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HYBRID MODE COUPLING FOR ENHANCED SENSING AND INTEGRATED
PHOTONICS

BY

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DISSERTATION

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Abstract

In this dissertation, we investigate the hybrid mode-coupling approach to enhance sensing and integrated photonic applications. The coupling of photonic elements is not new; the current demand is to further explore coupling strategies within photonic systems and complementary systems to meet or exceed design metrics and functionality. These strategies include the exploitation of material and structural design to enhance integration and coupling. We studied plasmonic-photonic coupling and high index contrast to enhance resonant and diffractive coupling, respectively.

Hybrid mode coupling benefits sensing for real-time quantitation, interrogation of low molecular weight, and nanoscale molecules by using a plasmonic-photonic coupling. A plasmonic-photonic coupling weds the key capabilities of highly localized fields at the metal interface with the resonant nature of high-quality-factor (Q) low-loss microcavities. This new class of hybrid sensor will advance the medical, pharmaceutical, defense, and environmental industries.

Conventional biosensing methods are tedious and have a long lead time for response. Furthermore, label-free optical detection of biomolecules does not generate a significant signal for detection. To address these limitations, we engineered a microring resonator-based sensor coupled to two gold concentric rings determined computationally. We report changes in the refractive index of the bulk medium and bio-monolayer at the corresponding sensitivities: 1340 nm/RIU and 105.3 fm/RIU for $\Delta n_{\text{biolayer}} = 0.2$ with a volumetric size of $1.0 \times 10^3 \text{ nm}^3$. The redshift of the resonance due to bulk sensing is a six-fold increase over the conventional microring resonator. Subsequently, we designed and conducted an experimental study of a plasmonic chain of gold bowtie nanostructures atop a microring resonator where the splitting of the resonant modes was observed.

Likewise, hybrid mode coupling advances integrated photonics applications where there is a demand to increase the performance of interconnects and components. As a requirement of the collaborative effort to build a photonic-electronic integrated circuit for energy-efficient computing, the photonic components had to be CMOS compatible. The grating coupler, a key integration component, is coupled to a vertical-cavity microlaser to power the optical circuit. For practical realization, the coupling is at normal incidence, and the grating coupler is buried within oxide to

ease flip-chip integration. To address the aforementioned constraints, we engineered an approach to design a high-efficiency grating coupler based on a high contrast overlay and apodization for fiber-to-chip that yields greater than 90% coupling efficiency over a broad bandwidth. The efficient diffractive coupling mechanism is due to the presence of a dual-layer grating and constructive interference between the grating teeth, i.e., scattering elements when mode matched with the source. Furthermore, we employed S-parameter analysis to determine the theoretical limits of this design. We then applied the approach towards a purely optical polymeric material system to enhance coupling efficiency from 7% to 62%.

This work advances our understanding of the coupling mechanisms to engineer devices for enhanced performance in sensing and integrated photonics applications. This work builds upon seminal past work and may serve as a building block for enhanced sensing and integrative, highly efficient photonics systems with unprecedented performance.

*Foremost, I dedicate this thesis to God.
Philippians 4:13; Psalm 18:1-2; Joshua 1:9; Jeremiah 29:11*

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List of Abbreviations

ALD	Atomic Layer Deposition
BOX	Buried Oxide Layer
CE	Coupling Efficiency
CHA	Carl Herrman Associates
CMOS	Complementary metal-oxide-semiconductors
CMT	Coupled-Mode Theory
DBR	Distributed Bragg Reflector
DUT	Device under Test
EBL	Electron Beam Lithography
FDTD	Finite-Difference Time-Domain
FEM	Finite Element Method
FWHM	Full-Width at Half-Maximum
GC	Grating Coupler
HCGs	High Contrast Gratings
HPC	High-Performance Computer
MNTL	Micro and Nanotechnology Laboratory
MRR	Microring Resonator
MRL	Material Research Laboratory
NOA	Norland Optical Adhesives
OI	Optical Isolator
OP	Optical Polarizer
PD	Photodetector
PECVD	Plasma Enhanced Chemical Vapor Deposition
PET	Polyethylene Terephthalate
PSQ	Polysilisiquioxane
Q	Quality Factor
RIE	Reactive Ion Etching
SEM	Scanning Electron Microscope
SOD	Spin-on Dielectric

SMF	Single Mode Optical Fiber
TE	Transverse Electric
TM	Transverse Magnetic
UV	Ultra-Violet
VCTL	Vertical Cavity Transistor Laser
VSCEL	Vertical Cavity Surface-emitting Laser
WGM	Whispering Gallery Mode

Chapter 1: Introduction

1.1 Importance of Hybrid Mode Coupling in Photonic Systems

Moore's law, which has served as the "rule of thumb" for the electronics sector since the advent of digital technologies, is approaching some fundamental limits. Photonics is widely viewed as a solution because of its ability to transmit data across arbitrary distances with low loss and high bandwidth [1]. Photonic technologies are increasingly becoming integrated into our society because the applications of photonics are ubiquitous: high-speed computing, telecommunications, and sensing. The technologies and applications are vital towards paving the way for quantum information processing and atomic-scale photonics. Photonics relies on leveraging the notable merits of light's speed and power density to advance the utility of integrated electronic-photonic applications.

Current state-of-the-art electronic devices rely upon the assembly of hundreds of electronic components coupled to achieve the desired functionality or figure of merit. Although coupling of photonic elements is not new, the demand to further explore coupling strategies within photonic systems and complementary systems to meet or exceed design metrics is driven by the emergence of electronic-photonic integration. Common building blocks of photonic circuits include waveguides, microring resonators, gratings, modulators, filters, and dividers. Presently, intensive investigations are underway to engineer unique material platforms [2], metamaterials, and metastructures to enhance coupling. In photonic systems, synergistic coupling between photonic elements and materials underpins integration as well as unlocking interesting phenomena to advance performance or extend functionality [3-7] as shown in Fig. 1.1. Mutual coupling involves an energy exchange between components such as couplers, switches, and filters. Under the law of conservation of energy, the coupled-mode theory can be applied towards the coupling of photonic elements and systems to gain insight into the hybrid nature of the modes. Hybrid mode coupling is a special class of mutual coupling in which the combined system exhibits supermodes, i.e., eigenmodes that contain non-negligible contributions from the individual modes of more than one of the isolated systems. Several works have demonstrated the advantages of hybrid mode coupling [8]. In Vollmer's work, the sensitivity of the proposed sensor was boosted by orders of magnitude

when integrating plasmonic nanostructures to a spherical microresonator and the hybrid device exceeded the upper limit of sensitivity for each component alone [9]. The significance of this coupling arrangement has ushered in the new era of ultra-sensitive detection to enumerate particles with low mass and small size such as small molecules. An on-chip plasmonic-photonic light concentrator was designed with a conversion efficiency of 92% and concentration field factor of 4.9 when coupling a plasmonic nanotaper to a silicon waveguide [10]. The team of Li et al. developed a phase-gradient metasurface possessing a small footprint, broadband operation, and low loss. As a result, their device can control light propagation and couple waveguide modes [11].

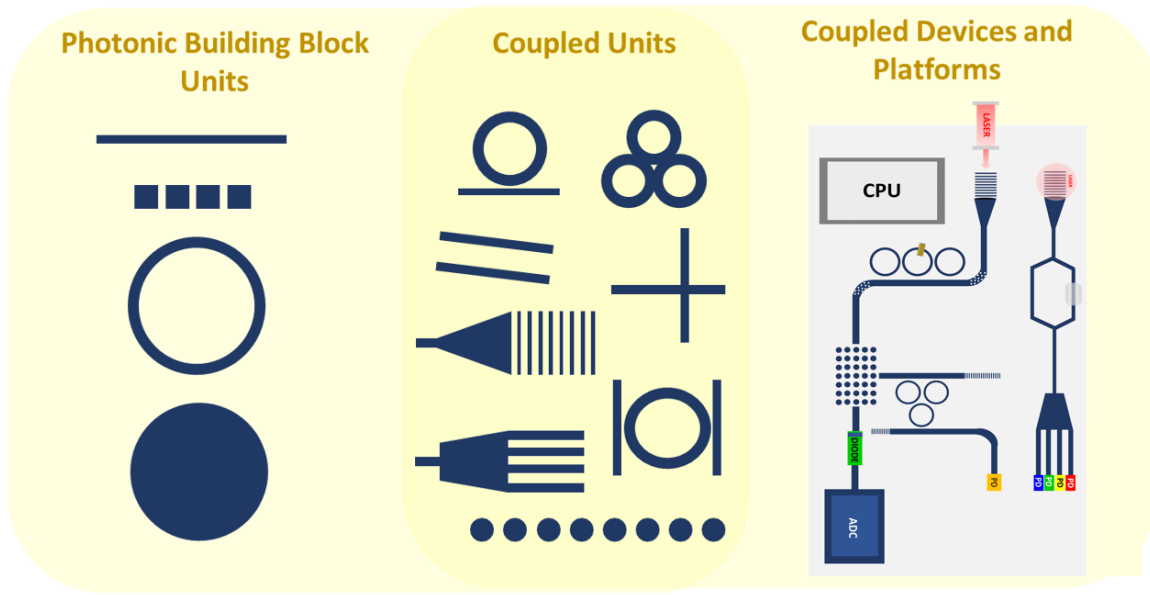


Figure 1.1. Schematic of passive photonic building blocks, units, devices, and platforms such as photonic integrated circuits [12-14]. The photonic building blocks units consist of waveguides, gratings, microring, and microdisk resonators. The coupled units are built by coupling the building blocks to achieve the desired functionality: isolating, filtering, coupling, directionality, and modulation. Coupled units and building blocks can be further enhanced by coupling various photonic structures to create advanced functionality and architectures.

1.2 Coupled Mode Theory

The coupling of optical structures can form a hybrid system where supermodes originate. To evaluate the supermodes in a hybrid system, coupled-mode theory (CMT) is applied to examine the propagation of light in a perturbed or weakly coupled system. It is also used to evaluate the exchange of optical energy in such a system. Using CMT, the modes representing the unperturbed

states must satisfy Maxwell's equations. Each local guided mode or resonant mode of a hybrid system is represented as a linear superposition of the unperturbed states. The resulting relationship is the approximate solution assuming a monochromatic, sinusoidal steady state solution. When the states are coupled, power between the optical or photonic structures is exchanged. Typically, the mode of one structure tends to dominate in coupling due to non-trivial realization.

In a two-state system, two types of supermodes emerge: even (symmetric) and odd (antisymmetric). They are the sum and the difference of the unperturbed states, respectively. These states can be viewed as constructive and destructive interference. Their average field amplitudes and field distributions are superimposed to approximate the hybrid mode coupling by computing the mode orthogonality or Poynting vector. Co-directional (parallel waveguides) and contra-directional (gratings) coupling are classic examples of hybrid mode coupling. In such systems, the mode coupling occurs when the propagation constants are matched. Coupled mode theory for these cases is based on spatially varying fields. The template for the canonical coupled mode theory is as follows [15]:

$$(\mathbf{E} \ \mathbf{H})(x, y, z) = \sum_k a_k (\mathbf{E}_k \ \mathbf{H}_k)(x, y, z) \quad (1.1)$$

The template represents the sum over each modal contribution, k , where $\mathbf{E}$ and $\mathbf{H}$ are the electric and magnetic field distributions, respectively. The template becomes a generalized eigenvalue problem to compute the eigenvalues and eigenvectors. The resulting CMT formulation is used in Maxwell's equations to derive the CMT equations of a hybridized system. For simplicity, a two-dimensional model based on symmetric modes is explored. The generalized form of the improved coupled-mode equations, in that case, becomes [16]:

$$\frac{d}{dz} a(z) = i\gamma_a a(z) + ik_{ab} b(z) \quad (1.2a)$$

$$\frac{d}{dz} b(z) = ik_{ba} a(z) + i\gamma_b b(z) \quad (1.2b)$$

where the average field amplitudes of the two modes being coupled are a and b , and they are coupled by loss or gain coefficients, γ_a and γ_b . The coupling matrix-elements are found k_{ab} and k_{ba} [17]. A supermode forms when the difference between the propagation constants is zero.

Systems containing a higher dimension necessitate computational means to arrive at a solution. Numerical or analytical approaches are applied to solve for the CMT equations for a given device structure. For this reason, CMT is especially useful in providing an approximate electromagnetic understanding of the coupled modes near resonances. CMT is typically utilized in the design of sensors [18], optical couplers, gratings [19], resonators, switches, and filters [16].

Similar to the spatially varying CMT formalism, the temporal coupled mode theory (TCMT) transforms the CMT framework into the time or frequency domain to study perturbed resonator systems. TCMT is useful to characterize resonant systems with two or more ports. In this framework, a supermode forms when two or more optical cavities or resonant fields are resonantly coupled (i.e., the difference in resonant frequencies is zero). In this work, only non-magnetic materials are considered ($\mu_r = 1$). In the frequency domain, the primary Maxwell's equations assuming no charge or current are:

$$\nabla \times H - i\omega\epsilon_0\epsilon E = 0 \quad (1.3a)$$

$$-\nabla \times E - i\omega\mu_0 H = 0 \quad (1.3b)$$

where ω is the angular frequency, ϵ_0 is the vacuum permittivity, and ϵ is the relative permittivity, respectively. The Maxwell wave equation in the frequency domain becomes

$$\frac{1}{\epsilon(r)} \nabla \times (\nabla \times E(r, \omega)) = \left(\frac{\omega}{c}\right)^2 E(r, \omega) \quad (1.4a)$$

In the context of optical cavities such as microresonators (microring, microdisk), photonic crystal, or fiber, the localized resonances serve as the basis fields. Therefore, the linear superposition of any resonant field contribution is utilized in a modified version of coupled mode theory for the frequency domain. Optical cavities or curved interfaces have the field solutions of cylindrical or spherical coordinates. For curved interfaces, the electromagnetic field has the form:

$$\psi(r, \theta, z) = (E H)(r, z) \exp(-i\gamma R\theta) \quad (1.4b)$$

$$(E H)(r, \theta, z) = a(\theta)\psi(r, \theta, z) \quad (1.4c)$$

The bend radius and the angular propagation are r and γ , respectively. Propagation is along the r - z plane along the bend. Its contribution as an independent modal element is represented in Equation 1.4.c where a presents its average field amplitude. For an optical cavity, the electromagnetic field of an independent eigenmode is shown in Equation 1.4d and as a modal element in Equation 1.4e, where a represents the field amplitude.

$$\psi(r, \theta, z) = (E H)(r, \theta, z) \quad (1.4d)$$

$$(E H)(r, \theta, y) = a [\psi(r, \theta, y)] \quad (1.4e)$$

The field amplitudes are unknown in the coupled or hybrid system. To solve for the unknown coupling coefficients and amplitudes, the following procedure, hybrid CMT, is applied [15].

1.3 Degeneracy in Hybrid Mode Coupled Systems

By further inspection of (Equation 1.4a), we formulate the Maxwell wave equation as an eigenvalue problem. Considering a 2D geometry, the Maxwell wave equation exemplifies the Schrödinger relationship for a traveling particle in a region with constant potential due to mathematical equivalence. By comparison, propagating, antiparallel electromagnetic waves have equal magnitude, and the general solution can be written as a linear summation of their independent contributions. For the eigenvalue problem, the operator acts on the electric field on the left side of the equation and the eigenfrequency is associated with the quantity $(\omega/c)^2$.

In the coupled mode analysis, the linear differential equations of 1.5a and 1.5b can be rearranged into a matrix-based eigenvalue problem:

$$Ax = \lambda x \quad (1.5a)$$

$$\text{where } A = (i\gamma_a \quad ik_{ab} \quad ik_{ba} \quad i\gamma_b) \quad (1.5b)$$

The solutions of the equation, λ and x , are the eigenvalues and eigenvectors, respectively. The eigenvalues can be real or imaginary and distinct or repeated. Interesting phenomena can arise in a hybrid mode coupled system to permit tuning of a device's responsivity [20]. The behavior of the coupled system is studied by inspection of the characteristic equation. The spectral position and widths associated with the eigenfrequency of the hybrid resonance system can be predicted. Note that the eigenvalues of the hybrid system can be complex when considering non-Hermitian cases (i.e., an open system). The eigenvectors represent the modal or resonant field.

An open system is denoted by having complex eigenvalues. Open systems are ubiquitous and are often solved as closed systems to simplify the complexity of the problem. However, non-Hermitian systems epitomize all physical systems. Traditionally, systems containing parity-time (PT) symmetry have been subject to intensive investigation as an exemplary experimental analog case for a non-Hermitian system exhibiting loss-induced gain [21]. More recently, several studies have demonstrated that non-Hermiticity can be achieved in passive and plasmonic systems [22-25, 4].

Non-Hermitian systems are denoted by negative imaginary components of the diagonal elements of the matrix representing losses or positive imaginary components representing a gain in the system. In the context of spatially varying fields, the wave vector is complex for a system evolving in space (e.g., a directional coupler). For temporally varying fields, the eigenfrequency is complex when the system is evolving in time (e.g., resonators). The real part of the complex eigenvalue represents the energy of a state while the imaginary part corresponds to the width of the state or to the decay rate or quality factor [26]. Consider an arbitrary two-state resonantly coupled system that has two complex eigenfrequencies, E_1 and E_2 :

$$E_1 = W_1 - \frac{i}{2}\Upsilon_1, \quad E_2 = W_2 - \frac{i}{2}\Upsilon_2 \quad (1.6)$$

The entire system is represented by Hamiltonian, $\mathbf{H}$, which is composed of two open states within a common environment.

$$H^2 = \begin{bmatrix} E_1 & a \\ b & E_2 \end{bmatrix} \quad (1.7)$$

where a and b represent the matrix coupling elements. From inspection of the Hamiltonian, no coupling occurs when a and b are both zero. Fully asymmetric coupling occurs when a or b equals zero, but the other is non-zero. When a equals b , there is a symmetric coupling. Otherwise, partially asymmetric coupling takes place when $|a - b| > 0$. To gain a better understanding of the behavior of the non-Hermitian systems, we calculate the eigenvalues and eigenvectors.

$$(E_1 - \lambda)(E_2 - \lambda) - ab = 0 \quad (1.8a)$$

$$E_1E_2 - \lambda E_2 - \lambda E_1 + \lambda^2 - ab = 0 \quad (1.8b)$$

The characteristic equation is:

$$\lambda^2 + \lambda(-E_2 - E_1) - ab + E_1E_2 = 0 \quad (1.8c)$$

By using the quadratic formula, the eigenvalues become:

$$\frac{-(-E_1 - E_2) \pm \sqrt{(-E_2 - E_1)^2 - 4(-ab + E_1E_2)}}{2} \quad (1.8d)$$

After simplification, the eigenvalues become:

$$\frac{(E_1 + E_2) \pm \sqrt{(E_1 - E_2)^2 + 4ab}}{2} \quad (1.8e)$$

And corresponding eigenvectors are:

$$V_1 = \left[\frac{1}{2b} \left(E_1 - E_2 + \sqrt{(E_1 - E_2)^2 + 4ab} \right), 1 \right] \quad (1.8f)$$

$$V_2 = \left[\frac{1}{2b} \left(E_1 - E_2 - \sqrt{(E_1 - E_2)^2 + 4ab} \right), 1 \right] \quad (1.8g)$$

The system can be described by the following characteristics of the discriminant:

$$X = \frac{\sqrt{(E_1 - E_2)^2 + 4ab}}{2} \quad (1.9)$$

Let us now analyze some characteristics of the system as the matrix elements change. First, when the diagonal elements E_1 and E_2 are real and the off-diagonal elements form a conjugate pair $a^* = b$, then the system is Hermitian. Hermitian systems have very well understood properties according to the spectral theorem, e.g., the matrix is diagonalizable with a unitary matrix, the eigenvalues are real, the eigenvectors of distinct eigenvalues are orthogonal, and we can still construct an orthonormal basis of eigenvectors even when there are degenerate eigenvalues. In this case of degenerate eigenvalues and orthogonal eigenvectors of a Hermitian system, a diabolic point appears in the spectrum. Now let us consider the more general case in which the system may be Hermitian, or it may be non-Hermitian. Level repulsion occurs when the real part of the discriminant (X) is positive. In this case, the real parts of the two eigenvalues, which we recall describe the positions of the two energy levels, will have a larger difference. Similarly, because the width, decay rate, or quality factor of the state are related to the imaginary part, these properties will become more dissimilar when the imaginary part of the discriminant (X) is positive. We say that the system has an avoided level crossing when the two eigenvalues are not equal ($\lambda_1 \neq \lambda_2$) despite the unperturbed energies being equal ($E_1 = E_2$). As evident from Equations (1.8e) and (1.9), this occurs when $X \neq 0$. Exceptional points (EP) appear when $X = 0$ (i.e., $-(E_1 - E_2)^2 = 4ab$). If the diagonal elements (E_1 and E_2) are complex, then the system is non-Hermitian. In a non-Hermitian (non-conservative) system, the eigenvalues and eigenvectors coalesce ($\lambda_1 = \lambda_2$ and $V_1 = V_2$) at an exceptional point. Consequently, the dimensionality of the eigenspace collapses into a single eigenvector and eigenvalue. This collapse enables a new degree of freedom. The two degeneracies, i.e., diabolic and exceptional points, are spectral singularities that possess unique attributes that we may use to engineer the response of the system. In particular, the Reimann

surface of a diabolic point creates a double cone topology and an exceptional point exhibits a square-root branch topology. Of great interest is the counterintuitive behavior of a non-Hermitian system operating near or at an exceptional point in which a Berry phase shift allows the system to return to its initial state. By Berry phase shift, we mean the global phase evolution of a complex vector as it is carried around a loop in its vector space. Along the loop, the eigenvalues and eigenvectors interchange. Additionally, greater eigenvalue splitting is found in a non-Hermitian (square-root dependence) compared to a Hermitian system (linear dependence). In contrast to the diabolic point (eigenvectors do not coalesce when $X = 0$), the eigenvectors coalesce, and this coincides with the EP.

$$V_1 = \left[\frac{1}{2b} (E_1 - E_2 + 2X^0), 1 \right] \quad (1.10a)$$

$$V_2 = \left[\frac{1}{2b} (E_1 - E_2 - 2X^0), 1 \right] \quad (1.10b)$$

To further evaluate the spectrum, the phase rigidity of the wavefunctions is considered. It is the ratio between the bi-orthogonality defined as $(V_1, V_1) = \langle V_1, V_1^* \rangle$ and orthogonality defined by the conventional inner product $\langle V_1, V_1 \rangle$. At or near an EP, the phase rigidity approaches a minimum. The lifetimes of the system bifurcate near the EP, which coincides with a phase rigidity of 1. This bifurcation indicates that the eigenvectors are orthogonal.

To consider coupling three optical systems, we propose a symmetrical 3x3 matrix. Due to reciprocity, matrix elements $a_{12} = a_{21}$, $b_{13} = b_{31}$, and $c_{23} = c_{32}$. Therefore, the subscripts are dropped, and the matrix elements can be referred to as a , b , and c .

$$H^{[3]} = \begin{vmatrix} E_1 - \lambda & a & b \\ a & E_2 - \lambda & c \\ b & c & E_3 - \lambda \end{vmatrix} \quad (1.11)$$

The characteristic equation becomes:

$$\begin{aligned} \lambda^3 - \lambda^2(E_1 + E_2 + E_3) + \lambda(E_1E_2 + E_1E_3 + E_2E_3 - a^2 - b^2 - c^2) \\ + E_1c^2 + E_2b^2 + E_3a^2 - E_1E_2E_3 - 2abc = 0 \end{aligned} \quad (1.12)$$

From the characteristic equation, we observe that the behavior of a 3×3 matrix system can enable a higher-order exceptional point to be obtained. In particular, it is known that in a k dimensional space, the levels can only cross at a manifold of dimension $k-2$ [27]. An exceptional point will occur when at least two of the eigenvalues and corresponding eigenvectors coalesce. In the case that all three eigenpairs coalesce, the eigenspace will exhibit a cube root topology, whereas when only two of the three eigenpairs coalesce, the eigenspace will also include square root topologies. As the splitting of the eigenvalues increases, the n^{th} root will rapidly increase, thereby making the system extremely sensitive to perturbations.

The narrow parameter space window of an EP makes it often difficult to perform a precise measurement of the system due to fabrication error and tool-dependent material properties. Very few works have experimentally demonstrated an EP in a passive and/or plasmonic system. Hence, we propose a thorough investigation of the neighborhood of an EP in tandem.

1.4 Dissertation Overview

The responsivity of a device or sensor can be engineered to operate at a degeneracy where the system becomes more sensitive to a perturbation or has extended tunability. The advantages of this approach can enable unprecedented photonic and optical technologies. Furthermore, it can extend the toolbox for integrated photonics applications. Recent works have demonstrated that exceptional points can be engineered with the use of artificial photonic materials and structures [28]. This dissertation investigates several hypotheses regarding resonators and couplers and is organized as follows.

In Chapter 2, we address optoplasmonic sensors based on the multi-coupling of resonances of whispering gallery mode resonators, and we hypothesize that plasmonic nanostructures can be engineered to possess improved sensitivity and LOD compared to their individual counterparts by operating at a degeneracy in the hybrid system.

In Chapter 3, we address the addition of a high contrast overlay on a lower index grating coupler, and we show that the overlay can enhance the performance of grating couplers aimed towards integrated photonic applications. A method to further increase the coupling efficiency and directionality of the grating coupler design containing Fabry-Perot cavities is to operate at a degeneracy of the system via a non-Hermitian coupling. The Fabry-Perot cavities are defined by an in-plane reflector, bottom reflector, and reflector at the source. The loss mechanisms are tuned by their phase and cavity length. New devices with enhanced performance are presented in this dissertation. CMT and exploration of degenerate systems will provide a better understanding of the supermodel properties and constraints that enable specific device performance.

In Chapter 4, we summarize the key conclusions of the dissertation. We discuss the lessons learned and suggest paths for future research.

1.5 References

- [1] Yamada, Koji. "Silicon photonics as a post-Moore photonic circuit technology." *2016 Asia Communications and Photonics Conference (ACP)*. IEEE, 2016.
- [2] Bettotti, Paolo. "Hybrid materials for integrated photonics." *Advances in Optics* 2014(2014).
- [3] Benyoucef, M., et al. "Quality-factor enhancement of supermodes in coupled microdisks." *Optics Letters* 36.8 (2011): 1317-1319.
- [4] Miri, Mohammad-Ali, and Andrea Alù. "Exceptional points in optics and photonics." *Science* 363.6422 (2019): eaar7709.
- [5] Othman, Mohamed AK, and Filippo Capolino. "Theory of exceptional points of degeneracy in uniform coupled waveguides and balance of gain and loss." *IEEE Transactions on Antennas and Propagation* 65.10 (2017): 5289-5302.
- [6] Chelladurai, Daniel, et al. "Low-loss hybrid plasmonic coupler." *Optics Express* 27.8 (2019): 11862-11868.

- [7] Özdemir, Ş. K., et al. "Parity–time symmetry and exceptional points in photonics." *Nature Materials* (2019): 1.
- [8] Thraskias, Christos A., et al. "Survey of photonic and plasmonic interconnect technologies for intra-datacenter and high-performance computing communications." *IEEE Communications Surveys & Tutorials* 20.4 (2018): 2758-2783.
- [9] Vollmer, Frank, and Stephen Arnold. "Whispering-gallery-mode biosensing: label-free detection down to single molecules." *Nature Methods* 5.7 (2008): 591.
- [10] Luo, Ye, et al. "On-chip hybrid photonic–plasmonic light concentrator for nanofocusing in an integrated silicon photonics platform." *Nano Letters* 15.2 (2015): 849-856.
- [11] Li, Zhaoyi, et al. "Controlling propagation and coupling of waveguide modes using phase-gradient metasurfaces." *Nature Nanotechnology* 12.7 (2017): 675.
- [12] Pal, U. (2017). Silicon photonics: Designing and prototyping silicon waveguides. [online] COMSOL Multiphysics. Available at: <https://www.comsol.com/blogs/silicon-photonics-designing-and-prototyping-silicon-waveguides/> [Accessed 4 Nov. 2019].
- [13] Khilo, Anatol, et al. "Photonic ADC: Overcoming the bottleneck of electronic jitter." *Optics Express* 20.4 (2012): 4454-4469.
- [14] Wu, Qi, Jeremiah P. Turpin, and Douglas H. Werner. "Integrated photonic systems based on transformation optics enabled gradient index devices." *Light: Science & Applications* 1.11 (2012): e38.
- [15] Agrawal, Arti, et al., eds. *Recent Trends in Computational Photonics*. Cham: Springer, 2017.
- [16] Chuang, Shun Lien. *Physics of photonic devices*. John Wiley & Sons, 2012.
- [17] Chuang, Shun-Lien. "A coupled mode formulation by reciprocity and a variational principle." *Journal of Lightwave Technology* 5.1 (1987): 5-15.

- [18] Bellanca, Gaetano, Piero Orlandi, and Paolo Bassi. "Assessment of the orthogonal and non-orthogonal coupled-mode theory for parallel optical waveguide couplers." *JOSA A* 35.4 (2018): 577-585.
- [19] Kehl, Florian, et al. "Design of a label-free, distributed Bragg grating resonator based dielectric waveguide biosensor." *Photonics*. Vol. 2.1. Multidisciplinary Digital Publishing Institute, 2015.
- [20] Gao, Zihé, et al. "Non-Hermiticity and exceptional points in coherently coupled vertical cavity laser diode arrays." *Applied Physics Letters* 114.6 (2019): 061103.
- [21] El-Ganainy, Ramy, et al. "The dawn of non-Hermitian optics." *Communications Physics* 2.1 (2019): 37.
- [22] Huang, Yin, Georgios Veronis, and Changjun Min. "Unidirectional reflectionless propagation in plasmonic waveguide-cavity systems at exceptional points." *Optics Express* 23.23 (2015): 29882-29895.
- [23] Kodigala, Ashok, Thomas Lepetit, and Boubacar Kanté. "Exceptional points in three-dimensional plasmonic nanostructures." *Physical Review B* 94.20 (2016): 201103.
- [24] Alaeian, Hadiseh, and Jennifer A. Dionne. "Non-Hermitian nanophotonic and plasmonic waveguides." *Physical review B* 89.7 (2014): 075136.
- [25] Pile, David. "Nano-optics: Exceptional plasmonics." *Nature Photonics* 11.1 (2017): 24.
- [26] Eleuch, Hichem, and Ingrid Rotter, "Exceptional Points in open and PT symmetric systems." *arXiv preprint arXiv: 1311.6320* (2013).
- [27] Landau, L. D., and E. M. Lifshitz. *Quantum Mechanics: Non-Relativistic Theory*. Pergamon Press, 1981.
- [28] Midya, Bikashkali, Han Zhao, and Liang Feng. "Non-Hermitian photonics promises exceptional topology of light." *Nature Communications* 9.1 (2018): 2674.

Chapter 2: Optoplasmonic Biosensors for the Detection of Human Performance Biomarkers

2.1 Narrative of the Problem

With the increasing dependence and integration of technologies into our daily lives and the advent of the information age, humans are bombarded with inordinate amounts of information daily. A report conducted by Basex found that "94% of [employees] felt overwhelmed by information to the point of powerlessness" [1]. Beyond the typical workplace setting, cognitive overload can compromise mission-critical operations such as air safety, military operations, spaceflight, and surgery. For example, during a drone attack in 2010, 23 Afghan civilians were killed due to the operator's inability to effectively assess information simultaneously received from instant messages, radio exchanges, and video feeds. It was cited that the cause was information overload [2]. Research suggests that the maximum capacity of humans to process information is 120 bits per second [3] which falls between the data transmission rates of the telegraph and the first telephone during the mid-1800s [4]. As a comparison, the internet operates at a speed of 11.5 Mbits/s [5].

Recent studies have shown that information overload can adversely affect cognitive ability and processing by altering the production of human performance biomarkers. Human performance biomarkers are measurable biologics such as proteins and hormones that indicate cognitive state and associated biochemical or immunological changes affecting the entire body [6, 7]. The extended onset of a stressor may lead to impaired cognition and chronic health issues, such as digestive problems, heart disease, and autoimmune disorders.

Cortisol, "the stress hormone", is a commonly used biomarker that screens for symptoms (e.g., fatigue, palpitations, muscle tension, etc.) and downstream side effects. Its concentration levels vary diurnally with the lowest levels occurring at night. Cortisol and other biomarkers can be detected in sweat, interstitial fluid, blood, saliva, hair and urine. In clinical settings, blood samples are commonly used in which the concentration range is between 2 $\mu\text{g/ml}$ and 25 $\mu\text{g/dL}$ [7, 8].

A definitive diagnosis of cognitive overload is challenging because the underlying stressors are not well correlated with symptoms. An enzyme-linked immunosorbent assay, known as ELISA, is a gold standard for protein concentration determination at picomolar concentrations and is used during diagnostic testing. Despite its wide adoption in a clinical setting, it is a tedious process that requires multiple steps, a trained specialist, along with costly and large sample volumes. Its size and processing do not permit miniaturization for at-home diagnostics [7, 8]. While several at-home stress kits that enable cortisol detection exist, they require that samples be sent to a laboratory for results that could take weeks to obtain [8, 9]. Moreover, determining the correlation between certain stressors and associated symptoms for each individual requires continuous monitoring of performance. To overcome this limitation, there has been an increased effort towards developing point-of-care (POC) devices based on label-free methods with high sensitivity, lower detection limits that enable a larger dynamic range, and rapid turn-around on results. Enhanced optical biosensors are a promising alternative for measuring the cognitive levels given their small footprint, portability, and high sensitivity.

There is an emerging class of optoplasmonic biosensors based on whispering gallery mode (WGM) resonators coupled to plasmonic nanostructures for enhanced detection sensitivity by orders of magnitude [9]. Microring resonators, a type of whispering gallery mode resonator, are suitable for this application due to their planar geometry that allows the exploration of a variety of complex plasmonic structures to further boost detection sensitivity. It is envisioned that coupling complex nanostructures to microring resonators could yield unprecedented sensitivity. An overview of the generation of surface plasmons and basics of microring resonators is now presented.

2.2 Background and Theory

Microring resonators are circular waveguides that confine light due to total internal reflection. They are of great interest for biosensing due to their small footprint and label-free detection scheme. In addition, they are simple to fabricate with high reproducibility using commercially available lithography and processing tools. In addition to these advantages, they are also relatively inexpensive to produce and easily integrated with microfluidics. Microring resonators are utilized

as a refractive index sensor for their high sensitivity [10].

For critical coupling, optical power is fed into a straight waveguide that is placed at an optimal distance from the microring. Resonance within the microring occurs when the following condition is met:

$$m\lambda = 2\pi r n_{eff} \quad (2.1)$$

where m is the azimuthal integer of multiple path lengths, λ is the operating wavelength, and n_{eff} is the effective mode index. There are only certain wavelengths of light that will propagate in the microring due to constructive interference, leading to resonance modes. Once resonance is achieved, the light will circumnavigate along the periphery of the microring with an optical path length equal to the integer multiple of the wavelength ($m\lambda$). The optical path length is defined as the product of the circumference and the effective mode index. The coupling of light from the microring resonator into the bus waveguide is represented by:

$$\begin{bmatrix} b_1 \\ b_2 \end{bmatrix} = \begin{bmatrix} t & i\kappa \\ i\kappa^* & t^* \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} \quad (2.2)$$

where a and b are the normalized amplitudes of the field, κ is the coupling coefficient, and t is defined as the transmission coefficient. The matrix is symmetric and reciprocal under lossless coupling, which gives the subsequent relationship:

$$1 = |t|^2 + |\kappa|^2 \quad (2.3)$$

The phase delay, θ , is from propagation around the microring, $2\pi n_{eff}L/\lambda$. The resulting amplitude is $a_2 = ab_2 e^{i\theta}$, where a is the loss coefficient. Solving the matrix expression (2.2) computes the power transmission, which is defined as:

$$T = \left| \frac{b_1}{a_1} \right|^2 = \frac{|t|^2 + a^2 - 2a|t|\cos(\theta - \theta_t)}{1 + |at|^2 - 2a|t|\cos(\theta - \theta_t)} \quad (2.4)$$

The coupling introduces a phase, θ_t , where $t = |t|\exp(i\theta_t)$. At critical coupling, $a = |t|$ [11]. Experimentally, the transmission is typically measured using either a spectrometer or a tunable laser where the dips in the spectra correspond to a resonance at which the transmission drops to its minimum. The optical mode is predominantly confined within the cavity, which limits the extent of the decay length and the strength of the evanescent field. The decay length corresponds to the lateral distance in which the strength drops to $1/e$ of its value of the evanescent tail [10].

A microring resonator with a single mode will have a theoretical quality factor, Q , defined as:

$$Q = 2\pi \frac{\text{energy storage of cavity}}{\text{energy lost per round trip}} \cong \frac{\omega}{\delta\omega} \quad (2.5)$$

The quality factor is a key figure of merit to determine how efficiently a resonator stores energy within its cavity. A higher quality factor indicates a better signal-to-noise ratio for sensing. Experimental quality factors tend to be lower than the computed theoretical values due to fabrication imperfections such as surface roughness. Surface roughness will scatter light from the cavity, thereby reducing its energy storage.

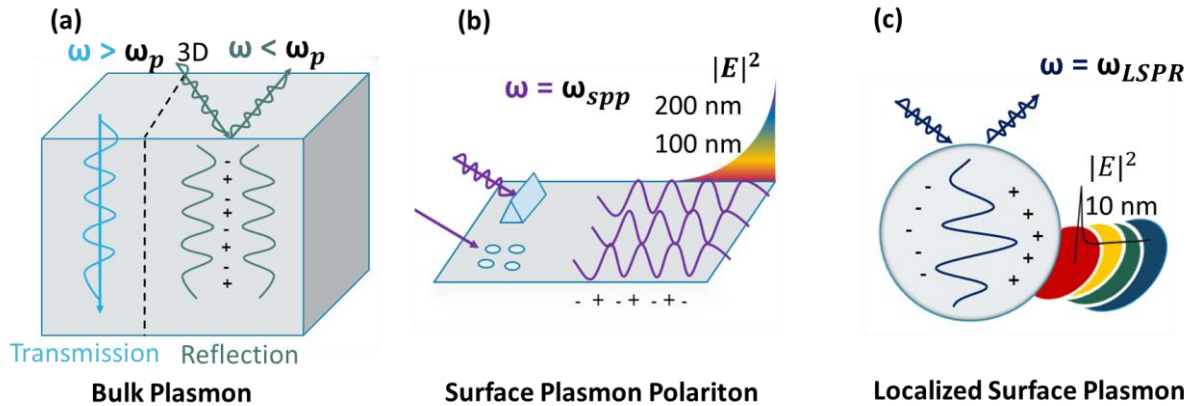


Figure 2.1. Adapted from [12]. Schematic of (a) bulk plasmon, (b) surface plasmon polariton, and (c) localized surface plasmon.

The free electrons in a metal can be described by the Drude model, which assumes that electrons behave as a free-electron gas. The Drude model is commonly used in the study of surface plasmons to relate the electron oscillations to the dielectric function of a metal. The effective electron mass

takes into consideration electron-electron interactions. When an external electric field (E) is applied to a metal, an electron is displaced by x , and its motion is governed by the equation of motion: $m\ddot{x} + m\dot{x} = qE$. The elementary charge is q and the damping term is represented by γ . Under the assumption that the electric field is a time-harmonic and taking the Fourier transform, the solution becomes $x(t) = qE/[m(\omega^2 + i\gamma\omega)]$. The frequency is represented as ω . This displacement is captured in the polarization, P , where $P(\omega) = -qx(\omega)N$. The number of electrons in each volume is represented by N . The polarization and electric flux density are related by the dielectric function: $D(\omega) = \epsilon(\omega)E(\omega) = \epsilon_0(\omega)E(\omega) + P(\omega)$. The dielectric function reduces to $\epsilon(\omega) = 1 - \omega_p^2/(\omega^2 + i\gamma\omega)$. The plasma frequency, ω_p , is then determined by the relationship, $\omega_p^2 = Nq^2/(\epsilon_0 m)$ [24], which corresponds to the bulk plasma frequency. For a bulk plasmon, light propagates through a volume when the eigenfrequency exceeds the plasma frequency. When the eigenfrequency is below the plasma frequency, light is reflected at the metal and dielectric boundary. A plasma polariton is a coupled state between a photon and a plasmon. In the case of the surface plasma polariton (SPP), light propagates along the metal dielectric interface when the eigenfrequency is between 0 and $\omega_p/\sqrt{2}$ when $|\epsilon|=-1$. Propagating electromagnetic waveguides couple to the non-radiative surface plasmons. For longitudinal surface propagation, the wave vector must be equal at the metal and dielectric boundary and excited by a p-polarized wave. Given this condition, an SPP cannot be excited on a planar surface in free space because the wave vector of free space is always lower than the surface plasmon frequency. Hence, several strategies have been employed to efficiently generate SPPs: Kretschmann configuration, scanning near-field optical microscopy (SNOM), and a grating. The surface plasmon resonance is satisfied when there are matching boundary conditions at the interface. The resulting dispersion relationship is:

$$\beta_{sp} = \frac{\omega}{c} \sqrt{\frac{\epsilon_d \epsilon_m}{\epsilon_d + \epsilon_m}} \quad (2.6)$$

where ϵ_d is the permittivity of the dielectric material, ϵ_m is the permittivity of the metal and β_{sp} is the propagation constant of the surface plasmon polariton. For comparison, the localized surface plasmon resonance (LSPR) is governed by the dipole resonance condition. If the size of the nanostructure is smaller than the incident wavelength, electrostatics is assumed based on the quasistatic approximation. Accordingly, charge accumulates at the surface of the nanostructure.

This produces a restoring force with resonance frequency, ω . Hence, the polarizability has a dominant effect on the localized surface plasmon resonance. This resonance is dependent on the material properties and geometry of the nanostructure. The excitations of the different surface plasmon resonances are depicted in Fig. 2.1. Figure 2.2 shows the added benefit of combining both, plasmonic and photonic waveguides to increase the field strength at the surface while maintaining a high Q. An arbitrary lossy metal material, an enhancement layer, is placed on top of a bare waveguide to demonstrate hybrid coupling using COMSOL software. The thickness of the enhancement layer is varied to find the optimal thickness for increased electric field at the surface. It is evident from the electric field profiles that the intensity shifts from the core-bottom cladding boundary to the core-enhancement layer interface. The electric field strength increased by 33% at 70 nm thickness.

