Photonic grating coupler designs for optical benching

Eng Wen Ong
University at Albany, State University of New York, eong@albany.edu

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Photonic Grating Coupler Designs for Optical Benching

by

Eng Wen Ong

A Dissertation
Submitted to the University at Albany, State University of New York
in Partial Fulfillment of the Requirements for the Degree of
Doctor of Philosophy
College of Nanoscale Science and Engineering
2018
Abstract

**Background:** Silicon photonics has been rapidly developing as a field. The primary reason for this is its lower operating costs and faster switching rates for use in big data centres. Instead of microns-wide copper lines to transmit signals, silicon photonic chips use waveguides, usually of silicon or silicon nitride. Photonic signals bypass the issues of resistive-capacitance lag (RC-lag) and resistive heating encountered by copper lines. Additionally, a single waveguide may transmit multiple signals along different carrier wavelengths.

Wafer-scale optical benching is one way of confirming the quality of these waveguides: the photonic wafer is placed in an optical bench, optical fibres are aligned on top of it, and photonic structures called ‘vertical grating couplers’ or ‘grating couplers’ diffract light from one vertical optical fibre into waveguides in the plane of the wafer, and then up into the second fibre.

Grating couplers are preferable to another photonic structure called ‘tapers,’ as the latter often requires dicing of the photonic wafer into individual dice prior to measurement.

In addition to waveguide-quality monitoring, grating couplers can also be used to transmit information off packaged dice.

**Research Interest:** One of the major problems is the interface between the optical fibre and the grating coupler, due to the size difference between the mode of the single-mode optical fibre ($\approx 100 \mu m^2$) and the waveguide ($\approx 0.1 \mu m^2$). The size difference causes a significant loss of power (and therefore signal quality) between the two structures, and therefore, it is of paramount importance to have a grating coupler which can efficiently convert the mode size between these two structures.
Another limitation of grating couplers is their alignment tolerance (microns), particularly when compared to their electrical counterparts (probe pads, hundreds of microns). Having a grating coupler with increased alignment tolerance would therefore help reduce operator skill requirements as well as improve machine-aligned throughput.

Lastly, the demand for cheaper devices will necessitate that photonic chips be fabricated on cheaper substrates. At present, a commonly used substrate is 220 nm silicon-on-insulator (SOI) (~ $1000 for a 300 mm wafer), but grating couplers based on new materials will be needed for bulk silicon substrates (~ $300).

**Objectives:** The aim of this work is threefold:

1) to design, fabricate and characterise a grating coupler that efficiently converts the mode size of a single mode fibre-28 (SMF-28, a standard for long-haul infrared telecommunications) to that of an on-chip photonic waveguide for the telecommunications C-band (1530–1565 nm),

2) to design, fabricate and characterise a grating coupler that increases the -1 dB alignment tolerance in the x-y plane from 2 μm × 2 μm to 10 μm × 10 μm for the C-band, and

3) to design, fabricate and characterise a grating coupler that does not require an SOI substrate for the C-band.
List of Publications

I, Eng Wen Ong, the dissertation author, was the lead researcher for these works:


Revised versions of these articles are being included because they were part of the programmatic line of research that comprised this dissertation and including them provides a coherent and appropriately sequenced investigation. They are included under the general permission from:

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I would like to acknowledge Elizabeth Lorenzini and Harry Lazier for their assistance with collecting the SEM images used in this thesis.

Thanks to my friends in capoeira who helped me maintain my sanity. Perhaps one day I will promote the rest of you to Supreme Ninja Dark Overlords.

I’d like to thank my family for their financial and emotional support, for raising me to be a good boy, and for enduring my practice talks.

To Ms Lim Syn Yin, I’m sorry for taking so long, Sayang. I will get you the flame-licked jewellery because that is your favourite colour. I know it.

Also, Eggy, if this thing works out, when we meet in heaven, remember to address me as ‘Dr.’, and I will salute you as ‘Sir’.
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1 Introduction

1.0. Chapter Overview

- The ‘Interconnect Bottleneck’ is the inability of copper lines to keep up with the demand of high speed data.
- Silicon photonics is a potential solution for these high data rates.
- The silicon photonics market is forecasted to be worth $3.5B USD by 2025, of which silicon photonic dice alone will be worth $560M [1]
- Grating couplers are photonic devices which bring data on/off photonic chips
- Generally, they can be designed:
  - to have high coupling efficiencies,
  - to have high misalignment tolerances, or
  - to have large bandwidths.

1.1. Background

1.1.1. The Interconnect Bottleneck

To connect ever smaller structures, copper line interconnects must be reduced in width. Thinner lines increase the resistance of these wires, while thinner dielectric spaces between lines increase the capacitance between these wires. Both effects increase the parasitic resistance-capacitance (RC) time delay of propagating a signal down the wire. Since 2001—despite architectural and material advancements in copper/low-K-dielectric technology—the RC delay caused by copper interconnects has been increasing, as seen in Fig. 1.1.1.1 [2]. In contrast, in
1980, the delay was limited to an electromagnetic wave travelling at the speed of light (typically 6.6 ps for a 1 cm Al line in SiO₂) [3].

Additionally, higher resistance increases Joule heating in the wires, which are thermally insulated by interlayer dielectric and are farther from the thermal sink of the Si substrate. The higher temperatures of these interconnects leads to faster electromigration and wire breakdown [3]. Fig. 1.1.1.2 illustrates the distribution of power dissipation in sample 180 nm technology.

![Design Rule](image)

Fig. 1.1.1.1 Trend in interconnect propagation delay (1 cm length) with technology linewidth and time for traditional aluminium metal and SiO₂ insulator; projected copper and low-k dielectric; and projected optical waveguide technologies. Reproduced with permission from [2] © 2002 IEEE.

![Pie chart](image)

Fig. 1.1.1.2 Pie chart distribution of power dissipation in 180 nm IC technology. Clock distribution is heavily power consuming because it is constantly switching at the highest rate, whereas signal wires have a switching activity of about 0.1–0.15 compared to clock. Reprinted from [3] by permission from Springer Nature: Springer Silicon Photonics by Pavesi and Lockwood © 2004.
In contrast to these issues, optical interconnects 1) do not face parasitic RC issues, 2) do not encounter resistive Joule heating, and 3) can send several signals simultaneously by wavelength-division multiplexing (WDM).

1.1.2. Wavelength Division Multiplexing (WDM)

In signal processing, ‘multiplexing’ means combining several separate streams of information into one consolidated signal. Signals can be multiplexed by space, frequency, amplitude, phase, time, polarisation and code. WDM is a subset of frequency division multiplexing and applies specifically to fibre optic (and now silicon photonic) technology.

In silicon photonics, signals of different wavelengths are combined (multiplexed, usually by photonic devices called ‘arrayed waveguide gratings’) together, travel across a single waveguide, and then are split (de-multiplexed, usually by ‘ring resonators’) into different photodetectors. There are generally three different regimes of WDM: normal WDM (uses 1310 nm and 1550 nm light), coarse WDM (CWDM) (20 nm spacings between signals), and dense WDM (DWDM) (0.8 nm spacing between signals).

