Figure 91(a) shows that if \( p(\text{NC}) = 0.9 \), and the \( \mu_C \) and \( \mu_{NC} \) are separated by 4, \( p_E = 0.01 \). Figure 91(b) shows for the same \( p(C) \) and \( p(\text{NC}) \), that the MDC (which bounds \( p_E \) at X) is a signal change of 5.6, a decrease compared with Fig. 90, and that \( T \) has moved closer to \( \mu_C \) (from 3 to 2.41). Figures 92 and 93 show that this trend continues as \( p_{NC} \) increases first to 0.99 and then to 0.9999. In fact, when \( p_{NC} = 0.9999 \) changing the MDC does not significantly affect the total error. Thus, the total error depends only on the probability distribution in the NC state.
**Figure 91:** Error probability for $p(\text{NC}) = .9$, $p(\text{C}) = 0.1$. Upper diagram (a) shows C-NC mean separation of $4\sigma$; lower diagram (b) shows separation of $5.6\sigma$, for which $p_E = 0.0014$.

**Figure 92:** Error probability for $p(\text{NC}) = .99$, $p(\text{C}) = 0.01$. Upper diagram (a) shows C-NC mean separation of $4\sigma$; lower diagram (b) shows separation of $4.6\sigma$, for which $p_E = 0.0014$. 
Figure 93: Error probability for $p(\text{NC}) = .9999$, $p(C) = 0.0001$. Upper diagram (a) shows C-NC mean separation of $4\sigma$; lower diagram (b) shows separation of $5.6\sigma$, for which $p_E = 0.0014$. 
Because the NC distribution determines \( p_E \), \( T \) is selected to keep the error probability below the error bound (\( p(C|NC) < X \)). For example, if \( T \) is set at \( 2\sigma_{NC} \) above the mean NC level, this results in \( p(C|NC) = 6.7\% \), and the same total error probability, \( p_E \). If the threshold is set at \( 3\sigma_{NC} \), this results in both \( p_E \) and \( p(C|NC) \sim 0.1\% \). For any probability bound, \( X (0 < X < 1) \),

\[
p(C|NC)\{T\} = \int_T^{\infty} \frac{1}{\sqrt{2\pi}\sigma_{NC}} \exp\left(-\frac{(x-\mu_{NC})^2}{2\sigma_{NC}^2}\right) dx \leq X
\]

\( T = \sigma_{NC} \text{ erf}^{-1}(0.5 - X) + \mu_{NC} \) (53)

where \( \sigma_{NC} \) is the standard deviation in the sensor output when a chemical is not present. \( \text{erf}^{-1} \) is the inverse of the standard error function associated with the Gaussian distribution:

\[
\text{erf}(S) \equiv \int_0^S \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} dx.
\] (54)

Having established the threshold based only on the probability distribution in the NC state, it remains only to determine the MDC. Two possible choices of MDC are discussed and one is selected. The first MDC is the minimum change in sensor output that keeps \( p_E \) the same regardless of the state of the sensor. Specifically, the mean signal change in response to chemical, \( \mu_C \), that keeps the measurement error constant would be the MDC. For a threshold of \( T = \mu_{NC} + N\sigma_{NC} \),

\[
p(C|NC) = p(NC|C)
\] (55)

\[
\int_T^{\infty} \frac{1}{\sqrt{2\pi}\sigma_{NC}} \exp\left(-\frac{(x-\mu_{NC})^2}{2\sigma_{NC}^2}\right) dx = \int_{-\infty}^T \frac{1}{\sqrt{2\pi}\sigma_C} \exp\left(-\frac{(x-\mu_C)^2}{2\sigma_C^2}\right) dx
\] (56)

\[
0.5 + \text{erf}(N) = 0.5 + \text{erf}\left(\frac{\mu_C - \mu_{NC} - N\sigma_{NC}}{\sigma_C}\right)
\] (57)

\[
\mu_C - \mu_{NC} = N(\sigma_{NC} + \sigma_{NS})
\] (58)

Under most sensing conditions, \( \sigma_{NC} \simeq \sigma_{NS} \); the two noise levels separated by the MDC have nearly the same noise performance. In this case, the threshold, \( T \), would be set to at \( 3\sigma_{NC} \) and the MDC would be \( 6\sigma_{NC} \). This definition of MDC is illustrated in Fig. 94.

The second choice of MDC is what seems to be implied in the literature. The sensitivities quoted do not differentiate between the threshold and the MDC, implying that they have
**Figure 94:** MDC specification which keeps the total probability of error, $p_E$, constant regardless of the state of the sensor. Here the MDC is 6 $\sigma$ above the mean level in the no chemical state (solid line).

*the same value.* However, this definition of MDC should be used carefully. If the MDC and threshold are set at $\mu_{NC} + 3\sigma_{NC}$, then, in the presence of the MDC, the error probability, $p(NC|C)$, becomes approximately 50%. That is, there is 50% probability of a false negative. This issue is shown conceptually in Fig. 95. Therefore, this sensitivity standard may not literally represent the MDC in practice. It is just a comparison measure. Actual sensor error probabilities in the presence or absence of an agent should be calculated, by taking into account the SNR implied by the MDC standard.

Having noted its limitations, but accepting that this comparison measure seems to be most common in the literature, the second definition is adopted. Therefore, *the MDC is the index or concentration change for which the sensor output changes by $3\sigma_{NC}$.* This facilitates the simplest comparison between different devices. We note that both Luff and Brandenburg [51] also specify a $3\sigma$ MDC.

Further, for a general chem or bio sensing system the integration time (effective bandwidth) directly impacts the MDC by reducing noise. This is only limited by the required response time. An increase in the integration time by a factor of $M$ reduces the system bandwidth by $1/M$, and the noise-induced standard deviation in the sensor output by $1/\sqrt{M}$, producing a corresponding decrease in the MDC. Thus, the MDC is only correctly
Figure 95: MDC specification in which the threshold and the MDC have the same value. In this case, \( p(\text{NC}|\text{C}) = 0.5 \). The chemical state distribution (dash-dot) has been magnified for illustration.

specified when the bandwidth or integration time is identified. For this work a bandwidth of 1 Hz is selected.

Note that all sensitivities quoted at the end of Ch. 6 have been specified using this 3\( \sigma \)MDC.

7.2 Noise in Chemical Sensing

Ignoring environmental noise temporarily, we can assess the intrinsic system noise and thereby determine the minimum sensitivity. The noise arises from source fluctuations, shot noise, read noise and noise associated with dark current, however it is desirable to operate in the shot-noise-limited regime. Typically the noise variance is quantified in terms of a noise current. CMOS detectors accumulate photo-generated electrons in a capacitive structure, termed a well. The number of photo-generated electrons, \( N \), is proportional to the optical power, \( P \), and the number of incident photons, \( N_{ph} \). In short, by choosing an integration time, we can specify the noise in terms of the number of electrons.