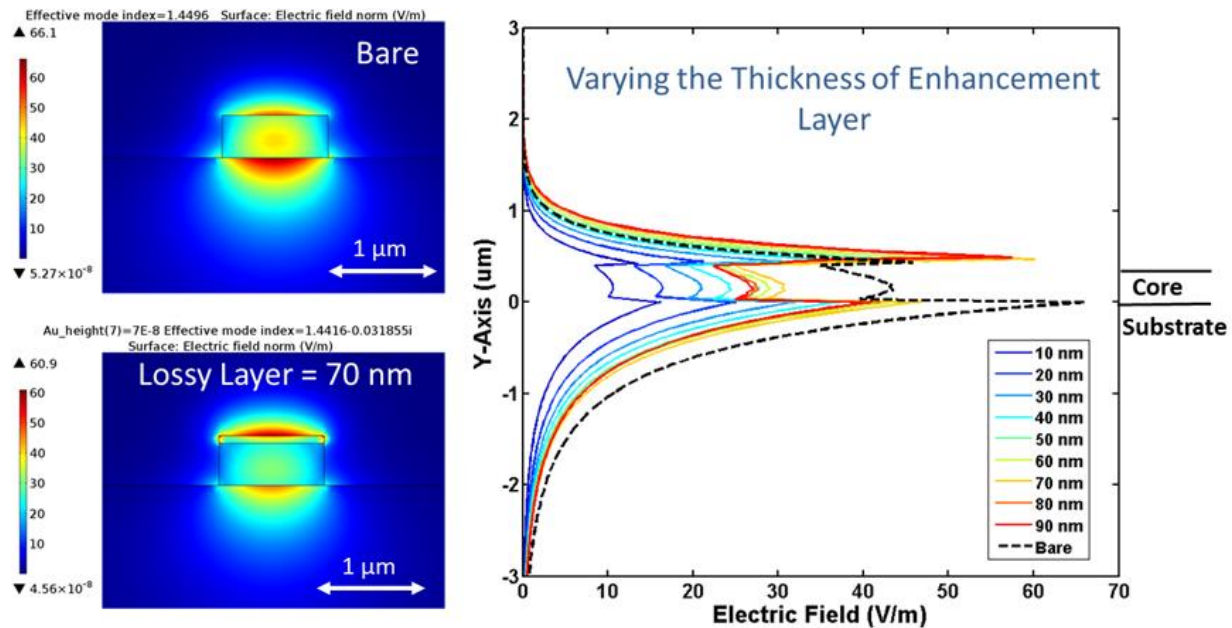


Figure 2.2 Plasmonic-photonic coupling scheme from [13] using a 2D waveguide computational via case study using Finite Element Method. A dielectric waveguide will have a single propagating mode in the core when the core has the highest refractive index compared to the upper and lower cladding (upper left). The surface plasmon mode forms at the dielectric-metal interface (bottom left). When the evanescent wave couples, a hybrid mode forms (right).

There are two key components of a biosensor: (1) a transducer element and (2) a biorecognition element. The transducer element generates optical or electrical feedback. The biorecognition element is entrapped, adsorbed, or covalently bonded to the surface within the biosensing region

[14]. There are typically two types of sensing methods: bulk and surface sensing. Bulk sensing involves detecting a refractive index shift in a superstrate or an aqueous environment; however, this method does not account for specificity. Initially, a surface refractive index change occurs, and the analyte alters the effective index of the propagating mode. Typically, this causes the resonance wavelength to red shift.

Evanescent field strength dictates the detection sensitivity and the ability to resolve the signal from a frequency shift from a nearby binding event. The detection limit of a microring has been experimentally determined to be 1.5 pg/mm² [10]. This is equivalent to roughly 500 bound IgG antibodies over a surface area of 66 μm² [10]. Mathematically, the relationship between a binding event and the shift in resonant wavelength can be shown using the reactive sensing principle below [15]:

$$\frac{\Delta\omega_r}{\omega_r} = \frac{\Delta\lambda_r}{\lambda_r} = \frac{|W_p|}{W_c} \cong - \frac{\alpha_{ex} |E_0(r_v)|^2}{2 \int \epsilon_0 |E_0(r_v)|^2 dV} \quad (2.7)$$

where $\Delta\omega_r$ is the shift in the resonant angular frequency, ω_r is the resonant angular frequency of the binding event, $\Delta\lambda_r$ is the shift in the resonant wavelength due to a binding event, λ_r is the resonant wavelength, W_p is the minimum energy needed to polarize the analyte (tends to be negative), W_c is the energy within the cavity, α_{ex} is the excess polarizability of the analyte, ϵ_0 is the permittivity of the cavity, and $|E_0(r_v)|^2$ is the amplitude of the electric field at the binding site. The corresponding denominator is the total electric amplitude throughout the cavity. A considerable frequency shift occurs when the analyte overlaps the evanescent field.

There are substantial efforts underway to engineer enhanced microring resonator and other microresonator biosensor platforms to substantially boost the sensitivity and specificity. Several amplification alternatives to the method proposed herein involve secondary detection probes. Furthermore, researchers have demonstrated sub-picogram per milliliter detection levels by co-immobilizing enzymes for signal amplification [10]. Despite the increase in sensitivity and specificity, there is a need for ultrasensitive, label-free detection of biomarkers with concentrations as low as the femtomolar range in complex media to pinpoint the early onset of cognitive overload

and associated adverse effects. This requirement was set forth by our funding agency, the Air Force Research Laboratory, for measurement of biomarkers in sweat and saliva for neurotransmitters. Another method involving the use of secondary reagents creates a different issue: the process changes the native structure of the analyte, which could alter its conformation required for binding, yielding false-negative outcomes [10].

To remedy the aforementioned limitations, one can deposit metal layers or nanostructures onto the sensor's surface to produce a surface electromagnetic wave that enhances the evanescent field strength to better resolve a wavelength shift. Hence, surface electromagnetic waves are very sensitive to the local environment, which makes them ideal for biosensing and potentially unprecedented detection sensitivity. Ideal enhancement layers or nanostructures should be composed of metals with the ability to generate surface plasmons at the metal-dielectric interface. SPPs form at the interface between the dielectric material, which has a positive dielectric constant, and the metal, which has a negative dielectric constant. In addition, note that the magnitude of the metal permittivity is greater than that of the dielectric. Increased light-matter interactions occur at the interface due to the coupling of the electromagnetic and electron oscillations [16].

Because the decay lengths of metals are often significantly less than those of dielectrics, the surface plasmon mode does not extend deeper into the metal thin film, thereby leading to the energy that is tightly confined at the interface. Subsequently, a larger fraction of the field will appear in the dielectric at subwavelength distances, creating an evanescent field. The evanescent field that extends into the superstrate is the sensing region. The propagating mode of the microring couples to the metal thin film, and surface charge density oscillations are generated. The characteristics of these oscillations vary with wavelength and are determined by the Drude model [12]. Optimization of geometry along with careful material selection is required to obtain conditions in which maximal enhancement and confinement of the evanescent field are achieved with minimal absorption loss due to the inherent nature of metals.

2.3 Microring Coupled Plasmonic Slot Waveguide Biomarker Sensor

Real-time quantitation and interrogation of biomolecules in their native state are of paramount importance for medical, pharmaceutical, defense, and environmental applications. The ability to continuously monitor the presence of ultra-low concentrations of these molecules in solution allows us to quickly probe key dynamic biological processes underpinning various disease etiologies such as neurological disorders, cancer, and cardiovascular disease. The main challenge in the label-free optical detection of biomolecules is that their relatively low molecular mass and sub-wavelength size do not generate a considerable change in the permittivity of the ambient environment. To circumvent this limitation, there has been a devoted effort towards the development of a new class of hybrid plasmonic–photonic biosensors based on whispering gallery mode (WGM) microresonators coupled to plasmonic resonant systems for enhanced detection sensitivity by orders of magnitude [17-21]. This synergistic coupling combines the notable advantages of highly localized fields at the metal interface with the resonant nature of high-quality factor (Q) low-loss microcavities. At resonance, the microcavity collectively excites an arrangement of plasmonic resonators that generates a surface plasmon at the metal-dielectric interface for increased nanoscale light-analyte interaction, albeit, it is intrinsically constrained by the free conduction electrons to sustain resonance. To further enhance detection sensitivity, several strategies have been exploited to increase the near-field electric strength because it largely dictates the sensitivity by coupling to multiple resonant structures [22]. Primarily, the plasmonic nanostructures are arranged in a dimer configuration [23], utilizing asymmetric patterns [24], and material properties are engineered to construct metal-insulator-metal (MIM)/insulator-metal-insulator (IMI) structures [25]. Additionally, the optical near-field can be further enhanced by extending the dielectric spacer thickness that elevates the plasmonic nanostructures [26]. Hence, the optical response can be tuned by tailoring the geometrical and material properties. The attractiveness of this hybrid resonant coupling approach is the ability to produce a significant measurable change per binding event well above the noise threshold of the optical microcavity. Typically, the bulk sensitivity for hybrid devices is around 700 nm/RIU with a limit of detection of 5.0×10^{-5} RIU and a theoretical quality factor of 3.0×10^3 [21]. In previous work, a microring coupled plasmonic slot waveguide biosensor offered a bulk sensitivity of 584 nm/RIU and a wavelength shift of 77 fm due to a single protein binding event [27]. In this work, we further

investigate the underlying coupling mechanisms that enhance the sensitivity by exploring the design space and we explore the detection of even smaller analytes.

Among the various innovative hybridized plasmonic-photonic approaches being investigated for increased surface electric near-field enhancement, planar cavity architectures constructed by coupling multiple planar resonant structures are ideal for practical realization. Microring resonators (MRRs) create a suitable whispering gallery mode platform for this approach because of their high-quality factor, scalability, and integrated planar architecture that is amenable to conjoining complex planar plasmonic nanostructures. A recent study has shown that patterning gold nanodisks periodically on top of a microring to couple the waveguide mode into the plasmonic nanostructures increases the bulk sensitivity to 176 nm/RIU by utilizing localized surface plasmon resonance (LSPR) resulting in a two-fold increase compared to a bare microring [28]. A separate study revealed that placing a silver nanorod on top of a microring resonator produced a bulk sensitivity of 497 nm/RIU by exploiting propagating surface plasmons [29]. For plasmonic design considerations, subwavelength slots show great promise for generating an enhanced electric near-field because of their increased confinement and exemplary electric field redistribution [30]. Of particular interest are plasmonic slot waveguides with transverse magnetic (TM) polarization that generate highly spatially confined fields at their surfaces through the excitation of surface polaritons, which are beneficial for biosensing applications. When a plasmonic slot waveguide forms a circular resonator, it can guide surface plasmons. It becomes easy to launch azimuthal surface plasmon polaritons (SPPs) at the interfaces that then behave as whispering gallery modes [20]. Recent works have shown that these engineered metallic rings can lead to maintaining surface polaritons [31, 32].

For proteins, the refractive index is estimated based on amino chemistry [33]. However, little is known for small molecules (<4-5 nm, mostly 1 nm) and they are therefore measured using dynamic light scattering (DLS) or nuclear magnetic resonance spectroscopy (NMR) [34, 35]. Both electrical and optoplasmonic plasmonic sensors have achieved single ion level detection [17]. To compare device performance, the selectivity, limit of detection (LOD), signal-to-noise (SNR), and repeatability are the common figures of merit. The electrical sensor's performance degrades in the presence of sub-optimal pH and salinity. For this reason, it is an active area of investigation to improve its biocompatibility. On the other hand, optical sensors are limited by their form factor

and lack of flexibility, prompting active investigations to determine alternative materials for conformability. In comparison, optical sensors can quantify size and mass of molecules whereas electrical (FETs) sensors cannot [36].

As shown in Fig. 2.3, we propose a coupled hybrid plasmonic slot waveguide/microring resonator sensing platform. The integrated sensor is composed of two gold concentric rings that are elevated by a silicon dioxide spacer layer atop a silicon nitride microring resonator on a silicon substrate. The microring dimensions are 1 μm wide, 400 nm thick, and 30 μm in radius. Gold is selected as an ideal plasmonic material given its biocompatibility, stability, and well-known surface functionality schemes [37]. The width of each gold ring is 80 nm and the interspacing between them is 20 nm. The thicknesses of the gold layer and of the silicon dioxide spacer layer will be varied to study their influence on the coupling between the plasmonic-like mode and photonic-like mode of the hybrid structure. The concentric gold rings are adhered to the silicon dioxide spacer layer using a 5 nm thick titanium adhesion layer. The effects of this metal adhesion layer are considered in this study because of their potential influence on the plasmonic enhancement. The superstrate is water. A 3 μm thick silicon dioxide layer forms the bottom cladding.

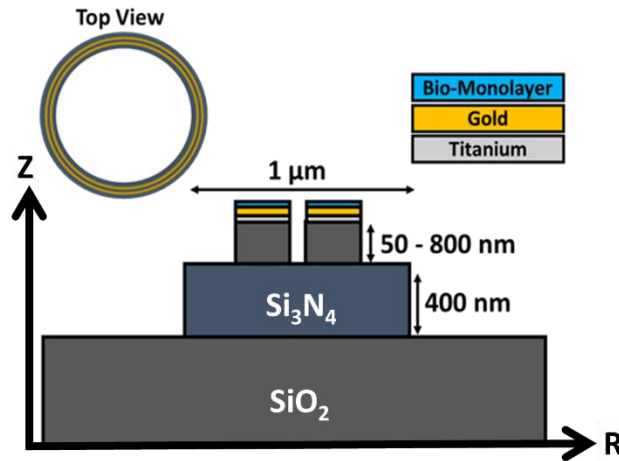


Figure 2.3. Cross-sectional diagram of the proposed hybrid plasmonic microring resonator for biosensing. Propagation is in the azimuthal direction. The cross section is the (R, Z) plane of the cylindrical coordinate system.

The resonant properties of the hybrid plasmonic-photonic sensor were studied using the finite element method model in COMSOL Multiphysics software. A mesh refinement study was

performed on the smallest dimension of the device, the adhesion layer. The parameter mesh checker indicates how many divisions there are across the thickness of the layer. As shown in Fig. 2.4., the frequency remains relatively constant as the number of divisions is increased.

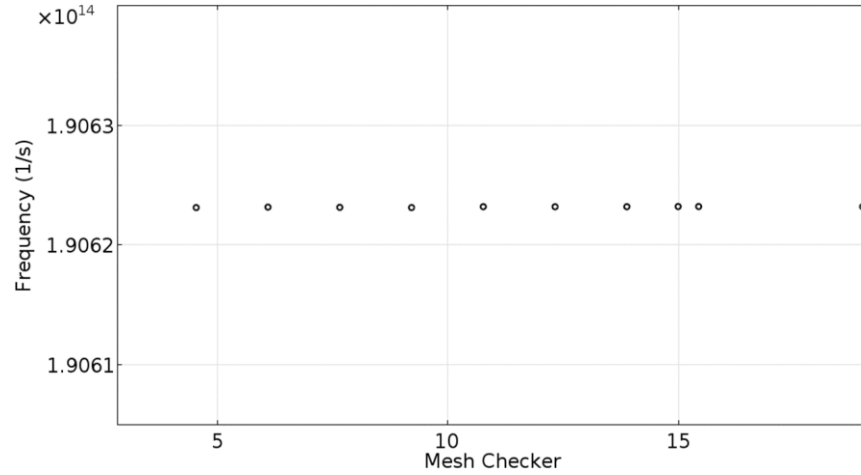


Figure 2.4. Mesh refinement study on the adhesion layer of the device.

The dielectric spacer thickness and gold thickness were optimized to pinpoint highly cooperative coupled resonant systems. Table 2.1 lists the refractive indices taken at 1550 nm.

Table 2.1. Refractive indices of the materials of the biosensor.

Features	Material	Refractive Indices		Ref.
		N	K	
Bottom Cladding	SiO ₂	1.428	0.00	38
Core	Si ₃ N ₄	1.977	0.00	38
Concentric Rings	Au	0.5241	10.742	39
Superstrate	H ₂ O	1.3180	9.9×10 ⁻⁵	40
Adhesion Layer	Ti	3.6845	4.6088	39

Rotational symmetry enables us to reduce the simulation to a 2D axisymmetric model. For a resonance around 1550 nm, the azimuthal order, m , was calculated to be 191 for the specified device geometry. A parametric study was performed to determine a suitable device geometry while optimizing the trade-offs between sensitivity and intrinsic detection limits. The spacer thickness

was varied from 50 nm to 800 nm. The gold thickness was varied from 40 nm to 100 nm. To provide generalized results, the change in refractive index was varied from 0.1 to 0.2. The sensitivity along the top gold surface was examined by placing a monolayer of biomolecules on the concentric rings' gold surface. This bio-monolayer thickness was kept at 10 nm. To truncate the simulation domain without introducing artifacts, perfectly matched layers PMLs were placed on the top, bottom, and outer radius with a width of 1.55 μm . In this simulation, the boundary conditions were set as perfect electric conductor (PEC) along the outer boundaries. The figures of merit for performance are the sensitivity ($S_{molecule}$) and intrinsic limit of detection ($iLOD_{molecule}$) adapted from [41]:

$$S_{molecule} = \frac{\Delta\lambda_{res}}{\Delta n_{biolayer}} * \frac{V_{molecule}}{V_{biolayer}} \quad (2.8)$$

$$iLOD_{molecule} = FWHM \frac{1}{S} = \frac{\lambda_{res}}{Q} \frac{1}{S} \quad (2.9)$$

where V is the volume, λ is the wavelength, $\Delta n_{biolayer}$ is the relative refractive index of the biomolecule compared to the water ambient, and FWHM is the full-width at half-maximum of the resonance. The device sensitivity (S) is defined as the change in the resonant wavelength ($\Delta\lambda_{res}$) per change in the refractive index of the ambient. This change in refractive index of the ambient can be approximated by ($\Delta n_{biolayer} V_{biolayer}/V_{molecule}$). The intrinsic limit of detection (iLOD) is the smallest quantity of biomaterial to produce a measurable change in the optical response. To accurately measure a spectral shift, the size of the shift needs to be large compared to the FWHM of the resonance. A value of 0.1% to 1% of the FWHM is typically assumed adequate to maintain sufficient signal-to-noise ratio [21]. Thus, iLOD is computed by dividing the FWHM by the sensitivity. There is a trade-off between achieving a high surface electric field enhancement due to plasmonic effects and maintaining a large quality factor that governs the overall performance of the optoplasmonic biosensor. To further boost the sensitivity of a hybrid plasmonic-photonic sensor, the dielectric spacer thickness can be elevated [42]. Inherently, our symmetric metal slot waveguide rings form a dimer-like configuration due to their concentric nature, which can significantly increase the detection sensitivity when compared to a single ring or plasmonic

element. Previous studies in this area have shown that the field strength of dimer type nanostructures increases as the inter-particle gap width decreases, following the "plasmon ruler" method [43].

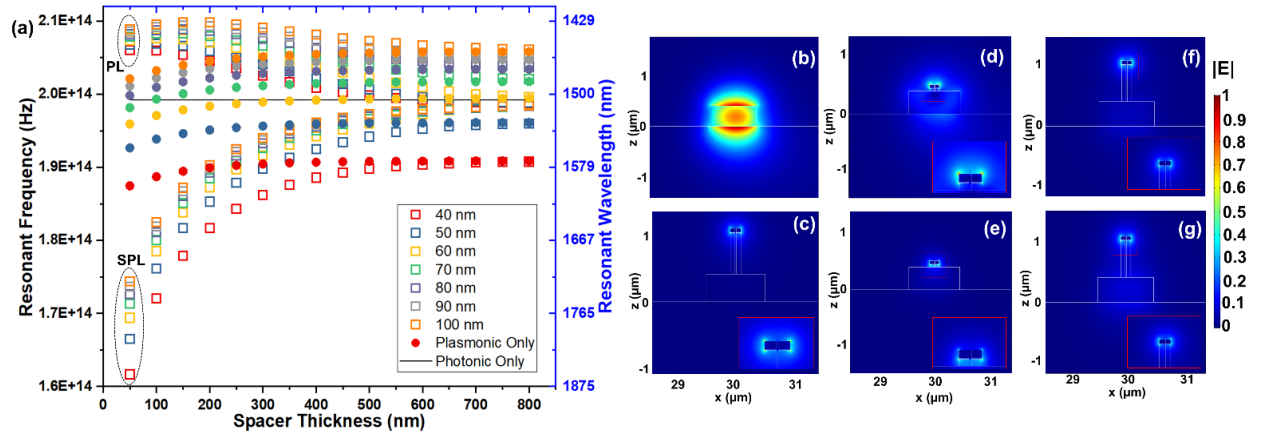


Figure 2.5. (a) The resonant frequencies as a function of dielectric spacer thickness for several gold thicknesses. SPL represents the surface plasmon-like and PL represents photonic-like mode. The electric field profiles of (b) bare waveguide with quasi-TM polarization, (c) pure plasmonic structure with $t_{\text{au}} = 60$ nm and $t_s = 600$ nm, (d,e) quasi-TM dominated and plasmonic dominated structures with $t_{\text{au}} = 60$ nm and $t_s = 50$ nm, and (f,g) hybrid-like structure with $t_{\text{au}} = 60$ nm and $t_s = 600$ nm.

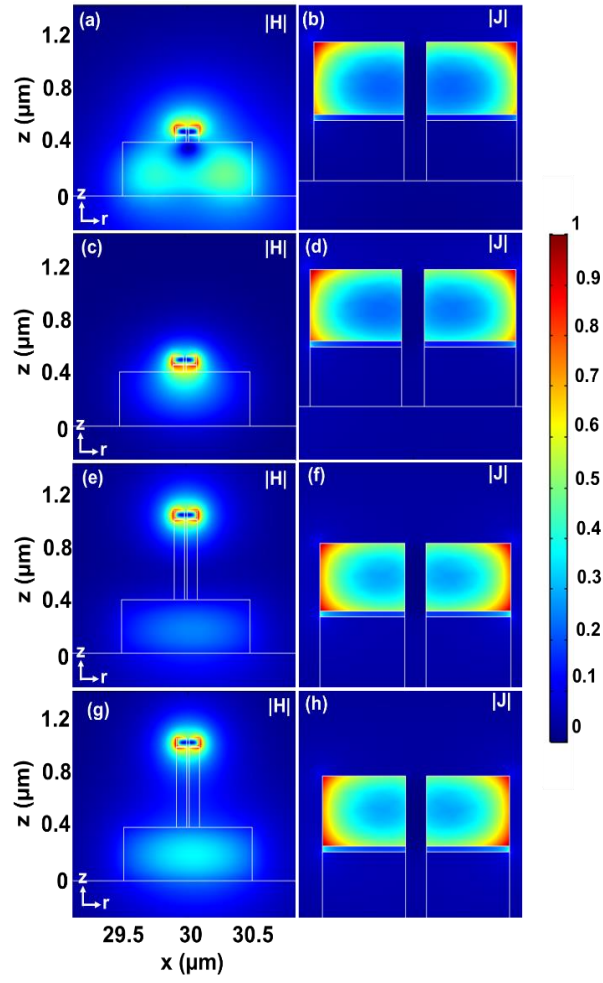


Figure 2.6. Magnetic field profiles and current density. (a, b) Quasi-TM dominated structure with $t_s = 50$ nm and $t_{au} = 60$ nm. (c, d) Plasmonic dominated structure with $t_s = 50$ nm and $t_{au} = 60$ nm. (e-h) Hybrid-like structure with $t_s = 600$ nm and $t_{au} = 60$ nm.

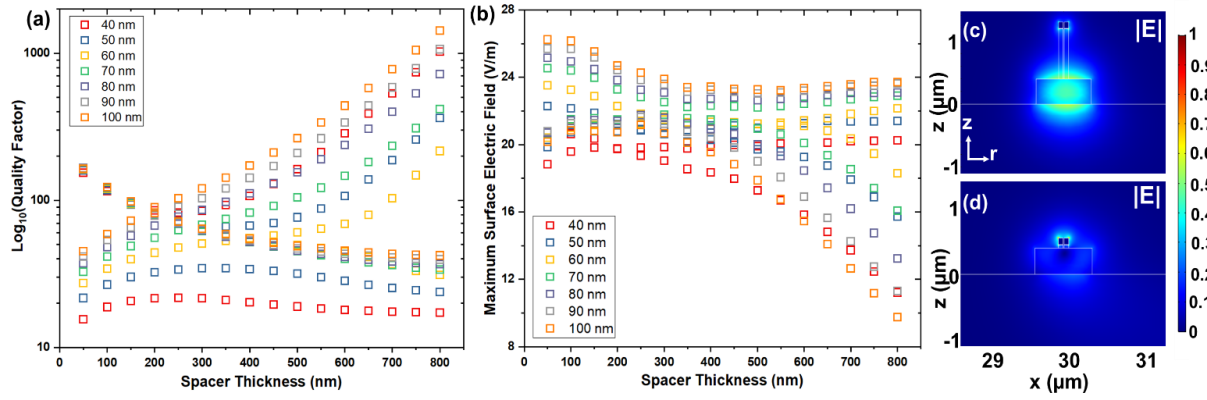


Figure 2.7. (a) Quality factor and (b) maximum surface electric field as a function of dielectric spacer thickness for several gold thicknesses. The normalized electric field profiles for (c) maximum quality factor and (d) maximum surface field.

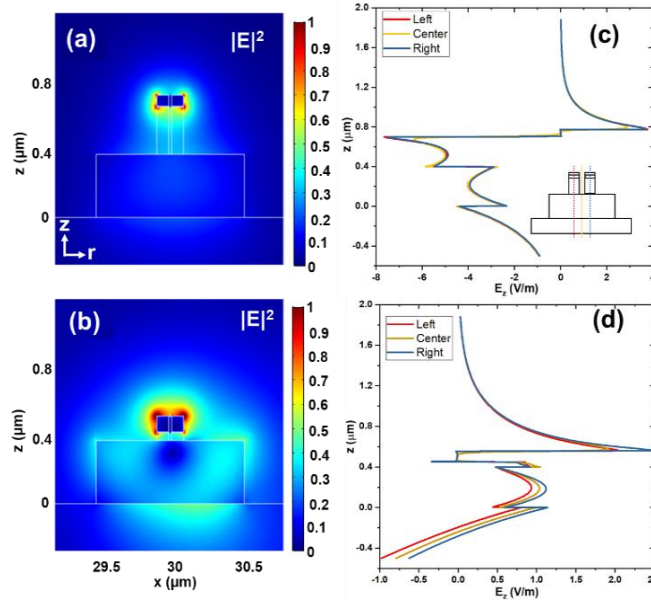


Figure 2.8. (a) H_{TM0} The hybrid design with $t_{\text{au}} = 70$ nm and $t_s = 300$ nm yielded maximum electric field intensity in z near the bottom corners of the gold. (b) H_{TM1} . The hybrid design with $t_{\text{au}} = 100$ nm and $t_s = 50$ nm.

To identify a resonant hybrid biosensor platform, we first consider the case without the bio-monolayer and screen for hybridized super modes of an optoplasmonic device. Figure 2.5 (a) depicts the resonant frequency of the hybridized plasmonic-like and hybridized quasi-TM guided (photonic-like) profiles as a function of spacer thickness for several gold thicknesses. The filled circles represent the resonance frequencies of a solitary plasmonic system with a spacer layer. As a result of the superposition of the pure photonic and plasmonic mode, there are two hybridized modes that exhibit most of the power flow residing within (1) the proximity of the metal region for the plasmonic-like mode or (2) the core for the photonic-like mode. The black line corresponds to the bare photonic mode for the bare microring without the gold rings atop. In comparison, the resonant frequencies of the plasmonic-like mode increase with increasing spacer thickness until they reach a horizontal asymptote. For thick spacer layers, the plasmonic-like mode exhibits very little coupling to the dielectric waveguide. With increasing gold thickness, there is a decrease in the resonant frequencies. For the photonic-like mode, as the dielectric spacer layer increases, the resonant frequency red shifts and approaches the resonance of a bare microring. As the gold thickness increases, the resonant frequencies decrease. The two regimes of plasmonic-like and photonic-like frequencies merge as the oxide spacer layer thickness increases. Interestingly, where the lines intersect with the plasmonic and photonic-like modes, hybridized super modes emerge from near resonantly coupled systems, H_{TM0} and H_{TM1} . For comparison, a pure quasi-TM polarized waveguide appears in Fig. 2.5 (b). In Fig. 2.5 (c), a solitary plasmonic system contains hotspots located mostly at the top outermost corners. The corner modes are coupled. In Fig. 2.5 (d-g), the electric field of the same structure at different frequencies indicates on-resonance coupling of the TM mode to the plasmonic mode and nearly plasmonic resonant structure with only the bottom corner modes excited, respectively. Although the hybrid mode of Fig. 2.5 (c) is not phase matched, there is evanescent coupling between the quasi-TM mode and the local surface plasmon resonances (LSPR). The LSPR coupling is independent of incident polarization; however, SPR requires phase matching with TM polarization. At the three-way intersection of the bare waveguide mode, the solitary plasmonic system ($t_{\text{au}} = 60$ nm), and the hybrid system ($t_{\text{au}} = 60$ nm and $t_s = 600$ nm), the electric fields of these modes (H_{TM0} , H_{TM1}) become nearly indistinguishable. In the latter case, the quasi-TM mode is coupled to the plasmonic system containing all four corner modes excited. The spatial superposition of the electric fields of the solitary plasmonic and bare photonic modes gives rise to the hybrid devices shown in Fig. 2.5 (c, d, f, g). Hence, as the spacer thickness increases

near the intersection of their resonant frequencies, the H_{TM0} concentrates optical energy around the metal structure while the H_{TM1} concentrates more energy within the waveguide. The near field coupling recycles optical energy from the plasmonic structure into the cavity. In the case of Fig. 2.5 (e), the H_{TM0} behaves as a localized mode as the spacer thickness decreases at lower frequencies. The lack of field enhancement within the gap can be explained by the dipole-dipole charge distribution caused by surface charges that are excited along the direction perpendicular to the axis of the slot waveguide. When the SiO_2 spacer increases in thickness, the photonic mode does not excite the plasmonic mode; consequently, the resonant frequency approaches that of a conventional dielectric mode. Given the two types of supermodes, there are two excitation approaches for measurement by free space excitation of H_{TM0} and coupling light from waveguide to plasmonic system for H_{TM1} [44, 45]. The enlarged field profiles of the gap region, shown in the insets, reveal a dipolar resonance that is characteristic of TM-polarized plasmonic slot waveguides.

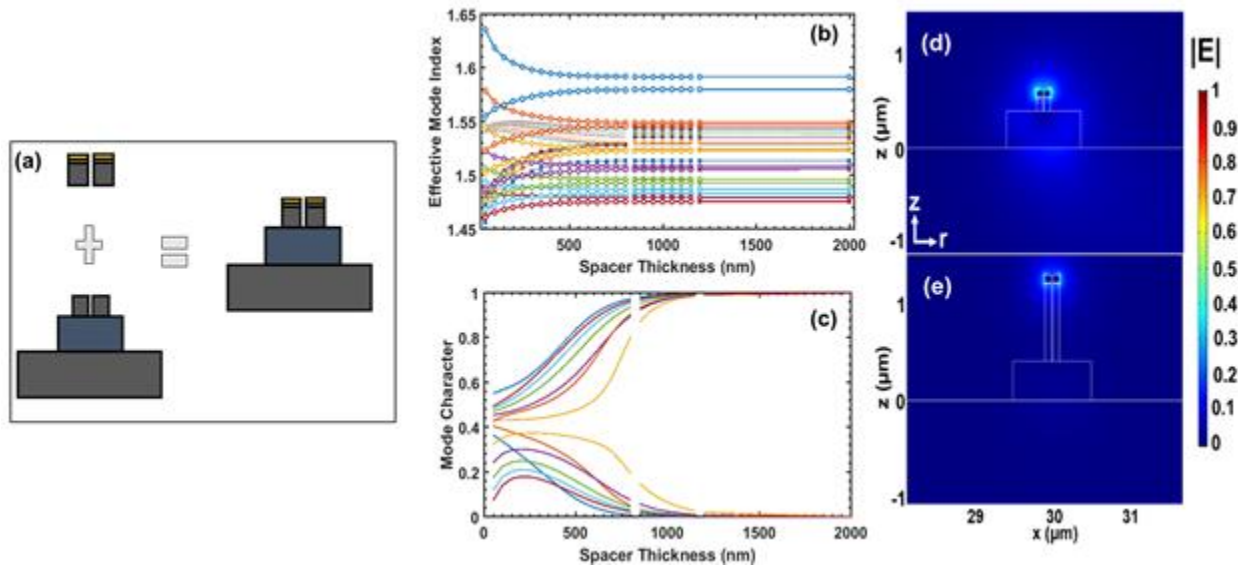


Figure 2.9. (a) Hybridization of two modes, (b) effective mode index and (c) mode character. The electric field profile of the structure with (d) 50% mode character and (e) maximum mode character.

In Fig. 2.8, the maximum surface enhancement for the plasmonic-like mode occurs at $t_s = 300$ nm and $t_{\text{au}} = 70$ nm. At $t_{\text{au}} = 40$ and 50 nm, the maximum surface electric field remains approximately the same for all spacer thicknesses. The increase in intensity arises from an increase in scattering

at the surface due to the direction of light polarization. The maximum surface electric field for the photonic-like mode occurs at 50 nm spacer thickness and gold thickness of 100 nm. The coupling distance is small, which increases the transfer of the evanescent field into a thick gold layer with a large surface area for increased interaction. The quality factor for both hybridized mode profiles increases continuously with increasing spacer thickness. The quality factor of the plasmonic guiding mode increases as the gold layer becomes thicker reaching a maximum near 1400 at a spacer thickness of 800 nm and a gold thickness of 100 nm, which is characteristic of thicker films' reduced ability to sustaining SPR, thereby reducing optical loss. These quality factors are higher than those of conventional SPR devices, because of the presence of a spacer, which permits optimal phase matching to tune the SPR excitation and analyte interaction. The decrease of the quality factor can be attributed to the increase in radiative and non-radiative losses associated with metal within proximity of higher refractive material. In the case of the photonic-like modes, the quality factor of the devices with gold films of 40 and 50 nm rises substantially while the quality factor slightly decreases for thicker films. The increase in quality factor indicates better limit of detection as a hybrid optical biosensor. To improve the spectral linewidth, we must identify a design with a small linewidth that increases the measurable index change, which influences the limit of detection, a key figure of merit.

The field profile of the magnetic field and current density of four designs (as in Fig. 2.3) are displayed in Fig. 2.6. It is evident that there is magnetic coupling with increased current density along with the top corners of each gold film when the spacer thickness is 50 nm. The area of magnetic field minimum appears as a void distorting the photonic mode and shifting the current density to the topside of the gold film. Analogous to the aforementioned device, there is a strong localized magnetic field around the gold structures with similar current density when the spacer thickness is 50 nm. When the spacer thickness is extended to 600 nm, the magnetic field of the H_{TM1} mode contains higher field confinement in the waveguide region than the H_{TM0} mode; however, the current density of H_{TM0} is slightly greater than the H_{TM1} mode. The field profile of Fig. 2.6 (e) does not appear to contain coupling, but is double resonant.

To gain insights into the coupling scheme, we plot the modal profile of the electric field and the vertical cross-sectional profile along the plasmonic slot waveguide and the waveguide core in Fig. 2.7. The presence of the thin metal film introduces a significant effect on the electric field

distribution and localization of the guided mode when the dielectric spacer is thin by redistributing the power flow. It is worth noting that the electric field is nearly homogeneous across the topside of the gold film, indicating that local sensitivity is uniform per binding event along the top surface.

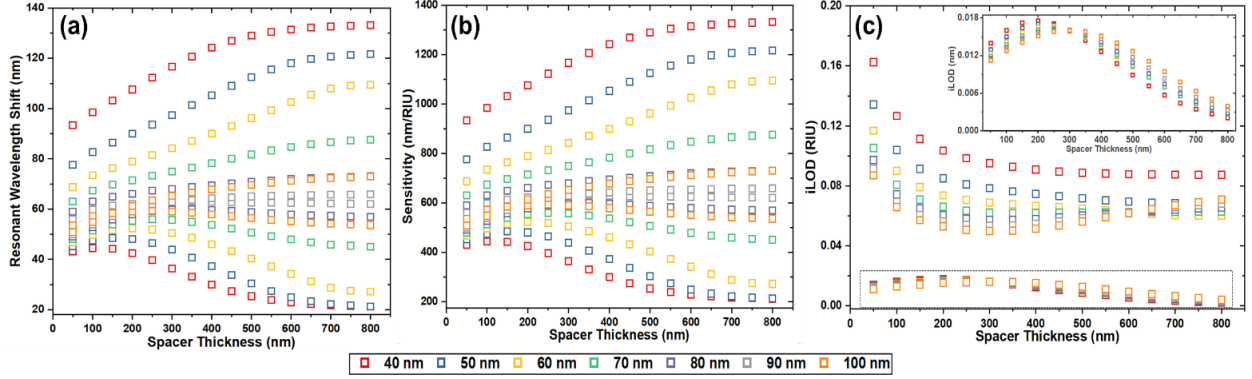


Figure 2.10. (a) Resonant wavelength shift, (b) bulk sensitivity, and (c) iLOD as function of spacer thickness for various gold thicknesses.

We then investigate the strength of the coupling between the plasmonic and photonic modes using coupled mode theory. The hybridized mode (ψ_{HPPS}) is a superposition of a quasi-TM polarized waveguide (ψ_{PL}) without the plasmonic nanostructure and surface plasmon resonance of the nanostructure (ψ_{SPL}) without the dielectric waveguide mode:

$$\psi_{HPPS} = a\psi_{PL} + b\psi_{SPL} \quad (2.10)$$

where a and b are the amplitudes of the hybridized modes, photonic-like (PL) and surface plasmon-like (SPL), respectively, and $|a|^2 + |b|^2 = 1$. The mode character, i.e., the degree of hybridization, is computed using the following relationship [46]:

$$|a|^2 = \frac{n_{HPPS} - n_{SPL}}{(n_{HPPS} - n_{PL}) + (n_{HPPS} - n_{SPL})} \quad (2.11)$$

The coupled mode amplitude ($|a|^2$) is a measure of mode character. If it is greater than 0.5, the mode is called photonic-like. Otherwise, it is called plasmonic-like. At $|a|^2 = 0.5$, the strongest hybridization occurs because the hybridized mode contains equal contributions of the photonic

and plasmonic modes representing mode-matching. To compute the effective mode index of each contribution, we utilized the COMSOL mode analysis module. We first computed the resonant frequencies using the eigenfrequency module in COMSOL. Next, we used the mode analysis module to extract the corresponding effective mode indices of the pure plasmonic mode, pure photonic mode and the plasmonic/photonic driven hybridized modes at their corresponding resonant frequencies. Figure 2.9 (a) displays the independent modes to be hybridized. The effective mode index and the mode character are shown in Fig. 2.9 (b, c). The effective mode of the plasmonic-driven hybridized modes decreases as the spacer thickness increases as a result of less modal overlap with the waveguide. Conversely, the effective mode index of the photonic driven hybridized modes increases as the spacer thickness increases because the modal overlap is reduced. At the maximum mode character, most of the field is concentrated around the plasmonic structure. The maximum surface electric field for either hybridized mode, H_{TM0} and H_{TM1} , has a mode character around 0.6 at gold thickness of 50 nm and 70 nm, respectively. The maximum quality factor occurs when the spacer thickness is the greatest $t_s = 800$ nm with $t_{au} = 100$ nm and 40 nm, respectively. Interestingly, the mode character being around 0.5 is the same for PL and SPL hybridized modes at $t_s = 50$ nm and $t_{au} = 70$ nm. Their electric modal field profiles are shown in Fig. 2.9 (d, e).

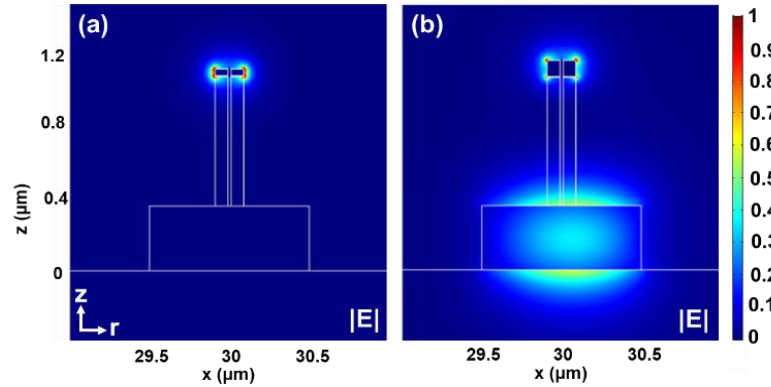


Figure 2.11. Electric field profile of the designs with (a) maximum sensitivity and (b) the coupled mode.

To determine which optoplasmonic design provides the best bulk sensitivity, we simulated the refractive index change of 0.1 RIU of the surrounding environment from water. For the H_{TM0} mode, the resonant shift per binding increases as the spacer thickness increases, and as the gold thickness

decreases. The optoplasmonic device with $t_s = 800$ nm and $t_{au} = 40$ nm produces the greatest resonant wavelength shift of 134 nm. Hence, it produces the greatest sensitivity of 1340 nm/RIU with an intrinsic limit of detection (iLOD) of about 0.1 RIU in Fig. 2.10. In the case of the H_{TM1} , the resonant binding shift increases with increasing gold thickness. The greatest resonance shift and sensitivity are about 73 nm and 730 nm/RIU with an iLOD of 0.004 RIU. This exceeds the sensitivity of bare microcavity based sensors, which typically have a sensitivity range of 50 to 200 nm/RIU [21]. The corresponding electric field distributions shown in Fig. 2.11 (a, b) reveal little to no coupling for the H_{TM0} . They also show mode-matching for the resonantly coupled photonic-like hybridized modes. Applying the LOD relationship of [21], the minimum LODs are 1.0×10^{-3} RIU and 4.0×10^{-5} RIU, respectively. The minimum LOD is calculated by multiplying the iLOD by 0.1.