1.1.3. The Break-Even Length

Photonic interconnects cannot replace copper interconnects at all levels and at all lengths; there is an inherent delay in converting the electrical signal of the transistors to an optical one, and reconverting an optical signal back into an electrical one (EOE conversion).

The break-even length is the distance for which the performance of an E-only transmitted and EOE converted signal are equal. The break-even parameter could be speed, power consumption, cost, or chip real estate [3]. Fig. 1.1.3.1 shows break-even length for speed (interconnect latency). Depending on calculations, the break-even length for speed ranges from 6 mm–3.7 cm. Therefore, photonic interconnects are usually used at or beyond this length scale.
Fig. 1.1.3.1. Estimated break-even length for speed performance according to measurements. The actual measured performance of the optical connection led to numerical values between 2.6 cm and 3.7 cm. However, according to estimated optimisation of the parameters, the length drops to 6 mm. Above the break-even length, the optical interconnect is expected to have better speed performance. Reprinted from [3] by permission from Springer Nature: Springer Silicon Photonics by Pavesi and Lockwood © 2004.

1.1.4. Silicon Photonics Market Forecast & Applications

The silicon photonics market is forecasted to be worth $3.5B by 2025, as shown in Fig. 1.1.4.1 [1], of which silicon photonic dice alone will be worth $560M ([1], not shown in graph).

Fig. 1.1.4.1. Forecasted silicon photonics market till 2025. Reproduced with permission from [1] © 2018 Yole Développement.
Because of its advantages, photonics are in demand in high-volume, large scale data-switching operations like data centres, high performance computing and fibre-to-the-home telecom [1]; in 2018, 40 Gigabit Ethernet (40GE)-capable switches are 97% of the 25 million x86 server units [4], with demand for 400GE being pushed primarily by cloud service providers Amazon, Microsoft and IBM, and secondarily by telecommunications providers [5]. It is also seeing demand in low-volume applications like autonomous cars (due to low latency), in-flight entertainment [1] and as core interconnections between processors in consumer-level products [6].

Specifically regarding rack-to-rack connections in data centres, silicon photonics enable switches to run faster (via WDM) and at cooler temperatures (no Joule heating), at length scales which far exceed the break-even length. Thus, end-user data centres are the primary economic driver of R&D in silicon photonics [7].

1.2. Photonic Testing

As photonic wafers are manufactured, they need to be tested at several processing steps to increase reliability and detect excursions. For passive photonic structures (straight waveguides, waveguide bends, ring resonators, etc.), testing usually involves coupling light from an external laser on to the wafer, through the passive structures, then off-wafer to an external optical power meter. Measuring the power lost through the passive structures provides information about their quality. Lost power is usually measured in a logarithmic decibel scale for power (not to be confused with the logarithmic decibel scale for signal):

\[
dB \text{ change} = 10 \log \left( \frac{P_{\text{output}}}{P_{\text{input}}} \right). \tag{1.2.1}
\]
There are generally two types of photonic structures (themselves also ‘passives’) which couple light: grating couplers and (regular/inverse) tapers. A third type of photonic structure—evanescent couplers—won’t be considered as they require a special optical fibre which has been stripped of its cladding.

(Inverse) taper devices typically require dicing of the wafer and polishing of the chip edge. This limits their use in wafer-scale testing. Furthermore, their alignment tolerance is about -3 dB (~ 50%) for ± 1–2.3 μm of misalignment [8–11]. Additionally, in the case of inverse tapers, the tip must be very narrow, e.g. 30 nm [12], resulting in a low-yield of inverse taper devices or in some cases, designs being incompatible with standard CMOS processes. Lastly, the taper’s resulting mode size is still smaller than a cleaved SMF28, generally requiring a lensed SMF28 to improve modal matching [13,14]. However, there are some designs capable of accepting a cleaved SMF28 [15–17].

1.2.1. The Grating Coupler Problem

In contrast to (inverse) tapers, grating couplers are not limited to chip-edge real estate, do not require wafer dicing (easily facilitating non-destructive wafer-scale testing) and are compatible with regular, cleaved SMF28 optical fibres. In this sense, optical grating couplers are the equivalent of electrical test pads in the electronics world. Fig. 1.2.1.1(a) illustrates an artists’ impression of aligning optical fibres over photonic circuitry to measure passive structures.

Ideally, a grating coupler would be able to couple in 100% of the light from the laser source into the photonic circuitry, across infinite bandwidth, and regardless of misalignment (whether lateral, tilt angle, or polarisation—arguably a form of axial rotation angular misalignment), In reality though, there must be a compromise between these attributes. Fig.
1.2.1.1 construes this tradeoff as a blue three-pointed star and lists the usual values for most half-etched grating couplers based on 220 nm silicon-on-insulator (SOI), which is a very common wafer platform for photonics.

![Diagram of the Grating Coupler Problem](image)

Fig. 1.2.1.1. The Grating Coupler Problem. Any real grating coupler has to balance the 3 vertices of the blue performance three-pointed star: there is a tradeoff between coupling efficiency, bandwidth, and misalignment tolerances. The values are given for the theoretical maxima for grating couplers based on 220 nm-thick SOI wafers, from [18]. The maximisation of area of the blue star is confined within the red star of design, which also has its own tradeoff between design complexity, reusability, throughput, fabrication tolerance, cost, and minimum feature size.

Trying to maximise the area of the blue three-pointed star, particularly towards the apices of coupling efficiency and bandwidth, is the goal of many research papers on grating couplers. However, for any cost-appropriate, industry-relevant design, this maximisation must be done within the apices of the red design hexagram, which itself has to work with its own tradeoffs:

- **Multi-purpose Reusability**: the design is reusable at different tilts, different fibre endings (e.g. cleaved vs angle-polished), different polarisations (e.g. using regular vs polarisation-maintaining fibres), and different wavelengths.

- **Design Complexity**: the ease at which a given grating coupler design can be repurposed for a different wavelength, tilt, layer / material change. Extremely
complex designs may not be able to turnaround in time to adapt to new photonic builds.

- **Minimum Feature Size**: 100 nm is the minimum feature size for the processes used in the fabrication of the grating couplers covered in this thesis. The grating couplers were manufactured at SUNY Polytechnic Institute’s Albany Nanotech Complex foundry in Albany, which utilises state-of-the-art ASML 193 nm DUV lithography. Grating couplers built in foundries with larger resolutions, e.g. 248 nm KrF excimer laser DUV might have a corresponding minimum feature size of 130 nm.

- **Cost/Zero Change**: the grating coupler only utilises pre-existing mask sets / layers, material recipes and integration.

- **Fabrication Tolerance**: the grating coupler’s performance is reproducible within and across wafers of the same route.

- **Device Throughput**: how rapidly a grating coupler can be fabricated; a thin, single-layer, single etch grating coupler can be manufactured much quicker than a more complex grating coupler.

The three apices of the blue three-pointed star of performance will now be discussed.