Although source fluctuations are often quantified in terms of relative intensity noise, RIN [53], the integration time of sensors requires that the source be quantified in terms of
low frequency fluctuations, i.e. drift. As a fully integrated sensor will include a feedback-stabilized laser, and as all images are normalized to constant intensity, these fluctuations are negligible.

Shot noise due to photon arrival is a Poisson process, and therefore the variance in the number of photons arriving within a given time scales as the mean number of arriving photons. That is, if the mean number of photons arriving within a set interval is $N_{ph}$, then after many of these intervals, the variance in the number of photons that arrived would have a magnitude of $N_{ph}$. If a well-based detector captures a mean of $N$ photoelectrons ($N = p N_{ph}$, where $p$ is the quantum efficiency of the detector), the detected shot noise variance (see Appendix A) is also, $N$ [54]. Specifically,

$$\sigma_{shot}^2 = N (e^-)^2. \quad (59)$$

Read noise is typically specified in terms of numbers of electrons, $e^-$, per read event. A larger well-size may be used to decrease the relative read noise. The read noise, which is estimated for a particular Si-CMOS array [55], is $\sigma_{RD}^2 = 185^2 (e^-)^2$. By averaging 10 frames with a 100 ms integration time, the effective bandwidth and thereby the read noise variance is reduced (by $1/10$).

The dark current produces captured electrons due primarily to thermal generation. For the same CMOS array [55], at $25^\circ C$, and for a 1 s total collection time, the dark current generates approximately $18750 (e^-)$. The associated dark current shot noise variance is $\sigma_{DK}^2 \simeq 137^2 (e^-)^2$. Both the read noise and dark current noise must be considered in relation to the total well size, which, is $2.125 \times 10^6 (e^-)$ for the specified array. Dark current and associated noise increases at higher temperatures and for longer exposure times.

### 7.3 Noise Measurements and Noise-limited Detection

The noise of a fully integrated sensor system includes the effects of a Si-CMOS linear array with a full well size of $\sim 2 \times 10^6 e^-$. The total system noise variance can be written as

$$\sigma_{total(1Hz)}^2 = N + \sigma_{RD}^2/10 + \sigma_{DK}^2 (e^-)^2. \quad (60)$$
The standard deviation, $\sigma_{total(1Hz)}$, developed by these noise sources, represents an ultimate goal to achieve in a fully integrated device.

Figure 96 depicts the noise performance of the experimentally measured sensor, and that of a fully integrated sensor, limited by fundamental noise sources. The triangles identify the observed noise performance of the non-integrated sensor system. As this noise level is well-above the level developed by the fully integrated sensor system (dashed line), the non-integrated system is not limited by the combined effect of shot noise, read noise, and dark current noise. The combined noise of a fully integrated sensor is dominated, except at very low numbers of captured photons, by photon shot noise. The linear behavior of the measured sensor noise (triangles) at higher intensities is consistent with signal fluctuation caused by drift or variations in positioning equipment. Thus, we can estimate the ultimate sensitivity of a fully integrated sensor by considering only the intrinsic noise of the system. When compared with the experimentally measured noise (triangles), a noise reduction of $5-6 \times$ and a corresponding reduction in MDC is possible.

![Figure 96: Comparison between the standard deviation, $\sigma$, and the power, $P$, of the measured sensor system, triangles, and the standard deviation estimated for a fully integrated sensor limited by fundamental noise sources (dashed line), essentially shot noise. This represents a 4-6× reduction in the noise.](image-url)
Figure 97: Simulated data (triangles) showing the effect of spatial resolution in the detected multimode pattern on device sensitivity. An increase in pixel pitch from 1.35 to 2.8 \( \mu m \) reduces sensitivity by \( \sim 2.1 \times \). Experimental sensitivity (\( \sim 1/3 \) of simulated data at the same spatial bandwidth) is indicated by ‘+’.

### 7.4 Other Factors

Two additional factors affect the sensitivity estimate of the fully integrated CMOS sensor: the pixel size and the guiding layer thickness. The pixel size determines the degree of spatial integration of the multimode pattern. In a fully integrated device, the CMOS array may be evanescently or grating coupled. The experimentally measured system, however, includes imaging optics that magnify the multimode pattern incident on the CCD array. The effective resolution experimentally, 1.4 \( \mu m \), is limited not by the actual camera pixel pitch, but by the numerical aperture of this imaging system. Simulated results (Fig. 97) show the sensitivity variation with spatial bandwidth for our 100-\( \mu m \) waveguides. Commercial Si-CMOS detector arrays are available with a pixel pitch of 2.8 \( \mu m \)[56]. Using an array with this pitch reduces sensitivity by 2.1\times.

The sensitivity may also be improved by thinning the guiding layer, increasing the evanescent field within the sensing layer, and thereby the index sensitivity coefficient, \( \frac{\partial n_{eff}}{\partial n_{SL}} \). A change from the current guiding layer thickness of 0.20 \( \mu m \) to the optimal thickness of \( \sim 0.13 \mu m \) improves sensitivity by 20%. This improvement requires an
input grating coupler for practical implementation. These two factors (assuming 2.8 \( \mu m \) pitch) create a net sensitivity reduction of 1.8 \( \times \).

7.5 Estimated Sensitivity of Fully-Integrated Si-CMOS Sensor

The sensitivities of a fully-integrated sensor on Si-CMOS, that is limited by the aforementioned fundamental noise sources, can be estimated by comparison with the measured sensitivities of a sensor on silicon (Table 6). By optimizing the guiding layer thickness, accounting for the pixel size, and operating in the shot noise limit, we estimate that the fully-integrated MDC will be reduced by a factor of 2.72. This suggests a methanol vapor sensitivity of smaller than 200 \( ppmv \), and an index sensitivity of better than 6 \( \times 10^{-7} \). For specific agents, the sensitivities as interpreted by both the optimal-ratio FOM, \( S \), and by \( RMSE_{1k} \) are listed in Tab. 7.

<table>
<thead>
<tr>
<th>Sensitivity</th>
<th>( S )</th>
<th>RMSE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methanol</td>
<td>180 ( ppmv )</td>
<td>110 ( ppmv )</td>
</tr>
<tr>
<td>( \Delta n_{SL} )</td>
<td>5.9 ( \times 10^{-7} )</td>
<td>4.0 ( \times 10^{-7} )</td>
</tr>
<tr>
<td>Isopropanol</td>
<td>7 ( ppmv )</td>
<td>5 ( ppmv )</td>
</tr>
<tr>
<td>Benzene</td>
<td>21 ( ppmv )</td>
<td>14 ( ppmv )</td>
</tr>
<tr>
<td>Water</td>
<td>77 ( ppmv )</td>
<td>55 ( ppmv )</td>
</tr>
</tbody>
</table>

Finally, environmental noise caused by fluctuations in chemical concentration or a variation of the index of the surrounding medium may ultimately limit performance. The sense layer may also absorb benign environmental chemicals and may be impacted by humidity. Further, as specified earlier, the sense layer index thermal sensitivity is \( -2.4 \times 10^{-4}/^\circ C \). Limiting the temperature dependence to maintain the MDC requires that the temperature be held constant to within \( \pm 0.004^\circ C \). Thus, in the absence of isothermal conditions, a reference sensor or other optical methods must be used to counter this temperature sensitivity.
Chapter VIII

CONCLUSION AND FUTURE WORK

In summary, this dissertation has demonstrated the sensitivity of a Si-CMOS-compatible multimode MZI-based EWS, and shown the key factors that determine its sensitivity. A sensitive modal pattern analysis strategy had been developed to quantify modal pattern change in response to index change on the sensing arm. Further, it has been shown that material effects do impact the sensitivity, and this effect has been quantified.