Because of their low mass or size, it is difficult to transduce a discernible shift in the refractive index of typical biomarkers. In addition, the refractive index values of biomarkers span a wide range. The reported values are often in terms of bulk refractive index for a given concentration. Therefore, we varied the refractive index change of the 10 nm monolayer on the topside of the gold surface. There is a negative shift in the resonance shift per binding event, which can be ascribed to anomalous dispersion dominating and its interplay with the dipolar resonance of the plasmonic system [46]. We observe the greatest sensitivity when $t_s = 700$ nm and the $t_{au} = 60$ nm. We found that this does not coincide with the maximum surface electric field, which is commonly used as an indicator of sensitivity for SPR sensors. Additionally, it does not possess the greatest coupling based on its mode character close to 1. The greatest spectrum shift of 21 fm was observed when the refractive index change was 0.1 RIU, and nearly half that shift was at a refractive index change of 0.1 RIU. At a refractive index change of 0.2, the sensitivity was 105 fm/RIU in Fig 2.12. These sensitivities are comparable to the high-Q microsphere and microtoroid based sensors for single particle and molecule detection [21]. The volumetric size of the molecule is 1.0×10^3 nm³. The advantage of the optoplasmonic sensor is evident in the spatial electric and magnetic field profiles of the hybridized modes with the greatest sensitivity in Fig. 2.13.

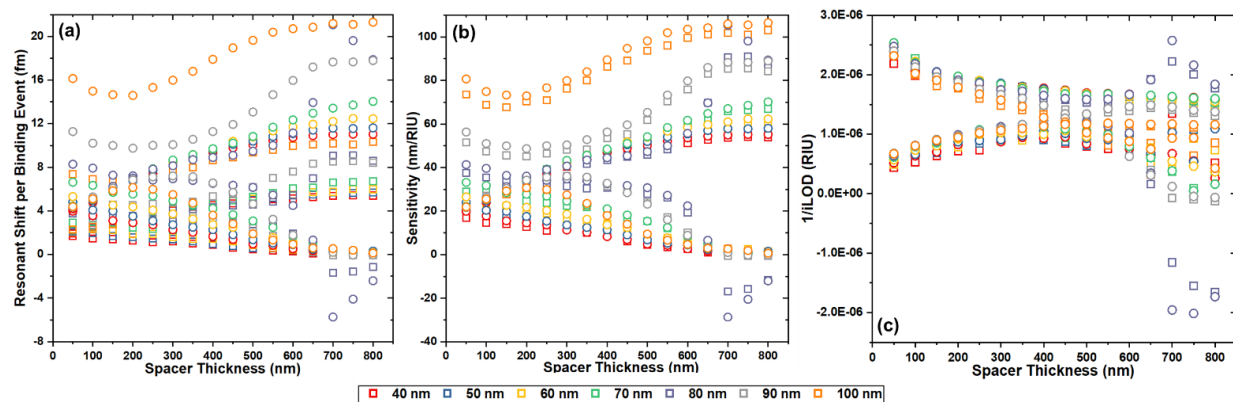


Figure 2.12. (a) Resonant wavelength shift per binding event, (b) sensitivity, and (c) the inverse of the iLOD.

For a biolayer of 10 nm, the maximum volume for a molecule is 0.39 nm. This size allows for a minimum of 76.8 million biomolecules. A bio-monolayer of 10 nm was placed along all sides of the gold structure. Fine meshing was applied with four tetrahedral elements along the thinnest direction. The total number of particles of the monolayer is dependent on the gold surface area as shown in Table 2.2.

Table 2.2. Number of Biomolecules per Biolayer Volume

Biolayer Thickness of 10 nm		
Gold Thickness (nm)	Volume of Biolayer (10^8 nm^3)	Number of Biomolecules (millions)
40	6.79	1.728
50	7.54	1.920
60	8.29	2.112
70	9.05	2.304
80	9.80	2.496
90	10.56	2.688
100	11.31	2.880

In summary, we have investigated the sensitivity and detection limit of a proposed biosensor design for the detection of biomolecules as a function of dielectric spacer thickness for various gold thicknesses. With this exemplary design, we can resolve changes in the refractive index of the bulk medium and single binding event at the corresponding sensitivities: 1340 nm/RIU and 105.3 fm/RIU for $\Delta n_{\text{biolayer}} = 0.2$.

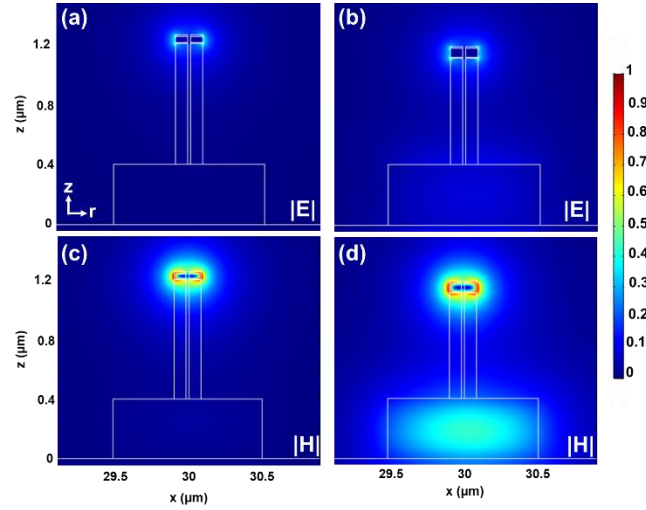


Figure 2.13. Electric field profile of the designs with maximum sensitivity of coupled modes (a) H_{TMO} and (b) H_{TM1} . The magnetic field profile of the designs with (c) maximum sensitivity and (d) maximum quality factor.

Table 2.3. Comparison of hybrid plasmonic-photonic device sensing qualities.

Sensor	Bulk Sensitivity (nm/RIU)	FOM (RIU ⁻¹)	Ref.
Plasmonic slot waveguide coupled MRR	1340	1000	This work
Gold Nanodisks periodically coupled to MRR	176	N/A	[28]
SOI racetrack-shaped ring resonators	70	900	[47]
Metal coated toroid microcavity	500	700	[48]
Double-slot silver hybrid racetrack MRR	687.5	133.24	[49]
Typical Hybrid sensors	700	20,000	[21]
Silver nanorod coupled MRR	497	N/A	[29]
Plasmon-Enhanced Colorimetric ELISA	100	N/A	[50]
SiON microring array	112	625000	[51]

ELISA testing is a fluorescence ensemble measurement that examines changes in intensity versus resonant wavelength shift. Conventional fluorescence measurements cannot resolve single-molecule detection. Hence, recent works have combined ELISA with plasmonic [50], paramagnetic beads [52], and nanofluidic [53] platforms to boost sensitivity and achieve single-molecule detection. Table 2.3 compares the optical sensors with enhanced ELISA methods. Our device has a relatively high bulk sensitivity and it is 13x more sensitive than the plasmon-enhanced colorimetric ELISA.

In practice, the rings are coupled to a bus waveguide which couples to the MRR. We assume that the coupling bus waveguide has a negligible coupling to the top gold concentric rings. As light propagates around the rings, energy is exchanged at every node. In the coupled system, the gold concentric rings will have a different intrinsic loss than that of the silicon nitride waveguide. Thus, the coupling between the vertically stacked rings can be analyzed as a circular directional coupler. For this reason, the transfer matrix can be applied to describe the evolution of the coupled mode at an interaction region at each node.

An ideal device will have a high Q-factor by alleviating radiative and non-radiative losses by optimizing device design and fabrication procedures. In [33], the authors demonstrated numerically, experimentally, and analytically that surface roughness on an optical microdisk resonator generates counterpropagating modes that can couple to form supermodes. The supermodes arise from the reactive and dissipative coupling. Their experimental data revealed that unbalanced doublets were better described by non-Hermitian physics. For simplicity, we assume for our hybrid sensor that the accumulative interaction effect can be approximated by average loss mechanism such as the surface roughness. Due to the intrinsic loss of gold concentric rings and bending loss in the MRR, the coupled optical cavity is an analog of an open quantum system. Therefore, the system can contain exceptional points where the eigenfrequencies and the eigenvectors coalesce. This is evident by the field profiles of the eigenvectors becoming indistinguishable when the resonant frequencies are identical. To better understand the phenomena, the problem is reformulated as a scattering matrix problem and the behavior of the system further examined for degeneracies.

The transfer matrix formalism is described by:

$$\begin{bmatrix} b_1 \\ b_2 \end{bmatrix} = \begin{bmatrix} t & k \\ -k^* & t^* \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} \quad (2.12)$$

The transfer matrix can be rewritten in couple mode expressions:

$$\frac{d\Lambda}{dt} = -iH\Lambda - \sqrt{\gamma}\mathbf{a}_n \quad (2.13)$$

$$H = \begin{bmatrix} \omega_o - \frac{1}{2}(\gamma_1) & k_{12} \\ k_{21} & \omega_o - \frac{1}{2}\gamma_2 \end{bmatrix}, \quad \Lambda = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} \quad (2.14)$$

The exceptional points occur when:

$$(\gamma_1 + \gamma_2) = 8k_{12}k_{21} \quad (2.15)$$

Intense computational simulations were performed to identify the region where exceptional points lie by finding regions where the resonant frequencies and quality factors are matched. In the resonant frequency space (computed from the real part of the eigenvalue space), the region of exceptional points begins at gold thickness of 57.02 nm and different resonant frequencies approach zero as the spacer thickness decreases as shown in Fig. 2.13 (a) and (b). The difference of the quality factor (computed from the imaginary part of the eigenvalue) is shown in Fig. 2.13 (c). The encircled regions are where the exceptional points lie, where the difference of the quality factors approaches zero; this is further observed in Fig. 2.13 (d) where the difference in quality factors approaches zero as the spacer thickness decreases. A key property of an exceptional point is that the real and imaginary components of the eigenvalues diverges from the exceptional point. This is evident in Fig. 2.14 as the resonant frequency difference and the quality factor diverge. It is indicative of operating near exceptional points. The proposed sensor provides high sensitivity due to its operation near an exceptional point. Although, the sensitivity of the device is remarkably high, it is difficult to fabricate under the constraint of 0.01 nm for accuracy and precision.

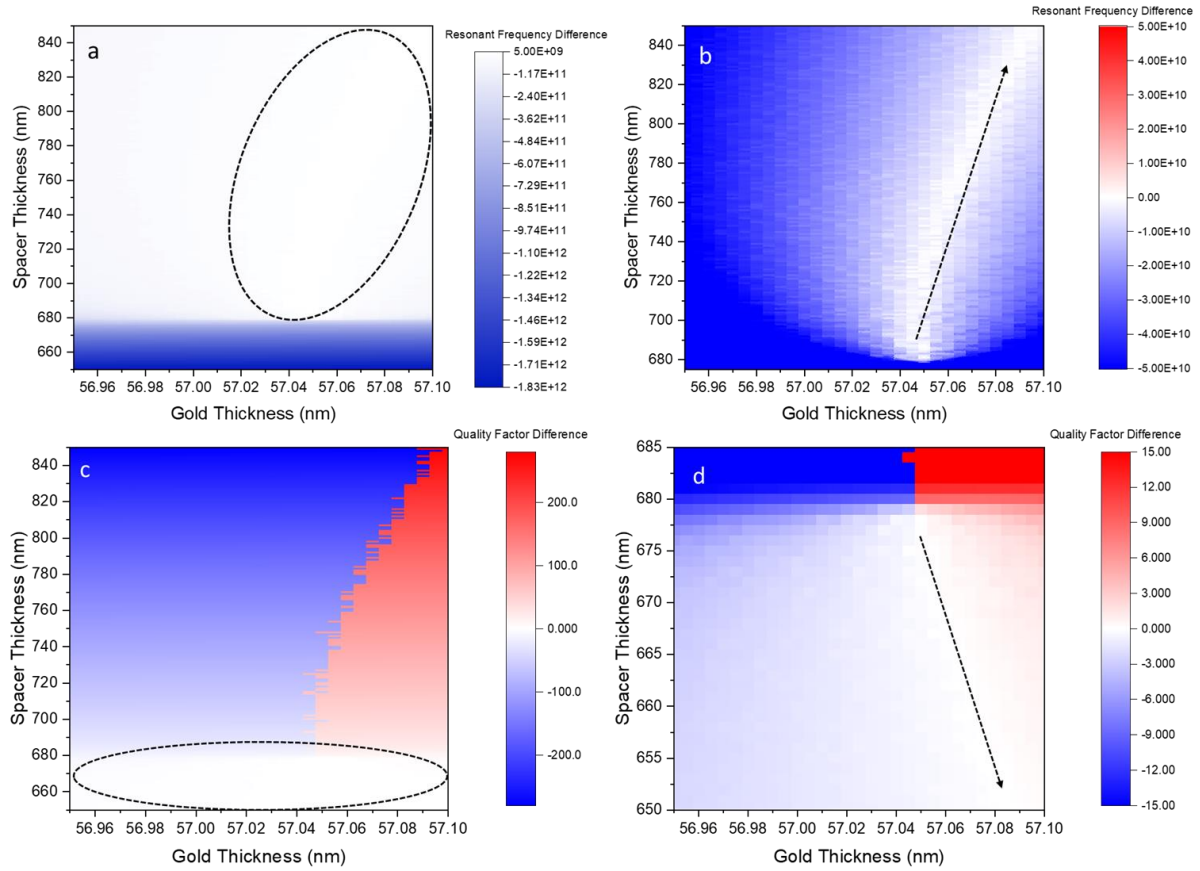


Figure 2.14. The difference in resonance frequencies of the photonic-like and plasmonic-like sensors (a) and zoomed in region encircled in (a) where exceptional points lie in (b). The difference in quality factors in (c) and zoomed in region encircled in (c) shown in (d).

2.4 Plasmonic Bowtie Nano-Antenna Coupled Microring Biosensor

The sensitivity of conventional whispering gallery mode-based sensors is limited by their high confinement factor restricting the amount of optical energy available in the evanescent field, thereby limiting light-matter interactions to quantitatively detect small molecules [54]. To overcome this limitation, high-quality-factor WGM microcavity ($\sim 10^{10}$) biosensors are employed to achieve high spectral resolution; however, these biosensors increase the footprint of the device and pose a challenge to resolving the signal given the thermal noise floor [55]. Concomitantly, plasmonic based sensing platforms have pushed the limits of sensitivity towards single molecule detection due to their high subwavelength field confinement within the evanescent field, but suffer from low quality factors due to their inherent metal losses. Optoplasmonic based approaches, a

hybrid of SPR and WGMs, have emerged to overcome the aforementioned limitations by combining their notable merits of high-quality factor and subwavelength field confinement. Of interest are localized surface plasmons (LSP), given their ability to further increase field enhancement, which suits them well for small molecule detection. To obtain the best sensing performance requires judicious inspection of highly cooperative plasmonic-photonic coupling [56-58]. Several works have demonstrated the powerful utility of the incorporation of metal nanoparticles onto WGM to boost sensitivity by orders of magnitude [59-66]. However, most LSPR based optoplasmonic devices include the addition of a single nanoparticle to WGM microcavity. Such approaches limit the number of detection opportunities (i.e. binding sites) of a single molecule. Present work in optoplasmonic sensing seeks to increase the detection opportunities by increasing the number of nanoparticles attached to the WGM [54, 56, 58].

An ongoing challenge lies in the fabrication of these optoplasmonic devices to secure robust measurements by utilizing top-down and bottom-up fabrication approaches that (1) permit repeatability at the cost of increasing fabrication complexity and (2) reduce fabrication complexity without sacrificing repeatability from device-to-device. Alternatively, much effort is devoted to the development of optoplasmonic sensors that meet or exceed the performance of conventional biosensors while exploring the incorporation of nanoparticles in a controlled fashion. Urbonas et al. demonstrated a refractive index sensor that consisted of a microring resonator patterned with a second order Bragg grating arrangement of gold nanodisks. In this work, they were able to obtain a sensitivity of 176 nm/RIU compared to a bare ring (70 nm/RIU) with quality factor of 300. Despite the sensitivity being lower than most optoplasmonic devices, impressively, the free spectral range is unlimited which indicates large spectral shifts are resolvable. This is achieved by engineering the dispersion to suppress unwanted resonances [65, 67]. Furthermore, several strategies have been employed to boost the sensitivity by using a dielectric spacer layer [68], dimer configuration [69], and metal-insulator-metal assembly [70].

Towards this aim, we plan to demonstrate how extending the principle of the 2nd order Bragg grating patterning of a circular array of plasmonic bowtie antennas in a DBR-dimer configuration atop a microring resonator can boost sensitivity (Fig. 2.15). The overall goal underpinning our proposed design: an array of gold bowtie nanoantennas to localize the field in the gap of the bowtie

pair and couple this plasmon resonance to the WGM resonance to magnify the effect of a binding event. We select the thickness, width, and separation of bowties and the thickness of the spacer layer to balance the tradeoff between increased sensitivity and lower Q. In this work, Dr. Xin Yu developed the fabrication recipe and fabricated the device. The thickness and size of bowtie nanostructures were extracted from the plasmonic slot-waveguide coupled microring resonator study. Several rounds of fabrication were completed by Dr. Xin Yu. Unfortunately, the fabrication process suffered from electron beam lithography proximity effect and layer-to-layer alignment issues. For these reasons, repeatability was difficult to achieve for key features such as microring resonator-bus waveguide gap and alignment of the bowtie nanostructures. Figure 2.16 shows the experimental testing setup. Figures 2.17 and 2.18 show experimental results. Figure 2.19 shows the SEM images.

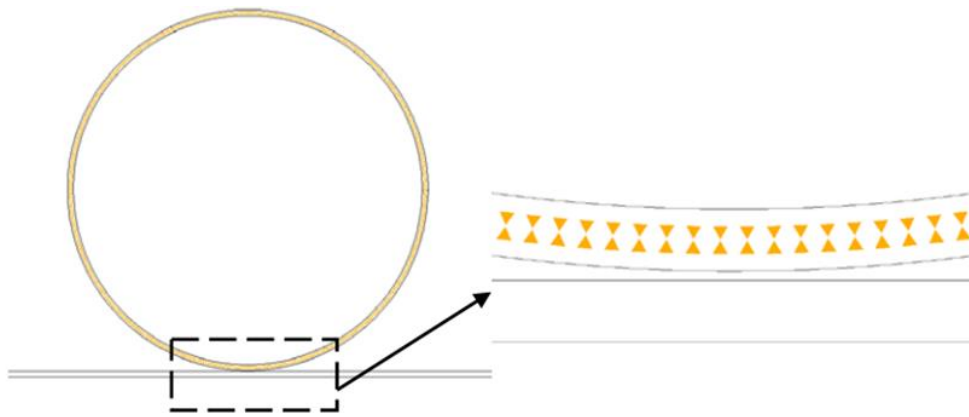


Figure 2.15. Schematic of the proposed sensor design and zoomed in region of the plasmonic bowties bound to the microring surface.

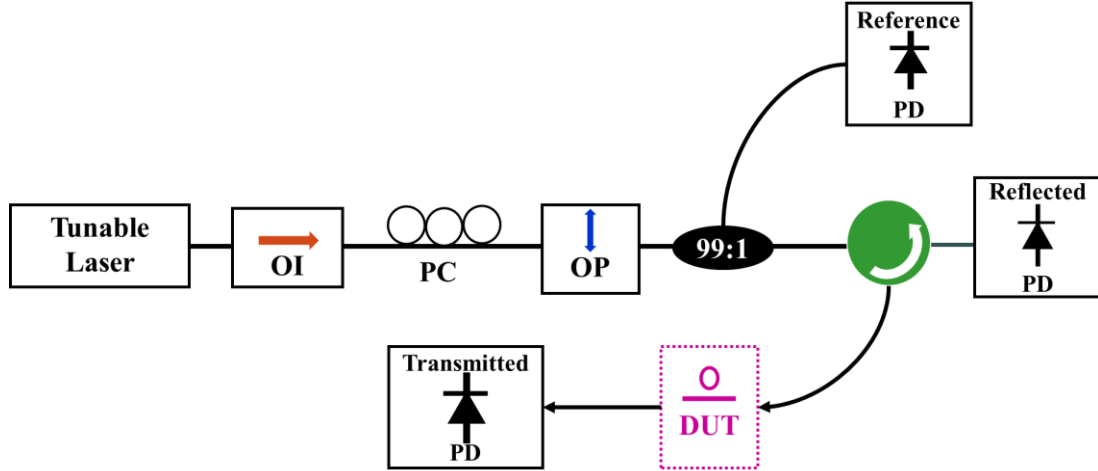


Figure 2.16. Schematic of the experimental test setup for measuring the transmission and reflection spectra of devices. OI: optical isolator, PC: polarization controller, OP: optical polarizer, PD: photodetector, and DUT: device under test. Adapted from Amir Arbabi's dissertation [71]

Preliminary findings display that the periodic arrangement of bowties on top of the microring causes mode-splitting in the spectra. For comparison, a TE-polarized bare microring with a gap of 300 nm produced a loaded quality factor exceeding 1.3×10^4 . The microring is critically coupled at longer wavelengths. The resonant wavelength is 1562 nm. For a TE-polarized bowtie coupled microring resonator, there are bowties located at the 386 anti-nodes. Resonance splitting was observed at 1515 nm when the gap length was 50, 100 and 150 nm. The splitting was on average 1 nm. The quality factor is around 4200 for these designs.

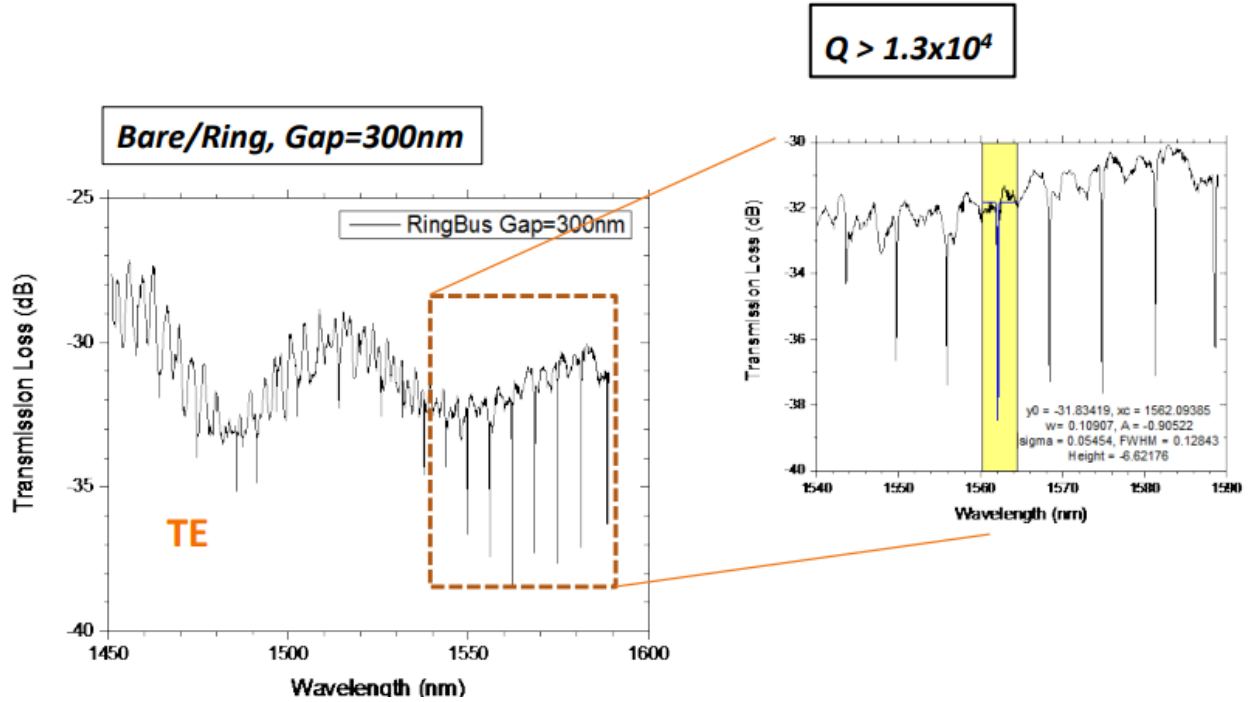


Figure 2.17. For TE polarization, the bare microring is critically coupled above 1550 nm with maximum resonance peak at 1562 nm.

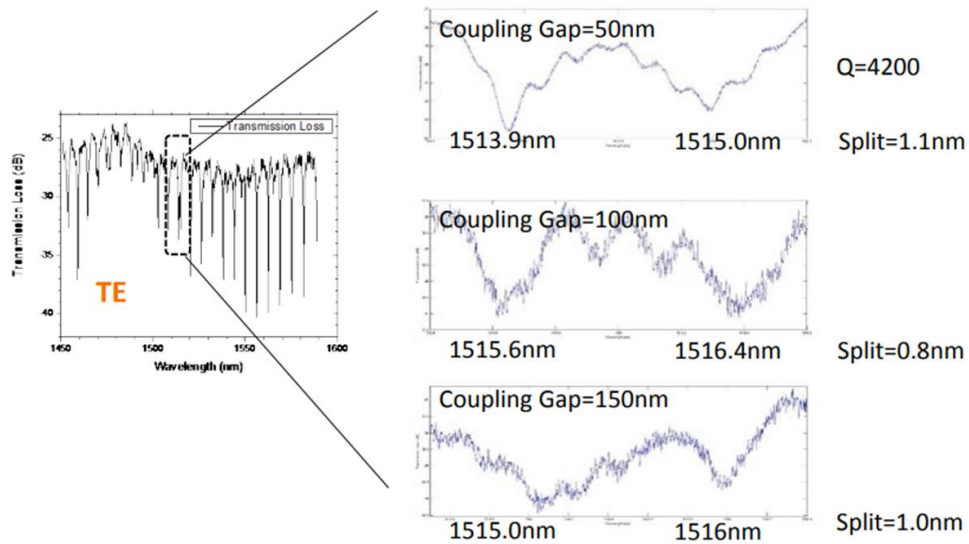


Figure 2.18. The bowtie-coupled MRR displays mode splitting around 1515 nm at the varying MRR gaps: 50, 100 and 150 nm. The bowtie length is 100 nm.

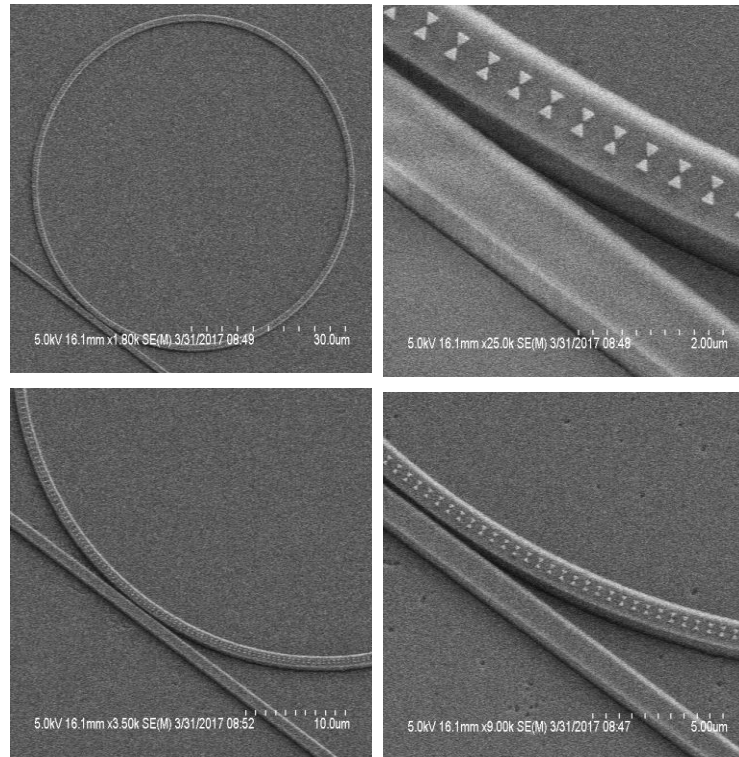


Figure 2.19. SEM of the best fabrication thus far for the DBR Bowtie study.

2.5 References

- [1] Spira, Jonathan." The Knowledge Worker's Day: Our Findings", BaseX Blog, 4 November 2010.
- [2] Blackhurst, Jack. "The Quantified Warriier," Armed Forces Journal, 1 December 2012.
- [3] Levitin, Daniel J. *The organized mind: Thinking straight in the age of information overload*. Penguin, 2014.
- [4] Didsbury, Howard F., ed. *21st century opportunities and challenges: An age of destruction or an age of transformation*. World Future Society, 2003.
- [5] Akamai Technologies. "Akamai's State of The Internet" (pdf). Retrieved 10 November 2014.
- [6] Strimbu, Kyle, and Jorge A. Tavel. "What are biomarkers?" *Current opinion in HIV and AIDS* 5.6 (2010): 463.
- [7] Kaushik, Ajeet, et al. "Recent advances in cortisol sensing technologies for point-of-care application." *Biosensors and Bioelectronics* 53 (2014): 499-512.

- [8] Murdock, Richard C., et al. "Optimization of a paper-based ELISA for a human performance biomarker." *Analytical chemistry* 85.23 (2013): 11634.
- [9] Shopova, S. I., et al. "Plasmonic enhancement of a whispering-gallery-mode biosensor for single nanoparticle detection." *Applied Physics Letters* 98.24 (2011): 243104.
- [10] Estrada, I. A., et al. "Multiplex detection of pathogen biomarkers in human blood, serum, and saliva using silicon photonic microring resonators." *SPIE Sensing Technology Applications*. International Society for Optics and Photonics, 2015.
- [11] Jin, Jian-Ming. *The finite element method in electromagnetics*. John Wiley & Sons, 2010.
- [12] Pitarke, J. M., et al. "Theory of surface plasmons and surface-plasmon polaritons." *Reports on progress in physics* 70.1 (2007).
- [13] Western, Condensed Matter Physics at. "Prof. Silvia Mittler." *The University of Western Ontario*, www.physics.uwo.ca/~smittler/evanescent.html, 1 June 2015.
- [14] S. Mohanty and E. Kougianos, "Biosensors: a tutorial review," *IEEE Potentials*, vol. 25, pp. 35-40, 2006.
- [15] Nadgaran, H., and M. Afkhami Garaei. "Enhancement of a whispering gallery mode microtoroid resonator by plasmonic triangular gold nanoprisms for label-free biosensor applications." *Journal of Applied Physics* 118.4 (2015): 043101
- [16] Polo, John, Tom Mackay, and Akhlesh Lakhtakia. *Electromagnetic Surface Waves: A Modern Perspective*. Newnes, 2013.
- [17] Treviño, Juan, et al. "Surface plasmon resonance immunoassay analysis of pituitary hormones in urine and serum samples." *Clinica Chimica Acta* 403.1 (2009): 56-62.
- [18] Wade, James H., and Ryan C. Bailey. "Applications of optical microcavity resonators in analytical chemistry." *Annual Review of Analytical Chemistry* 9 (2016): 1-25.
- [19] Xavier, Jolly, et al. "Advances in optoplasmonic sensors—combining optical nano/microcavities and photonic crystals with plasmonic nanostructures and nanoparticles." *Nanophotonics* 7.1 (2018): 1-38.
- [20] Arnold, S. "Taking single virus detection and sizing to the limit with molecular sensitivity: the birth of nanoplasmonic-microcavity hybrid sensors." *Frontiers in Biological Detection: From Nanosensors to Systems V*. Vol. 8570. International Society for Optics and Photonics, 2013.
- [21] Bozzola, Angelo, Sara Perotto, and Francesco De Angelis. "Hybrid plasmonic–photonic whispering gallery mode resonators for sensing: a critical review." *Analyst* 142.6 (2017): 883-898.
- [22] Lin, Linhan, and Yuebing Zheng. "Optimizing plasmonic nanoantennas via coordinated multiple coupling." *Scientific reports* 5 (2015).

- [23] Acimovic, Srdjan S., et al. "Plasmon near-field coupling in metal dimers as a step toward single-molecule sensing." *ACS nano* 3.5 (2009): 1231-1237.
- [24] Brown, Lisa V., et al. "Fan-shaped gold nanoantennas above reflective substrates for surface-enhanced infrared absorption (SEIRA)." *Nano letters* 15.2 (2015): 1272-1280.
- [25] Syahir, Amir, Kotaro Kajikawa, and Hisakazu Mihara. "Sensitive Detection of Small Molecule–Protein Interactions on a Metal–Insulator–Metal Label-Free Biosensing Platform." *Chemistry–An Asian Journal* 7.8 (2012): 1867-1874.
- [26] Dey, Dibyendu, et al. "A new generation of mid-infrared sensors based on quantum cascade laser." *SPIE Defense, Security, and Sensing. International Society for Optics and Photonics*, 2011.
- [27] Braswell, Shaneen, et al. "A computational study of a hybrid plasmonic-microring for label-free detection." *Photonics Conference (IPC), 2016 IEEE.*, 2016.
- [28] Urbonas, Darius, et al. "Ultra-wide free spectral range, enhanced sensitivity, and removed mode splitting SOI optical ring resonator with dispersive metal nanodisks." *Optics Letters* 40.13 (2015): 2977- 2980.
- [29] Zhang, Meng, Genzhu Wu, and Daru Chen. "Silicon hybrid plasmonic microring resonator for sensing applications." *Applied optics* 54.23 (2015): 7131-7134.
- [30] Cai, Wenshan, et al. "Elements for Plasmonic Nanocircuits with Three-Dimensional Slot Waveguides." *Advanced materials* 22.45 (2010): 5120-5124.
- [31] Steele, Jennifer M., et al. "Resonant and non-resonant generation and focusing of surface plasmons with circular gratings." *Optics Express* 14.12 (2006): 5664-5670.
- [32] Osowiecki, Gaël D., et al. "Vertically coupled plasmonic slot waveguide cavity for localized biosensing applications." *Optics Express* 22.17 (2014): 20871-20880.
- [33] Biasi, Stefano, et al. "Hermitian and Non-Hermitian Mode Coupling in a Microdisk Resonator Due to Stochastic Surface Roughness Scattering." *IEEE Photonics Journal* 11.2 (2018): 1-14.
- [34] Zhao, Huaying, Patrick H. Brown, and Peter Schuck. "On the distribution of protein refractive index increments." *Biophysical journal* 100.9 (2011): 2309-2317.
- [35] Ciulli, Alessio. "Biophysical screening for the discovery of small-molecule ligands." *Protein-Ligand Interactions*. Humana Press, Totowa, NJ, 2013. 357-388.
- [36] Keating, S. P. "On the refractive index of molecular fluids." *Molecular Physics* 48.4 (1983): 655-672.
- [37] Saha, Krishnendu, et al. "Gold nanoparticles in chemical and biological sensing." *Chemical reviews* 112.5 (2012): 2739-2779

- [38] Arbabi, Amir, and Lynford L. Goddard. "Measurements of the refractive indices and thermo-optic coefficients of Si₃N₄ and SiO_x using microring resonances." *Optics letters* 38.19 (2013): 3878-3881.
- [39] Johnson, Peter B., and R.-W. Christy. "Optical constants of the noble metals." *Physical Review B* 6.12 (1972): 4370.
- [40] Hale, George M., and Marvin R. Querry. "Optical constants of water in the 200-nm to 200- μ m wavelength region." *Applied optics* 12.3 (1973): 555-563.
- [41] Grist, Samantha M., et al. "Silicon photonic micro-disk resonators for label-free biosensing." *Optics express* 21.7 (2013): 7994-8006.
- [42] Chen, Hao, et al. "Design, fabrication, and characterization of near-IR gold bowtie nanoantenna arrays." *The Journal of Physical Chemistry C* 118.35 (2014): 20553-20558.
- [43] Hatab, Nahla A., et al. "Free-standing optical gold bowtie nanoantenna with variable gap size for enhanced Raman spectroscopy." *Nano letters* 10.12 (2010): 4952-4955.
- [44] Klusmann, Carolin, et al. "Identification of Dielectric, Plasmonic, and Hybrid Modes in Metal-Coated Whispering-Gallery-Mode Resonators." *ACS Photonics* (2018).
- [45] Luo, Ye, Maysamreza Chamanzar, and Ali Adibi. "Compact on-chip plasmonic light concentration based on a hybrid photonic-plasmonic structure." *Optics express* 21.2 (2013): 1898-1910.
- [46] Bian, Yusheng, and Qihuang Gong. "Tuning the hybridization of plasmonic and coupled dielectric nanowire modes for high-performance optical waveguiding at sub-diffraction-limited scale." *Scientific reports* 4 (2014): 6617.
- [47] Jung, Yun Suk, et al. "Blue-shift of surface plasmon resonance in a metal nanoslit array structure." *Optics Express* 17.18 (2009): 16081-16091.
- [48] K. De Vos, I. Bartolozzi, E. Schacht, P. Bienstman, R. Baets, *Opt. Express* 2007, 15, 7610.
- [49] Y. F. Xiao, C. L. Zou, B. B. Li, Y. Li, C. H. Dong, Z. F. Han, Q. Gong, *Phys. Rev. Lett.* 2010, 105, 153902
- [50] Chen, Si, et al. "Plasmon-enhanced colorimetric ELISA with single molecule sensitivity." *Nano Letters* 11.4 (2011): 1826-1830.
- [51] Guider, Romain, et al. "Sensitivity and limit of detection of biosensors based on ring resonators." *Sensing and bio-sensing research* 6 (2015): 99-102.
- [52] Chang, Lei, et al. "Single-molecule enzyme-linked immunosorbent assays: theoretical considerations." *Journal of immunological methods* 378.1-2 (2012): 102-115.
- [53] Shirai, Kentaro, et al. "A single-molecule ELISA device utilizing nanofluidics" *Analyst* 143.4 (2018): 943-948.

- [54] Xavier, Jolly, et al. "Advances in optoplasmonic sensors—combining optical nano/microcavities and photonic crystals with plasmonic nanostructures and nanoparticles." *Nanophotonics* 7.1 (2018): 1-38.
- [55] Zhao, Jing, et al. "Localized surface plasmon resonance biosensors." (2006): 219-228.
- [56] Klusmann, Carolin, et al. "Identification of Dielectric, Plasmonic, and Hybrid Modes in Metal-Coated Whispering-Gallery-Mode Res-onators." *ACS Photonics* (2018).
- [57] Liu, Jui-Nung, et al. "Nanoantenna–Microcavity Hybrids with Highly Cooperative Plasmonic–Photonic Coupling." *Nano letters* 17.12 (2017): 7569-7577.
- [58] Arbabi, Ehsan, et al. "Hybrid whispering gallery mode/plasmonic chain ring resonators for biosensing." *Applied Physics Letters* 105.23 (2014): 231107.
- [59] Dantham, Venkata R., et al. "Label-free detection of single protein using a nanoplasmonic-photonic hybrid microcavity." *Nano letters* 13.7 (2013): 3347-3351.
- [60] Shopova, S. I., et al. "Plasmonic enhancement of a whispering-gallery-mode biosensor for single nanoparticle detection." *Applied Physics Letters* 98.24 (2011): 243104.
- [61] Swaim, Jon D., Joachim Knittel, and Warwick P. Bowen. "Detection limits in whispering gallery biosensors with plasmonic enhancement." *Applied Physics Letters* 99.24 (2011): 243109.
- [62] Xiao, Yun-Feng, et al. "Strongly enhanced light-matter interaction in a hybrid photonic-plasmonic resonator." *Physical Review A* 85.3 (2012): 031805.
- [63] Kang, Tae Young, et al. "Plasmon-Coupled Whispering Gallery Modes on Nanodisk Arrays for Signal Enhancements." *Scientific reports* 7.1 (2017): 11737.
- [64] Schmidt, Markus A., et al. "Hybrid nanoparticle–microcavity-based plasmonic nanosensors with improved detection resolution and extended remote-sensing ability." *Nature communications* 3 (2012): 1108.
- [65] Urbonas, Darius, et al. "Ultra-wide free spectral range, enhanced sensitivity, and removed mode splitting SOI optical ring resonator with dispersive metal nanodisks." *Optics letters* 40.13 (2015): 2977-2980.
- [66] Arnold, Stephen, et al. "Periodic plasmonic enhancing epitopes on a whispering gallery mode biosensor." *Optics express* 20.24 (2012): 26147-26159.
- [67] Arbabi, Amir, et al. "Realization of a narrowband single wave-length microring mirror." *Applied Physics Letters* 99.9 (2011): 091105.

- [68] Chen, Hao, et al. "Design, fabrication, and characterization of near-IR gold bowtie nanoantenna arrays." *The Journal of Physical Chemistry C* 118.35 (2014): 20553-20558.
- [69] Acimovic, Srdjan S., et al. "Plasmon near-field coupling in metal dimers as a step toward single-molecule sensing." *ACS nano* 3.5 (2009): 1231-1237.
- [70] Hackett, Lisa P., et al. "Spectrometer-Free Plasmonic Biosensing with Metal–Insulator–Metal Nanocup Arrays." *ACS sensors* 3.2 (2018): 290-298.
- [71] Arbabi, Amir. *Selective mode coupling in microring resonators for single mode semiconductor lasers*. Diss. University of Illinois at Urbana-Champaign, 2013.

Chapter 3: High-Efficiency Grating Couplers for Photonic Integrated Circuit Applications

3.1 Motivation of the Problem

The advent of modern communication has driven industrial demands to increase data rates and bandwidth for communications and computing applications. Energy-efficient, optical interconnects for multi-chip high-performance computing applications necessitate ultra-fast, scalable, and low-loss capabilities to outperform conventional electrical interconnects that are limited in speed, scalability, and bandwidth. Integrated photonics have proven their utility in transmitting information around the world. Namely, the utilization of optic fiber cables for telecommunications and long-haul networks has prompted exploration of their use for shorter interconnect distances for on-chip, chip-to-chip and across the backplane to meet the ever continually increasing industrial demands [1-6]. To push the technological envelope, this entails achieving lower power consumption, increased bandwidth and lower latency of processors [7-9]. This trend, Moore's law, is driven by the desire to increase processor performance by downsizing the feature size to a 10 nm scale to further increase the transistor density. Consequently, conventional electrical interconnects cannot perform at such data transmission capacity. To date, copper-based electrical interconnects are commonly employed and have reached their bottleneck in scalability as signal frequencies increase, number of signal channels and components expand, and integration complexity grows [10]. Alternatively, optical interconnects can match and outperform high-speed electrical interconnects at predicted capacities, because electrical buses cannot perform at the projected capacity. Optical interconnects are less sensitive to latency and power dissipation concerns. Furthermore, optical interconnects are better suited for long interconnections and high density given that electrical interconnects are vulnerable to the inherent cross talk and parasitic capacitance associated with metal, thereby, making it them susceptible to electromagnetic interference [11]. A number of recent works have demonstrated optical interconnects as a viable approach [12, 13]; hence, current work is underway to replace copper wires with photonic components. For wide adoption, optical datalinks and interconnects

necessitate the performance of greater than 100 Gb/s for short-range links using vertical cavity surface-emitting lasers (VCSELs). Ongoing efforts are directed towards VCSELs in conjunction with optical interconnects to modulate bit rates close to 100 GB/s [14-16]. Towards this aim, the goal is to couple to the vertical cavity transistor laser (VCTL) developed by Professor Milton Feng's research group. They are working towards obtaining performance up to 300 Gb/s with bandwidth of ~ 150 GHz. To date, their uncooled VCTL operates at an efficiency of 1 Tb/J at a data rate of 50 Gb/s [17]. For practical realization, the VCTL will be coupled at normal incidence into the grating coupler to ease flip-chip integration. The schematic is shown in Fig. 3.1.