**1.2.1.1. The Mode Size Mismatch Problem**

As mentioned, Fig. 1.2.1.1.1(a) shows an artists’ impression of aligning optical fibres over photonic circuitry to measure passive structures. The lime-green circle in Fig. 1.2.1.1.1(b) is a drawn-to-scale expansion of the mode field diameter (MFD) of the single-mode optical fibre of Fig. 1.2.1.1.1(a). For 1550 nm light travelling in a Corning® SMF-28™ single-mode optical fibre, the MFD is 10.4 μm [19,20]. Meanwhile, the single mode strip waveguide it must be
confined to has h × w dimensions of \(220 \text{ nm} \times \sim 550 \text{ nm}\), drawn as the pink ‘SOI wire’ sitting atop 2 µm of white buried oxide (BOX). This difference in modal size between the two passive optical structures is one all grating couplers (and tapers) must overcome and is called the Mode Size Mismatch Problem.

The Mode Size Mismatch Problem is the primary reason for the non-unity coupling efficiency of grating couplers: within the length of the grating coupler (~10–20 µm), the grating coupler must confine/expand the mode of the SMF28/photonic waveguide over a scale of ~ 200 times.

**1.2.1.2. The Misalignment Tolerance Problem**

Wafer-level electrical probe pads are roughly 100 µm × 100 µm. When stepping between die, an electrical probe tester has within those tolerances to land the electrical probes on these test pads. In contrast, optical probe testers need to account for tolerances in 3 freedoms of motion: lateral, tilt, and axial rotation (polarisation).
1.2.1.2.1. Lateral Misalignment Tolerance

Although the lateral misalignment tolerances of 220 nm SOI SWG grating couplers are not generally published, they should be on a similar scale to that of a 220 nm SOI grating coupler with a 1 µm BOX, as shown in Fig. 1.2.1.2.1.1(a) [23], i.e. a -1 dB misalignment tolerance of ± 2.5 µm. For comparison to how the misalignment tolerance might vary, Fig. 1.2.1.2.1.1(b) [24] is the misalignment tolerance of a 250 nm SOI non-SWG grating coupler with a 3 µm BOX. Both pairs of axes have been relabelled to maintain consistent notation: the x-axis is along the direction of the waveguide; the y-axis is along the grooves of the grating coupler.

Generally, misalignment tolerance along the y-axis is slightly better (-1 dB for ±3 µm) than the x-axis and can be improved by increasing the width of the grating from 10 µm to 12 µm [25]. Practically speaking, this means that optical probe testers need to land single mode optical fibres repeatedly within x × y tolerances of 5 µm × 6 µm. Grating couplers are more tolerant to z-height misalignments [26].

Fig. 1.2.1.2.1.1 (a) Comparison of simulation and measurement results of the lateral alignment tolerances. The smooth curves are simulation results. The normalised coupling efficiency is shown as function of the lateral position of the fibre. The distance between fibre and grating is approximately 10 µm. The -0.5 and -1 dB contour are indicated on the figure. The SOI thickness is 220 nm and the BOX thickness is 1 µm. Reproduced with permission from [23] © 2006 JSAP. (b) The absolute coupling efficiency as a function of the lateral position of the fibre. The SOI thickness is 250 nm and the BOX thickness is 3 µm. Reproduced with permission from [24] © 2011 IEEE. The wavelength is 1550 nm and is TE-polarised in both figures.
Both pairs of axes have been relabelled to maintain consistent notation: the x-axis is along the direction of the waveguide; the y-axis is along the grooves of the grating coupler.

1.2.1.2.2. Tilt Misalignment Tolerance

Grating couplers are usually designed for a specific tilt of the optical fibre (usually defined as the angle between the optical fibre and the surface normal). If no tilt was implemented in the design, there would be secondary backscattering directly back into the laser source, causing out-of-phase destabilisation. Generally, for every 1° the peak wavelength will shift by 9 nm, but there is also a -0.5 dB penalty for ± 2° of tilt misalignment [23].

However, lateral and tilt tolerances are inversely related: larger lateral tolerances require a larger beam diffracted by the grating, but have a narrower power distribution in wave-vector space, and so have smaller tilt tolerances. Conversely, smaller diffracted beams are harder on lateral tolerances but more relaxed on tilt tolerances. Table 1.2.1.2.2.1 from [27] summarises spatial and angular alignment tolerances for grating couplers with different decay lengths being excited by their respective optimal input FWHM Gaussians.

Table 1.2.1.2.2.1 Spatial (Δx) and angular (Δθ) alignment tolerances for gratings with different decay lengths

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<th>Decay Length (µm)</th>
<th>FWHM_{opt} (µm)</th>
<th>-1.25 dB</th>
<th>-3 dB</th>
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<td>Δx (µm)</td>
<td>Δθ (°)</td>
<td>Δx (µm)</td>
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<td>6.22</td>
<td>± 1.5</td>
<td>± 0.8</td>
<td>± 2.5</td>
</tr>
<tr>
<td>12.44</td>
<td>± 3</td>
<td>± 0.4</td>
<td>± 5</td>
</tr>
<tr>
<td>24.88</td>
<td>± 9</td>
<td>± 0.2</td>
<td>± 10</td>
</tr>
</tbody>
</table>

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1.2.1.2.3. Axial Rotation Misalignment Tolerance (Polarisation Diversity)

Lastly, most grating couplers are designed to accept only one polarisation of light (transverse-electric [TE] or transverse magnetic [TM]). This is due to a consequence of birefrigence based on the grating coupler’s geometry. The difference in coupling efficiency between TE and TM is very high, around the order of ~ -30 dB. Usually, this is not an issue as
the other photonic circuitry components are designed with only one polarisation in mind. However, some photonic circuits are designed to be polarisation-diverse, and consequently, 2D polarisation-diverse grating couplers is an area of active research to accept unpolarised light from an optic fibre.

Practically speaking, even if the light from the optic fibre was polarised, there is a possibility of axial rotational misalignment of the optic fibre. To deal with this issue, sophisticated optical testers have polarisation controller modules to sweep the polarisation to obtain maximum coupling efficiency.

1.2.1.3. The Bandwidth Problem

As grating couplers are based on the phenomenon of diffraction, their coupling efficiency is wavelength-dependent. The Bragg condition is the basic principle upon which grating couplers operate: light waves of a given vacuum wavelength, \( \lambda_0 \), diffract off a periodic structure of pitch \( \Lambda \) and interfere constructively for diffraction order \( m \) at angle \( \theta_m \):

\[
\sin \theta_m = \frac{n_{\text{eff, grating}}(\lambda_0)}{n} + m \frac{\lambda_0}{n \Lambda},
\]

(1.2.1.3.1)

where \( n = \frac{n_{\text{substrate}}}{n_{\text{superstrate}}} \), a ratio of the refractive index between the substrate and superstrate;

\( n_{\text{eff, grating}} \) is the effective index of the grating coupler.