Specifically, the fundamental action of multimode sensing has been explained theoretically. The sensitivity enhancement has been shown to be simply related to the increased optical path length of the optical field under the SL. The material response to chemical and temperature change has been fully characterized. The impact of this material response on device sensitivity has been investigated along with potential mitigation techniques. The sensor has been simulated both in its full operation and to understand the modal coupling properties of the multimode y-junction. The sensor has been demonstrated at an index sensitivity of \(< 2 \times 10^{-6}\), and a methanol vapor concentration sensitivity \(< 500\text{ppbv}\). Corresponding sensitivities for other agents have also been estimated. Sensitivity estimation methods have been examined and one selected. The hardware noise parameters of a fully-integrated sensor have been compared with the measured noise of the sensor measurement to estimate the sensitivity of a fully-integrated Si-CMOS sensor at \(< 6 \times 10^{-7}\).

The following items could be investigated with the knowledge developed here:

- an input coupler that couples low order input modes to the highest order modes under the SL could be designed
- an output chirped grating coupler that separates the modes into different spatial areas would be desirable. This would essentially be a modal decomposition tool
- a temperature sensitive version of the interferometer could be designed
• this index-based sensor could be made agent-selective through agent-specific sensing layers

• alternately, a sensor chip with an array of sensors, each fabricated with a different sense layer, to increase selectivity [21] could be designed

• other EWS variants including resonant microcavities, or resonant cavity enhanced interferometry could be considered for enhanced path length under the sense layer
Appendix A

THE POISSON DISTRIBUTION AND SHOT NOISE

A.1 Postulates

The information in Sections A.1 and A.2 describe the Poisson distribution [57]. The postulates upon which the Poisson distribution are as follows:

1. The probability of one of more events occurring in an interval
   (a) is the same for equal size intervals,
   (b) is approximately proportional to the size of the interval, and
   (c) the approximation gets better for smaller intervals.

2. The probability of 2 or more events occurring in any one interval goes to zero as the interval gets smaller.

3. Events in non-overlapping intervals are independent of each other.

A.2 Derivation of Poisson Probability

By Postulate 1(b),

\[ p(1 \text{ or more events}) \simeq \lambda \Delta t \quad (61) \]
\[ p(0 \text{ events}) \simeq (1 - \lambda \Delta t) \quad (62) \]

where \( \lambda \) is a proportionality constant. So, what is the probability of zero events within the interval \([0, t + \delta t]\)?

\[ p_0(t + \delta t) \simeq p_0(t)(1 - \lambda \delta t) \quad (63) \]
\[ \frac{p_0(t + \delta t) - p_0(t)}{\delta t} \simeq -\lambda p_0(t) \quad (64) \]
\[ \frac{dp_0(t)}{dt} = -\lambda p_0(t) \quad (65) \]
By the same logic, what is the probability of exactly one event within the interval 
\[ 0, t + \delta t \]?

\[
p_1(t + \delta t) \simeq p_1(t)p_0(\delta t) + p_0(t)p_1(\delta t) \quad (66)
\]

\[
\simeq p_1(t)(1 - \lambda \delta t) + p_0(t)(\lambda \delta t) \quad (67)
\]

\[
p_1(t + \delta t) - p_1(t) \simeq -\lambda p_1(t)\delta t + \lambda p_0(t)\delta t \quad (68)
\]

\[
\frac{p_1(t + \delta t) - p_1(t)}{\delta t} \simeq -\lambda p_1(t) + \lambda p_0(t) \quad (69)
\]

\[
\frac{dp_1(t)}{dt} = -\lambda p_1(t) + \lambda p_0(t) \quad (70)
\]

Remembering Postulate 2, the probability of exactly two event within the interval 
\[ 0, t + \delta t \] may be described by the following:

\[
p_2(t + \delta t) \simeq p_0(t)p_2(\delta t) + p_2(t)p_0(\delta t) + p_1(t)p_1(\delta t) \quad (71)
\]

\[
\simeq p_0(t)(0) + p_2(t)(1 - \lambda \delta t) + p_1(t)(\lambda \delta t) \quad (72)
\]

\[
p_2(t + \delta t) - p_2(t) \simeq -\lambda p_2(t)\delta t + \lambda p_1(t)\delta t \quad (73)
\]

\[
\frac{p_2(t + \delta t) - p_2(t)}{\delta t} \simeq -\lambda p_2(t) + \lambda p_1(t) \quad (74)
\]

\[
\frac{dp_2(t)}{dt} = -\lambda p_2(t) + \lambda p_1(t) \quad (75)
\]

This may be continued for higher numbers, with the end result being that

\[
\frac{dp_N(t)}{dt} = -\lambda p_N(t) + \lambda p_{N-1}(t). \quad (76)
\]

These equations may be solved using an integrating factor, and the results are as follows:

\[
p_0(t) = e^{-\lambda t} \quad (77)
\]

\[
p_1(t) = \lambda t e^{-\lambda t} \quad (78)
\]

\[
p_2(t) = \frac{1}{2!}(\lambda t)^2 e^{-\lambda t} \quad (79)
\]

\[
p_N(t) = \frac{e^{-\lambda t}(\lambda t)^N}{N!} \quad (80)
\]
A.3 Mean and Variance of Poisson Process

Now, we find the mean value and variance [58] of a Poisson process like photon arrival. We begin by letting $\lambda t = a$, i.e.

$$P[x = k] = e^{-a} \frac{a^k}{k!},$$

(81)

which specifies the probability that exactly $k$ events will occur.