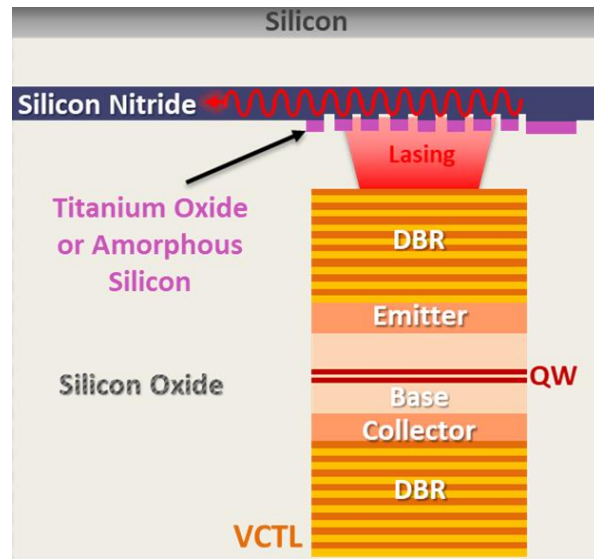


Figure 3.1. Schematic of the proposed integrated coupling scheme that artificially increases the effective mode index of Si_3N_4 by incorporating CMOS-compatible high contrast materials.

In Fig. 3.2, CMOS processing, memory, and electronic-photonic processor blocks are interfaced with silicon photonic optical switching. The micro-lasers, transistor laser, and light emitting transistor permit optical switching. Optical interconnects are placed throughout the integrated system to transfer information across various platforms. One key requirement of the optical interconnect block is to engineer a highly efficient grating coupler.

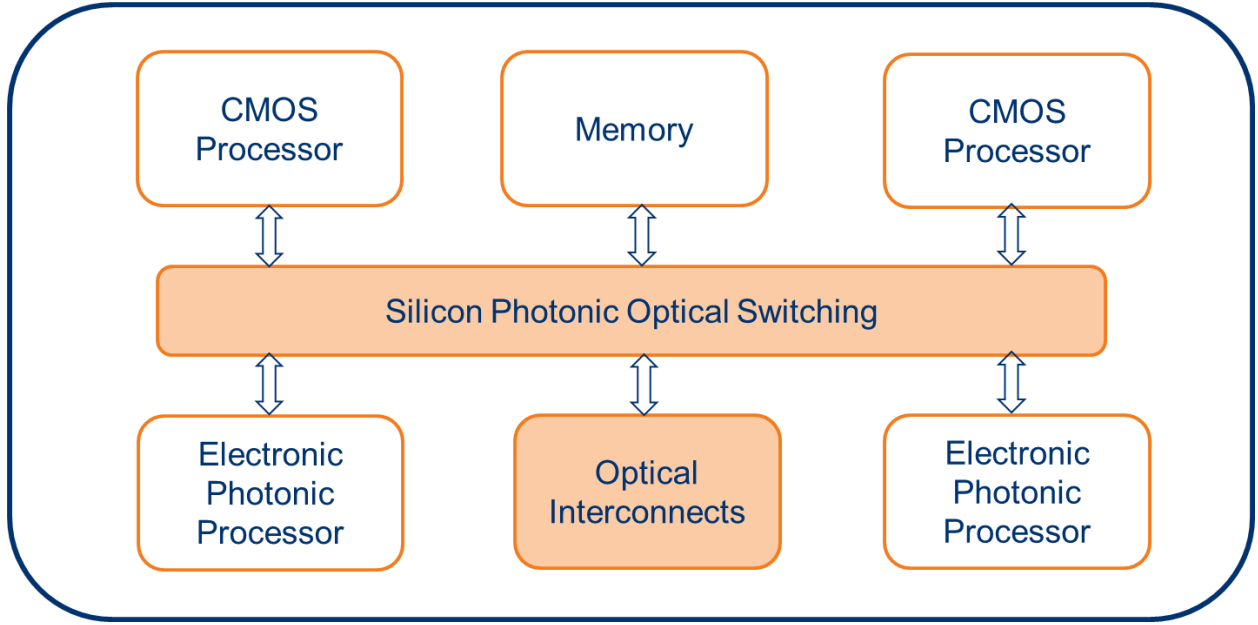


Figure 3.2. Simplified block diagram of the electronic-photonic integrated circuit. Adapted from the proposal to Energy-Efficient Computing: from Devices to Architectures (E2CDA). The contributions of this dissertation were a part of the Optical Interconnects research thrust.

3.2 Statement of the Specific Problem

The silicon-on-insulator (SOI) platform has emerged as the widespread technology utilized in photonic integrated circuit applications due to its notable merits: especially high refractive index contrast, which enables small footprint and compatibility with CMOS processes [18]. However, it is not suitable for telecom wavelengths below 1000 nm, i.e., the operating wavelength range of the VCTL, because of its high intrinsic absorption losses. An alternative CMOS-compatible candidate, silicon nitride, circumvents the aforementioned limitations of silicon by offering lower optical loss, low thermo-optic coefficient, and increased manufacturing flexibility [19]. Although silicon nitride possesses inherent advantages over silicon within this shorter wavelength telecom window, the lower refractive index contrast of silicon nitride makes it challenging to develop high-efficiency grating couplers. The coupling metrics are central wavelength, bandwidth, processing complexity, and size. Design engineers have employed several strategies to enhance the fiber-based coupling efficiency above the 40 - 50% of conventional grating couplers by incorporating bottom distributed Bragg reflectors (DBRs) [20], metal bottom reflectors [21], a staircase geometry [22], or a multi-layered device [23], but these modifications increase the fabrication complexity. The highest reported fiber-based coupling efficiency for silicon nitride grating coupler

is -1.3 dB [24]. The coupling efficiency is still lower than the result in silicon of -0.36 dB for an apodized bi-level grating consisting of SOI and silicon-nitride overlay [25].

To date, most silicon nitride grating couplers are designed for C-band or O-band with the highest experimental reported value of -1.3 dB and bandwidth of 80 nm at an oblique incident angle. Those reported with efficiencies above -1.3 dB are simulation based and are difficult to fabricate. The simulation of the proposed uniform HCG structure achieves CE of -0.72 dB with a bandwidth of 74 nm without apodization for 980 nm operation. As for SOI GCs, the reported coupling efficiency is above -0.7 dB for the C-band or O-band windows. Those higher than -0.46 (90%) are only in simulation, are hard to fabricate or have a metal back reflector, bottom DBR, bi-level grating or staircase. Very few works exist on laser-to-grating couplers, but most recently, Kumari et al. report -5.75 dB at 850 nm using SOI and bottom DBR. The structure, though, is multi-mode. Herein, we propose a high-efficiency silicon nitride grating coupler design with amorphous silicon overlay, which achieves an efficiency of -0.17 dB without a bottom reflector in simulations. Table 3.1 presents key coupler designs.

Table 3.1. Comparison of key silicon nitride based grating coupler designs from literature.

#	Coupling Efficiency	λ (nm)	Bandwidth (nm)	Design	Refs.
1	-4.2 dB	1545	67 nm	SiN waveguide buried in SiO ₂ with a silicon substrate	26
2	-1.74 dB	1310	NA	SiN waveguide buried in SiO ₂ with a silicon substrate	27
3	-1.3 dB	1536	80 nm	SiN waveguide buried in SiO ₂ and a partially etched silicon grating underneath with silicon substrate	28
4	~-2 dB	1310	80 nm	SOI/SiN grating	29
5	-2.5 dB	1567	65 nm	Multilayered grating with silicon nitride, silicon dioxide and silicon on sio2 box layer and a silicon substrate	30
6	-0.66 dB (sim)	1550	40 nm	Apodized silicon nitride staircase grating with air top cladding and silicon dioxide bottom cladding	31
7	-0.88 dB (sim)	1550	40 nm	SiN waveguide buried in SiO ₂ and a partially etched silicon grating underneath with silicon substrate	32
8	-2.5 dB	1490	53 nm	SiN waveguide buried in SiO ₂ with bottom DBR on a silicon substrate	33
9	-0.12 dB (sim)	980	74 nm	a-Si overlay on Si ₃ N ₄ waveguide with SiO ₂ bottom cladding and a silicon substrate.	This work

3.3 Background and Theory

A key component towards on-chip implementation is an optical grating coupler to couple power into the circuit and subsequent on-chip functionalities. There are two main coupling strategies for integrated photonic applications (Fig. 3.3): (1) butt-coupling and (2) surface grating coupling. Butt-coupling coupling consists of in-plane coupling from a free space source (i.e., optical fiber) into the side of a waveguide on a substrate. Despite its low loss coupling characteristic, it is prone to misalignment and constrains the number of devices to be tested at a given time. Alternatively, a surface grating coupling, a type of diffraction phase grating, relies on out-of-plane illumination from an optical source into a waveguide that contains a grating structure consisting of periodic notches of alternating refractive indices along the direction of propagation [34]. Each tooth acts as

a scatterer and the sum of their contributions in phase leads to constructive or destructive interference. At the interface, incident light is diffraction coupled into the waveguide. The efficiency of diffraction coupling relies upon the effective refractive index modulation scheme. This scheme is dependent on the grating parameters to satisfy the Bragg condition. The advantage of this vertical coupling approach (i.e., out of plane coupling) is lower losses due to the elimination of chip cleaving and polishing, thereby, making it amenable for dense, chip-scale architectures. In this way, surface grating couplers enable simultaneous testing of multiple devices given the denser arrangement of devices. Due to reciprocity, the equivalent surface grating coupler can be utilized for coupling optical energy into and out of a chip as shown in Fig. 3.4. Therefore, surface grating couplers are utilized for coupling between different photonic and electronic layers of an interposer [26, 35].

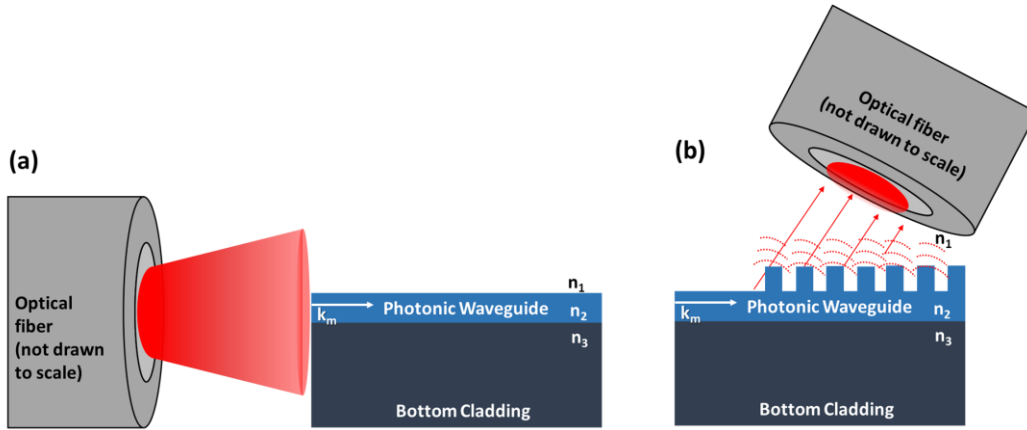


Figure 3.3. (a) Butt-coupling scheme and (b) surface grating coupling scheme.

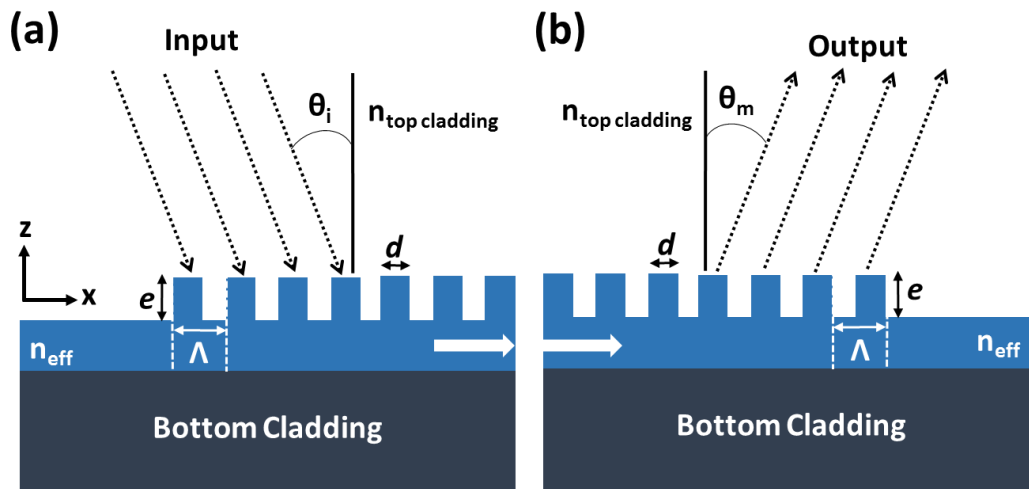


Figure 3.4. Schematic diagram of input and output grating coupling scheme of a binary grating.

The underlying operating principle of the surface grating coupler is governed by the diffraction equation which is based on the relationship between the incident angle of light, the effective index of the grating coupler, refractive index of the top cladding, diffraction order, and wavelength and grating period of an idealized grating [36]. The relationship is derived from incident light deflected into the m^{th} diffractive order with a corresponding wave vector, $\mathbf{k}_m$. The undiffracted wave vector is represented as $\mathbf{k}_i$. The grating vector is defined as $\mathbf{K}=2\pi/\Lambda$ where Λ is the period of the grating. The diffractive grating vector represents vector addition of the undiffracted wave vector to the integer multiple of the grating vector (Eq. 3.1). Therefore, it relates the index modulation of the grating with the incident phase velocity to meet the phase matching condition where the tangential component of the wave vector must be continuous according to Maxwell's equations. The vectors can be expressed as geometrical representation (Eq. 3.2-3.3). When substituted into Eq. 3.1 and reduced, the resulting relationship for the $\hat{x}$ component of the modified equation becomes the grating equation (3.4):

$$\mathbf{k}_m = \mathbf{k}_i - m\mathbf{K} \quad (3.1)$$

$$\mathbf{k}_m = \frac{2\pi}{\lambda} n_c (\sin \theta_m \hat{x} + \cos \theta_m \hat{z}) \quad (3.2)$$

$$\mathbf{k}_i = \frac{2\pi}{\lambda} n_{\text{eff}} (\sin \theta_i \hat{x} + \cos \theta_i \hat{z}) \quad (3.3)$$

$$n_{\text{clad}} * \sin \theta_m = n_{\text{eff}} - \frac{m\lambda}{\Lambda} \quad (3.4)$$

where n_c is the top cladding's refractive index, and n_{eff} is the effective refractive index of the grating structure. Based on Eq. 3.4, one can solve for the desired grating periodicity to first order approximation. For vertical coupling, second order ($m=2$) is desired to couple light perpendicularly. Typically, numerical methods such as finite element method (FEM) and finite-difference time-domain method (FDTD) are implemented to determine the optimal grating parameters for efficient coupling. Conventionally, the coupling efficiency is largely limited by the materials' refractive indices and index contrast between the grating teeth and top cladding. To circumvent this drawback, the weighted average of the tooth and groove regions can be varied to modulate the effective

refractive index to improve mode matching.

3.4 Design of a High Contrast Overlay Highly Directional Silicon Nitride Grating Coupler

The key parameters in designing a grating structure (binary design) are: the grating period, Λ , which is the interval encompassing a single tooth and notch, (2) the fill factor, ff , which is the duty cycle, and (3) etch depth, e , which is the vertical etched depth of the notch. Fig. 3.4 provides a schematic of the operating principle and the key grating parameters. In this work, a second order ($m=1$) grating structure is designed to operate at a center wavelength of 980 nm at normal incidence.

Apart from the key grating parameters, the selection of materials is very important due to its inherent limitations. The most mature photonic technology is based on silicon-on-insulator (SOI), which offers a large index contrast ($\Delta n \approx 2$). This increases the degree of integration density of optical components. Despite these characteristics, the high intrinsic absorption loss of silicon is not suitable for making waveguides for telecom wavelengths below 1000 nm. Similarly, many III-V semiconductor materials such as InP and GaSb are absorbing at these wavelengths. Although GaAs/AlGaAs, GaP, and GaN are each transparent in the 850-1000 nm window, they are quite expensive, especially considering that a special epitaxial growth must be done to define the core and cladding layers with an unintentional doping concentration below 10^{13} cm^{-3} to achieve waveguides with adequately low propagation loss. An alternative CMOS-compatible candidate, silicon nitride, circumvents the aforementioned limitations of silicon and III-V materials by offering lower optical loss, smaller thermo-optic coefficient, and increased manufacturing flexibility [37]. However, the lower refractive index contrast of silicon nitride on silicon dioxide ($\Delta n \approx 0.5$) makes it challenging to develop high-efficiency grating couplers. To improve the coupling efficiency of previous designs, high contrast overlays were considered. High contrast gratings (HCGs) have immense potential to enhance the performance of electronic-photonic integrated platforms. Therefore, CMOS-compatible HCG overlays, e.g., amorphous silicon (a-Si) and titanium dioxide (TiO_2), were explored to increase the coupling efficiency for vertical to in-plane coupling. The overlay material increases the effective mode index and the contrast with silicon oxide cladding. The high refractive index of amorphous silicon above 900 nm has

negligible absorption. The lossless material, titanium dioxide, has a large refractive index below 900 nm. Silicon carbide (SiC), an alternative to TiO₂, has the largest refractive index below 900 nm, but its high temperature fabrication process limits its utility.

Directionality is typically achieved by coupling light at a slight angle of incidence as shown in Fig. 3.3. For normal incidence, there is symmetry and therefore directionality is lost, because power is split evenly to the waveguides on either side. To achieve directionality, an in-plane distributed Bragg reflector (DBR) is added to reflect light back towards the output port. Interestingly, adding an in-plane DBR with the appropriate reflectivity on the output port creates a Fabry-Perot cavity that can have a higher coupling efficiency than just the single side DBR. This is because under the right conditions, the cavity can be critically coupled. The cavity is important because it creates multiple reflections that can mostly cancel out the fields going to undesired ports. This results in all of the power going to the desired output port.

3.4.1 Dimensions for a Single Mode Waveguide

Prior to determining the optimum grating parameters, the optimal waveguide (without grating) dimensions for single mode operation must be determined. Therefore, a mode analysis study of a Si₃N₄ waveguide buried in SiO₂ cladding was conducted to determine the optimal dimensions for single mode operation based on modal field profile, effective mode index, optical confinement, propagation, and attenuation loss. This was performed using the FEM software package from COMSOL, Inc. The key variables of interest are the effective mode index, propagation constant and the attenuation constant. COMSOL computes these variables using the expressions (3.5-3.7) where λ is the eigenvalue.

$$n_{eff} = \beta/k_o \quad (3.5)$$

$$\delta_z = \text{Re}(-\lambda) \quad (3.6)$$

$$\beta = \text{Im}(-\lambda) \quad (3.7)$$

The thickness of the waveguide was set to 400 nm, which is based on the substrate materials currently in stock in our lab. Therefore, the width of the waveguide was varied from 350 to 1200 nm during the simulation. The optimal dimensions of the waveguide are 900 nm by 400 nm. The optimized dimensions were determined by mode analysis to determine single mode regime with reasonable confinement factor and minimal attenuation in Fig. 3.5 and Table 3.2. Transverse electric polarization was selected for its higher confinement factor and lower attenuation loss. The electric field profiles of each polarization, transverse electric (TE) and transverse magnetic (TM), are shown in Fig. 3.6. The optimized dimensions of 400 nm in thickness and 900 nm in width give a confinement factor of 82%.

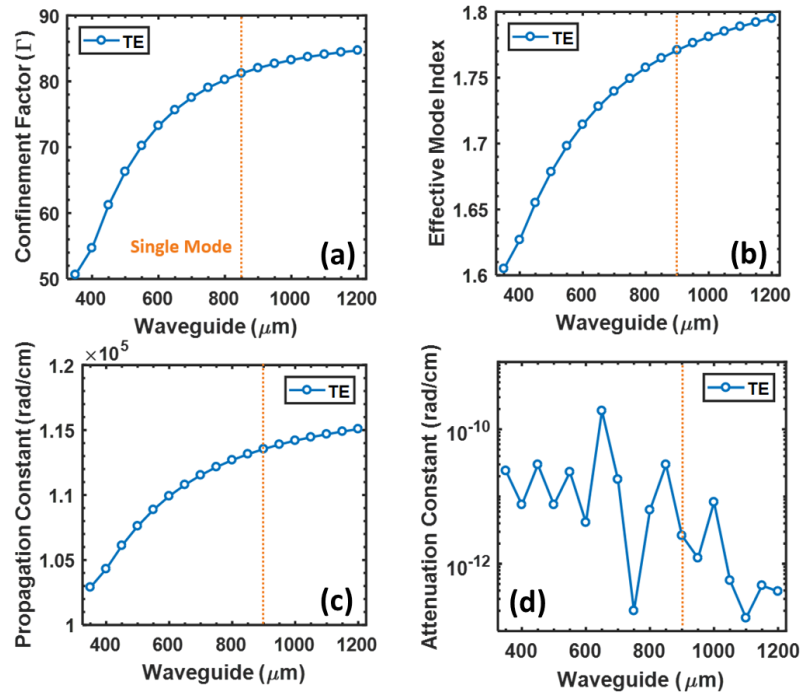


Figure 3.5. Single mode operation of a silicon nitride waveguide buried in silicon dioxide. (a) Confinement factor, (b) effective mode index, (c) propagation constant, and (d) attenuation constant as a function of waveguide width.

Table 3.2 Propagation characteristics of an optimal waveguide for each polarization.

Polarization	Effective Mode Index	Propagation Constant (rad/cm)	Attenuation (rad/cm)
TM	1.7239	1.105×10^7	7.66×10^{-11}
TE	1.72709	1.135×10^7	2.62×10^{-10}

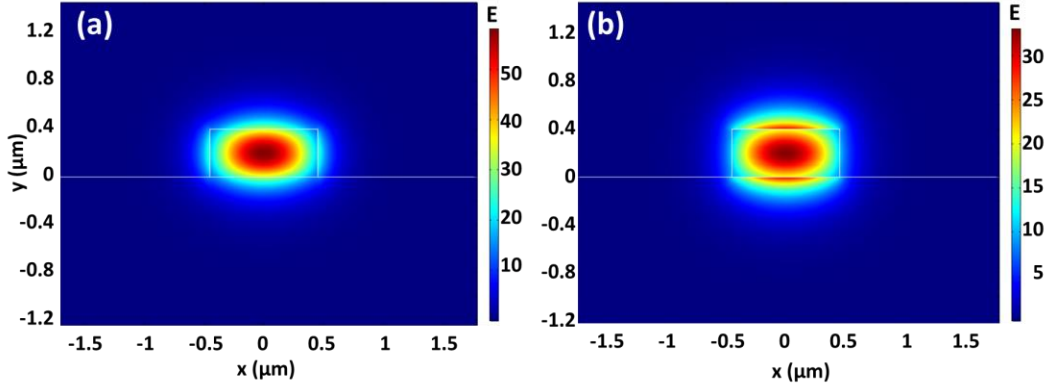


Figure 3.6. (a) TE polarization and (b) TM polarization of the optimized waveguide.

3.4.2 Design and Analysis of Non-Overlay Grating Couplers

The effective index, 1.77, of the grating structure is computed using mode solver in the COMSOL FEM software package. Given this information, the calculated grating period is roughly 553 nm based on Eq. 3.4 under the assumption of an infinitely long grating structure. The source is an optical fiber. It is placed 3 μm above the center point of the grating structure at normal incidence. The fiber source parameters are based on specifications of the fiber array manufacturer, Chiral Photonics. The source is a Gaussian beam with a diameter of 6.9 μm at 980 nm. The refractive indices of their fiber at the drawn end face are 1.444 and 1.449 for the cores and cladding, respectively. The numerical aperture is 0.12 and the air-glass reflectivity is -14.73 dB [38]. In Fig. 3.7, a 2D FEM simulation was performed to examine the effect of the grating pitch on the transmission for a silicon nitride grating structure with 50% fill factor and fully etched. For 980 nm light, the greatest efficiency occurs for the 2nd order grating condition, which occurs when the pitch is 600 nm. The local maximum at 1200 nm corresponds to the 4th order grating condition. Another simulation was performed to determine the optimal parameters of a silicon nitride grating

structure; the optimal grating parameters were grating period of 588 nm, fill factor of 53%, and etch depth of 253 nm. Additionally, a simulation was conducted using a pure amorphous silicon grating structure, which for a waveguide thickness of 220 nm, gave a coupling efficiency similar to a silicon nitride grating coupler. Amorphous silicon was selected as a material for comparison because of its negligibly low loss at 980 nm and its high refractive index. This finding is in agreement with the result of [39]. The optimal design parameters for both grating couplers from the 2D FEM model are presented in Table 3.3. Their electric field profiles are presented in Fig. 3.8.

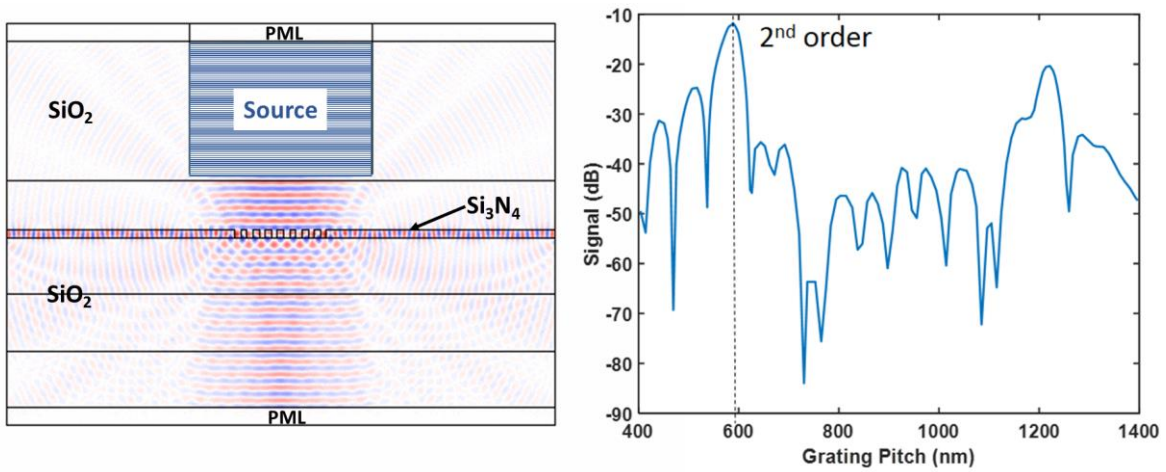


Figure 3.7. (a) Profile of the z-component of the electric field at 980 nm wavelength of a pure silicon nitride grating structure without directionality. (b) Coupling efficiency signal as a function of the grating pitch.

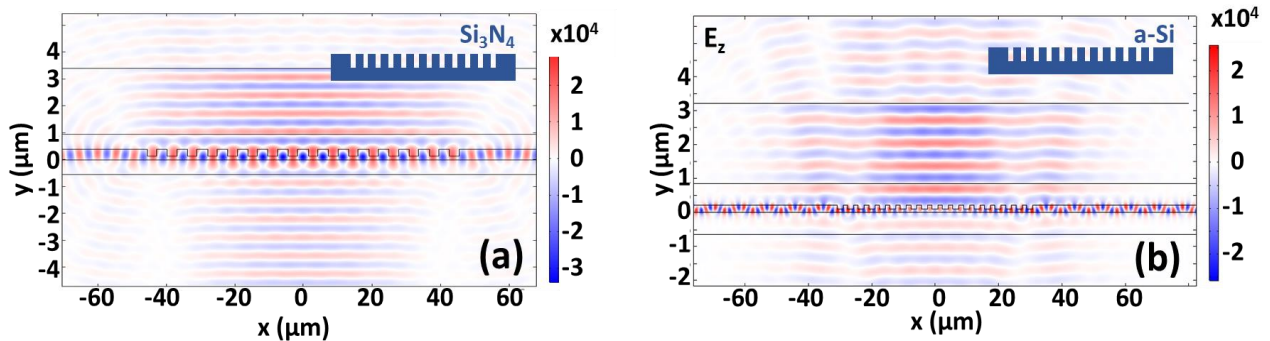


Figure 3.8. Profile of the z-component of the electric field at 980 nm wavelength of a grating structure made of (a) silicon nitride and (b) amorphous silicon.

Table 3.3. Comparison of grating coupler performance between pure amorphous silicon and silicon nitride core material for coupling.

	Pure a-Si Grating	Pure Si ₃ N ₄ Grating
Grating Period	332 nm	588 nm
Duty Cycle	43%	53%
Total Coupling Efficiency	52.6%	53.6%
Left	26.3%	26.8%
Right	26.3%	26.8%
Power Down	15.6%	34.8%
Power Up	18.2%	8.8%
Etch Depth	106 nm	253 nm
Waveguide Thickness	220 nm	400 nm
Effective Mode Index (TE)	3.1227	1.7709
Number of Periods	18	15

3.4.3 Design and Analysis of HCG Couplers

2D FEM simulations in COMSOL were performed to study high contrast grating coupler designs without side DBRs for directionality. A titanium dioxide overlay onto silicon nitride waveguide gave a coupling efficiency of approximately 56% total into both waveguides with substantial substrate loss near 33%. See Table 3.4. To further improve coupling efficiency and minimize substrate loss, amorphous silicon was utilized instead of titanium dioxide. The maximum achieved theoretical coupling efficiency of this design is 84.8% total into both waveguides. The corresponding 3-dB bandwidth of our amorphous silicon HCG design was 74 nm. This exceeds the performance of the experimentally demonstrated reflector-less grating coupler at 81.3% [40].

Table 3.4. Comparison of the design parameters and performance of titanium nitride and amorphous silicon high contrast overlays.

Uniform Design	TiO₂/Si₃N₄ Grating	a-Si/Si₃N₄ Grating
Grating Period	580 nm	548 nm
Duty Cycle	35%	22%
Etch Depth	200 nm	83 nm
Waveguide Thickness	400 nm	400 nm
High Index Layer Thickness	100 nm	172 nm
Effective Mode Index (TE)	1.7709	1.7709
Number of Periods	12	12
Total Coupling Efficiency	55.9%	84.76%
Left	27.95%	42.38%
Right	27.95%	42.38%
Power Down	33%	4%
Power Up	7.1%	9%

3.4.4 Design of the Side DBR for Directionality

A fully etched side DBR was incorporated for in-plane directionality [34]. The thicknesses of the interchanging low and high refractive structure are determined by Eq. 3.8. The number of DBR pairs was set to 34 to provide adequate reflectivity without significant reduction to the bandwidth.

$$d_{1,2} = \frac{\lambda}{4n_{1,2}} \quad (3.8)$$

Although the coupling efficiency to the left waveguide increases from 42.8% to 70.76% after adding the in-plane DBR, the total coupling efficiency is less than the original 84.76%. This decrease is because the amorphous silicon acts as a scattering center that re-radiates the light from the in-plane waveguide. As a result, more of the light is directed upward and this accounts for most of the drop in coupling efficiency. Therefore, we removed the high contrast material from the top of distributed Bragg grating. The coupling efficiency becomes roughly 79%.

3.4.5 Apodization for Mode Matching

To achieve mode matching of the light to the fiber, apodization was performed by varying the fill factor of one grating period at a time in sequential order from left to right. After varying the first five grating elements, the coupling efficiency to the left output waveguide increased from 79% to 85%. Afterwards, we continued varying the fill factor along the grating coupler, and the coupling efficiency increased to 88%. Based on the back reflections and substrate loss occurring at the waveguide extension, the waveguide extension was converted to two HCG grating periods and their fill factors were also varied. As a result, the coupling efficiency reached 92.6%. The DBR fill factor was varied by changing the width of the DBR tooth. Another parametric study was performed on each DBR element by adjusting the spacing and DBR fill factor to determine the optimal geometry of each element of the in-plane DBR. The elements were varied until the coupling efficiency remained constant. The maximum coupling efficiency reached 93.8%. This is the highest reported efficiency for silicon nitride. Table 3.5 shows the design optimization to improve coupling efficiency. The electric field profile in z of the best design produced so far is given in Fig. 3.9. The fill factor profile for this optimal design is given in Fig. 3.10

Table 3.5. Design optimization iterations of the high contrast grating overlay based on the designs noted above.

a-Si/Si₃N₄	Uniform GC	Uniform GC and Side DBR	Apodized GC and Side DBR	Apodized GC and Apodized DBR
Grating Period	544 nm	544 nm	N/A	N/A
Duty Cycle	22%	22%	N/A	N/A
Etch Depth	83 nm	83 nm	83 nm	83 nm
Waveguide Thickness	400 nm	400 nm	400 nm	400 nm
Number of Periods for GC	16	16	16	16
Si₃N₄ DBR Length	N/A	169 nm	169 nm	N/A
SiO₂ DBR Length	N/A	98 nm	98 nm	N/A
Number of Periods for DBR	N/A	34	34	34
Top BOX Thickness	3 μm	3 μm	3 μm	3.6 μm
Total Coupling Efficiency	84.8%	79%	92.6%	93.8%

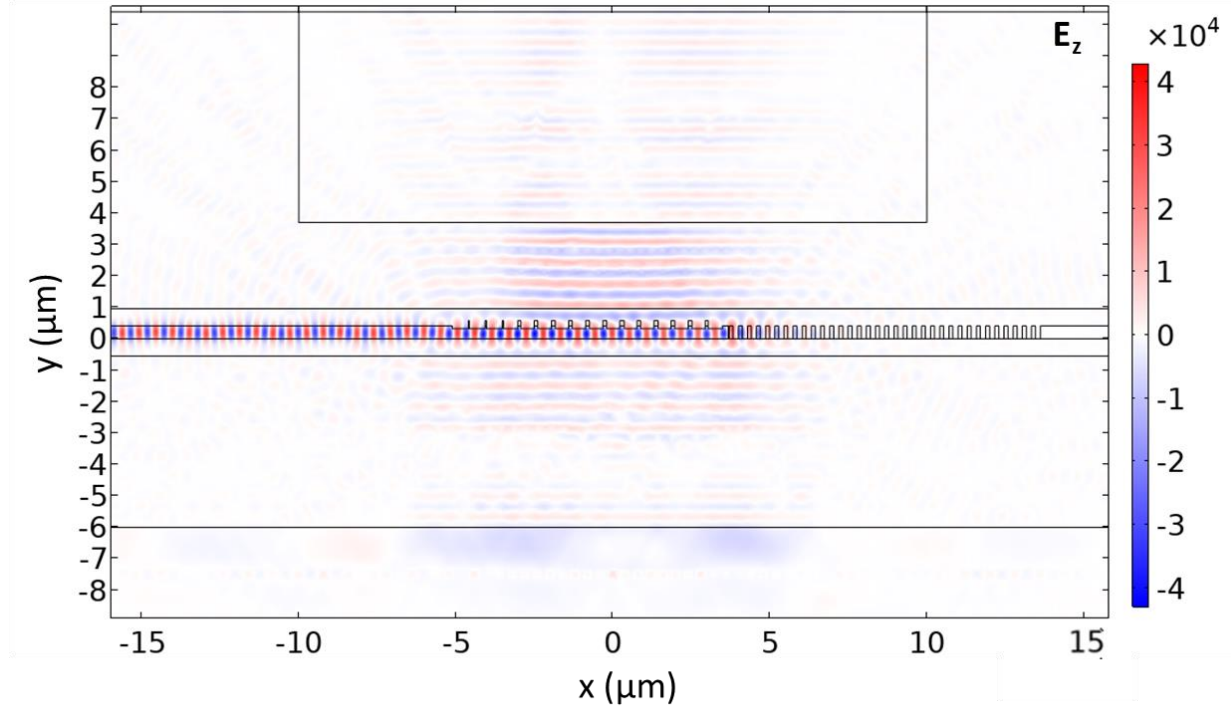


Figure 3.9. Optimal design of the high contrast overlay grating with the greatest coupling efficiency.

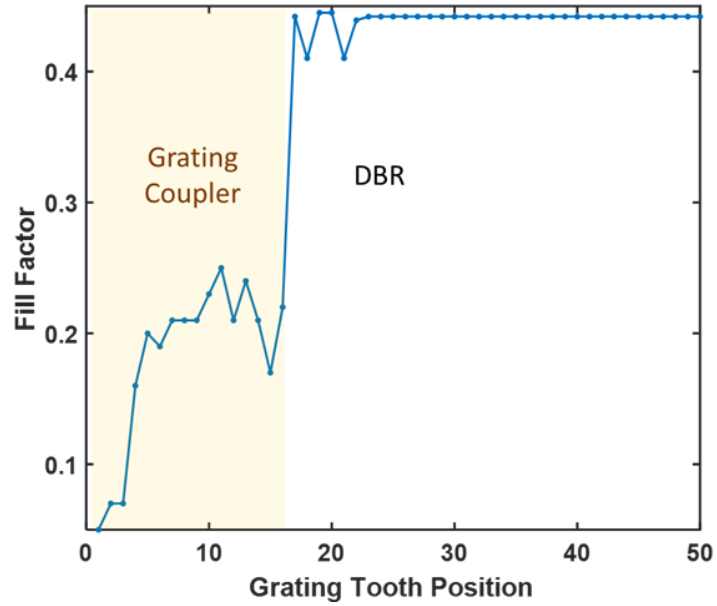


Figure 3.10. Fill factor of the apodized grating coupler and apodized DBR.

Another mesh refinement study was carried out as a result of the coupling efficiency exceeding 100% during a parameter sweep of the top oxide layer (see Fig. 3.11). The optimal top oxide thickness is 3.6 μm . The optimal HCG operates at a high coupling efficiency ($> 90\%$) over an extremely broad range of 930 nm to 1170 nm. The mesh refinement factor increased from 16 to 30 wavelength divisions to accurately capture the small grating teeth from apodization. The maximum coupling efficiency is 93.8% at mesh refinement factor of 30. A fabrication tolerance study was performed computationally to determine the robustness of the optimal grating coupler design. The grating parameters were varied by 5% as shown in Table 3.6. The results are plotted in Fig. 3.12. The coupling efficiency significantly drops below 20% when the grating period is varied by 5%. High coupling efficiency is maintained; however, the spectrum becomes redshifted when the a-Si thickness decreases by 5%. Between 800 nm and 1150 nm, the coupling efficiency is about the same as the baseline despite the 5% change in etch depth. Outside of this wavelength band, the coupling efficiency slightly increases with a 5% decrease in etch depth.

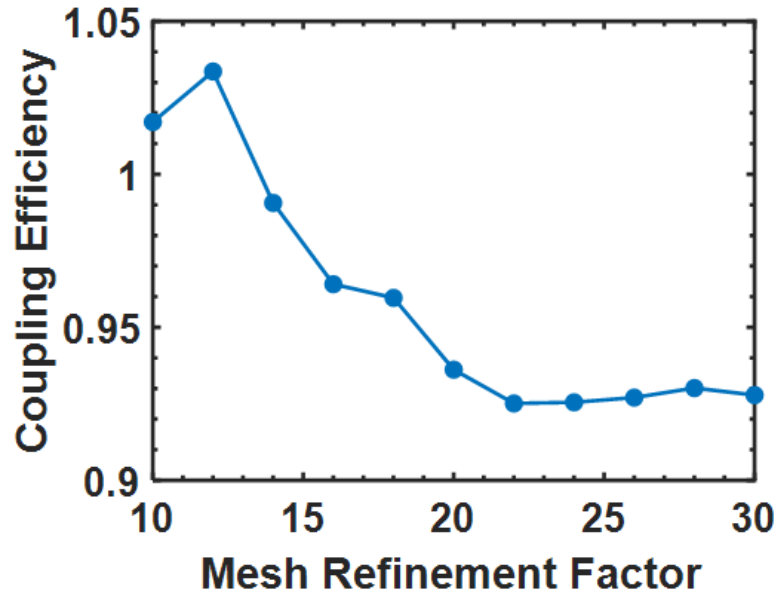


Figure 3.11. Mesh refinement study to determine a stable solution by monitoring the coupling efficiency.

Table 3.6. Fabrication Tolerances of Grating Parameters.