For \( m = -1 \), taking the derivative of the Bragg condition for \( \lambda \) with respect to \( \theta \) yields

\[
\frac{d\lambda}{d\theta} = \Lambda \frac{dn_{\text{eff}}(\lambda)}{d\lambda} \cdot \frac{d\lambda}{d\theta} - \Lambda n \cos \theta.
\]

(1.2.1.3.2)

To get an expression for the \( \Delta \lambda_{-1\text{dB}} \), the -1 dB bandwidth, Eq. 1.2.1.3.2 is multiplied by the coefficient for -1 dB bandwidth, \( \eta_{1\text{dB}} \), yielding
\[ \Delta \lambda_{1dB} = \eta_{1dB} \cdot \left| \frac{d\lambda}{d\theta} \right| = \eta_{1dB} \cdot \frac{n \cos(\theta)}{\left| \frac{1}{A} - \frac{dn_{eff}(\lambda)}{d\lambda} \right|}. \]  

(1.2.1.3.3)

Experimentally, \( \eta_{1dB} = 0.07 \) for an SMF28 fibre with 1550 nm light [28]. Theoretically, \( \eta_{1dB} \) is a function of the fibre position, height, numerical aperture, divergence angle, beam waist, centre wavelength, grating length and grating amplitude decay rate [29].

From Eq. 1.2.1.3.3, it is obvious that \( \Delta \lambda_{1dB} \) is a finite number that is limited by the coupling arrangement (fibre type, position, angle) and features of the grating coupler (n, \( \Lambda \)).

Bandwidth is commonly reported in the literature as a wavelength range where the coupling efficiency is within -1 dB (~80%) and -3 dB (~50%) of the peak coupling efficiency. For grating couplers based on 220 nm SOI which maximise coupling efficiency, the -1 dB bandwidth is \( \sim 41 \) nm, and the -3 dB bandwidth is \( \sim 64 \) nm [22,30].

### 1.3. Thesis Objectives

Given these challenges, the objectives of this thesis are three-fold:

#### 1.3.1. To Increase Lateral Misalignment Tolerance of Grating Couplers

Chapter 3 covers the design of a 220 nm SOI-based grating coupler with a significantly increased lateral misalignment tolerance. The -1 dB misalignment is \((x \times y) 21.4 \mu m \times 10.1 \mu m\) (cf. \(5 \mu m \times 6 \mu m\)). This grating coupler can be used for wafer-scale testing of photonic chips and could also be used in photonic packaging applications which require looser lateral misalignment tolerances.

#### 1.3.2. To Design a SiN\(_x\)-only Grating Coupler

Chapter 4 details the design of a SiN\(_x\)-only grating coupler with significantly higher coupling efficiency (-2.73 dB / 53.3%) compared to other SiN\(_x\)-only grating couplers designed
within similar parameters. Silicon nitride is an alternative design platform for photonics (for reasons outlined in Chapter 2).

Such a grating coupler can be used in testing silicon nitride photonic circuitry, in foundry-level device applications, and does not rely on more expensive SOI wafer substrates.

1.3.3. To Design a Zero-Change High Efficiency Grating Coupler

Chapter 5 discusses the design and fabrication of a zero-change grating coupler for SiNx circuitry that maximises coupling efficiency (-0.662 dB / 85.9%). A zero-change requirement ensures that the grating coupler only utilises existing mask levels and does not add further cost to the photonic wafer build. It therefore has real-world, beyond-academia, foundry-level applications where high-efficiency is crucial.

Compared to other zero-change grating couplers for SiNx circuitry, this design is amongst the world’s best.

1.4. Chapter Bibliography

5. Jeff Harris, *400 Gigabit Ethernet Is Here, but Who Benefits?* (Light Reading Group, 2017).
2 Grating Coupler Simulation and Design

2.0 Chapter Overview

- Finite difference time domain (FDTD) is a brute force algorithm suitable for designing grating couplers
- Grating couplers operate on the principle of the Bragg condition
- Advanced grating coupler design techniques can be categorised into:

| Table 2.0.1 Zero-Change-(In)Compatible Advanced Grating Coupler Design Techniques |
|---------------------------------|---------------------------------|
| Zero-Change-Compatible          | Zero-Change-Incompatible        |
| Apodisation                     | Extended Teeth                  |
| Back Reflectors                 | Optimised BOX & TOX thicknesses |
| Subwavelength Gratings (SWG)    | Cladding Engineering            |
| Bilayer Antennae                | High Contrast Gratings          |
| SiNx Material                   |                                 |
| Limited use of Mirrors          |                                 |
| Lateral Layout: Focusing Ellipses|                                 |
| Polarisation Diversity          |                                 |

2.1 Finite Difference Time Domain (FDTD) Background

There are several methods for computationally solving the propagation of electromagnetic (EM) fields in a structure. One method is finite difference time domain (FDTD), which—while computationally-intense—is suitable for complex geometric structures.

FDTD works by dividing the simulation space into discrete volumes called ‘Yee cells’ [1] (after applied mathematician Kane S. Yee). These Yee cells have an internal structure which record and propagate the x, y and z components of the E-fields (along the 3 cardinal axes) and H-fields (on the y-z, x-z and x-y planes) (cf. Fig. 2.1.1). At each discrete time step, a Yee cell will
solve Maxwell’s equations for the incoming E- & H-fields and pass on the solutions to its six neighbouring cells. It also receives the E- and H-field solutions of its neighbours and processes them for the next discrete time step.

The pertinent Maxwell’s equations are Faraday’s Law of Induction and Ampere’s Circuital Law (with Maxwell’s addition).

Faraday’s Law of Induction:

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}, \quad (2.1.1)$$

where $\nabla \times$ is the curl operator, $\vec{E}$ is the E-field, $\vec{B} = \mu \vec{H}$, $\mu$ is the permeability of the medium, and $\vec{H}$ is the H-field.

Ampere’s Circuital Law (with Maxwell’s addition):

$$\nabla \times \vec{H} = \vec{j} + \frac{\partial \vec{D}}{\partial t}, \quad (2.1.2)$$

where $\vec{j}$ is the conduction current (generally ignorable in non-conducting materials used in silicon photonics), $\vec{D} = \varepsilon \vec{E}$, and $\varepsilon$ is the permittivity of the material.
Eq. 2.1.1 solves for the curl of the E-field, while Eq. 2.1.2 solves for the curl of the H-field. Eqs. 2.1.1 and 2.1.2 are solved at interspaced half time-steps: using H-field values from the input EM wave, Eq. 2.1.1 is solved at $t=t_0$, and its E-field solutions are used to solve Eq. 2.1.2 at $t=t_{1/2}$, whose H-field solutions are fed back into Eq. 2.1.1 to solve for E at $t=t_1$, whose E-field solutions are fed back into Eq. 2.1.2 to solve for H at $t=t_{1/2}$. Thus, when an excitation EM wave is injected into the simulation space, it propagates through the Yee cells via this leap-frog method of solving Eqs. 2.1.1 and 2.1.2. In this sense, Yee cells can be thought of as 3-dimensional calculators solving Maxwell’s two curl equations through time. FDTD thus obtains its name from its method: it solves the finite difference in E- and H-fields through the time domain.