To find the mean and variance, we differentiate the Taylor series of $e^a$ wrt $a$.

$$e^a = \sum_{k=0}^{\infty} \frac{a^k}{k!}$$

(82)

$$e^a = \sum_{k=0}^{\infty} \frac{ka^{k-1}}{k!} = \frac{1}{a} \sum_{k=1}^{\infty} \frac{ka^k}{k!}$$

(83)

$$e^a = \sum_{k=1}^{\infty} \frac{zk(k-1)a^{k-2}}{k!} = \frac{1}{a^2} \sum_{k=1}^{\infty} \frac{k^2a^k}{k!} - \frac{1}{a} \sum_{k=1}^{\infty} \frac{ka^k}{k!}$$

(84)

And therefore by Eq. 83, the expected value of a Poisson process can be calculated as follows:

$$E\{x\} = e^{-a} \sum_{k=1}^{\infty} \frac{ka^k}{k!} = a,$$

(85)

and by Eq. 84, together with Eq. 83,

$$E\{x^2\} = e^{-a} \sum_{k=1}^{\infty} \frac{k^2a^k}{k!} = a^2 + a.$$  

(87)

As we know that the variance is specified by

$$\sigma^2 = E[(x - <x>)^2] = E[x^2 - 2x <x> + <x>^2] = E[x^2] - <x>^2,$$

(88)

this means that the mean and variance of the Poisson process are given by the following:

$$\mu_{\text{Poisson}} = a$$

(89)

$$\sigma^2_{\text{Poisson}} = a^2 + a - a^2 = a.$$  

(90)

Although these quantities can be considered unitless (i.e. numbers of things), if the items have charge or some other quantity, the units of $\mu$ are the same as a, but the units of $\sigma^2$ are in units of $a^2$. ‘a’ is only the magnitude of the number.
A.4 Mean and Variance of Captured Photoelectrons in Well-based Detector

For photon arrival times: If the average number of photons arriving within a time $t$ is given by $\lambda t$, then the probability of exactly $k$ photons arriving is given by

$$P[k \text{ in } t] = e^{-\lambda t} \frac{(\lambda t)^k}{k!}, \quad (91)$$

I.e. $a = \lambda t$. This means that the mean number of photons arriving is given by

$$\mu_{ph} = \lambda t, \quad (92)$$

and the variance in the number (i.e. if you measured many intervals of length $t$) is given by

$$\sigma^2_{ph} = \lambda t. \quad (93)$$

If then, these photons are read by a well-based detector with a Q.E. of $p$, $0 < p < 1$, then the mean number of captured photoelectrons in the interval, $t$, is given by

$$\mu_{pe} = p\lambda t, \quad (94)$$

and if you again measured many such intervals, the variance in the number of captured electrons would be

$$\sigma^2_{pe} = p\lambda t. \quad (95)$$

We choose the integration time such that the mean number of photons impinging on a photodetection site is $p\lambda t \simeq N_{tot}$, were $N_{tot}$ is the size of the well. In this case, the variance in the number of photons detected is simply $N_{tot}$. Thus, it is truly the number of electrons that governs both the mean and the variance of the shot noise for well-based detectors. The units of the mean are $(e^-)$ and of the variance are $(e^-)^2$.

Further, this variance does not depend on the bandwidth of the detector. It is simply some number. Although the current-based model of shot noise has a bandwidth dependence, this comes about because the shot noise electrons contribute to an analog current. Thus the shot noise of well-based detectors is correctly specified in terms of some number of captured electrons.
Appendix B

OBSERVING THE MULTIMODE PATTERN

This is just a formalization of the information required to create a multimode pattern via simulation. Assuming a time-harmonic guided mode in a waveguide in which the TE and TM modes are not coupled, the following may be derived. Beginning from Maxwell’s equations,

\[ \vec{E} = \frac{j}{\omega \varepsilon_0 n^2} \nabla \times \vec{H} \]  \hspace{1cm} (96)
\[ \vec{H} = \frac{j}{\omega \mu_0} \nabla \times \vec{E}. \]  \hspace{1cm} (97)

Continuing, we are interested in the x-directed magnetic field that will contribute to the forward-propagating Poynting vector.

\[ \vec{H} \cdot \hat{i} = -\frac{\beta}{\omega \mu_0} \vec{E}(x)e^{-j\beta z}. \]  \hspace{1cm} (98)

If there are multiple modes in the structure then the time average irradiance profile within the waveguide is given by

\[ < \vec{S}(z) > = \frac{1}{2} \text{Re} \left\{ \vec{E}_{tot} \times \vec{H}_{tot}^* \right\} \]
\[ = \frac{1}{2} \text{Re} \left\{ \sum_{t=1}^{N} \vec{E}_t(x)e^{-j\beta_t z} \times \sum_{s=1}^{N} \frac{-\beta_s}{\omega \mu_0} \vec{E}_s^*(x)e^{+j\beta_s z} \right\} \]  \hspace{1cm} (99)
\[ = \frac{k}{2\omega \mu_0} \text{Re} \left\{ \left( \sum_{t=1}^{N} \vec{E}_t(x)e^{-j\beta_t z} \right) \left( \sum_{s=1}^{N} \beta_s \vec{E}_s^*(x)e^{+j\beta_s z} \right) \right\}. \]

If this irradiance profile is integrated over the cross-section of the waveguide, then the orthogonality of the modes can be observed. Also, \( \beta \) is assumed to be real. The power
passing point, \( z \), is given by

\[
< \vec{P}(z) > = \frac{k}{2\omega_0} \int_{-\infty}^{\infty} Re \left\{ \left( \sum_{t=1}^{N} \vec{E}_t(x)e^{-j\beta_t z} \right) \left( \sum_{s=1}^{N} \beta_s \vec{E}_s^*(x)e^{+j\beta_s z} \right) \right\} dx
\]

\[
= \frac{k}{2\omega_0} \sum_{s=1}^{N} \sum_{t=1}^{N} \beta_s \int_{-\infty}^{\infty} \vec{E}_t(x)e^{-j\beta_t z} \vec{E}_s^*(x)e^{+j\beta_s z} dx \]

\[
= \frac{k}{2\omega_0} \sum_{s=1}^{N} \sum_{t=1}^{N} \beta_s \frac{2\omega_0 P_s}{\beta_s} \delta(t, s)
\]

\[
= \frac{k}{2\omega_0} \sum_{i=1}^{N} \beta_i \frac{2\omega_0 P_s}{\beta_s}
\]

\[
= k \sum_{i=1}^{N} P_s,
\]

as expected. The total power is given by the sum of the powers in the individual modes.
Appendix C

EXTRACTING MODAL AMPLITUDE AND PHASE FROM FIELD PATTERN

We begin this appendix from Eqs. ?? and ???. We wish to find the component of field, $a$, within some unknown field from the same waveguide, $\vec{E}_b(x)$, where

$$\vec{E}_b(x) = \sum_{i=1}^{N} s(i) \vec{E}_i(x), \quad (101)$$

where $s(i)$ is in general complex. If so, then we find the following:

$$\int_{-\infty}^{\infty} \vec{E}_b(x) \vec{E}_i^*(x) \, dx = \int_{-\infty}^{\infty} \{ \sum_{i=1}^{N} s(i) \vec{E}_i(x) \} \vec{E}_i^*(x) \, dx = \int_{-\infty}^{\infty} \{ s(1) \vec{E}_1(x) \vec{E}_1^*(x) + \cdots + s(i) \vec{E}_i(x) \vec{E}_i^*(x) \} \, dx \quad (102)$$

$$\int_{-\infty}^{\infty} \vec{E}_b(x) \vec{E}_i^*(x) \, dx = s(i) \frac{2\eta_0 P_i \mu_0}{n_{eff}^2}. \quad (103)$$