Grating Parameter	Baseline (nm)	+5% (nm)	-5% (nm)
Pitch	544	516	572
Etch depth	83	78.9	87.2
Si ₃ N ₄ DBR Length	172	163	181

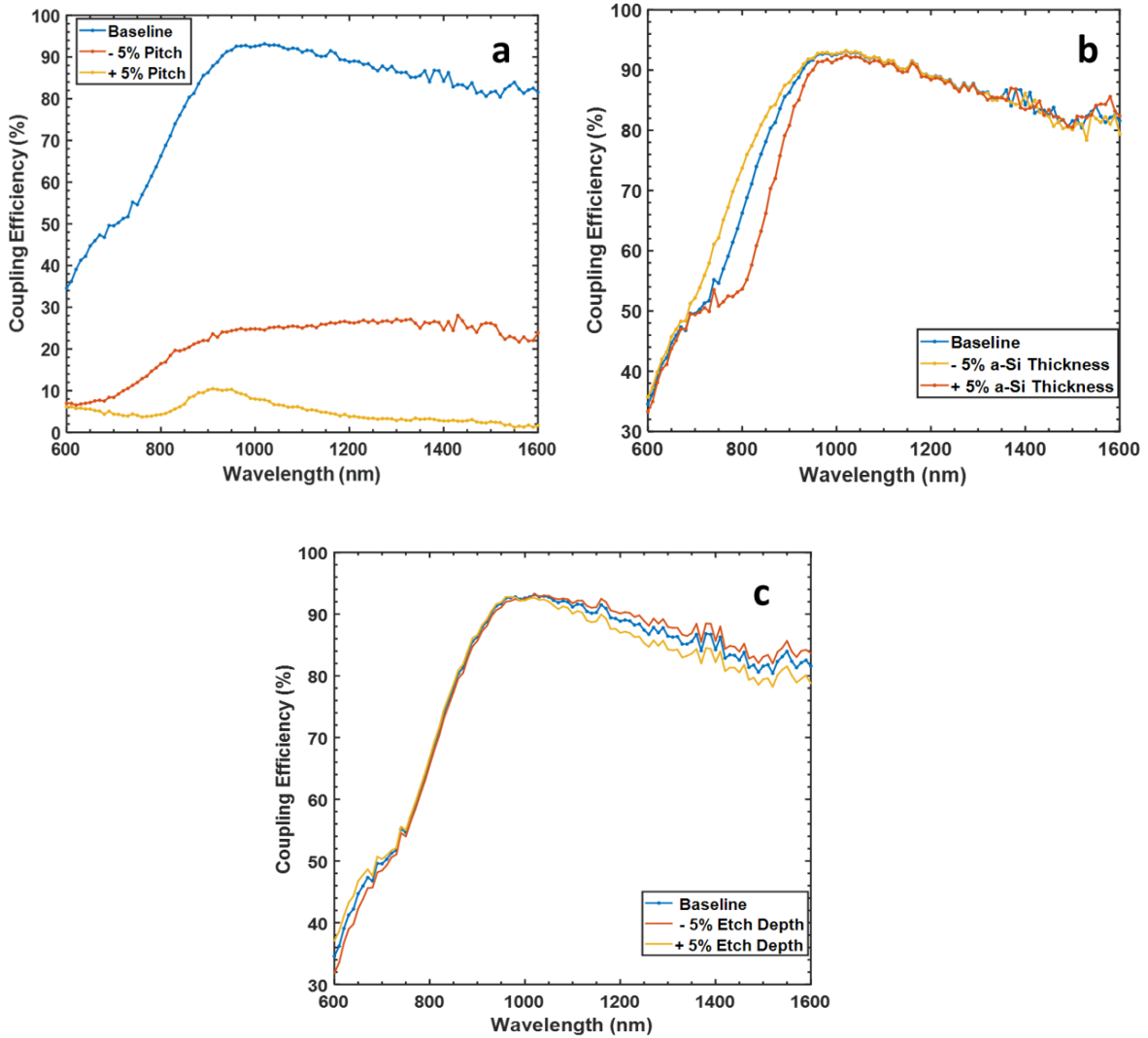


Figure 3.12. Fabrication tolerance of $\pm 5\%$ of grating parameters: (a) pitch, (b) amorphous silicon layer thickness, and (c) etch depth.

3.4.6 S-matrix Optimization

The aforementioned results required intensive simulation to find the optimal design in the multi-parameter design space. A closed form analytic solution that guides the design process would be more desirable. In Appendix B, we present preliminary results using the S-matrix formulation. This formulation makes several assumptions about the properties of the grating coupler, e.g., that the system can be faithfully represented with only four modes—the fiber input, two in-plane waveguides, and the substrate (i.e., scattering and radiation modes are negligible and the modes are matched when light passes through the HCG)—and that the system is lossless and thus can be represented by a unitary matrix. In practice, the simulations show that these properties do not strictly hold; however, the S-matrix formulation appears to still be useful for providing some intuition for making good initial guesses for beginning the numerical optimization.

3.5 Fabrication Process

In this project, the high efficiency grating coupler was fabricated at the Singh Center for Nanotechnology at the University of Pennsylvania. For quality control throughout the process, optical microscopy, scanning electron microscopy (SEM), and profilometry were used to characterize the results of each fabrication steps in attaining a grating coupling tolerance within 3% of the target design. The total fabrication process was carried out in 12 key steps, listed in Table 3.7, which include two electron beam lithography (EBL) steps with minimal misalignment. The mask with the layouts for the test devices is shown in Fig. 3.13.

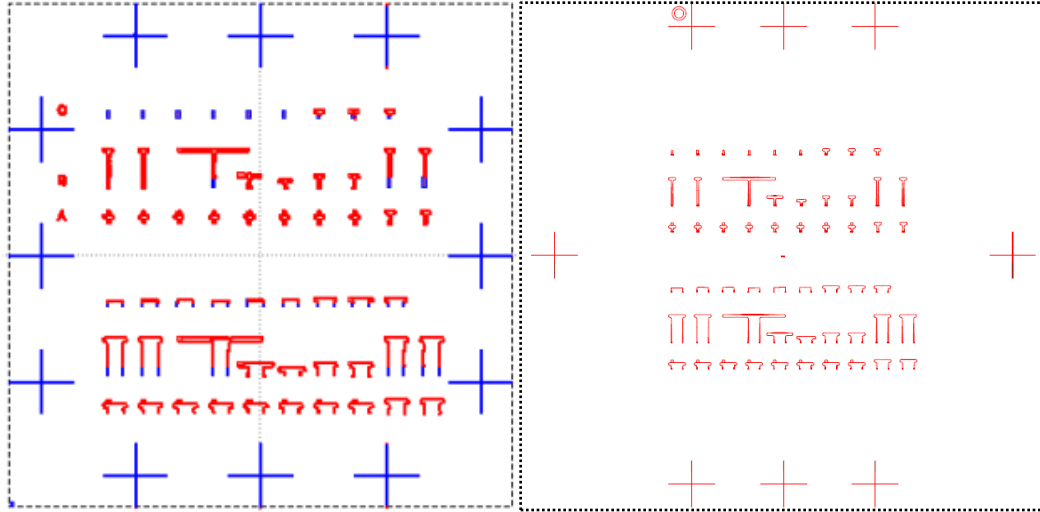


Figure 3.13. AutoCAD mask of the pattern of initial layout (left) and final layout (right).

A key fabrication objective is to reduce the number of EBL steps. The approach is to selectively etch the amorphous silicon. Prior to the start of fabrication, the EBL masks undergo fracturing and proximity correction using the software programs Beamer and Tracer, developed by the company, Genisys, Inc. The starting substrate is a 6- μm thick SiO_2 bottom cladding on a 500- μm thick Si substrate. The sample is cleaved to 2.2 cm x 2.2 cm and cleaned with acetone, isopropyl alcohol, and deionized water and dried with nitrogen flow.

Table 3.7. Fabrication Process

Fabrication Process		
Step	Tools	Objective
1	Sandvik LPCVD/Oxidation/Anneal Furnace	LPCVD Nitride
2	Oxford PlasmaLab 100 PECVD	Deposit amorphous silicon
3	Elionix E-beam Writer	Lithographically define the first pattern layer
4	Lesker 75 PVD with DC/RF Sputterer	Nickel deposition
5	Ultrasonicate Water Bath	Metal lift-off

Table 3.7. Continued

6	Oxford Cobra ICP Etcher	Dry etch amorphous silicon and silicon nitride
7	Elionix E-beam	Lithographically define the second pattern layer
8	Denton Vacuum Explorer 14	Chromium deposition
9	Ultrasonicate Water Bath	Metal lift-off
10	Oxford Cobra ICP Etcher	Dry etch silicon nitride
11	Heated Water Bath	Chromium/nickel etch in a covered glass dish
12	Oxford PlasmaLab 100 PECVD	Deposit silicon oxide

The fabrication flow diagram is provided in Fig. 3.14.

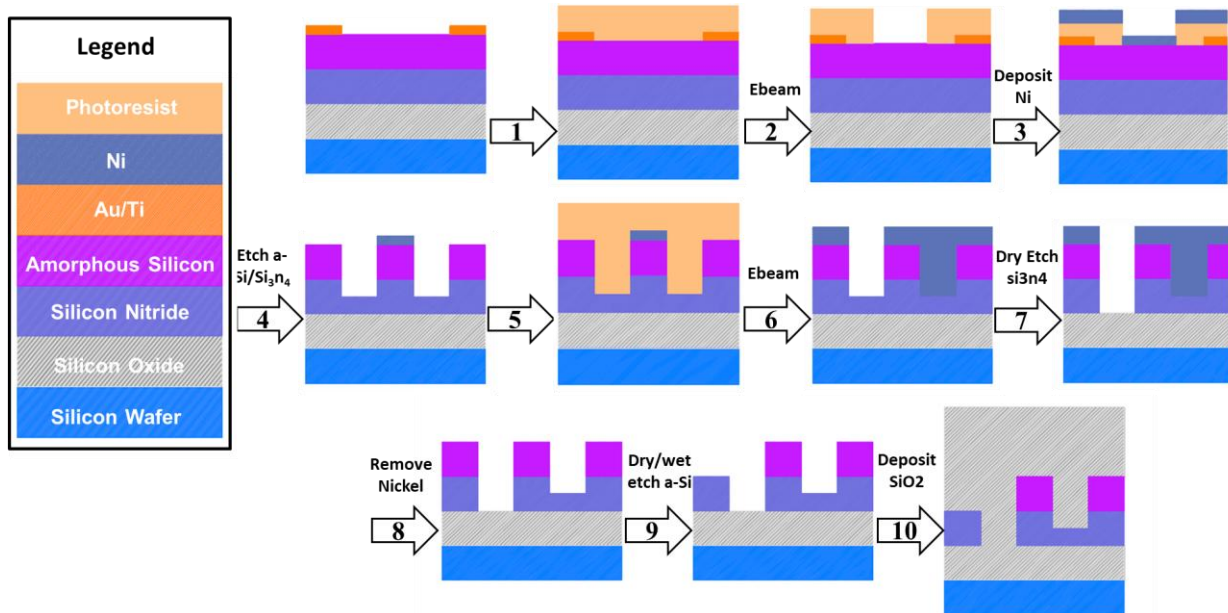


Figure 3.14. Fabrication flow diagram of the high contrast overlay grating coupler.

In the first step of fabrication, stoichiometric silicon nitride was deposited onto a silicon wafer using the Sandvik low-pressure chemical vapor deposition (LPCVD) furnace. The silicon wafer contained a thermal wet oxide prepared at a thickness of 6 μm . Prior to LPCVD deposition, all

wafers were cleaned using the RCA cleaning method. Details regarding the RCA cleaning method can be found at the following URL: <https://www.seas.upenn.edu/~nanosop/Furnace.htm>.

Occasionally, excess silicon nitride was deposited on the wafers due to variability in the deposition rate. This excess material was removed using the Oxford 80 Plus RIE. To remove excess silicon nitride, CHF_3/O_2 served as the etchant of the deposition recipe, in which the etch rate was 0.94 nm/minute with uniformity of 1.5%. Further information on the operation parameters of the etch recipe is displayed in Table 3.8.

Table 3.8. Excess Silicon Nitride Etch Recipe

Oxford 80 Plus	
CHF_3	100 sccm
O_2	45 sccm
Pressure	50 mT
RF Power	150 W
Capacitors	60/80%
Temperature	15 °C

Following this, the Oxford PlasmaLab 100 PECVD was used to deposit amorphous silicon as the high contrast layer onto the silicon nitride film using the following protocol provided by (https://repository.upenn.edu/scn_tooldata/43/); the amorphous silicon deposition rate was 52.74 nm/min. The parameters are listed in Table 3.9 for further reference.

Table 3.9. Amorphous Silicon Deposition Recipe

Oxford PlasmaLab 100 PECVD	
Silane (10 % SiH_4 in Helium) flow rate	200 sccm
Argon (Ar) flow rate	800 sccm (80% of 1000 sccm)
Pressure	1800 mT
High Frequency RF Power	75 W
Low Frequency LF Power	0 W
Capacitor starting points 1/2	77%/26%
Electrode temperature	350 °C

To alleviate the edge effect from deposition due to the inherent non-rotational configuration, amorphous silicon was deposited onto a whole wafer and subsequently diced to retain pieces that are uniform. Figure 3.15 is an optical image of the completed amorphous silicon deposition.



Figure 3.15. Optical image after amorphous silicon deposition.

After the amorphous silicon deposition, the first pattern of the grating coupler was defined lithographically using the Elionix EBL tool. To successfully complete this step of the fabrication, the EBL process was optimized through several series of quality control studies to obtain the ideal patterning of features. First, the ZEP520A, a positive e-beam resist, was used as the electron lithography resist to develop high-resolution features. In this process, it was diluted with anisole at a ratio 1:2 to create a thin layer of ZEP520a based resist. Then, a 100 nm thin layer of ZEP520a: anisole resist was spin-coated onto the sample at 1500 rpm for 1 minute and then, soft baked at 180 °C for 90 seconds. After soft bake processing, a thick layer of the anti-charging agent, Discharge H₂O, was spun at the same conditions as the resist. After exposure, the sample was generously rinsed with distilled water for a minute to remove the Discharge H₂O and placed in o-xylene at room temperature for 70 seconds to develop the resist. Then, the sample was generously rinsed with isopropyl alcohol for 30 seconds. Following the rinsing, the plasma descum process was applied to the patterned sample for 15 seconds (~10-15 nm removal) to remove residual resist from the exposed regions and produce neat metal lift-off. The descum recipe is set to a power of 50 W and etched for 15 seconds.

Second, a dose and bias study was devised to obtain the optimal dose-to-clear and desired pattern dimensions, respectively. The studies were designed using the BEAMER software using a reduced pattern from the original full mask that was created in AutoCAD.

For the dose study, an array of lines at relevant feature sizes was imported into BEAMER and looped to create an array of the line arrays at varying dose levels to determine the dose to clear value. Similarly, a flow process created using BEAMER imports the CAD file and loops through the pattern to create an equally spaced array with varying biased dimensions as shown in Fig. 3.16. The bias feature scales the dimensions of the pattern by a specified length.

For bias optimization, a study was conducted to determine the correct bias to closely reproduce the desired grating dimensions. The cad drawing contains devices with rectangular and focused grating structures in triplicate. There are 8 negative biases ranging from 0 to 14 nm. Fracturing and proximity effect correction are applied to improve the e-beam rastering process and edge correction, respectively. The design and the final bias design are shown in Fig. 3.16 and 3.17. A negative bias of 4 nm was found to be optimal with a 3% PEC correction and a dose of 150 $\mu\text{C}/\text{cm}^2$. Figures 3.18 and 3.19 show optical and SEM images of the test patterns from the dose test study. Figure 3.20 shows how the bias affects the linewidth of the grating coupler, DBR, and spacer. Figure 3.21 shows high-resolution SEM images of the optimal design structure.

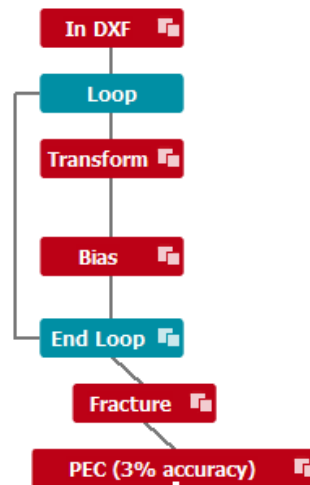


Figure 3.16. The flow diagram in BEAMER for the bias study.

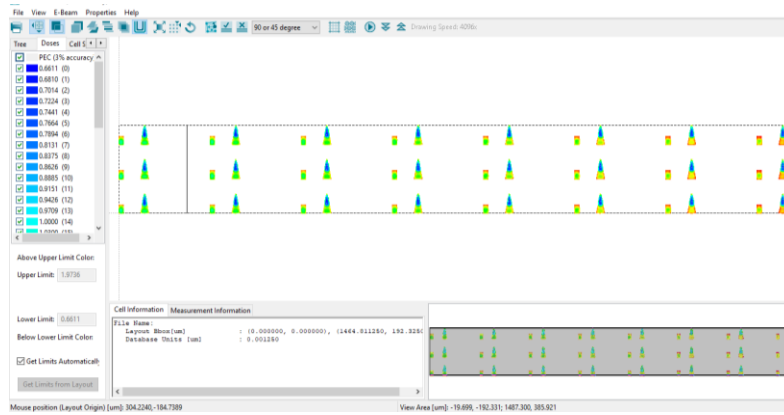


Figure 3.17. The E-BEAM pattern generated using the loop function over bias and position. The color scale is based on dose scale.

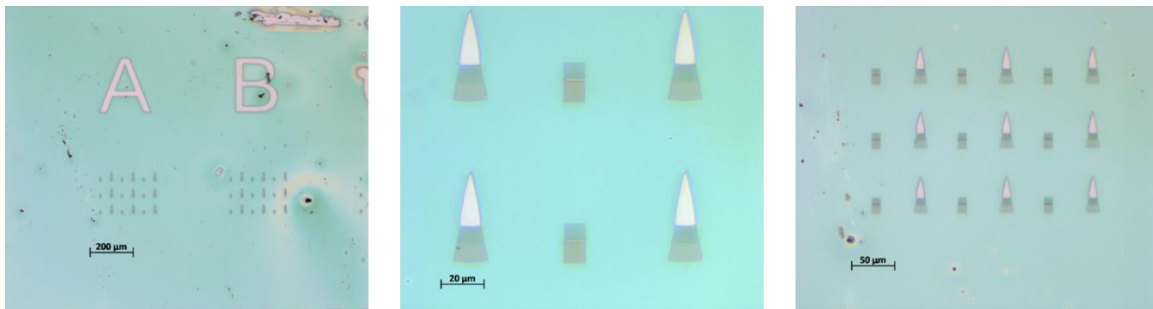


Figure 3.18. Optical image of a test pattern for dose study.

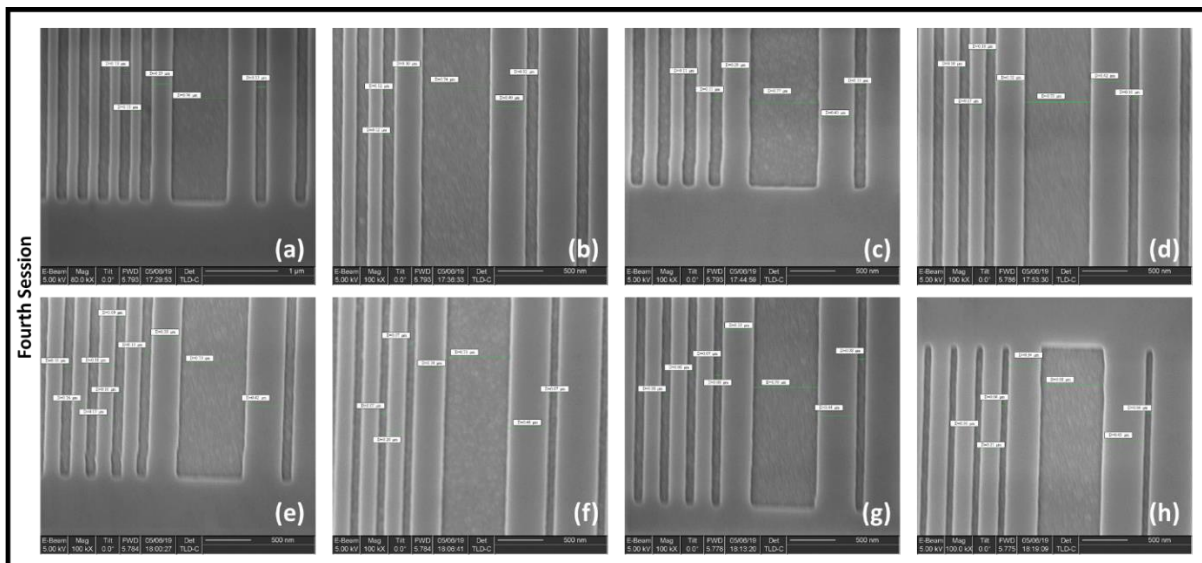


Figure 3.19. Scanning electron micrograph of the bias study.

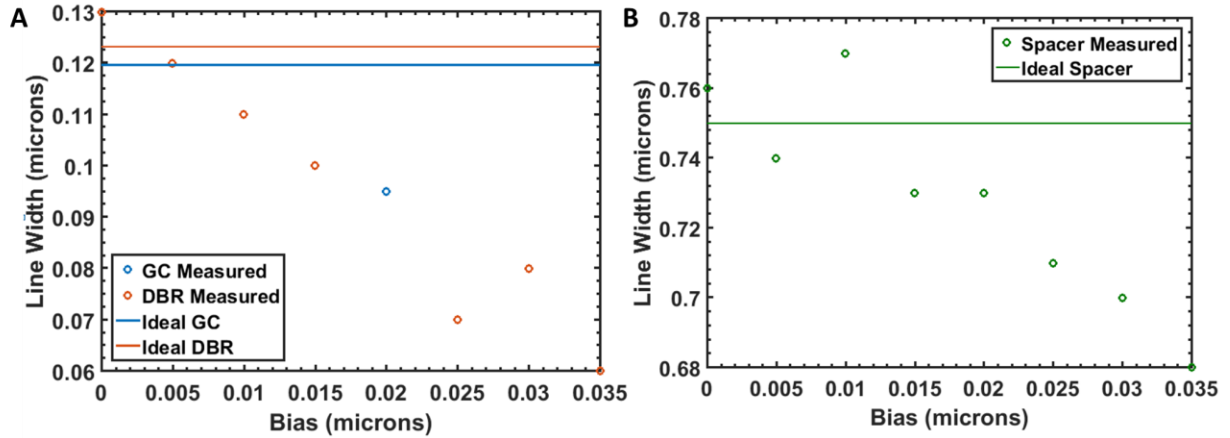


Figure 3.20. Bias study of (a) grating coupler and distributed Bragg reflector (DBR) and (b) spacer.

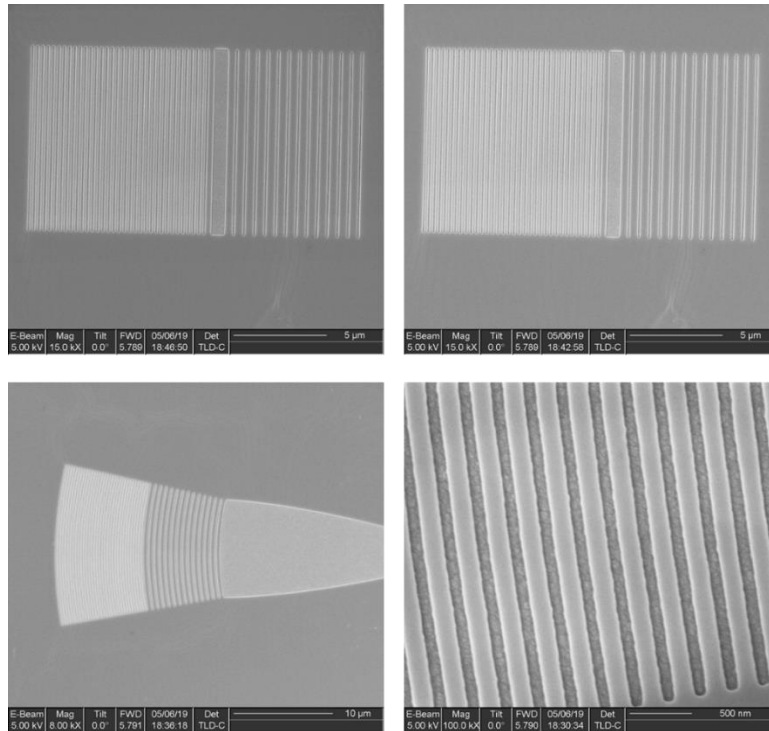


Figure 3.21. Scanning electron micrograph using ultra-high-resolution TLD-S of optimal biased design.

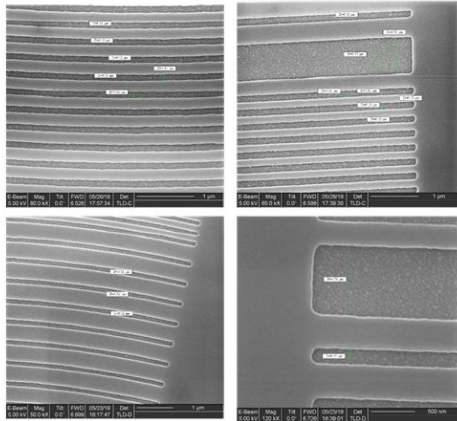
Separately, the write times were optimized by adjusting the current and proximity correction. A reduced write time decreased the number of dislocations, granularity, and overlapping regions in the after exposure. The write times for one chip are listed in Table 3.10. The difference in write times for PEC was ~ 10 -15 minutes. The current is the major driver.

Table 3.10. Write times based on field size, current, and proximity edge correction.

Field Size (microns)	Current	PEC (%)	Write Time (one chip)
300	100pA	3	3.1 hours
600		3	2.4 hours
600	200 pA	3	1.4 hours
		5	1.6 hours
600	500 pA	5	1.1 hours

An exposure with 500 pA with a 10 nm shot pitch and 1000 pA with 20 nm was further explored at the same bias. The 500 pA with 10 nm shot pitch produced a smoother line edge for the curved grating, but the bias required adjustment. The objective lens aperture of the 1000 pA (30 μm) is double the size for 100 pA and 500 pA exposures. For the 1000 pA with 20 nm shot pitch, the dimensions of the grating matched the desired dimensions well; however, the edges were rough for the curved gratings (see Fig. 3.22).

500 pA, 10 nm shot pitch, 600 μm field



1000 pA, 20 nm shot pitch, 600 μm field

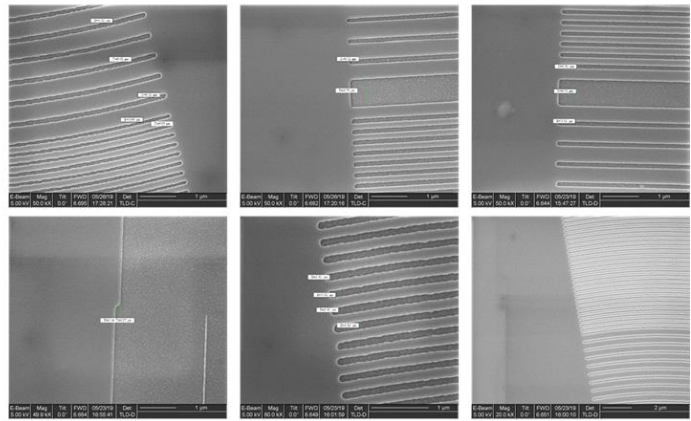


Figure 3.22. SEM of 500pA/10nm (Left) shot pitch and 1000 pA/20 nm (right).

Afterwards, a 30 nm layer of nickel was deposited onto the sample using Lesker 75 PVD with DC/RF Sputterer. The parameters for nickel deposition are listed in Table 3.11.

Table 3.11. Nickel deposition parameters

Lesker 75 PVD with DC/RF Sputter	
Power	400 W
Rotation	10 RPM
Pressure	10 mTorr

The nickel layer is utilized as a hard mask to etch amorphous silicon and produce a partial etch into the silicon nitride. The etch rates of silicon nitride and amorphous silicon were first determined using tetrafluoromethane (CF₄) as an etchant. The Filmetric 50 was utilized to collect spatial information of the etch rate across the sample surface. The etch rate increases near the edge of the sample. Hence, an 8 mm edge exclusion was carefully chosen for measurement. Next, the etch rate of silicon nitride using CF₄ gas was determined. The mean etch rate for silicon nitride and amorphous silicon is 3.28 nm/s and 2.417 nm/s, respectively.

To check the quality of the CF₄ etch, samples from the e-beam optimization study were used. The focused ion beam (FIB) lithography tool was used to mill regions on the sample to determine the etch rate and obtain a cross section view of the near-vertical side profile. See Figs. 3.23, 3.24, and 3.25.

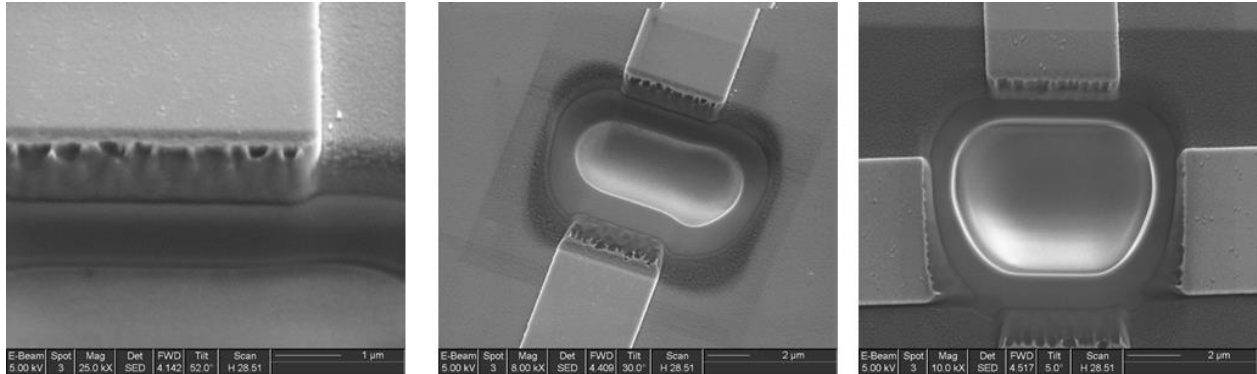


Figure 3.23. Electron beam imaging of FIB etched regions waveguide (left, middle) and alignment marker (right). The figures show from the top layer to bottom layer: nickel hard mask, amorphous silicon, silicon nitride, and part of the thick silicon oxide layer.

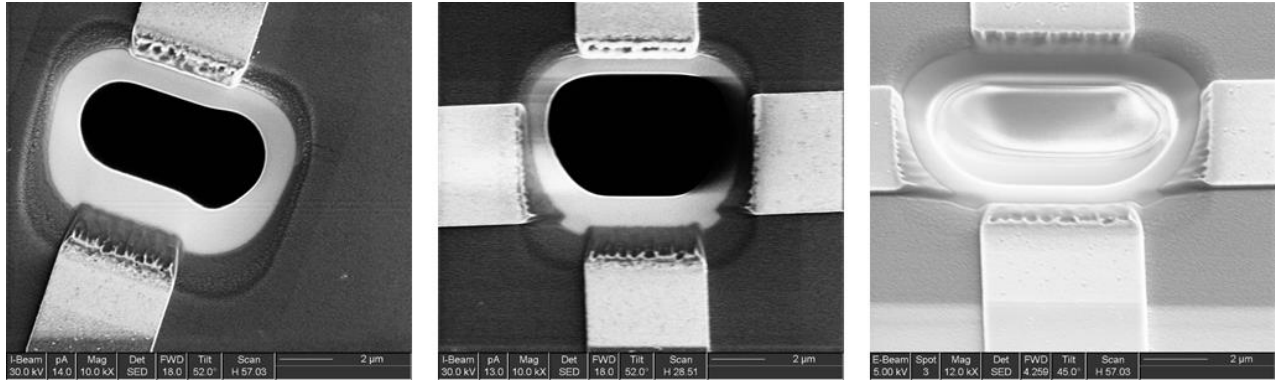


Figure 3.24. Focused ion beam images of the FIB etch regions of a waveguide (left) and an alignment marker (middle, right).

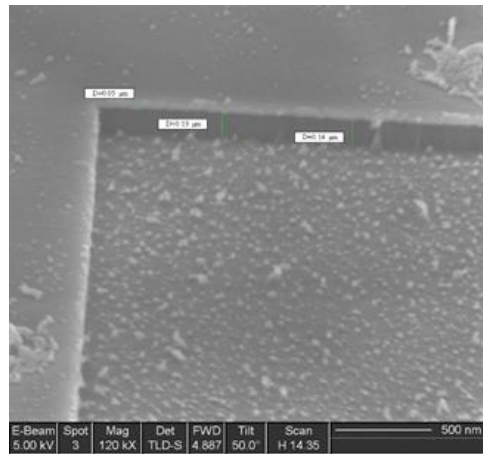


Figure 3.25. Scanning electron microscopy image at 50° tilt of post-etch of the right lower quadrant of an alignment marker.

The last image of Fig. 3.26 compensates for tilt and gives an etch depth of 130 to 140 nm after 60 seconds of etching. The rough surface may be due to the poor-quality amorphous silicon deposition.

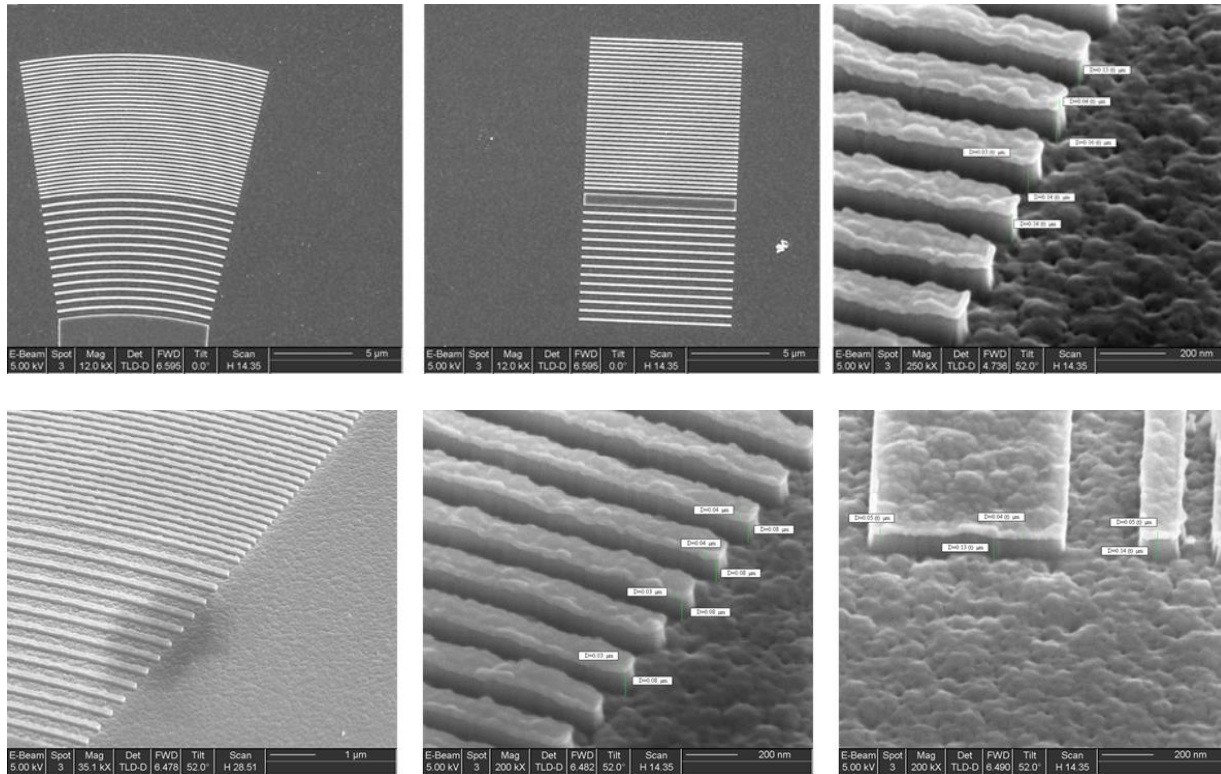


Figure 3.26. Partial etch using CF_4 etchant for 60 seconds.

Then, the etchant, sulfur hexafluoride (SF_6), was explored. SEM images were taken after a 60 second etch. The SF_6 recipe did not yield a quality etch. There appears to be undercutting of the features in Fig. 3.27 (a, b). Next, the SF_6 with argon gas was explored. SEM images were taken after a 60 second etch. The SF_6 with argon recipe also did not yield a quality etch. There also appears to be undercutting of the features in Fig. 3.28.

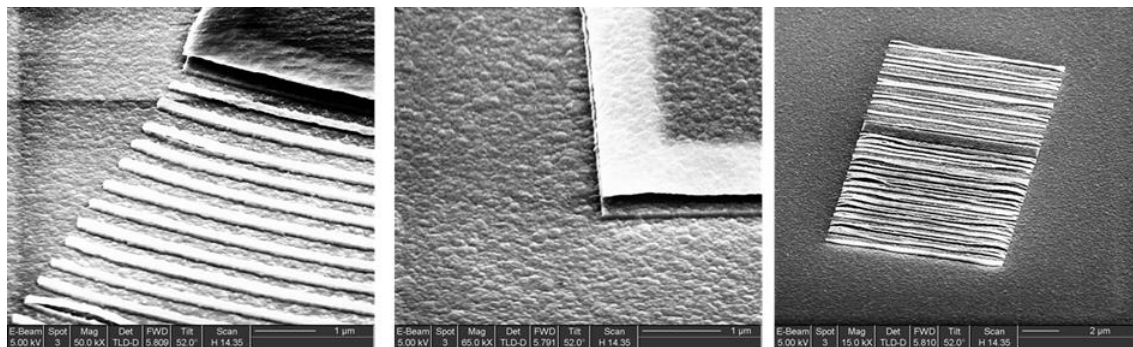


Figure 3.27. Partial etch with SF_6 etchant after 60 seconds of the rectangular grating coupler. The etchant aggressively attacks amorphous silicon while the silicon nitride layer below remains intact.

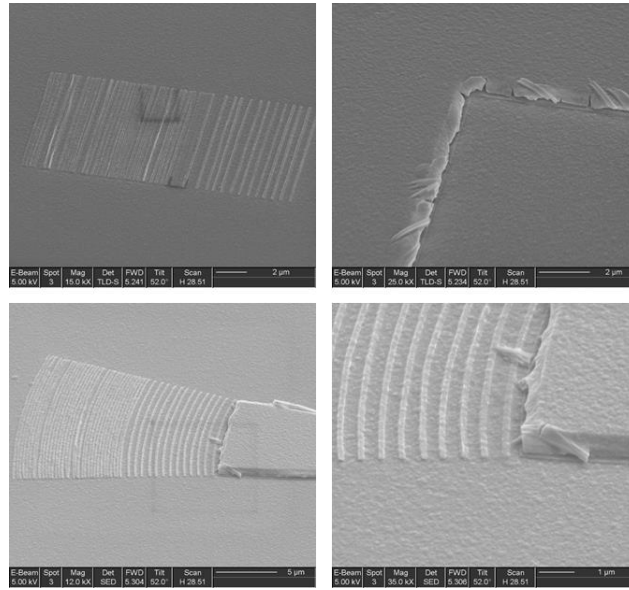


Figure 3.28. Scanning electron micrograph of SF_6 -Ar etchant of amorphous silicon for 60 seconds. From the micrograph, the etchant aggressively attacks the amorphous silicon and the undercut erodes the grating structure. The metal mask around the edges collapses to undercutting.

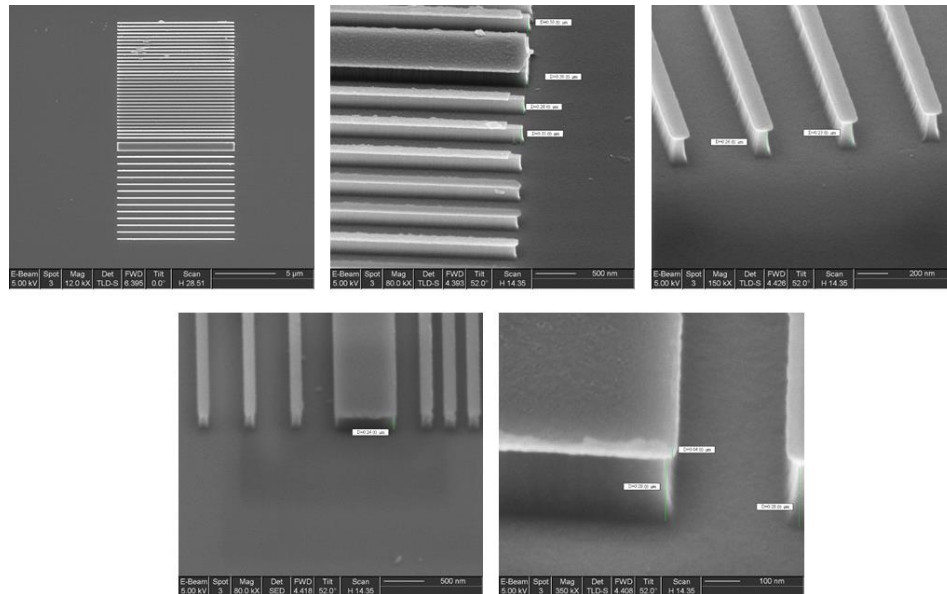


Figure 3.29. Scanning micrograph of CF_4 etchant of silicon nitride after 60 seconds. (a) Top down view of rectangular grating and (b-e) zoomed-in views of the grating coupler. There is a slight undercut, but the features remain intact.

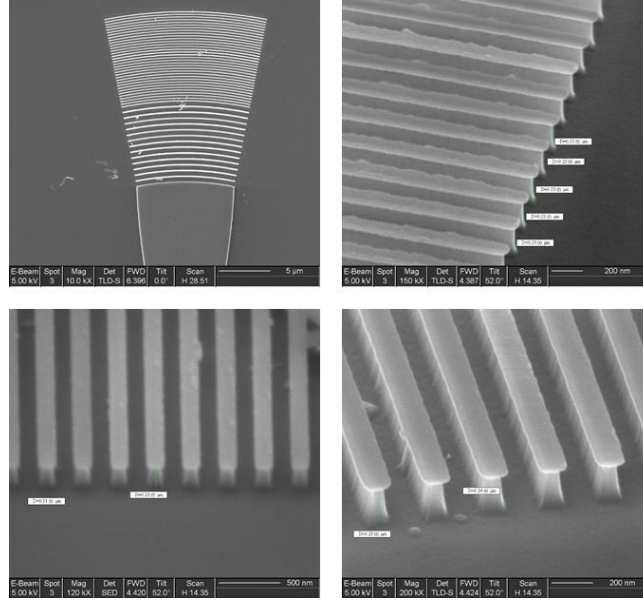


Figure 3.30. Scanning micrograph of CF_4 etchant of silicon nitride after 60 seconds. (a) Top down view of focused grating and (b-d) zoomed regions of the DBR.