2.1.1 Strengths and Weaknesses of FDTD

There are several strengths of FDTD which lends itself to solving photonic structures of complex geometry:

- The spatial meshing of Yee cells around any geometry allows FDTD to model photonic devices with complex geometries.
- FDTD is a time-domain technique (as opposed to a frequency-domain technique), so the results from a broadband pulse can be solved in one simulation.
- As a time-domain technique calculating the E- and H-fields as they evolve in time, FDTD can be intuitively understood by new users, and lends itself to producing animations of the E- and H-field movement through the structure.
- FDTD allows the user to specify the material properties (refractive index, extinction coefficient) at all points within the simulation space, thereby allowing the modelling of structures comprised of different dielectric materials.

However, FDTD also suffers from weaknesses as a simulation method, such as:
• FDTD requires that the entire simulation space be meshed with Yee cells, and the computation time of the simulation scales inversely with the size of the Yee cells to the fourth power \((1/dx^4)\). Thus, FDTD’s greatest weakness as a ‘brute force’ simulation method is its potentially long computation times, and user experience is required to minimise this without sacrificing model accuracy.

• Additionally, FDTD is not suitable for modelling photonic structures which have simple geometries but are comparatively large, such as waveguides or tapers.

• As a time-domain technique, an FDTD simulation will continue running as long as a significant amount of the energy from the original impulse remains in the system. This increases the required number of time-steps significantly, making FDTD unsuitable for modelling resonating photonic structures such as ring resonators, whispering gallery microdiscs, Fabry-Perot resonators, or photonic crystal cavities.

• There is no unique way to determine the E- and H-fields at interfaces, as the fields can be discontinuous. Different FDTD software have their own patented methods for dealing with this issue.

2.1.2 Lumerical FDTD

Lumerical FDTD is a commercial grade, fully-vectorial FDTD solver from Lumerical Inc. It was chosen as it is industry-proven and has been cited in over 8000+ academic publications since 2010.

It alleviates some of the weaknesses mentioned previously via graded meshes (i.e. reduced mesh size near interfaces), conformal mesh technology (avoiding a ‘staircase’ permittivity mesh by accounting for subcell features through solving Maxwell's integral
equations near structure boundaries), parallel use of multi-core processors, and symmetric arguments to halve or quarter the simulation space.

2.2 Comparative Simulations with Grating Couplers in the Literature

The proceeding section compares simulations—and if possible, measured results—between select grating couplers from the literature and their replicated simulations with Lumerical FDTD. The published simulations were replicated with Lumerical FDTD to:

1) confirm the validity of Lumerical FDTD as a product to design grating couplers that will accurately transfer to actual fabricated devices’ measured characteristics (due to the restrictive costs of lithographic chrome masks),

2) develop expertise with Lumerical FDTD,

3) understand the different design strategies used to produce a grating coupler with given properties,

These grating couplers use different advanced designs, the mechanisms of which are further covered in Section 2.4.

Selvajara, Vermeulen et al. 2009 [2] designed a grating coupler which utilised two distributed Bragg reflectors (DBRs, Section 2.4.6 Mirrors) using a simulation program called CAvity Modelling FRamework (CAMFR) [3], a … “full-vectorial Maxwell solver based on a combination of eigenmode expansion and advanced boundary conditions like perfectly matched layers (PML),” developed by the photonics group of the Department of Information Technology (INTEC) at Ghent University in Belgium. Fig. 2.2.1(a) presents the CAMFR simulation of their ideal DBR grating coupler (blue) and the simulation of their design-rule-constrained fabricated grating coupler (red). The replicated Lumerical FDTD simulations of the same structures are
shown in Fig. 2.2.1(b), demonstrating similar peak efficiency wavelengths and bandwidth profiles.

Fig. 2.2.1 From [2]. Comparison simulation for grating coupler utilising two Distributed Bragg Reflectors (DBRs). (a) Simulation of optimal design (blue line) and measured structure (red line) for 1550 nm. © 2009 OSA (b) Replicated simulation with Lumerical FDTD. The peak wavelengths and coupling efficiencies are similar. (c) The measured structure (TEM, not shown) has a thinner SOI and SiO$_2$ buffer layer. (d) Profile of structure with DBR mirror (blue inset) © 2009 OSA.

Roelkens, van Thourhout et al. 2006 [4] explored the effects of polysilicon extended teeth (Section 2.4.8.1 Extended Teeth) on a grating coupler’s upward directionality (i.e. the power diffracted upwards in an outgoing grating coupler) for 1550 nm light. Fig. 2.2.2(a) presents their simulated results using CAMFR while Fig. 2.2.2(b) shows the replicated simulation in Lumerical FDTD. The deviations at lower directionalities, particularly for “610 nm, 175 nm” and “580 nm, 175 nm” are attributed to Lumerical operator inexperience. They then simulated their design’s fibre-to-chip coupling efficiency (Fig. 2.2.3(a)) and tolerance to fabrication variations in overlay thickness (Fig. 2.2.4(a)) and etch depth (Fig. 2.2.4(b)). Fibre-to-chip coupling efficiency is a smaller percentage of the directionality, depending on the modal overlap (see Section 2.4.1 Apodisation—Non-uniform Grating Couplers).
Fig. 2.2.2 From [4]. Comparison simulation of grating coupler utilising extended polysilicon teeth. Directionality is the ratio of the upwards diffracted power. (a) Directionality as a function of the grating coupler period and overlay thickness, t ©2006 OSA. (b) Replicated simulations with Lumerical FDTD. Peak directionals coincide with appropriate etch depths. (c) Structure profile showing the poly-Si extended teeth (blue). Image modified from [4].

Fig. 2.2.3 From [4]. Apodised polysilicon extended teeth grating coupler fibre-to-waveguide coupling efficiency. Fibre-to-waveguide coupling efficiency is determined by both directionality and mode matching between the fibre and the grating coupler. Both the (a) published simulation ©2006 OSA and the (b) replicated simulation have peak coupling efficiency at 1.57 μm, similar efficiencies of ~75% and similar -3 dB bandwidths of ~35 nm.
Fig. 2.2.4 From [4]. Comparison simulation of polysilicon extended teeth grating coupler performance as a consequence of fabrication variations. (a) Fibre-to-waveguide coupling efficiency affected by different overlay thicknesses, t. (b) Fibre-to-waveguide coupling efficiency affected by different etch depths. ©2006 OSA. (c)–(d) Replicated simulations in Lumerical FDTD.