With this, we can extract the amplitude and phase coefficient, $s(i)$, by performing the following computation.

$$\int_{-\infty}^{\infty} \vec{E}_b(x) \vec{E}_i^*(x) \, dx = s(i) \frac{2\eta_0 P_i \mu_0}{n_{eff}^2} \quad (104)$$

To recreate the field, we simply reverse the decomposition as follows:

$$\vec{E}_b(x) = \sum_{i=1}^{N} s(i) \vec{E}_i(x) \quad (105)$$
Appendix D

ESTIMATION OF THE MULTIMODE PATTERN

‘REPETITION RATE’

We expect that there will be some index change in the cover layer at which the phases of the modes will become approximately equal again. This estimation accounts for the changing effective indices of the modes with index change, but does not account for the potentially changing numbers of modes. This effect may be present, but to gain an initial understanding of the repetition, we neglect it for now.

We consider the simplest conceptual interferometer. Two identical, adjacent planar waveguides, each of length, $Z$, that are illuminated with an identical multimode irradiance profile at free space wavelength, $\lambda_0$. This profile is assumed to couple equally, some significant amount of power into each of the $M$ guided modes of each waveguide. In addition, an output coupler is assumed that can add the electric fields of the two waveguides perfectly without inducing modal coupling between any modes, guided or radiation. In this case, we can write the sum of the fields in these two waveguides immediately after recombination as follows:

$$\overrightarrow{E}_{\text{tot}}(x, Z) = \overrightarrow{E}_{\text{sns}}(x, Z) + \overrightarrow{E}_{\text{ref}}(x, Z).$$

(105)

In either arm, the electric field of one transverse TE-like mode may be written as follows:

$$\overrightarrow{E}_{\text{sns/ref}}(x, Z) = \sum_{m=0}^{M} a_m E_m(x)e^{j\frac{2\pi Z}{\lambda_0}(n_m^{\text{eff}} + \frac{\partial n_m^{\text{eff}}}{\partial n_c} \Delta n_c)},$$

(106)

where $n_m^{\text{eff}}$ is the effective index of the $m^{\text{th}}$ mode of the waveguide in question, and $\Delta n_c$ is the index change in the cover layer. The complex field coefficient, $a_m$, represents the amplitude and phase effects of the input coupling. $E_m(x)$ is a real TE-like mode field profile in the $x$-direction. The waveguide layer structure is designed so that the index sensitivity coefficient for modes in the reference arm, $\frac{\partial n_m^{\text{eff}}}{\partial n_c}$, is zero. In the sense arm, however, these coefficients are designed to be as high as possible. In general, transverse higher order modes
will have a greater $\frac{\partial n_{mf}}{\partial n_{c}}$. Although this is not precisely the case, we approximate that in the absence of chemical, the two adjacent waveguides have exactly the same layer structure. This should allow us to learn about the repetition rate without unnecessary complication.

The corresponding equation for the magnetic fields of the transverse TE-like modes are

$$\overrightarrow{H}_{sns/\text{ref}} \cdot \hat{i}(x, Z) = \sum_{m=0}^{M} - \frac{a_m(n_{mf}^m + \frac{\partial n_{mf}}{\partial n_{c}} \Delta n_c)}{\eta_0} E_m(x) e^{j \frac{2\pi Z}{\lambda_0} (n_{mf}^m + \frac{\partial n_{mf}}{\partial n_{c}} \Delta n_c)}, \quad (107)$$

where $\eta_0$ is the impedance of free space.

We wish to find the value of $\Delta n_c$ at which the full multimode pattern becomes very similar to the pattern at $\Delta n_c = 0$. To answer this question, we must find the irradiance profile at the output of the this idealized MZI. We ignore for now, additional modes that might be created as the index of the guiding region slightly increases. To create the irradiance profile, we find the net electric and magnetic fields, and the find the Poynting vector. The combined electric field can be written

$$\overrightarrow{E}_{tot}(x, Z) = \sum_{m=0}^{M} a_m E_m(x) e^{j \frac{2\pi Z}{\lambda_0} (n_{mf}^m + \frac{\partial n_{mf}}{\partial n_{c}} \Delta n_c)} + \sum_{m=0}^{M} a_m E_m(x) e^{j \frac{2\pi Z}{\lambda_0} n_{mf}^m}$$

$$= \sum_{m=0}^{M} 2a_m E_m(x) e^{j \frac{2\pi Z}{\lambda_0} n_{mf}^m} e^{j \frac{2\pi Z}{\lambda_0} \Delta n_c} \cos(\frac{\pi Z \partial n_{mf}^m}{\lambda_0 \partial n_c} \Delta n_c)$$

(108)

The corresponding combined magnetic field can be written

$$\overrightarrow{H}_{tot} \cdot \hat{i}(x, Z) = \sum_{m=0}^{M} - \frac{a_m(n_{mf}^m + \frac{\partial n_{mf}}{\partial n_{c}} \Delta n_c)}{\eta_0} E_m(x) e^{j \frac{2\pi Z}{\lambda_0} (n_{mf}^m + \frac{\partial n_{mf}}{\partial n_{c}} \Delta n_c)} + \sum_{m=0}^{M} \frac{a_m n_{mf}^m}{\eta_0} E_m(x) e^{j \frac{2\pi Z}{\lambda_0} n_{mf}^m}$$

$$= \frac{-1}{\eta_0} \sum_{m=0}^{M} a_m n_{mf}^m E_m(x) e^{j \frac{2\pi Z}{\lambda_0} n_{mf}^m} \left\{ [1 + \frac{\partial n_{mf}^m}{\partial n_c} \Delta n_c] e^{j \frac{2\pi Z}{\lambda_0} \frac{\partial n_{mf}^m}{\partial n_c} \Delta n_c} + 1 \right\} \quad (109)$$

$$\simeq \frac{-2}{\eta_0} \sum_{m=0}^{M} a_m n_{mf}^m E_m(x) e^{j \frac{2\pi Z}{\lambda_0} n_{mf}^m} e^{j \frac{2\pi Z}{\lambda_0} \frac{\partial n_{mf}^m}{\partial n_c} \Delta n_c} \cos(\frac{\pi Z \partial n_{mf}^m}{\lambda_0 \partial n_c} \Delta n_c),$$

assuming $(\partial n_{mf}^m/\partial n_c) \Delta n_c/n_{mf}^m << 1$. For our case, this term has a value $\leq 1 \times 10^{-3}$, for changes in methanol vapor concentration changes of less than 350 ppbv.
Now, we may compute the output irradiance profile based on Eq. ??,

\[
\langle \mathbf{S} \rangle (x, Z) \hat{k} = \frac{\hat{k}}{2} \Re \left\{ \sum_{m=0}^{M} a_m E_m(x) e^{j \frac{2\pi Z n_m}{\lambda_0} \Delta n_c} e^{j \frac{2\pi Z}{\lambda_0} \frac{\partial n_m}{\partial n_c} \Delta n_c} \cos \left( \frac{\pi Z}{\lambda_0} \frac{\partial n_m}{\partial n_c} \Delta n_c \right) \right\}.
\]