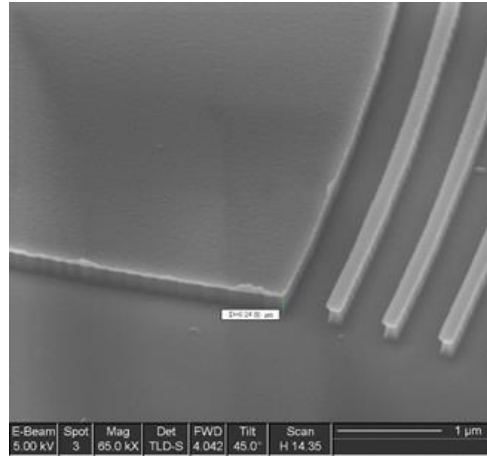


Figure 3.31. SEM image of CF_4 etch of silicon nitride after 60 seconds.

Overall, the CF_4 produced the best etch quality as can be seen in Figs. 3.29, 3.30, and 3.31. The etch rates for amorphous silicon and silicon nitride are 135 nm/min and 240 nm/min, respectively. Given that the etchant C_4F_8 was not available, the well-known photonic etch recipe for silicon-based materials could not be used. The etchants SF_6/O_2 and SF_6/Ar worked well for silicon nitride but performed poorly for the amorphous silicon. The etch rate for SF_6 with Ar is 280 nm/min for silicon nitride (nm/min).

After successful etching of amorphous silicon and silicon nitride (partial etch), the second e-beam pattern is lithographically defined using the same sample preparation for EBL. The second mask layer is designed to accommodate misalignment of 50 nm over the grating pattern.

A thin layer of chromium is deposited using the Denton Vacuum Explorer 14 as the second metal hard mask for preserving the partial etch and etching the remaining silicon nitride to form waveguide structures. The remaining silicon nitride (317 nm) is etched leaving the desired bi-layer structure. The nickel hard mask is removed using the nickel etchant, TFB, from Transene, Inc. The undesired amorphous silicon is selectively removed by using the Xactix XeF₂ etcher. Both metal hard masks, nickel, and chromium, are removed using nichrome etchant. The final step of the process is to deposit 3 μm of silicon dioxide onto the sample as the top cladding. The recipe is provided in Table 3.12.

Table 3.12. The deposition parameters for silicon oxide

Oxford PlasmaLab 100 PECVD	
Silane flow rate	265 sccm
Nitrogen oxide (N ₂ O) flow rate	800 sccm
Nitrogen (N ₂) flow rate	500 sccm
Pressure	60/80%
High-frequency RF power	140 W
Low frequency LF power	0 W
Capacitor #1 start point	60%
Capacitor #2 start point	26%
Electrode temperature	350 °C

The refractive indexes of the deposited materials were characterized using Woollam VASE ellipsometer in Table 3.13. The measurement was repeated for amorphous silicon using the Filmetric 50 to determine the refractive index at 950 nm, which is the upper limit of the tool. The measured refractive index is $n=3.582$ and $k=0$.

Table 3.13. Refractive index measurement

Material	850 nm		980 nm	
	n	k	n	k
Stoichiometric Silicon Nitride	2.0188	0	2.0017	0
Silicon Dioxide	1.4506	0	1.4534	0
Amorphous Silicon	---	---	3.909	0.00803

To create designs that could work at nearby wavelengths, simulations were performed using COMSOL by adjusting the grating pitch to reach the maximum coupling efficiency at 1030 and 1100 nm. The duty cycle, etch depth, and thickness of the amorphous silicon layer were held constant at 22%, 83 nm, and 172 nm, respectively. The limitations were determined by the need to fabricate devices on the same substrate. Table 3.14 shows the grating period and DBR thicknesses from the simulation. The letter corresponds to the row of unique design parameters and the number corresponds to the column which accounts for fabrication errors by scaling the

design. Table 3.15 displays the various design iterations of the EBL mask. The mask consists of two layers with the second layer containing regions to mask only the grating coupler structure. There are four key designs with different bending coupling structures between grating couplers: horseshoe and three varying corner radii. There are three different tapers: focused parabolic, linear with length of 100 μm and linear with length of 500 μm . The purpose of the taper is to facilitate an efficient adiabatic transition from grating coupler into waveguide. A subset of the designs contains a microring with a radius of 30 μm and varying gap sizes. Additionally, there are double tapers to determine the efficiency of the taper in Fig. 3.32 (d). In total, there are five design studies: wavelength (980, 1030, and 1100 nm), taper (focused, linear 100 μm , and linear 500 μm), bend radius (10, 14, and 18.5 μm), taper width (10 and 20 μm), and microring resonator (MRR) with varying gaps (150, 300, 450, and 600 nm). Devices are spaced by 350 μm x and y. The design includes back-to-back grating couplers used as the input and output for transmission measurements. The various designs are shown in Fig. 3.32. The first round of fabrication helped pinpoint any fabrication concerns.

Table 3.14. Varied the GC and DBR period based on waveguide extension design.

λ (nm)	Λ (nm)	ff (%)	DBR Length Si ₃ N ₄ (nm)	DBR Length SiO ₂ (nm)	CE (%)
980	544	22	98	168.9	81
1030	580.7	22	129.5	177.5	76.6
1100	635	22	138.3	189.6	71.4

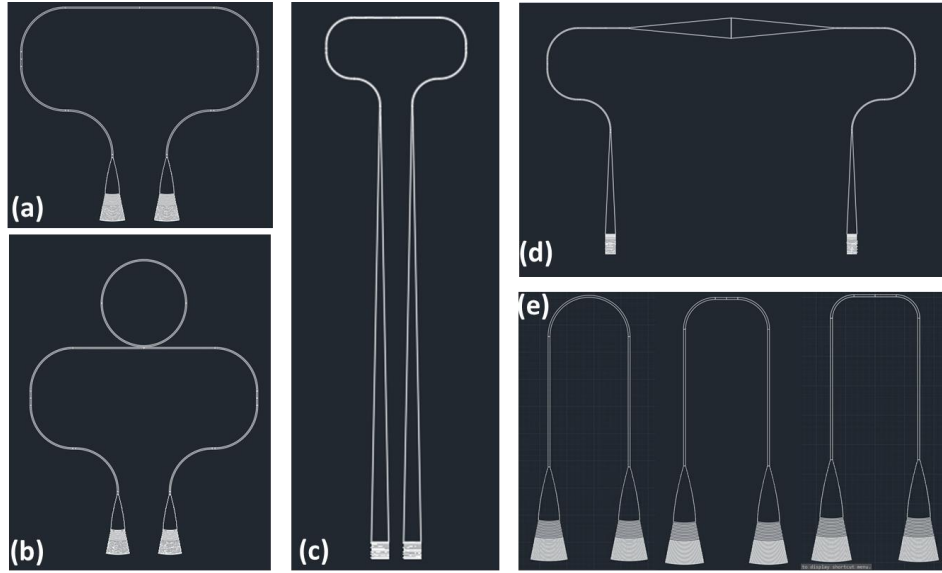


Figure 3.32. (a) Horseshoe + Taper 1 (focused) + varying GC/DBR, (b) Horseshoe + Taper 1 (focused) + varying GC/DBR + MRR (980, 1030, 1100).

Table 3.15. AutoCAD design layout of the first fabrication round. MRR = microring resonator, g = gap and wg = waveguide. The spacing in x and in y is 350 nm.

Row 3 (1120 tall)				
AB	0	980	1	horseshoe plain wg
AA	1	1030	1	horseshoe plain wg
Z	2	1100	1	horseshoe plain wg
R	10	1030	1	half circ 18.5 plain wg
Q	11	1030	1	half circ 14 plain wg
P	12	1030	1	half circ 10 plain wg
O	13	980	1	half circ 18.5 plain wg
N	14	980	1	half circ 14 plain wg
M	15	980	1	half circ 10 plain wg
Row 2 (1120 tall)				
Y	3	980	3	horseshoe plain wg
X	4	1030	3	horseshoe plain wg
W	5	980	2	horseshoe plain wg
V	6	1030	2	horseshoe plain wg
U	7	1030	1	horseshoe 2 tapers
T	8	1030	2	horseshoe 2 tapers
S	9	1030	3	horseshoe 2 tapers
L	16	1030	3	horseshoe plain wg, TW=10um
K	17	980	3	horseshoe plain wg, TW=10um
Row 1 (560 tall)				
J	18	1030	2	horseshoe plain wg, TW=10um
I	19	980	2	horseshoe plain wg, TW=10um
H	20	1030	1	horseshoe MRR, g=600 nm
G	21	1030	1	horseshoe MRR, g=450 nm
F	22	1030	1	horseshoe MRR, g=300 nm
E	23	1030	1	horseshoe MRR, g=150 nm
D	24	980	1	horseshoe MRR, g=600 nm
C	25	980	1	horseshoe MRR, g=450 nm
B	26	980	1	horseshoe MRR, g=300 nm
A	27	980	1	horseshoe MRR, g=150 nm

To optimize the fabrication process, the fabrication can be carried in the Material Research Laboratory (MRL) and the Micro and Nanotechnology Laboratory (MNTL). The first EBL step and metal liftoff were completed at the Singh Nanofabrication facility. To continue the fabrication, a descum operation using the Diener O2 descum tool was performed. The sample was dry etched to remove the a-Si/Si₃N₄ using (PECVD) Plasmalab Freon using the etchant SF₆ to remove 173

nm a-Si and 83 nm of Si₃N₄ (partial etch). A second EBL step was performed to define the rectangular region that covers the grating coupler and extends an extra 50 nm into the taper and into the DBR. Next, chromium is deposited using CHA Evaporator with a target thickness of ~20-30 nm. Metal lift off is repeated with acetone at 80 °C to remove undeveloped electron lithography beam resist. The combined metal masks are used to deep etch the remaining 317 nm of Si₃N₄ using Plasmalab Freon with SF₆. Wet etching is performed to remove nickel with etchant, nickel etch TFB. A timed dry etch of a-Si is carried out to remove undesired region above the taper, waveguide and DBR which is approximately 150 nm. Then, the remaining a-Si is wet etched and undercut ~50 nm on the edges of Cr mask using the developer, AZ 826 MIF. A SiO₂ layer as top cladding is deposited using Trion PECVD or PlasmaLab PECVD. Finally, the sample was cleaned with isopropyl alcohol, deionized water, and nitrogen flow.

3.6 Device Characterization

3.6.1 Experimental Set-up

Once fabrication is completed, the devices will be tested by collecting the transmission spectrum. The experimental test setup consists of a tunable laser with a wavelength range of 1450 to 1590 nm. A schematic of the experimental test station is given in Fig. 3.33. The output from the laser is fed into an optical isolator (OI). The output isolated from the optical isolator is connected to the polarization controller (PC) and then to an optical polarizer (OP) to isolate the polarized signal of interest. The signal is split 90:10 where the lesser amount of the signal goes to the reference photodetector (PD) to monitor the input power. The remaining power enters a 3-port circulator which has three ports: input, transmission, and reflection. The signal exiting the transmission port enters the device under test (DUT) and measures its output on another photodetector for transmission. The reflection port of the 3-port circulator is subsequently measured by another photodetector to determine the amount of reflected light. For the DUT, a grating coupler test station was built to test devices at normal incident light. It includes a custom sample holder, optical microscope, and a 2D pitch reducing optical fiber array (PROFA-2D) for optical coupling.

To test the surface grating coupler devices, an optical test station for vertical coupling was constructed. Professor Goddard and I designed and built the optical test station with

recommendations from the Air Force Research Laboratory (AFRL). See Appendix A for assembly of the optical test station for surface grating-based devices.

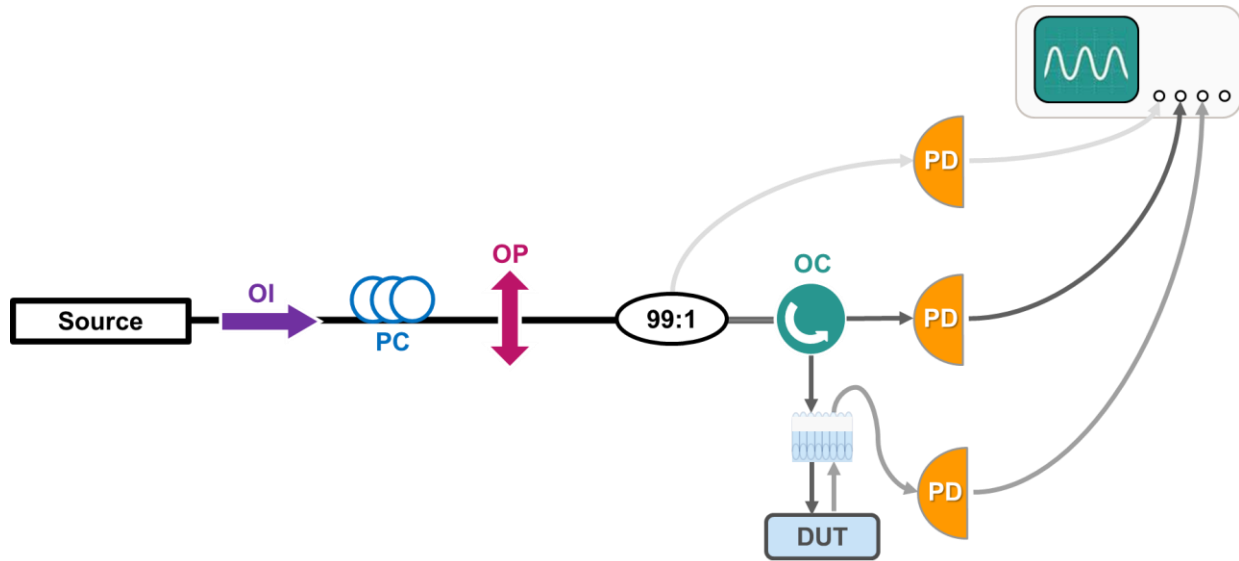


Figure 3.33. Schematic of the optical test station.

Like the edge coupling method, the optical fiber array is connected to the optical network for a device under testing. The light sources utilized for testing are the 1460-1590 nm tunable laser, a 1310 nm laser, a 980 nm laser, an 850 nm laser, and a 1030 nm super luminescent diode. When operated below threshold, the lasers act like a light emitting diode and have a broad emission spectrum. Right above threshold, the laser spectrum includes this broad spontaneous emission spectrum plus a peak from laser emission whose measured width depends on the resolution of the spectrometer. The vertical grating coupler is the device under test. The optical spectral analyzer (OSA) is an Agilent 86141B. The OSA can measure 600-1700 nm with a user settable resolution of 0.08, 0.1, 0.2, 0.5, 1.0, 2.0, 5.0, or 10.0 nm and a wavelength span that is typically chosen as 100x the resolution. When the 1460-1590 nm tunable laser is used, a simple DET01CFC photodetector plus logarithmic amplifier is used instead of the OSA. The PDA100A photodetector and a fiber coupled red laser diode are used for system alignment but neither is used for testing. Their operating characteristics are found in tables 3.16 and 3.17.

Table 3.16. Table of photodetectors utilized in optical testing station

Photodetector	Wavelength Range	Peak Wavelength	Gain Adjusted Range	Detector
PDA100A	400-1100 nm	970 nm	70 dB	Silicon PIN
DET01CFC	800-1700	1550 nm	N/A	InGaAs PIN

Table 3.17. Optical sources utilized for testing of the grating couplers. The spectral coverage is defined as the wavelengths for which the light source creates a signal on the OSA that is at least 20 dB above the noise floor.

Optical Sources	Type	Spectral Coverage	Threshold Current Typical	Threshold Current Max	Optical Output Power
850 nm	Diode	800-870 nm	20 mA @ 852 nm	50 mA @ 857 nm	40 mW
980 nm	Diode	950-1020 nm	10.9 mA	---	18 mW
1030 nm	SLED	900-1200 nm	-----	250 mA (operating)	6 mW
1310 nm	Diode	1200-1400 nm	N/A	N/A	1 mW
1550 nm	Tunable	1460-1590 nm	N/A	N/A	1 mW

3.6.2 Device Results

The data was collected with the help of student Raman Kumar. The high contrast grating coupler was designed for 1030 nm with a uniform grating period, a side DBR, and a waveguide extension. The grating coupler was tested over a wavelength ranging from 800 nm to 1500 nm. The noise floor was the average of the spectra from 950 nm to 100 nm and 1100 nm to 1150 nm on a linear scale. Then, the average spectra were normalized to the source. In Fig. 3.34, the maximum transmission with the 850 nm laser occurs at 840.3 nm and the insertion loss was 36.6 dB. Unfortunately, the transmission was not significantly above the noise floor. It was difficult to determine the bandwidth due to multiple neighboring narrow peaks of a few nanometers in width.

Between the wavelength range of 900 nm and 1200 nm, there was a broad bimodal peak with a maximum at 1113 nm and an insertion loss of 45.4 dB, shown in Fig. 3.35. The bimodal peaks in the grating transmission are due to the broad bimodal peak of the super-luminescent diode. After subtracting off the source, the insertion loss of the grating coupler is relatively flat. The second peak was at 1034.4 nm with the insertion loss of 44.8 dB. The bandwidth of the bimodal peaks was 88.8 nm. Over the range 1100 nm to 1500 nm, there was another peak at 1308 nm with the insertion loss of 42.7 dB in Fig. 3.36. The sharp peak arose from the laser signal. The bandwidth was less than a nanometer. For the measurements with the 1310 nm laser source, the insertion loss was around 42 dB.

Table 3.18 shows the comparison of the simulation and experimental results. The experimental results showed significantly more loss than predicted even assuming the aSi layer was over etched. There may be several reasons for this discrepancy. First, the PROFA fiber array was manufactured and optimized for 850 nm, but we utilized it for testing across the entire wavelength range. There is good light transmission in the fiber at wavelengths below 1200 nm, but we attribute about 5-10 dB of the observed loss to the PROFA above 1200 nm. Second, the properties of the PECVD deposited amorphous silicon such as the refractive index and extinction coefficient likely deviated from those in the published result of Pierce et al. [41, 42]. For this reason, the grating characteristics for the fabricated device differ from those used in simulation. A non-zero extinction coefficient in the amorphous silicon significantly increases the grating coupler loss. Furthermore, not achieving the desired refractive index would affect the optimal grating parameters such as grating pitch and thickness of the high index layer. These two differences could have redshifted and reduced the overall spectral response. To explore these hypotheses, a 2D sensitivity simulation was conducted to study the effect of common fabrication errors and the results are shown in Figs. 3.37 and 3.38.

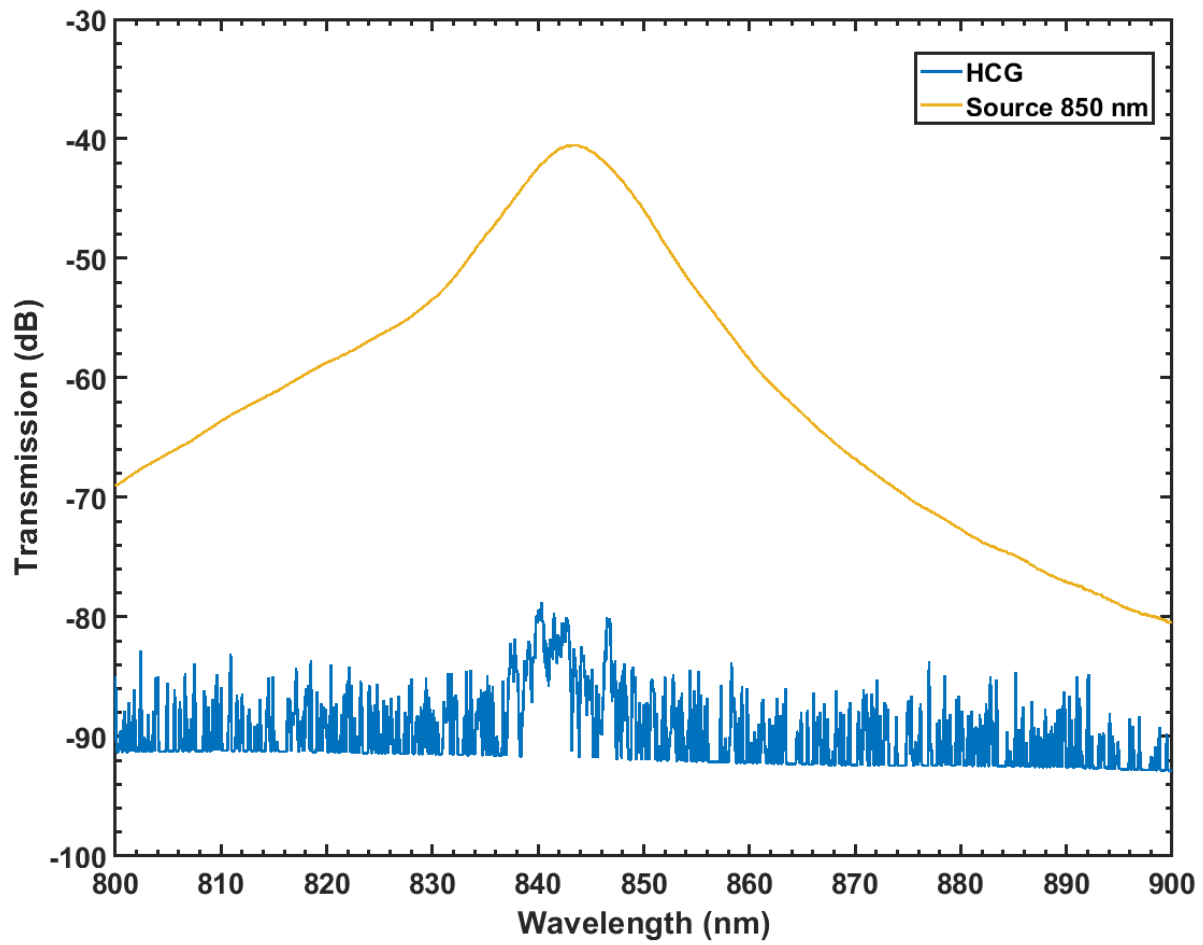


Figure 3.34. Measured spectra of the grating coupler with a source wavelength of 850 nm when the spectrum analyzer is set to a resolution of 0.2 nm.

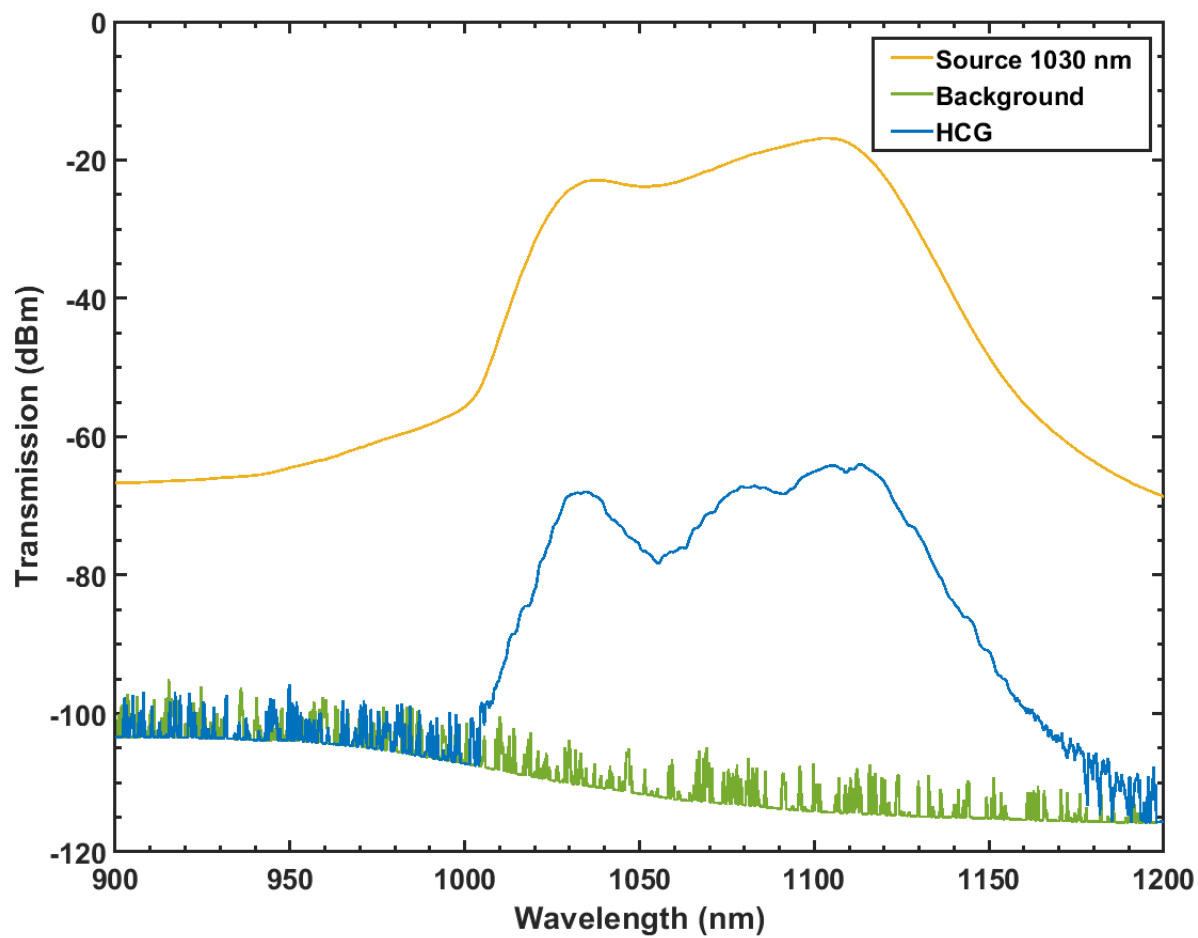


Figure 3.35. Measured spectra of the grating coupler with a source wavelength of 1030 nm when the spectrum analyzer is set to a resolution of 5 nm.

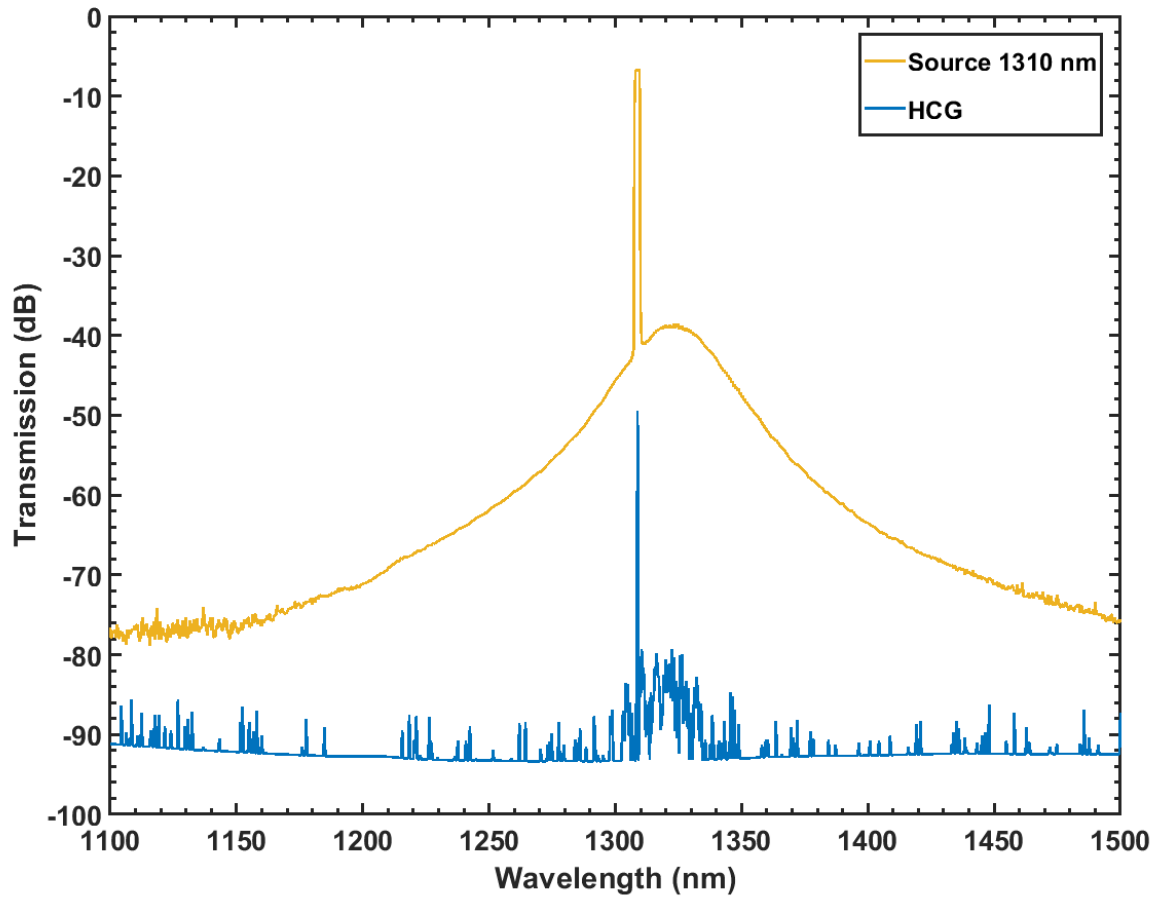


Figure 3.36. Measured spectra of the grating coupler with a source wavelength of 1310 nm when the spectrum analyzer is set to a resolution of 0.2 nm.

Table 3.18. Comparison of peak transmission spectra of experimental and simulation data.

#	Experimental		Comsol 2D Fully Etch		Lumerical 2D Fully Etched		Lumerical 3D Fully Etched	
	λ (nm)	Transmission (dB)	λ (nm)	Transmission (dB)	λ (nm)	Transmission (dB)	λ (nm)	Transmission (dB)
1	840.3	-36.6	840	-297.1	840.7	-5.7	840.7	-14.9
2	1034	-44.8	1035	-24.9	1034.1	-6.6	1034.1	-15.3
3	1113	-45.4	1110	-21.1	1113.2	-20.3	1113.2	-18.4
4	1308	-42.7	1310	-317.4	1308.5	-26.6	1308.5	-25
5	1323	-38.5	1320	-323.7	1322	-26	1322	-24.5

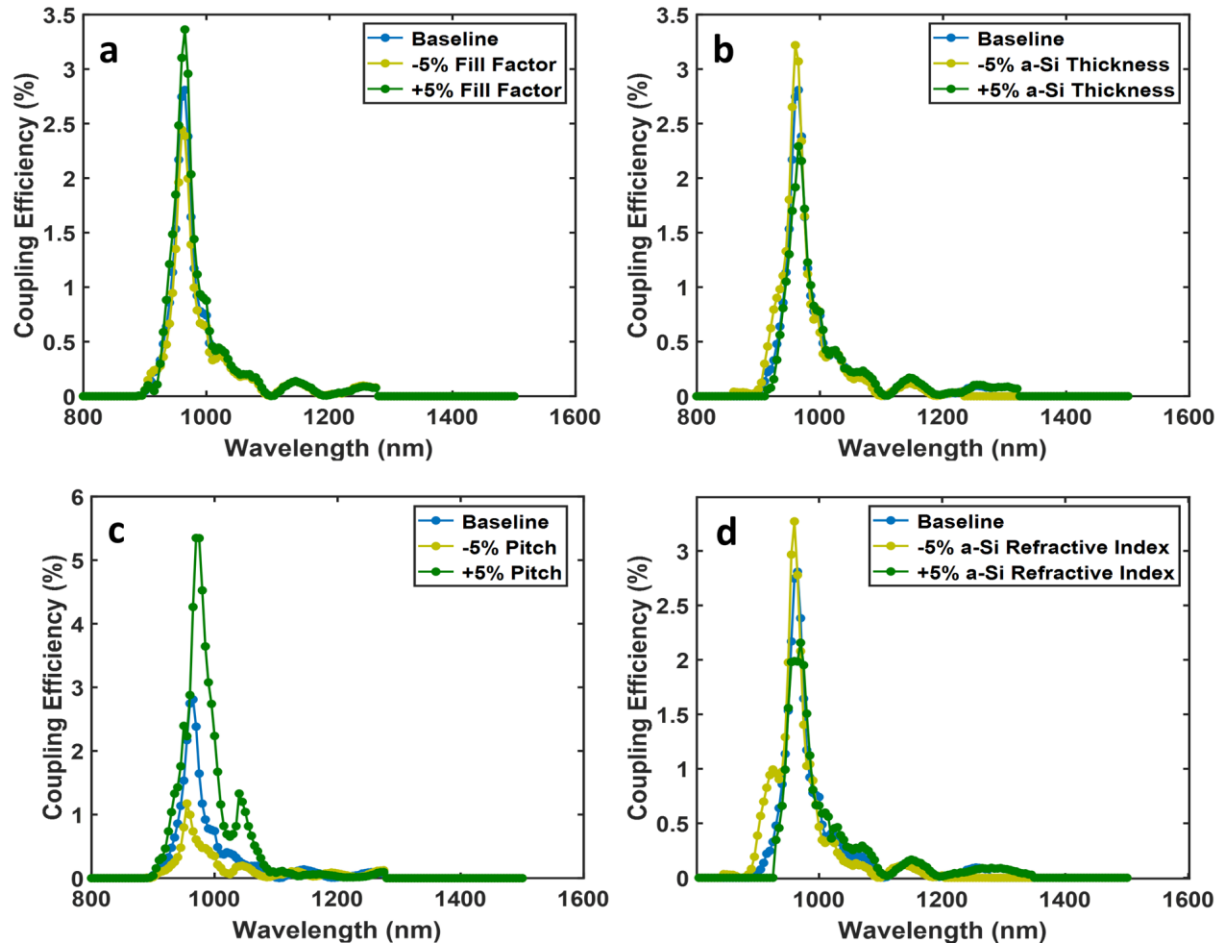


Figure 3.37. 2D Comsol simulation to study the fabrication tolerance of 5% applied to grating parameters: (a) fill factor, (b) amorphous silicon thickness, (c) pitch, and (d) refractive index of amorphous silicon. The baseline assumes the silicon nitride layer is fully etched.

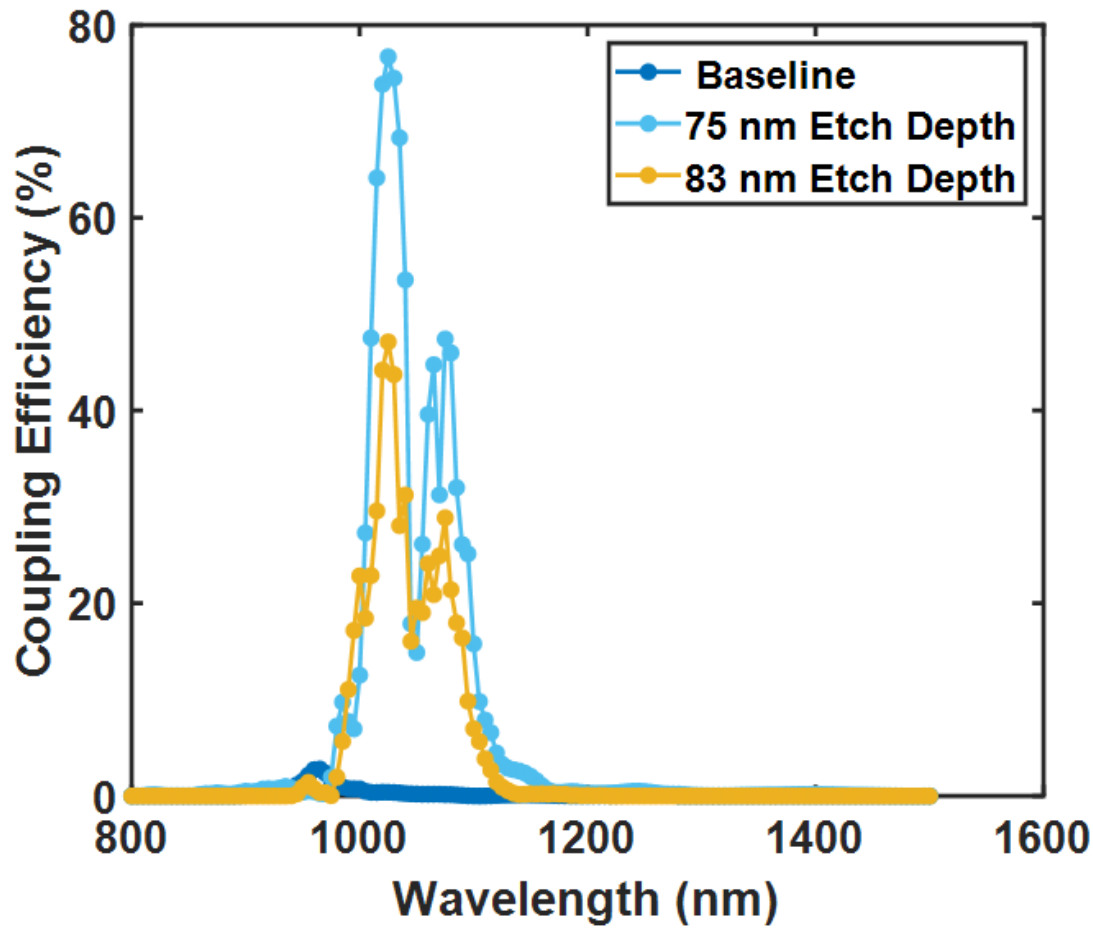


Figure 3.38. 2D Comsol simulation of the coupling efficiency of the grating coupler device: fully etched baseline (400 nm), optimal 75 nm etch depth, and 83 nm etch depth into silicon nitride.

While 2D simulations are instrumental to quickly determining the baseline features, 3D simulations provide a more realistic representation of the physical problem. Typically, large 3D simulations are performed in Finite-Difference-Time-Domain (FDTD) given its exceptional speed at the expense of accuracy. The FDTD relies on time-domain Maxwell equations implementation for computational electromagnetics. Hence, Lumerical's FDTD solver is utilized to compute the performance of grating coupler in 3D. As a direct comparison, the 2D simulations are performed in Lumerical and COMSOL shown in Fig. 3.39. Figure 3.40 shows the 2D and 3D cross sections of the grating coupler in the Lumerical software.

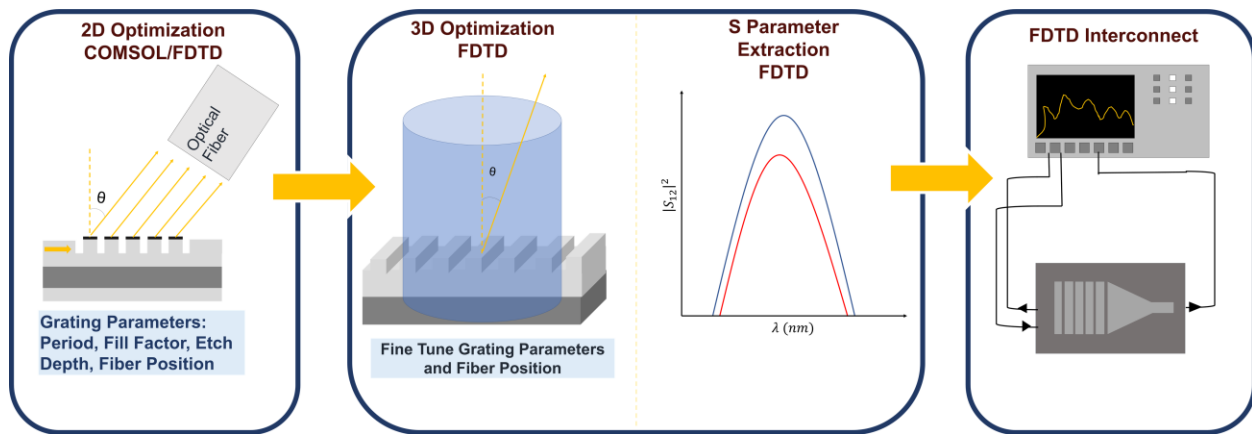


Figure 3.39. Grating coupler optimization using 2D and 3D simulations. Post 3D optimization, extract the s-parameters and model using the Interconnect PDK module provided by Lumerical.

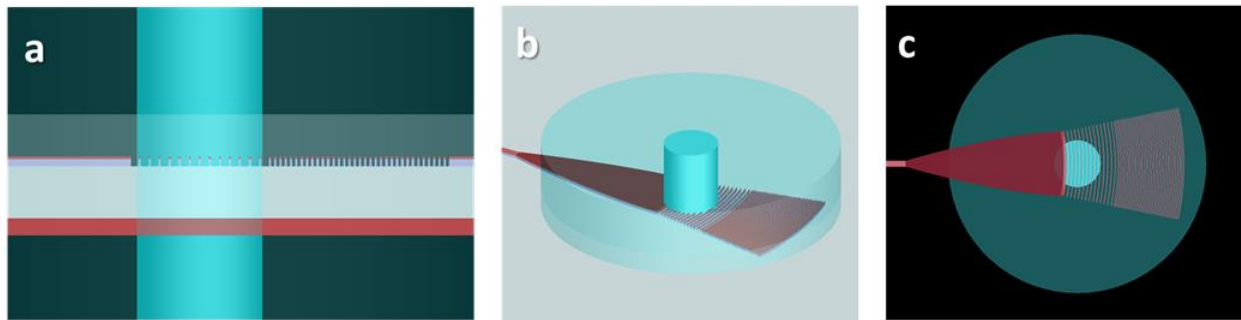


Figure 3.40. Simulation of a fiber to grating coupler. (a) 2D cross section of a grating coupler from the 2D FDTD solver, (b) 3D grating coupler, and (c) top down view of 3D coupler in 3D FDTD solver.