Benedikovic, Cheben et al. 2015 [5] designed a subwavelength grating (SWG) grating coupler (Section 2.4.3 Subwavelength Gratings). They simulated their design with FDTD and Fourier-eigenmode expansion method (F-EEM). Only the FDTD and experimental results are shown in Fig. 2.2.5(a). Due to their non-uniformity in the third dimension, SWG GCs usually perform poorer than their 2D simulations would suggest. The replicated Lumerical FDTD simulation is shown in Fig. 2.2.5(b) with comparable efficiencies to the 2D FDTD simulations of Benedikovic, Cheben et al., but makes a better distinction of the shift in peak coupling efficiency wavelengths (~15 nm) between the 2-step apodised and continuously apodised designs. Fig. 2.2.5(c) shows the group’s simulation result for an SWG grating coupler for 1300 nm (no experimental data), while Fig. 2.2.5(d) is the replicated Lumerical FDTD simulation.
Doerr, Chen et al. 2010 [7] designed a silicon-nitride-only grating coupler (see Section 2.4.5 SiN$_x$ Grating Coupler) using 2D FDTD. The simulated (light green) and experimental (dark green) results are shown in Fig. 2.2.6(a). The replicated simulation is shown in Fig. 2.2.6(b).

Fig. 2.2.5 From [6]. Comparison simulations of subwavelength grating (SWG) grating couplers. (a) and (c) Simulations of the SWG GCs for 1550 nm and 1310 nm respectively. ©2015 SPIE. (b) and (d) Replicated simulations in Lumerical FDTD showing similar peak coupling wavelengths and efficiencies for all four designs. (e) Structure profile of SWG GC ©2015 SPIE.

Fig. 2.2.6 From [7]. Comparison simulation of SiN$_x$ grating coupler. (a) Simulated (light green) and measured (dark green) coupling efficiencies of a SiN$_x$-only grating coupler. Image modified from [7]. (b) Replicated simulation with Lumerical FDTD using the artificial indices as stated in the original paper. The red-shifted peak wavelength and reduced coupling efficiency are attributed to using a cleaved SMF-28 instead of an 8°-polished SMF-28 as stated in the original paper.
Wade, Kumar et al. 2014 [8] designed a displaced bilayer crystalline silicon / polysilicon grating coupler (see Section 2.4.4 Bilayer Antenna) using FDTD. Their simulated 3D FDTD results of the optimal design (red dotted) is shown in Fig. 2.2.7(a). Due to design rules, their fabricated design had slots (hazel dotted [simulation] and hazel solid [measured]). Fig. 2.2.7(b) shows the replicated 3D FDTD results in Lumerical. Note that the replicated simulation accurately predicts the peak wavelength of the fabricated grating coupler. The reduced peak coupling efficiency is attributed to substituting the adiabatic taper in the actual design (dimensions not given) with a $6.35 \times 25.24 \, \mu m$ isosceles triangle linear taper (Fig. 2.2.7(d)).

Sacher, Huang et al. 2014 [9] designed a displaced bilayer crystalline silicon / silicon nitride grating coupler using FDTD. Their simulated and measured results are shown in Fig. 2.2.8(a). The replicated Lumerical FDTD results are shown in Fig. 2.2.8(b). The peak coupling
wavelength is similar. The lower coupling efficiency and narrower bandwidth in the Lumerical FDTD simulation is attributed to using a cleaved SMF-28 instead of a 21°-polished SMF-28, as stated in the original text.

Fig. 2.2.8 From [9]. Comparison simulation of a SiN$_x$-on-SOI bilayer grating coupler. (a) Simulated and measured coupling efficiency of the zero-change SiN$_x$-on-SOI bilayer grating coupler. ©2014 OSA. (b) Replicated simulation with Lumerical FDTD where the refractive index of Si$_3$N$_4$ was artificially set to 2.0, as stated in the original paper. (c) Structure profile of the SiN$_x$-on-SOI grating coupler. Note that the input source is a 21°-polished SMF-28. ©2014 OSA.

The proceeding several sections will deal with individual design strategies and will mention, where appropriate, the respective literature which utilises said design strategy.

2.3 Basic Grating Coupler Design

2.3.1 The Bragg Condition

Grating couplers work on the principle of the Bragg condition: when EM radiation of a given wavelength encounters scattering structures of comparable spacing, it scatters off in-phase in only a few directions, as only these directions have a difference of an integer number of wavelengths between path lengths. In these directions, the reflected waves interfere
constructively. Usually, the Bragg condition is explained from the vantage of an ‘outgoing’ grating coupler (i.e. from a photonic waveguide, into a grating coupler, into free space, and then into a single mode fibre): For an EM wave of given wavelength $\lambda$ moving in the positive $x$-direction (rightwards across Fig 2.3.1.1), between a substrate and superstrate whose refractive indices are $n_{\text{substrate}}$ and $n_{\text{superstrate}}$ respectively, and encountering point-like scatterers of pitch $\Lambda$ and averaged refractive index $n_{\text{eff}}^{\text{grating}}$, a diffraction order of integer $m$ (usually, $m = 1$) will scatter at angle $\theta_m$, such that

$$\sin \theta_{m}^{\text{sup}} = \frac{n_{\text{eff}}^{\text{grating}}}{n_{\text{superstrate}}} - \frac{m\lambda_0}{n_{\text{superstrate}}\Lambda}. \tag{2.3.1.1}$$

In the literature, $\theta_{m}^{\text{sup}}$ is the angle of the optical fibre from the surface normal, and is usually $8^\circ < \theta_{m}^{\text{sup}} < 15^\circ$. If the fibre were perfectly vertical (i.e. $\theta_m = 0^\circ$), there would be a second-order back-reflection back into the waveguide (for an outgoing grating coupler), or (in the case of an incoming grating coupler) back into the optical fibre and thus back into the external laser cavity [10]. This is avoided to prevent de-stabilising the laser with an out-of-phase back-reflection which would possibly reduce its lifespan.

One important assumption for the Bragg condition is that the scatterers are 1-dimensional point scatterers. This is valid to a first approximation in designing silicon photonic circuitry as the thickness of the guiding layer (e.g. $220 \text{ nm} \times n_{\text{Si}} (=3.47) = 763.4 \text{ nm} < 1550 \text{ nm}$) is less than the wavelength of the scattered light. However, as real grating couplers do have a finite thickness, and the scattering teeth are usually etched in from the top, the diffracted angle has to be solved numerically, and the diffracted power is not equi-distributed between superstrate and substrate.
2.4 Advanced Grating Coupler Design

2.4.1 Apodisation – Non-uniform Grating Couplers

Apodisation, from Latin, can be loosely translated as ‘removing the foot’. In optical design, it refers to intentionally changing the transmission intensity profile so that it is no longer an exponential decay (cf. Figs. 2.3.1.1 & 2.4.1.2) and thus approaches zero at the edges (hence, to ‘remove the foot’ of the profile).