As we are interested in the irradiance profile and not simply the power, mode orthogonality cannot be invoked. Thus, we must evaluate every term in the sum as follows:

\[
\langle \mathbf{S} \rangle (x, Z) \hat{k} = \frac{2\eta}{\lambda_0} \Re \left\{ \sum_{m=0}^{M} \sum_{s=0}^{M} a_m a_s^* E_m(x) E_s^*(x) e^{j \frac{2\pi Z}{\lambda_0} (n_m^e - n_s^e)} e^{j \frac{\pi Z}{\lambda_0} \frac{\partial n_m^e}{\partial n_c} \Delta n_c} \cos \left( \frac{\pi Z}{\lambda_0} \frac{\partial n_m^e}{\partial n_c} \Delta n_c \right) \cos \left( \frac{\pi Z}{\lambda_0} \frac{\partial n_s^e}{\partial n_c} \Delta n_c \right) \right\}.
\]

We further assume that all \( E_m(x) \) and \( n_m^e \) are real. We may simplify this expression further by applying the trigonometric identity,

\[
\cos(A)\cos(B) = 1/2 \{ \cos(A + B) + \cos(A - B) \}.
\]

Then we find the following:

\[
\langle \mathbf{S} \rangle (x, Z) \hat{k} = \frac{\hat{k}}{\eta_0} \Re \left\{ \sum_{m=0}^{M} \sum_{s=0}^{M} a_m a_s^* E_m(x) E_s(x) e^{j \frac{2\pi Z}{\lambda_0} (n_m^e - n_s^e)} e^{j \frac{\pi Z}{\lambda_0} \frac{\partial n_m^e}{\partial n_c} \Delta n_c} \cos \left( \frac{\pi Z}{\lambda_0} \left( \frac{\partial n_m^e}{\partial n_c} + \frac{\partial n_s^e}{\partial n_c} \right) \Delta n_c \right) + \cos \left( \frac{\pi Z}{\lambda_0} \left( \frac{\partial n_m^e}{\partial n_c} - \frac{\partial n_s^e}{\partial n_c} \right) \Delta n_c \right) \right\}.
\]

Rewriting the complex coefficient product, \( a_m a_s^* = A_{ms} e^{j \phi_{ms}} \), allows us to separate the real and imaginary parts of this expression as follows:

\[
\langle \mathbf{S} \rangle (x, Z) = \frac{\hat{k}}{\eta_0} \Re \left\{ \sum_{m=0}^{M} \sum_{s=0}^{M} A_{ms} E_m(x) E_s(x) \left[ \cos \left( \frac{\pi Z}{\lambda_0} \left( \frac{\partial n_m^e}{\partial n_c} + \frac{\partial n_s^e}{\partial n_c} \right) \Delta n_c \right) + \cos \left( \frac{\pi Z}{\lambda_0} \left( \frac{\partial n_m^e}{\partial n_c} - \frac{\partial n_s^e}{\partial n_c} \right) \Delta n_c \right) \right] e^{j \frac{\pi Z}{\lambda_0} \frac{\partial n_m^e}{\partial n_c} \Delta n_c + \frac{2\pi Z}{\lambda_0} (n_m^e - n_s^e) + \phi_{ms}} \right\}.
\]
\[ < \vec{S} > (x, Z) = \frac{\hat{k}}{\eta_0} \left\{ \sum_{m=0}^{M} \sum_{s=0}^{M} A_{ms} E_m(x) E_s(x) \right\} \]

\[
\begin{align*}
&\left[ \cos\left( \frac{\pi Z}{\lambda_0} \left( \frac{\partial n_{eff}^m}{\partial n_c} + \frac{\partial n_{eff}^s}{\partial n_c} \right) \Delta n_c \right) + \cos\left( \frac{\pi Z}{\lambda_0} \left( \frac{\partial n_{eff}^m}{\partial n_c} - \frac{\partial n_{eff}^s}{\partial n_c} \right) \Delta n_c \right) \right] \\
&\cos\left( \frac{\pi Z}{\lambda_0} \left( \frac{\partial n_{eff}^m}{\partial n_c} - \frac{\partial n_{eff}^s}{\partial n_c} \right) \Delta n_c + \frac{2\pi Z}{\lambda_0} (n_{eff}^m - n_{eff}^s) + \phi_{ms} \right) \right\}. 
\end{align*}
\]

\[ < \vec{S} > (x, Z) = \frac{\hat{k}}{\eta_0} \left\{ \sum_{m=0}^{M} \sum_{s=0}^{M} A_{ms} E_m(x) E_s(x) \right\} \]

\[
\begin{align*}
&\left\{ \cos\left( \frac{\pi Z}{\lambda_0} \left( \frac{\partial n_{eff}^m}{\partial n_c} + \frac{\partial n_{eff}^s}{\partial n_c} \right) \Delta n_c \right) \cos\left( \frac{\pi Z}{\lambda_0} \left( \frac{\partial n_{eff}^m}{\partial n_c} - \frac{\partial n_{eff}^s}{\partial n_c} \right) \Delta n_c + \frac{2\pi Z}{\lambda_0} (n_{eff}^m - n_{eff}^s) + \phi_{ms} \right) \right\} \\
&\frac{1}{2} \left[ \cos\left( \frac{2\pi Z}{\lambda_0} \left( \frac{\partial n_{eff}^m}{\partial n_c} - \frac{\partial n_{eff}^s}{\partial n_c} \right) \Delta n_c + \frac{2\pi Z}{\lambda_0} (n_{eff}^m - n_{eff}^s) + \phi_{ms} \right) + \cos\left( \frac{\pi Z}{\lambda_0} (n_{eff}^m - n_{eff}^s) + \phi_{ms} \right) \right] \right\}. 
\end{align*}
\]

\[ < \vec{S} > (x, Z) = \frac{\hat{k}}{2\eta_0} \left\{ \sum_{m=0}^{M} \sum_{s=0}^{M} A_{ms} E_m(x) E_s(x) \right\} \]

\[
\begin{align*}
&\left\{ \cos\left( \frac{2\pi Z}{\lambda_0} \left( \frac{\partial n_{eff}^m}{\partial n_c} \Delta n_c + \frac{2\pi Z}{\lambda_0} (n_{eff}^m - n_{eff}^s) + \phi_{ms} \right) + \cos\left( \frac{2\pi Z}{\lambda_0} \left( \frac{\partial n_{eff}^s}{\partial n_c} \Delta n_c - \frac{2\pi Z}{\lambda_0} (n_{eff}^m - n_{eff}^s) - \phi_{ms} \right) \right) \right\} \\
&\left[ \cos\left( \frac{2\pi Z}{\lambda_0} \left( \frac{\partial n_{eff}^m}{\partial n_c} - \frac{\partial n_{eff}^s}{\partial n_c} \right) \Delta n_c + \frac{2\pi Z}{\lambda_0} (n_{eff}^m - n_{eff}^s) + \phi_{ms} \right) + \cos\left( \frac{\pi Z}{\lambda_0} (n_{eff}^m - n_{eff}^s) + \phi_{ms} \right) \right] \right\}. 
\end{align*}
\]