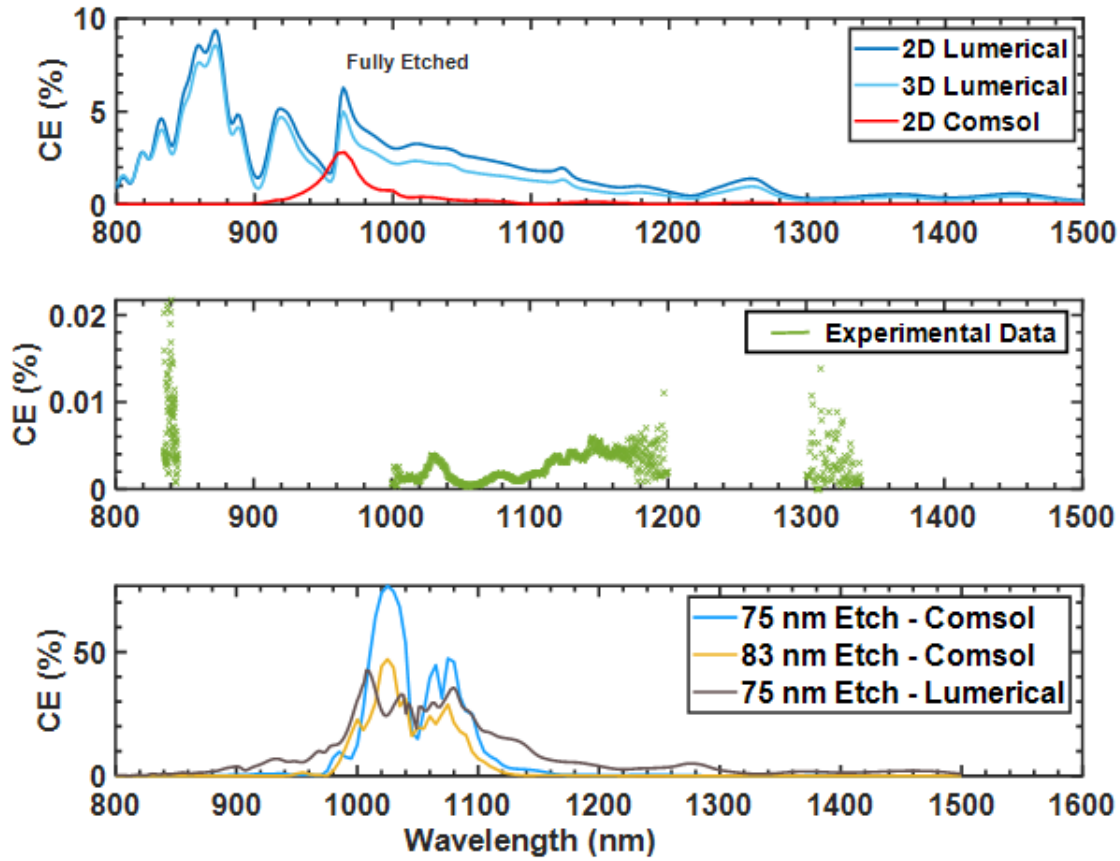


Figure 3.41. Comparison of spectra from simulation and experimental data of the grating coupler. (a) 2D and 3D simulation of a fully etched grating coupler and partially etched grating coupler in Comsol and Lumerical, (b) experimental results, and (c) 2D simulations for different etch depths.

The worst-case scenario was explored in which the grating coupler is fully etched. As a result, the coupling efficiency significantly dropped as shown in Fig. 3.41.

3.7 Design of a High-Efficiency Flexible Grating Coupler

Optical polymers have garnered a huge amount of interest as an ancillary material system in integrated photonic applications given their low-cost, versatility, rapid mass-producibility and flexibility. Particularly, these organic materials, utilized as passive components, are widely employed to assist on-chip adiabatic tapering, array waveguiding, and intra- and inter-connects [43, 44]. Their salient features noted above enable a broad range of applications: imaging, sensing, solar cells, display technologies and wearable devices. Flexible optical waveguide and coupling

structures can significantly improve the spatial arrangement on integrated photonic chips shown in Fig. 3.42. Despite these characteristics, a major drawback that impedes their wide adoption in integrated photonics is their low index contrast. The low index contrast lowers the optical confinement for waveguiding and precludes further reduction in footprint thereby inhibiting high integration density. The refractive indices of polymers are typically, 1.3 to 1.7 [45]. To cope with the low index contrast, high index nanoparticles can be incorporated in the polymer matrix. However, they can degrade functionality given the uncontrolled modification. Jointly, the fabrication processes can greatly affect the device performance due to cracks and surface roughness. The device can be slightly heated above its glass temperature to allow thermal reflow to alleviate cracks and roughness to create a smooth and uniform surface.

To date, most on-chip photonic devices are composed of rigid structures, which are limited in scalability potential, are non-conformable, and are not cost-effective for large-scale manufacturing [46]. To power an on-chip flexible optical device requires grating couplers to efficiently provide in-coupling and out-coupling of light [47]. Alternatively, polymer based 45° mirrors are used to couple light, but suffer from numerical aperture mismatch which requires a lens to compensate at the expense of substantially increasing the size and cost. The coupling efficiency has a strong dependence on the various geometrical parameters of the grating structure [19]. Due to the low index contrast of polymer systems, the theoretical coupling efficiency is extremely low at 30%. For this reason, several works have explored the introduction of high index layers to boost the index contrast. However, high index layers increase the complexity of fabrication to meet design tolerances. In this work, the all-polymer surface grating is apodized in the vertical direction by varying the height of each tooth and groove linearly along the grating.

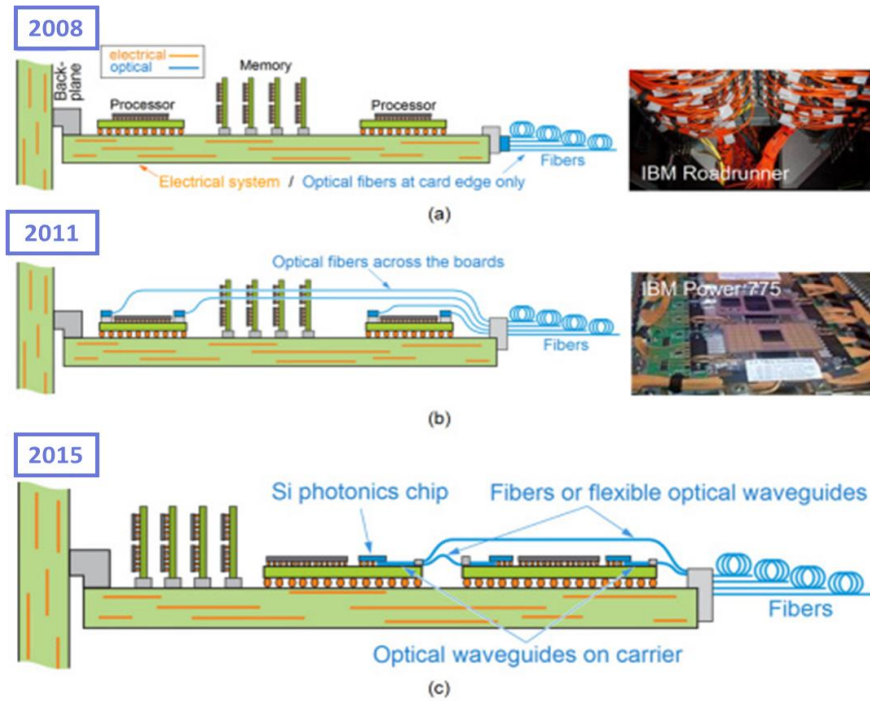


Figure 3.42. Roadrunner, a supercomputer developed by IBM that does not contain optical interconnects (a). Fibers connected to IBM's HPC system, Power 775 (b). Flexible optical waveguides connecting chips and board edge (c) [43].

Since its inception, there have been many technological advances in data and optical communications to address the growing demands for high data speeds and carrying capacity. A key issue is efficiently coupling optical signals into waveguides. The coupling efficiencies of polymer grating couplers are very low. The highest coupling efficiencies of polymer grating structures resulted from the inclusion of a high index material. These works are provided in Table 3.19. Therefore, this work focuses on developing an all-polymer grating coupler to retain its flexible nature. Optical communications wavelengths are 1310 and 1550 nm because they minimize dispersion and attenuation, respectively, for optical fiber. Given the available equipment in our lab, 1550 nm was designated as the operating wavelength.

Table 3.19 Comparison of polymer and hybrid polymer grating structures demonstrated in the literature.

#	CE (dB)	λ (nm)	Tilt (°)	Design	Δn	Refs.
1	-4.5	1550	45	Polyimide waveguide with SiN overlay and SiO ₂ bottom cladding	0.19	43
2	-0.86	800	0	Hypothetical high index waveguide material (n=1.8) with metal mirror and SiO ₂ for top cladding and substrate	0.34	44
3	-6	633	43.4	High index (polyvinyl-chloride-based) on thin high index inorganic layer on low index (acrylate-based) on PET substrate	0.2	45
4	-1.74	633	N/A	A focusing blazed grating with poly - methylstyrene waveguide on PMMA	0.5	46
5	-9.27	1550	45	liquid polysilisiquioxane (PSQ) resin high RI waveguide and low RI liquid polysilisiquioxane (PSQ) resin with Si ₃ N ₄ overlay	0.07	47
6	-4.9	1550	10	Air-Suspended SU-8 grating	0.57	48
7	-2.1	1550	0	Apodized high index polymer grating with air cladding	0.64	This work

An all-polymer material system was carefully chosen that possesses a high index contrast. In this work, UV-curable polymers by Norland product, NOA 164, were selected for their high refractive index as waveguide material. The choices for the bottom cladding are a spin-on dielectric: IC1-1000 or NOA 1315. IC1-1000 requires thermal curing. Previously, silicon dioxide and porous dioxide were considered as the bottom cladding, but were excluded due to their rigidity. Their refractive indices are in Table 3.20. Polyethylene terephthalate (PET), a plastic substrate, is chosen as the substrate [49].

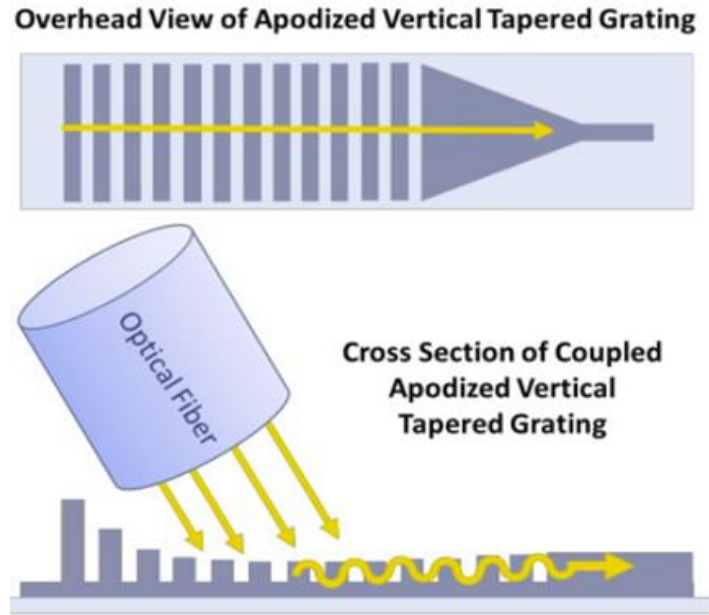


Figure 3.43. (top) Overhead view of the polymer grating structure. (bottom) Optical fiber coupled into a vertically apodized polymer grating structure.

Table 3.20. Refractive indices of the optical polymers considered for this study

Polymer	Refractive Index	Ref.
NOA 170	1.7	50
NOA 164	1.64	51
NOA 1315	1.315	51
SOD (IC1-1000)	1.433	52
PET	1.575	53

The single mode regime is determined for the grating system with SOD and NOA 1315 as the bottom cladding. The optimal waveguide thickness is 700 nm with a BOX layer thickness of 10 μm . Following identification of a single mode polymer waveguide dimensions, 2D FEM simulations of the grating coupler shown in Fig. 3.43 were performed using COMSOL to optimize the grating parameters. The initial results shown revealed little coupling into the structure when fully etched. The highest coupling efficiency of this grating coupler is around 7%, which is comparable to measure coupling efficiencies of all-polymer gratings. Therefore, another study performed varying the etch depth to boost the coupling efficiency by 35%. For directionality, an

in-plane DBR was appended to the grating coupler and apodized as performed above. The design is given in Table 3.21. The apodized grating structure reached a coupling efficiency of nearly 62%. This is the highest reported coupling efficiency for an all-polymer system. The field profile for this simulation is shown in in Fig. 3.44.

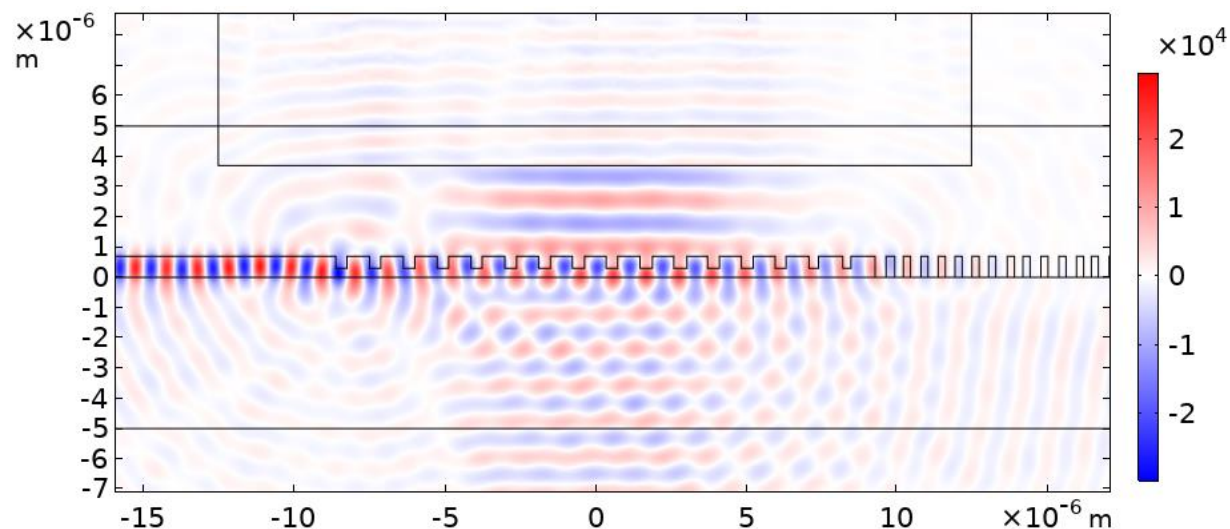


Figure 3.44. Profile of the z-component of the electric field for the design with the best efficiency.

Table 3.21. Optimal grating parameters of the flexible grating coupler.

GC Properties	Designs				
Grating Parameters	Full Etch	Partial Etch	Side DBR	Apodized GC	Apodized GC and Apodized DBR
Grating Period (nm)	1100	1122	1122	1122	1122
Etch Depth (nm)	700	414	400	400	400
Fill Factor (%)	60	67	67	67	67
Coupling Efficiency (%)	6.56	41.57	37.12	58.18	61.67

3.7.1 Fabrication Process and Experimental Set-up

The fabrication entails depositing the bottom cladding with a low refractive index onto the PET

substrate. The thickness should be at least 5 μm . Depending on the bottom cladding material, the curing may be thermal or using ultra-violet [UV] illumination. Afterwards, a submaster mold is created using gray-scale electron lithography to define the grating coupling pattern. A thin film layer of aluminum oxide is deposited onto the submaster mold using atomic layer deposition (ALD) to ensure the demolding process is efficient. The liquid waveguide material is then dispensed onto the submaster with the inverted substrate (bottom cladding/PET). The sample is UV cured with the high index material for waveguiding sandwiched between the substrate and submaster mold. The sample is demolded from the submaster mold. A conformal layer of high index material is dispensed on top of the sample and UV cured. If the desired film properties are achieved, the high index top cladding will be spun on using a spin coater, and subsequently cured using UV illumination. The resulting sample may be slightly heated to smooth the rough surface. The fabrication process is shown in Fig. 3.45. The optimization of the bottom cladding is found in Appendix C. For optimal device performance, consistent and reproducible thickness of spun-coated films for waveguiding and cladding layers is required [54]. For grayscale lithography using EBL, a dose calibration curve was determined for ZEP520a in Fig. 3.46. ZEP520a is a positive electron beam resist with high resolution and high sensitivity which makes it ideal for grayscale patterning.

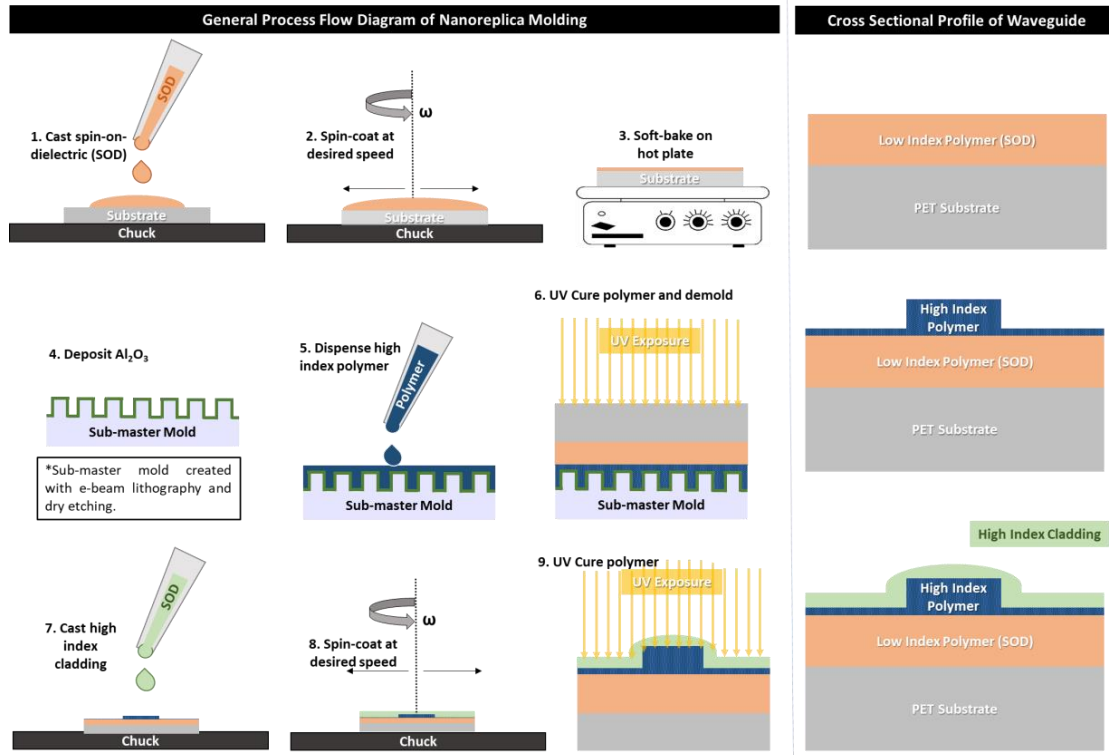


Figure 3.45. Process flow diagram of the all-polymer grating structure.

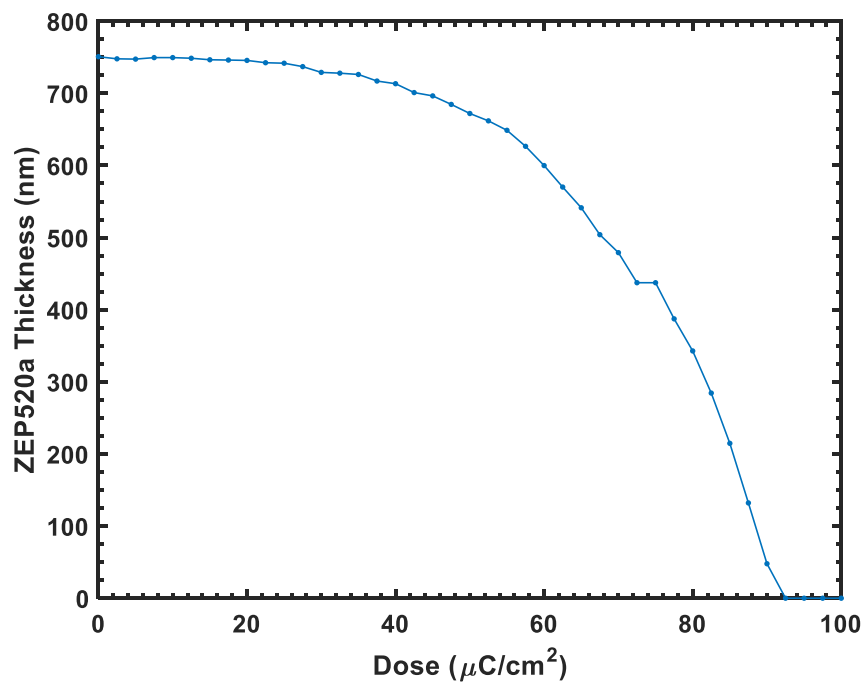


Figure 3.46. Dose calibration curve of ZEP520a for grayscale lithography. It is linear between 50 and 90 $\mu\text{C}/\text{cm}^2$.

3.8 S-matrix Optimization for Vertical Grating Couplers

Surveying the entire geometric parameter space by the "brute-force" approach to obtain the maximum device performance is inefficient and requires substantial computational resources (i.e., cluster computing). Furthermore, expanding the number of free parameters to explore nonlinear and topological spaces further increases the complexity and demand for computational resources. Those approaches often necessitate computationally intensive algorithms. Spurred by the need to alleviate the computational load, inverse design approaches are under intense exploration to optimize device performance based on pre-determined key metrics. Despite recent major advancements in photonics, the bar is as high as one sets it and subject to local maxima or minima entrapment. To gain insight regarding the upper performance limit of a device, several analytical methods have been proposed relying on coupled mode theory, S-matrix optimization, transfer matrix, and tight binding method. Recent works have demonstrated the vitality of analytical approaches towards exploring possible designs before intense computational effort ensues. Several studies have demonstrated the use of S-matrix formalism to determine the ideal coupling efficiency of various grating couplers, thereby enabling a pre-screening of useful designs and guiding design choices. Bunkowski et al. [55] developed an analytical framework based on S-matrix formalism to evaluate the performance of a three-port reflection grating for interferometric applications. In their S-matrix formalism, they assume the system is unitary and reciprocal. Building upon this work, Demeter et al. [56] adapted the three-port approach to explore the performance of a vertical grating coupler without substrate loss. In their work, modest improvement in the coupling efficiency was attained for a previously reported study of a grating coupler and subsequently verified by numerical simulations. Applying their approach to the proposed amorphous silicon HCG yields a coupling efficiency of 99.99% and backward reflection is 1.2×10^{-7} which is equivalent to approximately 69 dB of return loss. This represents the upper limit of coupling efficiency.

To mirror the practical embodiment of the HCG, we expound upon the aforementioned models to consider substrate loss and its effect by considering a 4-port model approach. A 4-port S-matrix

formalism is constructed to investigate the underlying physics and determine whether device coupling efficiency can be further enhanced. The light source is at normal incidence at Port 2. To add directionality, an in-plane distributed Bragg reflector (DBR) is placed at Port 1 to break the symmetry. Hence, the incident light is guided towards Port 3 with substrate loss at Port 4. The scattering matrix (S-matrix) is assembled considering reciprocity, symmetry, and unitary properties. The first case addresses loss towards the substrate without a substrate-induced Fabry-Perot cavity effect. We therefore assume there is no reflection from Port 4 back into Ports 1, 2, and 3. While the ideal case is studied, in practice, a fiber couples to a grating coupler where additional loss may arise from back-reflection into different diffraction orders. In addition, the field profile is not symmetrical when switching the input ports of a 4-port system due to mismatch between fiber and waveguide inputs. Despite the loss or change in modal profile, the power transfer between the modes is reciprocal.

The general scattering matrix is as follows to be adjusted to investigate substrate loss:

$$\mathbf{S} = \begin{bmatrix} r_{11} & t_{12} & t_{13} & t_{14} \\ t_{21} & r_{22} & t_{23} & t_{24} \\ t_{31} & t_{32} & r_{33} & t_{34} \\ t_{41} & t_{42} & t_{34} & r_{44} \end{bmatrix}$$

A system of equations is established based on the summed contributions at each port consisting of the complex free space field propagation factors multiplied by the reflection and transmission coefficients. Given the properties and material constraints of the grating coupler, the optimal parameters for each port transmission and reflection can be determined numerically. See Appendix B. Then, a grating coupler system can be designed to match these port parameters. This procedure is significantly faster than performing a parameter sweep of 2D or 3D simulations. However, the procedure does not guarantee that a design with these port parameters can be realized and so care must be taken to pick reasonable port parameters.

As a specific example, the cases in which there are reflective boundaries at Port 1, Port 2, and Port 3 are examined. To maximize the forward reflection and minimize back-reflections into the light source, a reflective boundary is placed at the input port to represent the effect of having a microlaser like a VCSEL present which contains a DBR to prevent light reflected into the laser

cavity. Light reflected towards the laser can damage the laser and generate unreliable output. The industry standard is less than 60 dB reflection. In simulation, a PEC boundary is placed at Port 2. The geometry is shown in Fig. 3.47. Results are discussed in Appendix B.

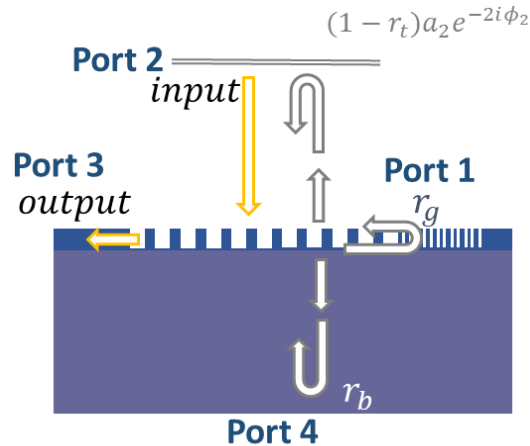


Figure 3.47. Modified 4-port approach containing 3 Fabry-Perot cavities.

3.9 References

- [1] Schmatz, M. B. J. O. K. V. "Optical Interconnects: Intra-system data transfer with light, 2005."
- [2] M. Paniccia, "The 50Gbps Silicon photonic Link," Intel.com, 2010. [Online]. Available: <http://blogs.intel.com/intellabs/2010/07/23/50g-link/>.
- [3] Biberman, Aleksandr, et al. "Broadband silicon photonic electrooptic switch for photonic interconnection networks." IEEE Photonics Technology Letters 23.5 (2011): 504.
- [4] Hino, Tomoyuki, et al. "A 10 Gbps x 12 channel pluggable optical transceiver for high-speed interconnections." Electronic Components and Technology Conference, 2008. ECTC 2008. 58th. IEEE, 2008.

- [5] Vlasov, Yuri A. "Silicon integrated nanophotonics for on-chip optical interconnects." European Quantum Electronics Conference. Optical Society of America, 2009.
- [6] Lifante, Ginés. Integrated photonics: fundamentals. John Wiley & Sons, 2003.
- [7] Horowitz, Mark, Chih-Kong Ken Yang, and Stefanos Sidiropoulos. "High-speed electrical signaling: Overview and limitations." *IEEE Micro* 18.1 (1998): 12-24.
- [8] D. A. B. Miller, "Physical Reasons for Optical Interconnection," Special Issue on Smart Pixels, *Int'l J. Optoelectronics* 11 (3), 155-168 (1997).
- [9] Miller, David AB. "Device requirements for optical interconnects to silicon chips." *Proceedings of the IEEE* 97.7 (2009): 1166-1185.
- [10] Pavesi, Lorenzo, and Gérard Guillot. "Optical interconnects." *Springer series in optical sciences* 119 (2006).
- [11] Bohr, Mark T. "Interconnect scaling-the real limiter to high performance ULSI." *Electron Devices Meeting, 1995. IEDM'95., International. IEEE, 1995.*
- [12] Cai, Shisheng, et al. "Review on flexible photonics/electronics integrated devices and fabrication strategy." *Science China Information Sciences* 61.6 (2018): 060410.
- [13] Atabaki, Amir H., et al. "Integrating photonics with silicon nanoelectronics for the next generation of systems on a chip." *Nature* 556.7701 (2018): 349.
- [14] K. Szczerba, T. Lengyel, M. Karlsson, P. A. Andrekson, A. Larsson, 94-Gbps 4-PAM using an 850-nm VCSEL, pre-emphasis, and receiver equalization, *IEEE Photon. Technol. Lett.* 28, p. 2519-2521, 2016.

- [15] Xie, Chongjin, et al. "Single-VCSEL 100-Gb/s short-reach system using discrete multi-tone modulation and direct detection." *2015 Optical Fiber Communications Conference and Exhibition (OFC)*. IEEE, 2015.
- [16] Kuchta, Daniel M., et al. "A 71-Gb/s NRZ modulated 850-nm VCSEL-based optical link." *IEEE Photonics Technology Letters* 27.6 (2015): 577-580, 201.
- [17] Feng, Milton, et al. "Current and future trend of energy/bit for high speed uncool optical links (50 Gb/s and 75° C)." *Photonics Society Summer Topical Meeting Series (SUM)*, 2017 IEEE. IEEE, 2017.
- [18] Rahim, Abdul, et al. "Expanding the silicon photonics portfolio with silicon nitride photonic integrated circuits." *Journal of Lightwave Technology* 35.4 (2017): 639-649.
- [19] Baets, Roel, et al. "Silicon Photonics: silicon nitride versus silicon-on-insulator." *Optical Fiber Communications Conference and Exhibition (OFC)*, 2016. IEEE, 2016.
- [20] Taillaert, Dirk, Peter Bienstman, and Roel Baets. "Compact efficient broadband grating coupler for silicon-on-insulator waveguides." *Optics letters* 29.23 (2004): 2749-2751.
- [21] Zaoui, Wissem Sfar, et al. "Cost-effective CMOS-compatible grating couplers with backside metal mirror and 69% coupling efficiency." *Optics express* 20.26 (2012): B238-B243.
- [22] Chen, Yang, et al. "High-efficiency apodized-imaging chip-fiber grating coupler for silicon nitride waveguides." *Optics letters* 41.21 (2016): 5059-5062.
- [23] Larrea, R. A., et al. "Compact focusing grating couplers for silicon horizontal slot waveguides." *Optics letters* 42.3 (2017): 490-493.
- [24] Xu, Pengfei, et al. "Fabrication-friendly high-efficiency silicon nitride grating coupler." *Lasers and Electro-Optics Pacific Rim (CLEO-PR)*, 2017 Conference on. IEEE, 2017.

- [25] Notaros, Jelena, et al. "Ultra-efficient CMOS fiber-to-chip grating couplers." Optical Fiber Communications Conference and Exhibition (OFC), 2016. IEEE, 2016.
- [26] Doerr, Christopher R., et al. "Wide bandwidth silicon nitride grating coupler." IEEE Photonics Technology Letters 22.19 (2010): 1461-1463.
- [27] Maire, Guillaume, et al. "High efficiency silicon nitride surface grating couplers." Optics Express 16.1 (2008): 328-333.
- [28] Sacher, Wesley D., et al. "Multilayer silicon nitride-on-silicon integrated photonic platforms and devices." Journal of Lightwave Technology 33.4 (2015): 901-910.
- [29] Wilmart, Q., et al. "A hybrid SOI/SiN photonic platform for high-speed and temperature-insensitive CWDM optical transceivers." Silicon Photonics XIII. Vol. 10537. International Society for Optics and Photonics, 2018.
- [30] Xu, Pengfei, et al. "Fabrication-friendly high-efficiency silicon nitride grating coupler." Lasers and Electro-Optics Pacific Rim (CLEO-PR), 2017 Conference on. IEEE, 2017.
- [31] Y. Chen, R. Halir, Í. Molina-Fernández, P. Cheben, and J. J. He, "High efficiency apodized-imaging chip-fiber grating coupler for silicon nitride waveguides," Opt. Lett., vol.41, pp. 5059-5062, October 2016.
- [32] J. Zou, Y. Yu, M. Ye, L. Liu, S. Deng, and X. Zhang, "Ultra efficient silicon nitride grating coupler with bottom grating reflector," Opt.Express vol. 23, 26305-26312, September 2015.
- [33] H. Zhang, C. Li, X. Tu, J. Song, H. Zhou, X. Luo, Y. Huang, M. Yu, G.Q. Lo, "Efficient silicon nitride grating coupler with distributed Bragg reflectors", Opt. Express, vol. 22, pp. 21800-21805, September 2014.

- [34] Taillaert, Dirk, et al. "An out-of-plane grating coupler for efficient butt-coupling between compact planar waveguides and single-mode fibers." *IEEE Journal of Quantum Electronics* 38.7 (2002): 949-955.
- [35] Mekis, Attila, et al. "A grating-coupler-enabled CMOS photonics platform." *IEEE Journal of Selected Topics in Quantum Electronics* 17.3 (2011): 597-608.
- [36] Apostolopoulos, Dimitrios, et al. "Photonic integration enabling new multiplexing concepts in optical board-to-board and rack-to-rack interconnects." *Optical Interconnects XIV*. Vol. 8991. International Society for Optics and Photonics, 2014.
- [37] Baets, Roel, et al. "Silicon Photonics: silicon nitride versus silicon-on-insulator." *Optical Fiber Communications Conference and Exhibition (OFC)*, 2016. IEEE, 2016.
- [38] Email communication with Chiral Photonics. Aug. 11, 2017
- [39] Kang, JoonHyun, et al. "Amorphous-silicon inter-layer grating couplers with metal mirrors toward 3-D interconnection." *IEEE Journal of Selected Topics in Quantum Electronics* 20.4 (2014): 317-322.
- [40] Marchetti, Riccardo, et al. "Reflector-less Grating-Coupler with a-0.9 dB Efficiency Realized in 260-nm Silicon-On-Insulator Platform." *Integrated Photonics Research, Silicon and Nanophotonics*. Optical Society of America, 2017.
- [41] D. T. Pierce and W. E. Spicer, Electronic structure of amorphous Si from photoemission and optical studies, *Phys. Rev. B* 5, 3017-3029 (1972).
- [42] Palik, Edward D., ed. *Handbook of optical constants of solids*. Vol. 3. Academic press, 1998.

- [43] Dangel, Roger, et al. "Polymer waveguides for electro-optical integration in data centers and high-performance computers." *Optics express* 23.4 (2015): 4736-4750.
- [44] Zhang, Ziyang, et al. "Hybrid photonic integration on a polymer platform." *Photonics*. Vol. 2. No. 3. Multidisciplinary Digital Publishing Institute, 2015.
- [45] Liu, Jin-gang, and Mitsuru Ueda. "High refractive index polymers: fundamental research and practical applications." *Journal of Materials Chemistry* 19.47 (2009): 8907-8919.
- [46] J. Hu, et al. "Flexible integrated photonics: where materials, mechanics and optics meet." *Optical Materials Express* 3.9 (2013): 1313-1331.
- [47] A. Mekis, et al. "A grating-coupler-enabled CMOS photonics platform." *IEEE Journal of Selected Topics in Quantum Electronics* 17.3 (2011): 597-608.
- [48] Bruck, Roman, and Rainer Hainberger. "Efficient coupling of narrow beams into polyimide waveguides by means of grating couplers with high-index coating." *Applied optics* 49.10 (2010): 1972-1978.
- [49] Pollard, M. E., et al. "Polymer waveguide grating couplers for low-cost nanoimprinted integrated optics." *Integrated Optics: Devices, Materials, and Technologies XVI*. Vol. 8264. International Society for Optics and Photonics, 2012.
- [50] *Light Sources and Technical Reports. Norland Products*,
www.norlandprod.com/adhesiveindex2.html. Accessed 6 June 2020.
- [51] Wang, Linghua, et al. "A polymer-based surface grating coupler with an embedded Si₃N₄ layer." *Journal of Applied Physics* 111.11 (2012): 114507.
- [52] Email communication from the company, Futurrex, Inc. (<http://futurrex.com/en/>).

- [53] *Polymer Properties Database*, Crows Polymer Science, 2020, polymerdatabase.com/polymer%20physics/Ref%/20Index%20Table2%20.html. Accessed 20 May 2020.
- [54] F. Song, et al. "Elastomeric polymer resonant waveguide grating based pressure sensor." *Journal of Optics* 16.6 (2014): 065702.
- [55] A. Bunkowski, O. Burmeister, K. Danzmann, and R. Schnabel, "Input-output relations for a three-port grating coupled Fabry-Perot cavity," *Opt. Lett.* 30(10), 1183–1185 (2005).
- [56] Demeter-Finzi, Anat, and Shlomo Ruschin. "S-matrix absolute optimization method for a perfect vertical waveguide grating coupler." *Optics Express* 27.12 (2019): 16713-16718.

Chapter 4: Summary and Future Work

4.1 Summary of Work and Contributions to the Field

The objective of this dissertation was to investigate different coupling mechanisms that could enhance the performance of sensing and integrated photonic devices. Particularly, we explored the tradeoffs of a hybridized system that enable highly sensitive optoplasmonic sensors when there is a multi-resonant coupling between a whispering gallery mode resonator, surface plasmon polaritons, localized surface plasmon, and/or plasmonic chain resonator. The sensitivity of the device was greatest when operating near an exceptional point and with transverse magnetic polarization giving rise to anti-symmetric electric field coupling between the concentric rings. The plasmonic slot waveguide microring resonator gives a bulk and binding sensitivity of 1340 nm/RIU and 105.3 fm/RIU, respectively, in water. The work builds upon the recent report of a 35 fm shift due to a binding event on the surface of the microsphere with a plasmonic chain of gold nanorods [1]. In comparison, the proposed sensor design in this work provides a three-fold increase of sensitivity, albeit the microspheres have a higher quality factor than microring resonators. Figure 4.1 puts the results of this work in context relative to the roadmap of other technologies. This technology could be utilized by several biological, environmental, and chemical sensing companies where silicon microring resonators are utilized as the foundation. Such coupling of multi-resonant systems can benefit quantum plasmonics, quantum sensing, optoelectronics, nanoplasmonics, and solar cell technologies. In 2018, Scientific American listed plasmonic sensing as one of the top ten emerging technologies [2]. Coupling plasmonic devices to photonic devices bring together the notable merits of highly confined electric fields and low loss.

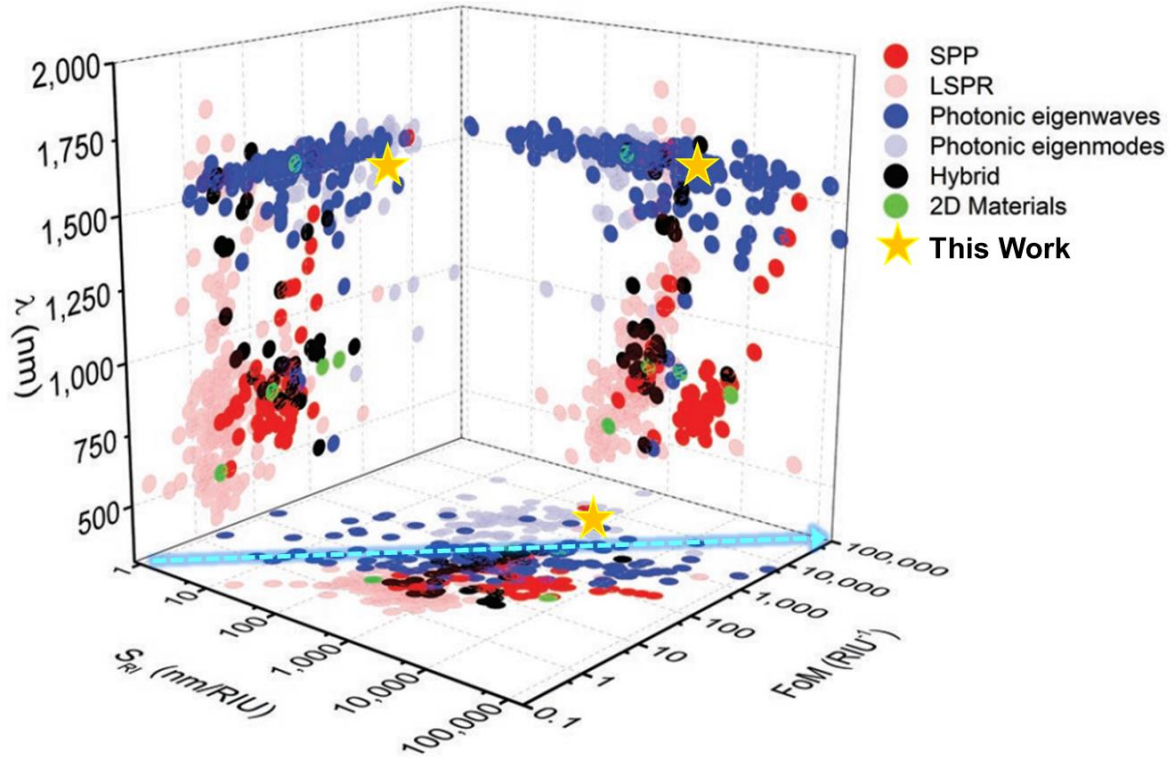


Figure 4.1. Adapted technology map comparing the sensitivity and figure of merit (FOM) of various optical refractive index sensors. The plasmonic slot waveguide microring resonator device is represented by the yellow star. The light blue dash line points towards the desired direction of higher sensitivity and FOM. A desirable optical refractive index sensor possesses high sensitivity and a large figure of merit [2].

A major contribution of this dissertation is the increased coupling efficiency of a grating coupler by varying the effective index of each grating period cell by overlaying with a high contrast material or by varying the vertical height of each grating tooth. This enabled the creation of high-efficiency couplers in normally low index contrast material systems such as Si_3N_4 and polymers. Mode matching was achieved by apodization sequentially from the output of the waveguide towards the in-plane distributed Bragg reflector. The simulated coupling efficiencies of 93.8% and 62% were achieved for inorganic and all-polymer material systems, respectively. These are the highest reported values for their respective material systems. To alleviate back reflections into the optical source, an optimized partially reflective in-plane distributed Bragg reflector was placed on the opposite of the grating coupler (near output). This method can be adapted for coupling to microcavity lasers such as a light-emitting transistor, vertical cavity transistor laser, and vertical-cavity surface-emitting laser. Having a fabricable robust method to significantly boost coupling

efficiency independent of wavelength and materials can significantly benefit the photonics industry and make progress towards photonic-electronic integration. Furthermore, it does not require computationally intensive algorithms to identify a high-performance grating coupler design. This simple, robust approach can be implemented on a personal computer.

4.2 Lessons Learned and Future Work

Due to time constraints and limited resources, not all simulated works were fabricated and tested. Several key directions are discussed to continue the work of this dissertation.

At the time of the fabrication of the bowtie nanostructure coupled to microring resonator, fabrication was challenging due to the electron lithography misalignment and proximity correction. To continue fabrication, there is now an electron- and laser-beam lithography software, Genisys BEAMER, where these issues are easily alleviated along with bias on size. Furthermore, we would have greatly benefited from an automated end coupling test station to reduce the time of data collection. This could be achieved by incorporating automated motor controllers and creating a program in LabVIEW to pinpoint the location of the greatest intensity for input and output. For biosensing measurements, an enclosure of the sensor under testing will permit better temperature control and prevent the evaporation of solvents. This could be achieved by fabricating a microfluidic chamber to house the sensor and permit a continuous flow of solution under testing as shown in Fig. 4.2.