The coupling efficiency of a grating coupler can than be calculated as the modal overlap between the grating coupler’s E-field profile and the complex conjugate of the SMF-28’s H-field profile with the integral [12]
\[ \eta = \left| \int_S E \times H_{\text{fibre}}^* \, dS \right|^2, \quad (2.4.1.1) \]

where the fibre mode is normalised and surface S is the facet of the fibre. The fibre mode is approximated by a Gaussian beam with a beam diameter of \(2w_0 = 10.4 \, \mu\text{m}\). Using the following axial orientation (which will be used throughout the remainder of this thesis): x-axis as the direction along the grating; y-axis as the lateral direction to the grating; z-axis as the vertical direction, Eq. 2.4.1.1 becomes

\[ \eta = \left| \int E(y)E(z = 0, x)Ae^{-\frac{(x-x_0)^2+(y-y_0)^2}{2w_0^2}} \times e^{in_fib \times \frac{2\pi}{\lambda} x \sin \theta} \, dx \, dy \right|^2, \quad (2.4.1.2) \]

where constant A is the normalisation of the Gaussian beam and \(n_{\text{fib}} = 1.46\). In regard to apodisation, most grating coupler research is concerned with the field overlap in the x-direction. As Eq. 2.4.1.2 can be separated into an x-dependent term and a y-dependent term, it can be expressed as

\[ \eta = \xi \left| \int E(z = 0, x)Ae^{-\frac{(x-x_0)^2}{2w_0^2}} \times e^{1.46i \times \frac{2\pi}{\lambda} x \sin \theta} \, dx \right|^2, \quad (2.4.1.3) \]

where constant \(\xi\) is a correction factor for the y-axis when calculating the overlap integral from a 2D problem to 3D. It depends on the design of the grating coupler in the y-dimension and is usually, \(\xi \sim 0.90–0.97\) [13]. As mentioned in the previous section, the output E-field profile of a uniform grating coupler is usually an exponential decay whose power output is

\[ P = P_0 e^{-2a \alpha}, \quad (2.4.1.4) \]
where $\alpha$ is the scattering strength of the grating. As such, a uniform grating coupler has a theoretical maximum coupling efficiency of $\sim 80\%$ [14]. In an apodised grating coupler, $\alpha$ is a function of $x$ and to produce a Gaussian output E-field, needs to obey [15]

$$2\alpha(x) = \frac{G^2(x)}{1 - \int_0^x G^2(t)dt}.$$ \hspace{1cm} (2.4.1.5)

Fig. 2.4.1.1 plots the ideal power distribution, $G^2(x)$; the integral of the ideal power distribution, $\int G^2(x) \, dx$; and the required scattering strength, $\alpha(x)$ ($\mu$m$^{-1}$).

$\alpha$ can be adjusted by varying the etch depth or, more practically, the duty cycle (the ratio of the unetched grating tooth to grating period) of the grating coupler. Linearly varying the duty cycle 1) reduces the optical power radiated by the earlier periods (thus improving mode matching) and 2) improves the optical impedance matching between waveguide and grating (thus reducing back
reflections) [16]. One method of linear ramping of the duty cycle (sometimes called ‘chirping’) [17] is

\[ \text{duty cycle} = 0.9 - R \cdot x, \]  

(2.4.1.6)

where \( x \) is the direction of propagation along the grating, 0.9 refers to the duty cycle of the first period, and \( R \) is the linear apodisation factor. For a 220 nm-thick SOI grating coupler with 110 nm etch depth, \( R = 0.0275 \, \mu m^{-1} \).

However, the reduction in duty cycle decreases the \( n_{eff} \) of the later grating periods, so those period lengths need to be extended to maintain phase-matching in the Bragg condition of Eq. 2.3.1.1. The extended period lengths can be calculated as [17,18]

\[ \Lambda_i = \left| \frac{\lambda}{n_{eff,i} - \sin \theta_m} \right|_{i=1-k}, \]  

(2.4.1.7)

where \( k \) is the maximum number of periods in the grating coupler and

\[ n_{eff,i} \approx \text{duty cycle} \cdot n_{Si} + (1 - \text{duty cycle}) \cdot n_{etched}. \]  

(2.4.1.8)

Fig. 2.4.1.2. plots the upward output E-fields of optimal [16] uniform (blue) and apodised (red) grating couplers based on 220 nm SOI / 2 \( \mu m \) BOX platform, as well as a fitted Gaussian function (black dotted) representing an SMF-28. As mentioned in the previous section, the uniform grating coupler’s E-field decays exponentially, which minimises its modal overlap with the SMF28. Conversely, by manipulating the duty cycle and period lengths, one can increase the modal overlap from 53.7% to 64.65%. Theoretically, if the maximal overlap between an exponentially decaying field and a Gaussian function is 0.81D, then apodising the grating coupler can improve the overlap to about D [19].

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Fig. 2.4.1.2. Upwards E-field profile of a uniform (blue) and apodised (red) grating coupler simulated from Lumerical FDTD. The dimensions were optimal for a 220 nm-thick SOI with a 2 µm BOX platform from [16]. A 5.2 µm-radius Gaussian (dotted line) shows the increased modal overlap of the E-field of the non-uniform/apodised grating coupler.

After linear apodisation, one can further improve apodisation by mutative refinement [16] using optimisation algorithms. Generally, there are two numerical methods, as shown in Fig.
2.4.1.3: chip-to-fibre, where a waveguide mode source is diffracted upwards by an output grating coupler and the radiated mode matched to the Gaussian mode of an optical fibre; or fibre-to-chip, where the Gaussian mode of an optical fibre impinges on an incoming grating coupler and diffracts into an on-chip waveguide. As both waveguide and optical fibre are usually single mode, and Maxwell’s equations are time-reversal invariant, both these methods usually converge on the same final design. The former method has been used in [13,20–31]; the latter in [14,16–18,32–34].

2.4.2 Back Reflectors

To effectively couple light upwards to an SMF-28, a grating coupler should ideally scatter all of its light within the fibre’s mode field diameter (MFD, 10.4 μm for an SMF-28 @ 1550 nm). From Eq. 2.4.1.4, we define $L_c^{\text{grat}}$, the coupling length of a grating coupler as [35]

$$L_c^{\text{grat}} = \frac{1}{2\alpha}.$$  \hspace{1cm} (2.4.2.1)

Meanwhile, the optical fibre’s MFD, $2w_0$, is related to its coupling length, $L_c^{\text{fib}}$, by [35]

$$\text{MFD} = 2w_0 = 2.74L_c^{\text{fib}} \cos \theta.$$  \hspace{1cm} (2.4.2.2)

If $L_c^{\text{grat}} > L_c^{\text{fib}}$, additional periods past the fibre will continue to scatter light, but such light won’t efficiently couple to the SMF-28. This occurs because a grating’s scattering strength, $\alpha$, is not high enough, which is common in low-index-contrast platforms like Si$_3$N$_4$ ($n = 1.9963$) /SiO$_2$ ($n = 1.444$) (cf. Section 2.4.5).

Instead of continuing with more scattering periods, a reflector grating could be placed behind a regular grating coupler (cf. Fig. 2.4.2.1). A reflector grating works on the same principle as the Bragg condition (Eq. 2.3.1.1), but here we are trying to maximise the back-
reflection, which occurs when the path length difference between successive reflections is an integer of $\lambda$, the minimum value of which is $m = 1$. Manipulating Eq. 2.3.1.1,

$$\Lambda = \frac{m \lambda_0}{n_{\text{eff}} - n_{\text{superstrate}} \sin \theta_m}.$$  \hspace{1cm} (2.4.2.1)

Here, $\theta_m = -90^\circ$. Hence, Eq. 2.4.2.1 reduces to:

$$\Lambda = \frac{\lambda_0}{n_{\text{eff}} + n_{\text{superstrate}}}.$$  \hspace{1cm} (2.4.2.2)

For a SiN$_x$/SiO$_2$ grating coupler, $n_{\text{eff}}^{\text{grating}} \approx 1.55$, so $\Lambda \approx 520$ nm, which is relevant to the back-reflector dimensions obtained in Chapter/Section 5.5.