Now, when do the net phase differences in each of the cosine terms in either Eq. 117 or Eq. 118 become some multiple of 2\pi. In Eq. 117, it appears as if there is a slowly varying envelope and a faster “carrier”. We will use this representation. In this case, the pattern created by any two modes will approximately repeat for

\[ \Delta n_c \simeq \frac{2\lambda_0}{\eta_0} \]
For our materials and layer structure, and assuming two high order modes, this has a value of about

\[ \Delta n_c \simeq \frac{2 \times 0.84/2000}{.42 + .42} = 0.001 \]  \hspace{1cm} (120)

For two of the lower-order transverse modes, this value would be closer to 0.0014.

Now to extend this to the entire pattern, we must find the lowest common multiple of \( \Delta n_c \) in order for this to be satisfied for each and every possible pair of modes. Thus it should be
EWSs rely only on an index change in a chemically or biologically sensitive cladding layer. Thus, the sensitivity constant, $\partial n_{eff}/\partial n_c$, of these devices governs their sensitivity. Estimation of the sensitivity has traditionally relied on numerical or experimental methods. Here, a quasi-analytical method is described to estimate the index sensitivity coefficient for TM modes.

The 3-slab TM Eigenvalue Equation treats the case of a semi-infinite cover and substrate layer surrounding a finite film layer. The modal effective index, $n_{eff}$, depends on the layer indices and thicknesses, through the upper cladding layer index, $n_c$, the guiding layer thickness, $h$, the film index, $n_f$, the substrate index, $n_s$, the transverse modal phase constant, $\kappa_f$, the cover and substrate transverse field decay constants, $\gamma_c$, and $\gamma_s$, and the free space wavenumber, $k_0$. The index sensitivity coefficient for a semi-infinite, three-slab TM waveguide may be derived starting from Eq. 121.

$$\tan (h\kappa_f) = \frac{\kappa_f \left[ \frac{n_f^2}{n_s^2} \Gamma_s + \frac{n_f^2}{n_c^2} \Gamma_c \right]}{\kappa_f^2 - \frac{n_f^2 \Gamma_s \Gamma_c}{n_c^2 n_s^2}}$$  \hspace{1cm} (121)

The modal effective index is defined by $n_{eff} \equiv \beta/k_0$. The transverse mode constants are defined by $\gamma_c = k_0 \sqrt{n_{eff}^2 - n_c^2}$, $\Gamma_s = k_0 \sqrt{n_{eff}^2 - n_s^2}$, and $\kappa_f = k_0 \sqrt{n_f^2 - n_{eff}^2}$. 

131
Taking the partial derivative of Eq. 2 with respect to \( n_c \) and rearranging terms produces Eq. A2. To make this equation readable, we define additional parameters \( A \equiv n_f^2 - n_{eff}^2; B \equiv n_{eff}^2 - n_c^2; \) and \( C \equiv n_{eff}^2 - n_s^2. \)

\[
\frac{\partial n_{eff}}{\partial n_c} =
\]

\[
\frac{\frac{1}{2} n_{eff}^2 \frac{n_{eff}}{n_f} + n_{eff}^2 C^{1/2}}{n_f^2 B^{1/2}} \left( \frac{A}{A - \frac{B^{1/2} n_s C^{1/2}}{n_f}} \right)^2 - \frac{\frac{1}{2} n_{eff}^2 \frac{n_{eff}}{n_f} + n_{eff}^2 C^{1/2}}{n_f^2 B^{1/2}} \left( \frac{A}{A - \frac{B^{1/2} n_s C^{1/2}}{n_f}} \right)^2
\]
INDEX MIXING RULES APPLIED TO THERMAL EXPANSION

F.1 Index Mixing Rules

Index mixing rules have been studied in the literature \[29\] \[30\]. They describe the weighting of bulk material indices when in mixtures to attain the index of refraction of a composite material. Specifically, Mehra \[29\] compares experimental results with the indices of refraction estimated using four different index mixing rules for binary mixtures of hexadecane and heptadecane with n-alkanols at different temperatures. Pandey et al. examine ternary and quaternary mixtures. The index mixing rules, which are based on a weighting of the bulk index, are now listed.

For example, the Lorentz-Lorenz (LL) mixing rule (for two components) can be written as

\[
\frac{n_{12}^2 - 1}{n_{12}^2 + 2} = \phi_1 \frac{n_1^2 - 1}{n_1^2 + 2} + \phi_2 \frac{n_2^2 - 1}{n_2^2 + 2},
\]

where \(\phi_1(\phi_2)\) is the volume fraction of substance 1 (substance 2) in the mixture.

The Gladstone-Dale (G-D) relation can be written as

\[
\frac{n_{12} - 1}{n_{12}} = W_1 \frac{n_1^2 - 1}{n_1} + W_2 \frac{n_2^2 - 1}{n_2},
\]

where \(W_i\) represents the weight fraction of the \(i^{th}\) component of the mixture.

Another option is the Weiner (Wn) relation which applies to isotropic bodies of spherically symmetric shape,

\[
\frac{n_{12}^2 - n_1^2}{n_{12}^2 + 2n_1^2} = \phi_2 \frac{n_2^2 - n_1^2}{n_2^2 + 2n_1^2}.
\]

Pandey states that the LL and Wn relations give identical results if the mixing process is accompanied by neither contraction nor expansion.
The Heller (H) relation can be written as

$$\frac{n_{12} - n_1}{n_1} = 3 \frac{m^2 - 1}{2 \phi_2 m^2 + 2}$$

(126)

where \(m = n_2/n_1\).