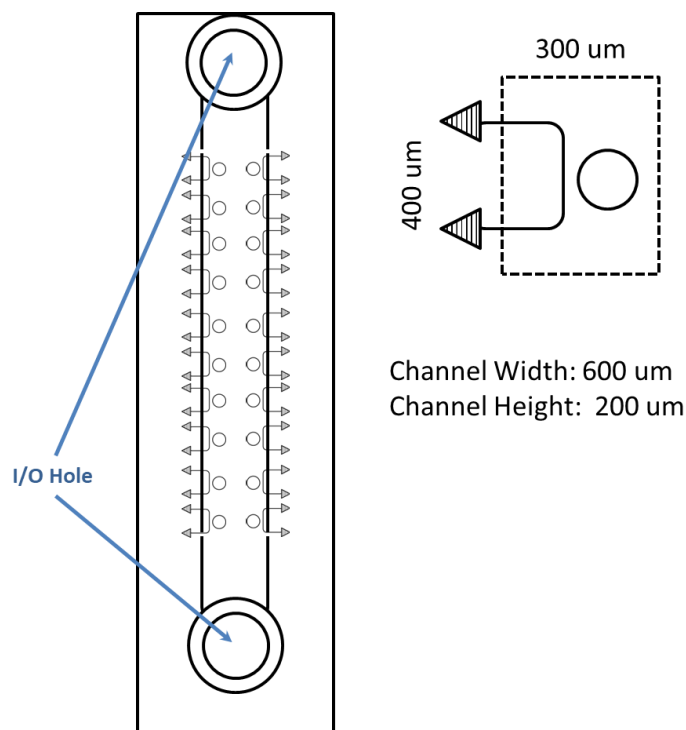


Figure 4.2. Possible microfluidic layout (not drawn to scale) for the biosensing of the coupled plasmonic chain-microring resonator device. The I/O hole represents the inlet and outlet.

To expand on the plasmonic nanostructure coupled microring resonators, different nanostructures should be explored to identify highly sensitive plasmonic nanostructures and their arrangement. This includes exploring topology optimization of the plasmonic layer to refine the resonant coupling. When plasmonic dimers are present, optical trapping is possible. Optical trapping will attract nearby molecules of interest, reducing the time for a binding event to occur.

Due to the electron beam lithography becoming unavailable on campus, fabrication work resumed at the Singh Nanotechnology Center at the University of Pennsylvania. While at the University of Pennsylvania, I trained on all tools including electron beam lithography to fabricate the grating coupler. Having trained on all tools provided in-depth insight into practical aspects to consider for computational simulation. Moving forward, the next step for the high-efficiency grating coupler work is to demonstrate heterogeneous integration of the device with a vertical transistor cavity laser or vertical-cavity surface-emitting laser. To facilitate the integration of the grating coupler to a microcavity laser, the grating coupler must be buried in several microns of oxide, and followed by the application of the planarization technology of chemical and mechanical polishing (CMP).

An epoxy such as benzocyclobutene (BCB) can be spun onto the surface as an interlayer for adhesive bonding. The most important element of integration is the alignment in x and y positions to coincide with the coupling efficiency computed from simulations. This can be achieved by modifying the current test station with additional micropositioners and a custom holder for the microcavity laser to align to the grating coupler. Also, a temperature controller needs to be affixed to the stage of the test station. Once the optimal position is determined, the adjoined samples are heated to cure the adhesive bond. The optimal amount of adhesive must be determined before integrating the final devices.

4.3 References

- [1] Arbabi, Ehsan, et al. "Hybrid whispering gallery mode/plasmonic chain ring resonators for biosensing." *Applied Physics Letters* 105.23 (2014): 231107.

- [2] Xu, Yi, et al. "Optical refractive index sensors with plasmonic and photonic structures: promising and inconvenient truth." *Advanced Optical Materials* 7.9 (2019): 1801433.

Appendix A: Construction of Optical Test Station for Vertical Grating Coupling

The optical test station comprises an optical stereo microscope, Thorlabs motorized translation stage with kinesis k-cube stepper motor controller, a custom sample holder, fiber array holder platform, and a custom v-groove fiber array. See Figs. A.1 and A.2.

Amscope 2x-225x Trinocular Boom Stand
Stereo Zoom Microscope + 9MP Camera

Thorlabs XYZ Motorized Translation Stage
with Kinesis® K-Cube Stepper Motor
Controller (**25mm** travel distance with
5 μ m absolute position repeatability and a
theoretical min step size of **0.5nm**)

Custom Sample Holder Platform

Custom V-groove Array Holder (not
pictured)



Sample Holder Cover to hold
samples in place



Milled out rectangle with two edges
allows us to repeatably position the
sample relative to fiber (fixed)

Since grating coupler will be patterned at
a specific offset from the sample corner,
alignment will be very quick

Figure A.1. Surface grating test station (on the left) and custom sample holder (on the right).

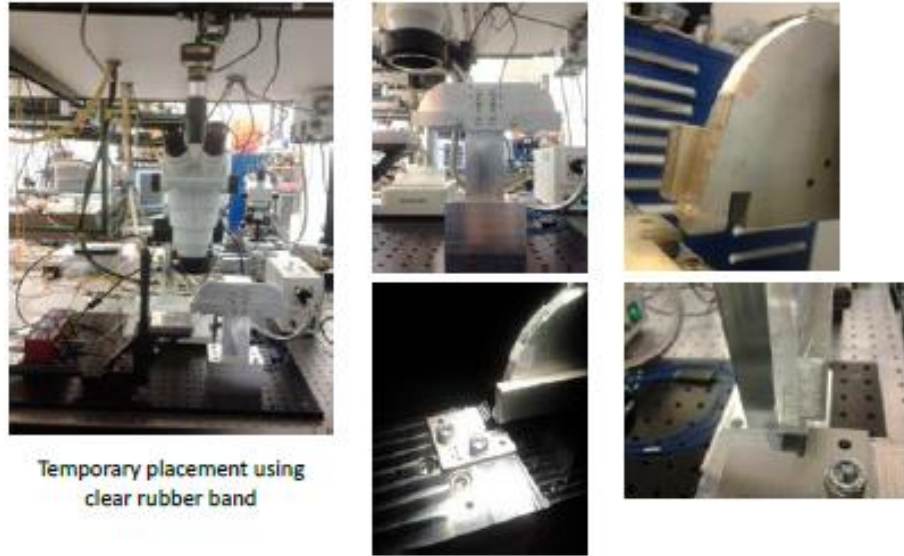


Figure A.2. Snapshots of surface grating test station with custom v-groove array and holder. Close up of the v-groove optical fiber and custom holder.

The optical microscope is an Amscope 2x-225x trinocular zoom stand stereo microscope with a 9 MP camera. The motorized controller contained a travel distance of 25 mm, absolute position repeatability of 5 μm , and a minimum theoretical step size of 0.5 nm. The custom sample holder consists of a machined aluminum rectangular platform with a milled cover piece to hold the sample in place. The optical fiber array contained eight-channel optical fibers with interspacing of the optical fibers are 250 μm . For wavelengths of 850 nm, 980 nm, and 1550 nm, the mode field diameter of the fiber core is 5, 6, and 8 μm , respectively. The diameter of the mode field profile scales linearly with wavelength.

The stage control of x, y, and z positions was manually controlled using the legacy software, APT (Advanced Positioning Technology) software package, provided by Thorlabs. To test the controller system, a photochemically etched sample was provided by Aditi Udupa. The gallium arsenide sample contained a 200- μm by 200- μm feature with a 10° etched slope. In this test, I aligned the sample to optical fiber manually by using the greatest voltage region to find the region which had the greatest optical output in Fig. A.3. The reflection results are plotted in Fig. A.4.

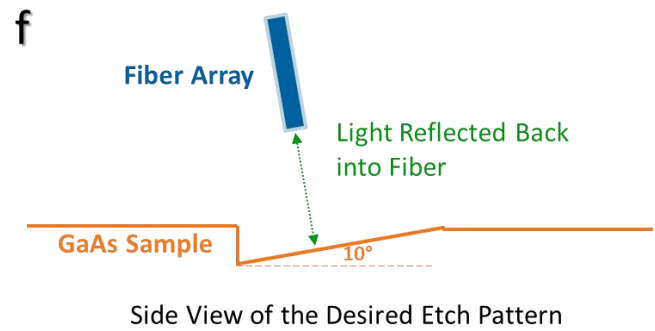
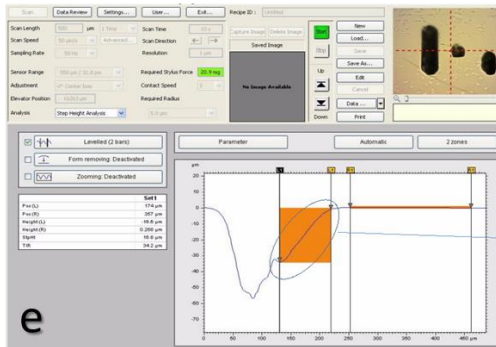
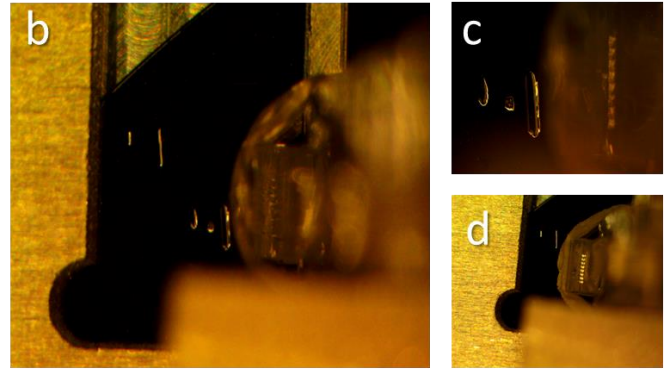
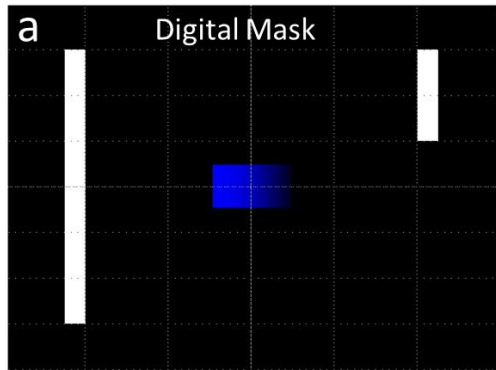


Figure A.3. (a) Digital mask of a photochemically etched sample. (b-d) Optical image of the device under testing with fiber array. (e) Profilometry of the sample after being photochemically etched. (f) Sketch of the side profile of the sample under test.

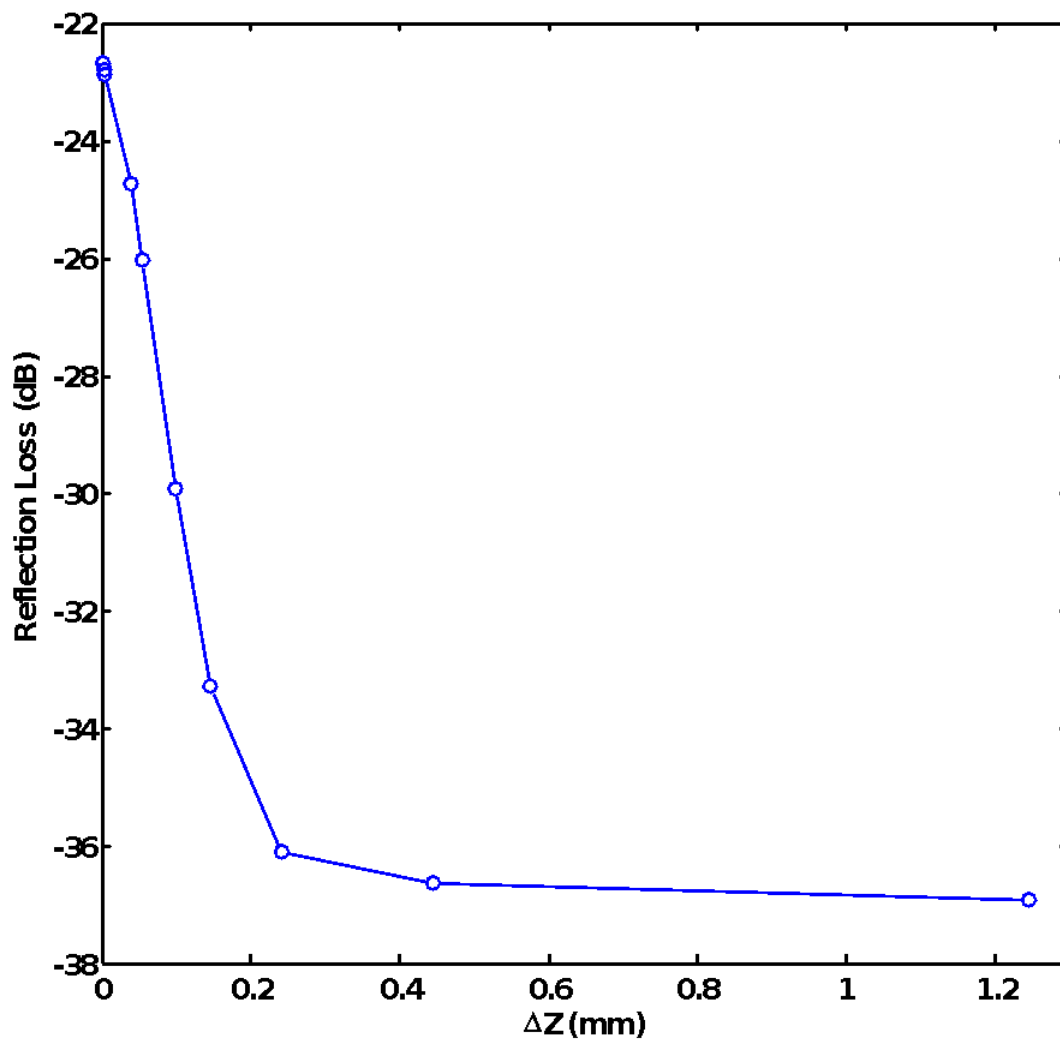


Figure A.4. Reflected loss as a function of change in z distance from the sample.

To automate testing and improve alignment, Professor Goddard wrote LabVIEW programs that controlled x, y, and z positions using an X-Box controller to find the lateral region with the greatest transmission. In Fig. A.5, there is a snapshot of the Labview program and key bindings of the X-Box controller.



Figure A.5. LabVIEW program to automate control of x, y, and z positions of the stage using an X-box joystick controller. The bottom left computer screen shows a truncated image from a sample under the microscope that has the word "transmission" on it. The X-box joystick controller with corresponding programmed actions (on the right).

For testing of the devices, the optical test station was later modified to contain an improved fiber array holder, side mirror, and interchangeable fiber arrays designed for certain wavelengths. The optical fiber array utilized for testing was the PROFA optical fiber array for 850 nm. The mode field diameter was $5.5 \mu\text{m}$ at a wavelength of 780 nm. The interspacing between the seven channels of optical fibers is $37 \mu\text{m}$.

Appendix B: S-matrix Optimization for Vertical Grating Couplers

The Fabry-Perot effect is investigated by considering the substrate (see Fig. B.1). Due to the presence of the silicon substrate, a Fabry-Perot cavity will form between the grating and the substrate. In our grating coupler design, the substrate is silicon. To improve the substrate-induced Fabry-Perot cavity, a purely reflective boundary at Port 4 is considered as a best-case approximation; however, silicon is very absorptive. We achieve a low loss reflective boundary by incorporating a vertical DBR stack as a bottom mirror ($r_b=1$). To optimize the forward transmission, two Fabry-Perot cavities are incorporated into the 4-port grating coupler at Port 1 and Port 3. The reflective boundaries are located at the in-plane DBR and the silicon substrate.

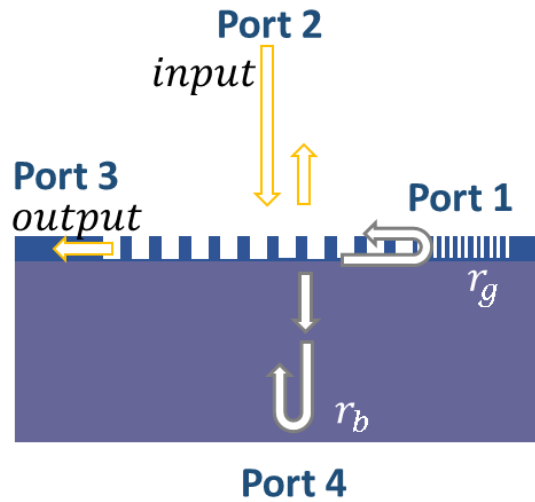


Figure B.1. 4-port approach to consider substrate effect.

An ideal surface grating coupler for photonic integration should meet the following objectives: (1) minimize back reflection into the light source, (2) minimize transmission into substrate, and (3) maximize the coupling efficiency. A vertical grating coupler alone cannot meet the aforementioned objectives. To achieve those aims, a vertical grating coupler can be inserted within a Fabry Perot cavity enclosed by a partially reflective DBR and a highly reflective DBR. The analytical approach was derived in collaboration with Professor Goddard. The partially reflective DBR is placed at

front end of the grating coupler that enters the desired waveguide port. A bottom DBR reflector is carefully placed below the grating to achieve ideal reflection as shown in Fig. B.2. These elements are judiciously engineered to achieve near 100% coupling efficiency.

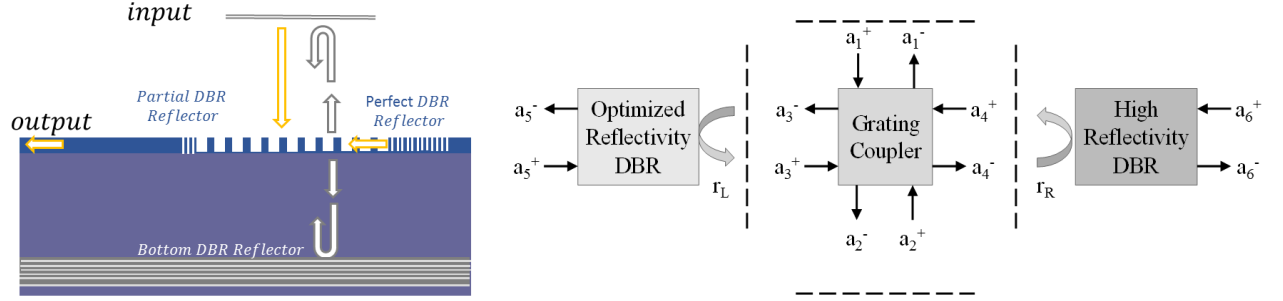


Figure B.2. Schematic of grating coupling (left) and equivalent S-matrix formalism (right).

The 4-port scattering matrix for a general grating coupler is given below.

$$\begin{pmatrix} a_1^- \\ a_2^- \\ a_3^- \\ a_4^- \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} & S_{13} & S_{14} \\ S_{12} & S_{22} & S_{23} & S_{24} \\ S_{13} & S_{23} & S_{33} & S_{34} \\ S_{14} & S_{24} & S_{34} & S_{44} \end{pmatrix} \begin{pmatrix} a_1^+ \\ a_2^+ \\ a_3^+ \\ a_4^+ \end{pmatrix} \quad (\text{B.1})$$

where we have used the fact that the matrix is symmetric because the grating coupler is a passive and made of reciprocal materials. Note that we do not assume the matrix is unitary because the system may be lossy, i.e., there might be light scattering into higher order waveguide modes or into free space and these are not included in the four defined ports.

The embedded vertical grating coupler between two in-plane DBRs is analogous to an add-drop microring resonator system whereby the critical coupling can occur and 100% of the light gets coupled from the input to the through the port at resonance. For the embedded vertical grating coupler, all light is coupled into the waveguide at Port 3 when the DBR mirrors have appropriately chosen reflectivity for the given grating coupler efficiency and no light is lost to the substrate. We assume the in-plane DBRs are lossless and can be represented by the 2x2 symmetric unitary

matrices below with complex coefficients r_L , t_L , r_R , and t_R . This specific choice of phase for the matrix elements is possible because we can move the locations of the output reference planes for ports 5 and 6.

$$\begin{pmatrix} a_3^+ \\ a_5^- \end{pmatrix} = \begin{pmatrix} r_L & j|t_L| \\ j|t_L| & r_L^* \end{pmatrix} \begin{pmatrix} a_3^- \\ a_5^+ \end{pmatrix} \quad (\text{B.2})$$

$$\begin{pmatrix} a_4^+ \\ a_6^- \end{pmatrix} = \begin{pmatrix} r_R & j|t_R| \\ j|t_R| & r_R^* \end{pmatrix} \begin{pmatrix} a_4^- \\ a_6^+ \end{pmatrix} \quad (\text{B.3})$$

Combining these with the generalized scattering matrix and solving yields:

$$\frac{a_5^-}{a_1^+} = j|t_L| \frac{S_{13} + r_R(S_{14}S_{34} - S_{13}S_{44})}{1 - r_L S_{33} - r_R S_{44} + r_R r_L (S_{33}S_{44} - S_{34}^2)} \quad (\text{B.4})$$

$$\frac{a_6^-}{a_1^+} = j|t_R| \frac{S_{14} + r_L(S_{13}S_{34} - S_{14}S_{33})}{1 - r_L S_{33} - r_R S_{44} + r_R r_L (S_{33}S_{44} - S_{34}^2)} \quad (\text{B.5})$$

$$\frac{a_2^-}{a_1^+} = S_{12} + \frac{r_L S_{13}(S_{23} + r_R S_{24}S_{34} - r_R S_{23}S_{44}) + r_R S_{14}(S_{24} + r_L S_{23}S_{34} - r_L S_{24}S_{33})}{1 - r_L S_{33} - r_R S_{44} + r_R r_L (S_{33}S_{44} - S_{34}^2)} \quad (\text{B.6})$$

$$\frac{a_1^-}{a_1^+} = S_{11} + \frac{r_L S_{13}^2(1 - r_R S_{44}) + r_R S_{14}^2(1 - r_L S_{33}) + 2r_L r_R S_{13}S_{14}S_{34}}{1 - r_L S_{33} - r_R S_{44} + r_R r_L (S_{33}S_{44} - S_{34}^2)} \quad (\text{B.7})$$

We want to not direct any light to the right, so we set $t_R = 0$. Thus, we can choose $r_R = e^{j\varphi}$ for some angle φ . Given the parameters of the scattering matrix, and noting that $|t_L| = \sqrt{1 - |r_L|^2}$, we can find the optimal r_L numerically that maximizes the coupling efficiency $T = \left| \frac{a_5^-}{a_1^+} \right|^2$ from the fiber to the output waveguide. From this result, the number of DBR pairs and the length of the phase shifting waveguide extensions can be computed.

Figures B.3 and B.4 show the field profile for the a-Si HCG and the plain Si₃N₄ grating couplers. Tables B.1 and B.2 provide the values for the respective scattering matrices. From this data, the side DBRs can be designed.

Table B.1. S-Parameter matrix of a-Si HCG with uniform periodicity.

a-Si Uniform Grating				
	Port 1	Port 2	Port 3	Port 4
$S_{1\#}$	0.027123-0.095613i	-0.64235-0.065145i	-0.64235-0.051444i	-0.065514+0.13997i
$S_{2\#}$	-0.63769+0.093064i	0.089771+0.38014i	0.20435-0.47700i	0.009756-0.09390i
$S_{3\#}$	-0.63770+0.093064i	-0.20435-0.4770i	0.089761-0.38015i	0.009754-0.093405i
$S_{4\#}$	0.084300+0.12395i	-0.047954-0.065145i	-0.047950-0.065142i	0.55274-0.44781i
Absorption	0.13703	0.15634	0.15634	0.44723

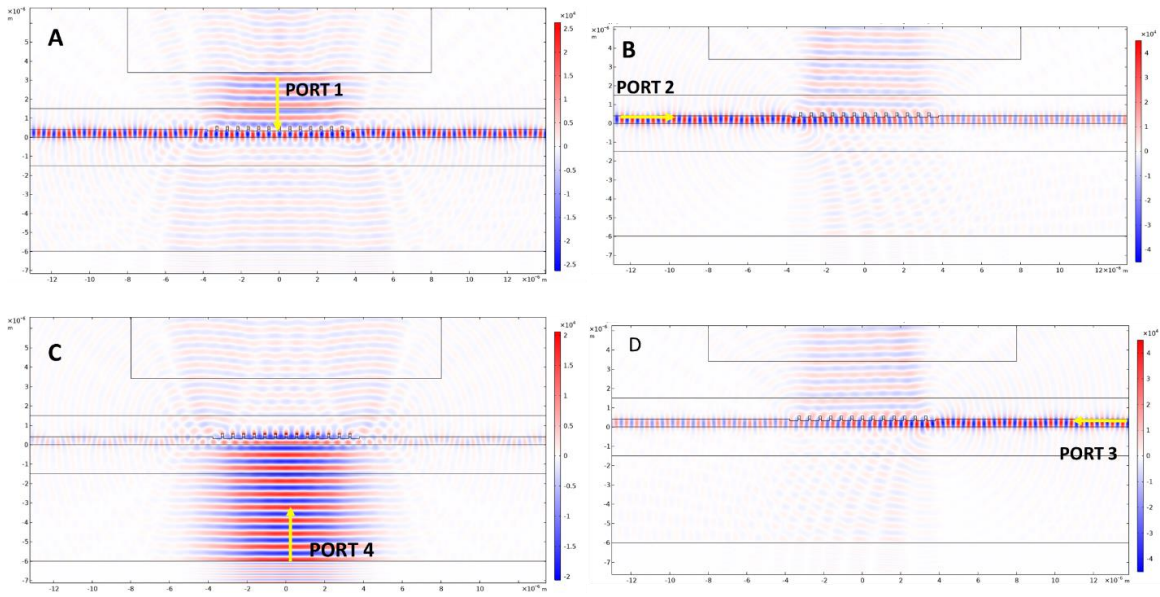


Figure B.3. Electric field profile, E_z , for the HCG without side DBRs for the cases where the incident field is at port (a) 1, (b) 2, (c) 3, and (d) 4.

Table B.2. S-Parameter matrix of silicon nitride with uniform periodicity.

Si ₃ N ₄ Uniform Grating				
	Port 1	Port 2	Port 3	Port 4
$S_{1\#}$	0.19598+0.17023i	0.51369-0.056162i	-0.55617-0.028086i	-0.055617+0.028086i
$S_{2\#}$	0.48856-0.17024i	0.094363+0.17787i	-0.11198-0.37159i	0.24655-0.27167i
$S_{3\#}$	0.48856-0.17033i	-0.11198-0.37159i	0.094332+0.17790i	0.24655-0.27168i
$S_{4\#}$	-0.27666+0.48721i	-0.034127-0.37566i	-0.034127-0.37566i	-0.0071276-0.59327i

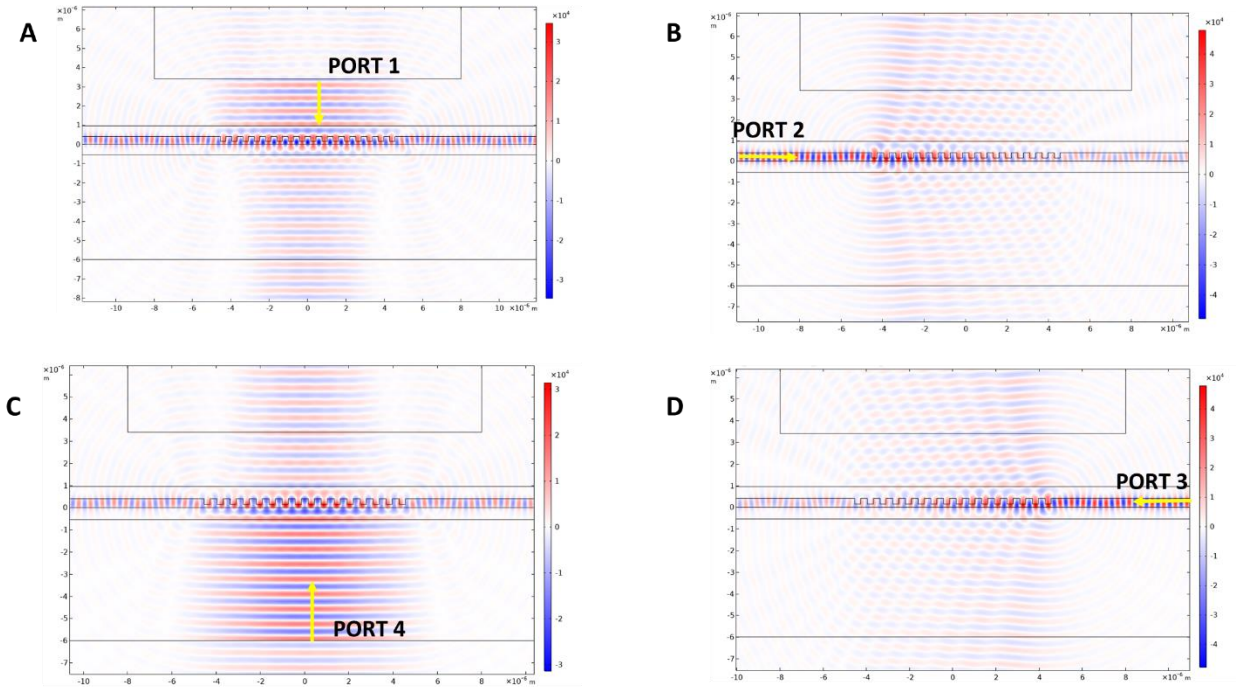


Figure B.4. Electric field profile, E_z , for the pure silicon nitride grating coupler without side DBRs for the cases where the incident field is at port (a) 1, (b) 2, (c) 3, and (d) 4.

Appendix C: Preliminary Flexible Grating Coupler Fabrication

The fabrication entails depositing the bottom cladding with a low refractive index onto the PET substrate. The thickness should be at least 3 μm . Depending on the bottom cladding material, the curing may be thermal or using ultra-violet illumination. Afterwards, a submaster mold is created using gray-scale electron lithography to define the grating coupling pattern. A thin film layer of aluminum oxide is deposited onto the submaster mold using atomic layer deposition (ALD) to ensure the demolding process is efficient. The liquid waveguide material is then dispensed onto the submaster with the inverted substrate (bottom cladding/PET). The sample is UV cured with the high index material for waveguiding sandwiched between the substrate and submaster mold. The sample is demolded from the submaster mold. A conformal layer of high index material is dispensed on top of the sample and UV cured. The high index top cladding will be spun on using a spin coater, and subsequently cured using UV illumination. The resulting sample may be slightly heated to smooth the rough surface. The fabrication process is shown in Fig. C.1.

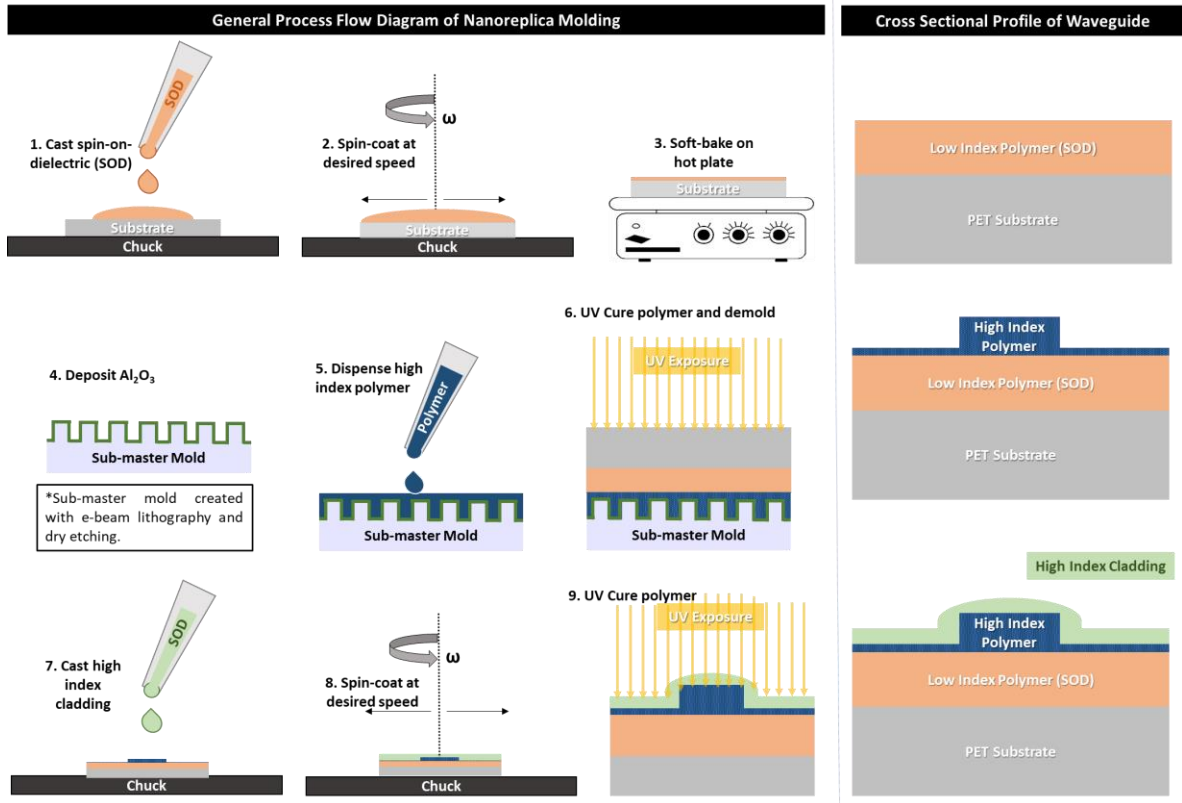


Figure C. 1. Process flow diagram of the all-polymer grating structure.

The first step of the fabrication was studied, which is to deposit the bottom cladding with optimal thickness and minimum roughness. Commonly, spin-coating is employed to apply a uniform thin film to a substrate using centrifugal force. It is a widely used technique to create thin films in the microelectronics industry and is currently adapted to produce flexible electronic and photonic devices. For optimal device performance, the consistent and reproducible thickness of spun-coated films for waveguiding and cladding layers is required [1]. The fabrication steps include initially spin-coating the bottom cladding, spin-on-dielectric, onto a substrate. Herein, the key parameters for the spin-coat process are determined and a model is established using a fractional factorial experiment.

Table C.1. Proposed Fractional Factorial Design

Factor	Parameters	Low - 1	Center 0	High + 1
X₁	Spin Rate (rpm)	2000	2500	3000
X₂	Soft Bake (°C)	100	150	200
X₃	# Spin Coats	1	3	5
X₄	Time (s)	40	50	60
X₅	# Droplets	7	11	15

A 2^{5-2} fractional factorial design, as tabulated in Table C.1, is performed using JMP statistical software package to determine the main effects due to the factors: spin rate, spin duration, soft bake temperature, volume, and number of spin-coated layers. The response variable is thickness. A resolution III design was selected to pinpoint the main effects only, ignoring the interaction effects. Each experiment consists of 8 conditions and 3 center points with a total of 11 samples. Center points were included to check for systemic error and nonlinearity.

An 8" silicon wafer was cleaved into 11 squares of 2 cm by 2 cm area to serve as the substrate. Varied volumes between 7 and 15 drops of spin-on-dielectric solution, ICI-1000, were applied and spun at different spin rates and durations. The acceleration ramp was kept at 500 rpm/s for all runs. Afterwards, the spun samples were placed on a hot plate of different temperature settings between 100 °C to 200 °C for one minute. Additionally, the number of layers applied to the substrate varied from 1 to 5 layers to determine scalability and consistency. Thin film measurements were performed using the SemiconSoft Mprobe 40 system over a wavelength range of 400-1000 nm at normal incidence. The Cauchy model based on planar two-layer (thin film, substrate) system was used to compute the thicknesses.

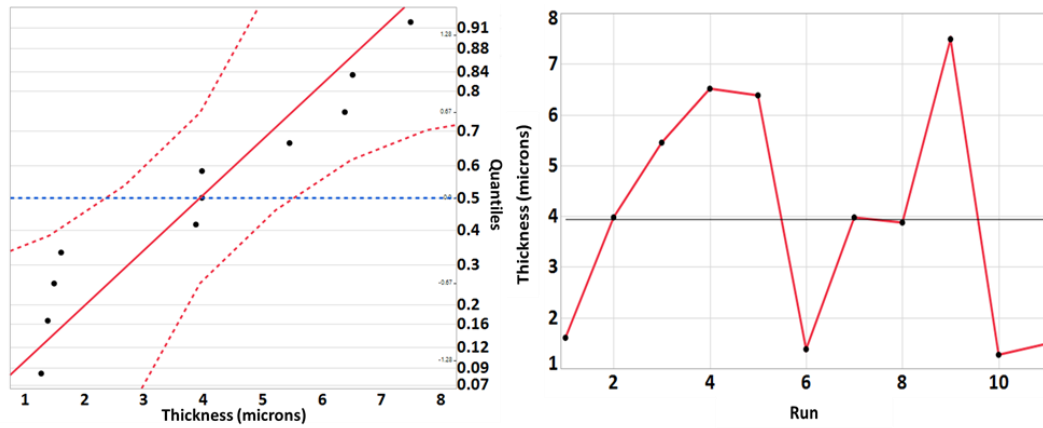


Figure C.2. Normal quantile (left) and time series (right).

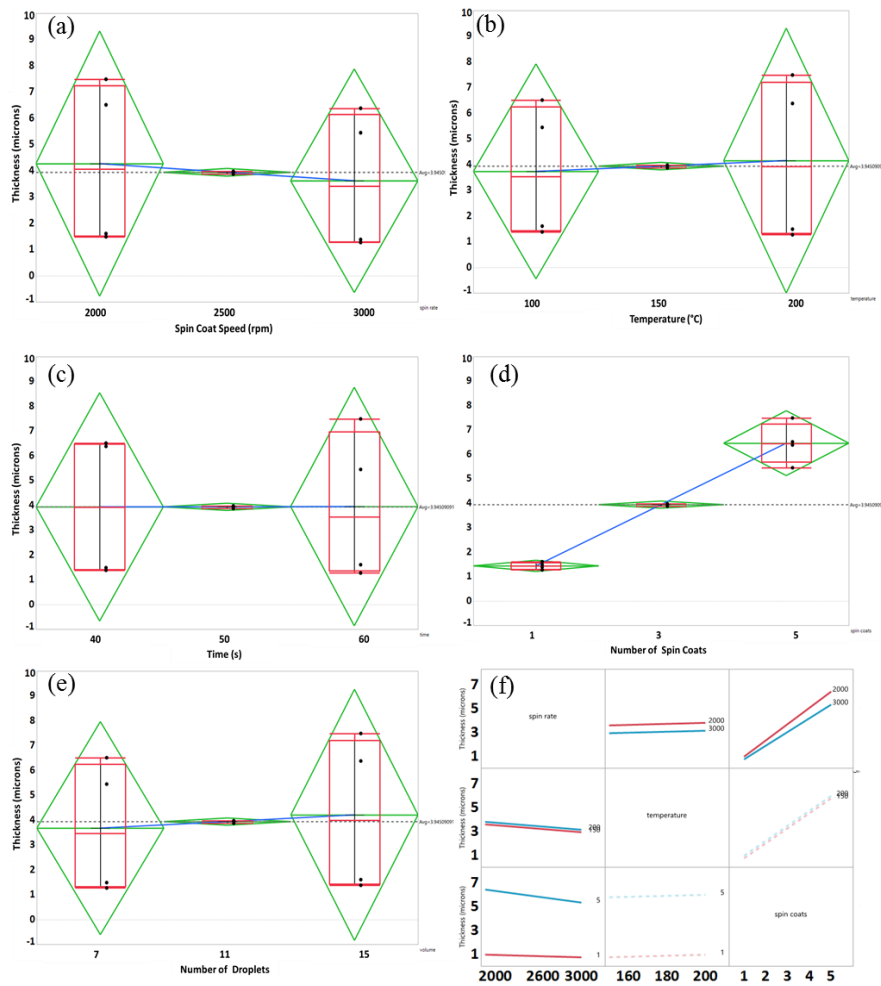


Figure C.3. Boxplot exhibiting variation of (a) spin coat speed, (b) temperature, (c) time, (d) number of spin coats, and (e) volume (number of droplets). Interaction effects plotted in (f).

The normal quantile plot in Fig. C.2 shows that the data comes from a normal distribution due to the points roughly following a straight line. The run order series indicates that there may be periodicity. In Fig. C.3 (a-e), the boxplots exhibit low variability between the low and high settings for spin coat speed, temperature, spin time, and volume. By visual inspection, it appears these parameters have little impact on film thickness; however, spin coat speed, spin time, and volume are statistically significant. There is a strong positive linear relationship between the number of spin coats and film thickness. In Fig. C.3 (f), the interaction effect profile indicates interaction between spin rate and a number of spin coats attributable to their intersection. The coefficient estimates are in Table C.2, and the resulting prediction model is in (C.1) based on ANOVA and the 95% confidence interval test. Furthermore, there is not enough evidence at $\alpha=5\%$ level to conclude that there is a lack of fit in the model given $p=1.0$.

$$Y = 3.353 - 0.329*X_1 + 0.105*X_2 + 2.512*X_3 + 0.017*X_5 - 0.216*X_1X_3 \quad (C.1)$$

Table C.2. Beta coefficients of the model and their 95 % Confidence Interval.

Term	Estimate	Std. Error	Lower 95%	Upper 95%
Intercept*	3.353	0.058	3.169	3.537
Spin Rate*	-0.329	0.019	-0.389	-0.269
Soft Bake *	0.105	0.009	0.078	0.132
# Spin Coats*	2.512	0.017	2.458	2.566
Time	0.007	0.017	-0.047	0.061
# Droplets*	0.017	0.001	0.013	0.020
Spin Rate* Soft Bake	-0.002	0.009	-0.029	0.025
Spin Rate*Spin Coats*	-0.216	0.017	-0.270	-0.162

Based on the 2^{5-2} fractional factorial experiment, the number of spin coat layers, spin coat speed, spin time, volume, and the intercept are statistically significant in determining the thickness of the spin-on-dielectric. Additionally, the interaction term between spin rate and the number of spin coats is statistically significant. To fine tune the thickness, an additional fractional factorial experiment with one layer of thickness is needed.

C.1 References

[1] F. Song, et al. "Elastomeric polymer resonant waveguide grating based pressure sensor." *Journal of Optics* 16.6 (2014): 065702.