The Arago-Biot (A-B) rule suggests that the mixture index is given by

$$n_{12} = \phi_1 n_1 + \phi_2 n_2.$$  

(127)

### F.2 Index Mixing Rules with Thermal Expansion

**F.2.1 Into Lorentz-Lorenz**

If we then put these volume fractions into the Eq. 123, we find the predicted effect on the composite index of the temperature change.

$$\frac{n_{12}^2 - 1}{n_{12}^2 + 2} = \frac{1}{1 + \alpha \Delta T} \frac{n_1^2 - 1}{n_1^2 + 2} + \frac{\alpha \Delta T}{1 + \alpha \Delta T} \frac{n_2^2 - 1}{n_2^2 + 2}.$$  

(128)

If in addition, \(n_2 \sim 1\), then this may be simplified to the following:

$$\frac{n_{12}^2 - 1}{n_{12}^2 + 2} \approx \frac{1}{1 + \alpha \Delta T} \frac{n_1^2 - 1}{n_1^2 + 2}.$$  

(129)

**F.2.2 Into Weiner**

If we apply the volume changes to Eq. 125, we find

$$\frac{n_{12}^2 - n_1^2}{n_{12}^2 + 2n_1^2} = \frac{\alpha \Delta T}{1 + \alpha \Delta T} \frac{n_2^2 - n_1^2}{n_2^2 + 2n_1^2}.$$  

(130)

This simplifies if the increase in volume results in an increase in vacuum \((n_2 = 1)\) to

$$\frac{n_{12}^2 - n_1^2}{n_{12}^2 + 2n_1^2} = \frac{\alpha \Delta T}{1 + \alpha \Delta T} \frac{1 - n_1^2}{1 + 2n_1^2}.$$  

(131)

**F.2.3 Into Heller**

If we incorporate the same volume calculations into Eq. 126, we find the following:

$$\frac{n_{12}^2 - n_1}{n_1} = 3 \frac{\alpha \Delta T}{2 + \alpha \Delta T} \frac{(\frac{n_2}{n_1})^2 - 1}{(\frac{n_2}{n_1})^2 + 2}.$$  

(132)

$$\frac{n_{12}^2 - n_1}{n_1} = 3 \frac{\alpha \Delta T}{2 + \alpha \Delta T} \frac{(\frac{1}{n_1})^2 - 1}{(\frac{1}{n_1})^2 + 2}.$$  

(133)
F.2.4 Into Arago-Biot

If we incorporate the same volume calculations into Eq. 127, we find the following:

$$n_{12} = \frac{1}{1 + \alpha \Delta T} n_1 + \frac{\alpha \Delta T}{1 + \alpha \Delta T} n_2,$$

and simplifying for $n_2 = 1$,

$$n_{12} = \frac{1}{1 + \alpha \Delta T} n_1 + \frac{\alpha \Delta T}{1 + \alpha \Delta T}.$$
Appendix G

DERIVATION - CONSTRAINED TO UNCONSTRAINED CTE

First, the conventional symbol for the volume CTE is $\alpha$, which has units of $1/K$. The conventional symbol for the linear CTE is $\beta$, which also has units of $1/K$.

A rectangular prism containing isotropic material is considered. It has a room temperature, $T$, volume given by

$$V_0 = X_0 \times Y_0 \times Z_0.$$  \hfill (136)

The rectangular prism has an unconstrained coefficient of the thermal expansion, $\alpha$. If the temperature increases to $T + \Delta T$, then the volume of the prism increases to

$$V(\Delta T) = V_0(1 + \alpha \Delta T) = X_0Y_0Z_0(1 + \alpha \Delta T).$$  \hfill (137)

As the material is isotropic, the expansion is equal in all three dimensions. Therefore each dimension expands by

$$(1 + \alpha \Delta T)^{1/3}.$$  \hfill (138)

As $\alpha \Delta T$ is small, this may be approximated by the first term in its Taylor series.

$$(1 + \alpha \Delta T)^{1/3} \simeq (1 + \frac{\alpha}{3} \Delta T).$$  \hfill (139)

We thus define the unconstrained linear coefficient of thermal expansion as

$$\beta \equiv \alpha/3.$$  \hfill (140)

We now perform the following steps to investigate the constrained expansion of thin films on silicon:
1. allow the prism's volume to increase in response to a temperature change, $\Delta T$.

$$V(\Delta T) = V_0(1 + \alpha \Delta T)$$

$$= X_0(1 + \alpha \Delta T)^{\frac{1}{2}}Y_0(1 + \alpha \Delta T)^{\frac{1}{2}}Z_0(1 + \alpha \Delta T)^{\frac{1}{2}}$$

$$\simeq X_0(1 + \beta \Delta T)Y_0(1 + \beta \Delta T)Z_0(1 + \beta \Delta T)$$

2. compress the film in the $XY$-plane back to the original area

$$\epsilon_X = \frac{X_0 - X_0(1 + \beta \Delta T)}{X_0(1 + \beta \Delta T)} = \frac{-\beta \Delta T}{1 + \beta \Delta T}$$

$$\epsilon_Y = \epsilon_X$$

3. calculate the increase in $Z$ as a result

$$Z(\Delta T) = Z_0(1 + \beta \Delta T)(1 + \nu \{-\epsilon_X\})(1 + \nu \{-\epsilon_Y\})$$

$$Z(\Delta T)/Z_0 = (1 + \beta \Delta T)(1 + \nu \frac{\beta \Delta T}{1 + \beta \Delta T})^2$$

$$= (1 + \beta \Delta T)(1 + \nu \beta \Delta T)^2$$

$$= \frac{(1 + \beta \Delta T + \nu \beta \Delta T)^2}{(1 + \beta \Delta T)^2}$$

$$= \frac{(1 + \nu \beta \Delta T)(1 + (1 + \nu)\beta \Delta T)}{(1 + \beta \Delta T)^2}$$

$$\simeq 1 + (1 + \nu)\beta \Delta T + \nu \frac{\beta \Delta T(1 + \beta \Delta T)^2}{1 + \beta \Delta T}$$

$$Z/Z_0(\Delta T) \simeq 1 + (1 + 2\nu)\beta \Delta T$$

We now attempt to relate the constrained CTE, $\beta_C$ (that is easily measured with ellipsometry) with the true unconstrained CTE, $\beta_U$, first in the linear case:

$$(Z_0 + \Delta Z(\Delta T))/Z_0 \simeq 1 + (1 + 2\nu)\beta_U \Delta T$$

$$\Delta Z(\Delta T)/Z_0 \simeq (1 + 2\nu)\beta_U \Delta T$$

$$\beta_C \Delta T \simeq (1 + 2\nu)\beta_U \Delta T$$

$$\beta_C \simeq (1 + 2\nu)\beta_U$$

Another relation between constrained and unconstrained linear CTE’s is [32]

$$\beta_C = (1 - \nu)/(1 + \nu)\beta_U.$$  

(145)
This relations provide similar corrections. In the theoretical limit of \( \nu = 1 \), an expected correction factor of \( 1/3 \) is observed from Eq. 144. In the limit of \( \nu = 0 \), both expressions provide a correction factor of 1.
REFERENCES


A. Papoulis and S. Pillai.
VITA

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