![Fig. 2.4.2.1 Back Reflector grating for a low-index-contrast SiN$_x$/SiO$_2$ platform. The reflector grating period is half the effective wavelength ($\lambda/n_{\text{eff}}$). A phase-adjusting gap ensures the forward propagating 20% wave and the backward propagating 20% wave interfere constructively. Percentage values are merely examples to give the reader an impression of the effectiveness of the Back Reflector design strategy. Inset: Operating principle of Back Reflector.](image)

### 2.4.3 Subwavelength Gratings

By fabricating structures with periodicity significantly smaller than the coupled wavelength in the $y$-direction (cf. Fig. 2.4.3.1(a)–(b)), one can tune the equivalent index of a period $j$ ($n_{\text{SWG},j}$) to a desired value (Fig. 2.4.3.1(c)). Grating couplers which employ these structures are called Subwavelength Grating Grating Couplers (SWG GCs).
Silicon-on-Insulator (SOI) wafers are a common substrate to design SWGs on as crystalline silicon has a very high refractive index in the C-band (3.47 @ 1550 nm @ 300 K), whereas the etched portions can be filled with silicon dioxide (1.444 @ 1550 nm @ 300 K). This gives a tuneable index of between ~3–1.8, keeping in mind that the smallest structures fabricable by the processes used in the fabrication of this thesis’ grating couplers are 100 nm.

The equivalent index is a monotonically continuous function of the refractive indices of the two materials and their respective ratios. SWG refractive index graphs—such as Fig. 2.4.3.1(c)—are used by designers to determine $f_y$ values, and are commonly generated by second order effective medium theory (EMT) [36–50]. However, 2nd order EMT breaks down at large $\Lambda_y$ as the curve $\Lambda_y = 600$ nm is no longer monotonic.

Typically, SWGs only require one mask, so there is no concern with inter-mask alignment. Additionally, the buried oxide (BOX) layer serves as a natural etch-stop for RIE. However, SWG holes of different enough sizes might result in RIE lag issues.
There are numerous SWG GC designs in the literature (further cited in Chapter 3). [37,40,48,51] provide overviews of SWG photonic devices (including grating couplers) and their operating principles.

### 2.4.4 Bilayer Antenna

Bilayer antenna grating couplers are based on the principle of phased array antennae. The first layer is often SOI while the second layer is usually polysilicon [8,31,52,53], SiN$_x$ [9,54–56], or a unique double-etch of the SOI [57,58]. Based on first principles, the grating coupler is modelled as two 1-dimensional Bragg grating couplers (as described in Section 2.3.1, offset from each other by $\frac{1}{4}\lambda$ in the x and z direction.

![Fig. 2.4.4.1 Bilayer antenna grating coupler based on SOI (blue) and polySi or SiN$_x$ (green) grating layers. Red dots indicate the scattering points on the layers. Inset: operating principle. (Inset adapted from [8])](image)

The inset of Fig. 2.4.4.1 shows how the offset produces constructive interference upwards and destructive interference downwards: The waveguide mode scatters of point 1 first, producing an upwards wavefront (blue arrow on 1). When the wavefront has travelled $\lambda/4$ in z, the original waveguide mode has travelled $\lambda/4$ in x and now scatters off point 2, producing another upwards wavefront (tiny blue arrow on 2). As both wavefronts have travelled $\lambda/4$ (one in z, the other in x), there is no relative phase between them and they interfere constructively. Conversely, the downwards wavefront on 1 (green arrow) will have travelled $\lambda/4$ downwards in z.
before the waveguide mode scatters off point 2. The downwards wavefront on 2 (tiny green arrow) is now $\lambda/2$ behind the downwards wavefront from 1, and so interfere destructively.

A traditional through-etch design is vertically symmetric and so has an upwards directionality of 50%. This double through-etch strategy increases the directionality to 70%. Apodisation increases the modal matching to ~80% [9]. However, the bilayer grating coupler’s performance is very dependent on inter-mask alignment.

### 2.4.5 SiN$_x$ Grating Coupler

Silicon nitride can be deposited on a silicon wafer as stoichiometric Si$_3$N$_4$ via Low Pressure Chemical Vapour Deposition (LPCVD) at ~800°C or as non-stoichiometric SiN$_x$ via Plasma-Enhanced Chemical Vapour Deposition (PECVD) at ~400°C [59]. One major advantage of PECVD SiN$_x$ over LPCVD Si$_3$N$_4$ is the lower heat budget required, enabling deposition of SiN$_x$ during front-of-the-line fabrication where the lower temperature will not interfere with dopant profiles.

Regardless, there are several benefits to designing a grating coupler out of either variant of silicon nitride:

- The thermo-optic coefficient of Si, $\frac{dn_{Si}}{dT} = 1.86 \times 10^{-4}/K @ 300K$ [60,61], whereas for Si$_3$N$_4$, $\frac{dn_{Si3N4}}{dT} = 2.45 \times 10^{-5}/K @ 300K$ [62] (~ 7 times less).

- Temperature dependence can be approximated as $\beta = \frac{1}{n} \frac{dn}{dT}$, which for silicon is $5.2 \times 10^{-5}/K$ [63–65], while for Si$_3$N$_4$ is $1.2 \times 10^{-5}/K$. Effectively speaking, the wavelength shift in Si photonic structures is ~ 0.1 nm / K, while in Si$_3$N$_4$ structures is ~ 0.02 nm / K [7]. Thus, Si$_3$N$_4$ structures have a lower (⅕) temperature dependence.
The refractive index of Si$_3$N$_4$ @ 1550 nm is 1.9963 [66], while that of Si$_x$N$_y$ can be tuned ~ 2 depending on the specific recipe (Si-rich: higher index; N-rich: lower index) [67]. The refractive index is sufficiently higher than SiO$_2$ (1.4440 @ 1550 nm, 293.15 K), enabling the design of high modal confinement photonic waveguides, while being significantly lower than Si (3.47) that fabrication tolerances are relaxed. The reduced modal confinement of a SiNx/SiO$_2$ waveguide reduces waveguide losses caused by sidewall and top roughness [59].

As per the Bragg condition (Section 2.3.1), i.e.

$$\Lambda = \frac{m\lambda}{\sin\theta_m - \frac{n_{eff}(\lambda)}{n}},$$

(2.3.1.1)

the lower the effective refractive index of the grating coupler ($n_{eff}$), the larger the pitch of the grating coupler ($\Lambda$). Bear in mind that both the numerator and denominator are negative as $m$ is usually = -1. The larger pitch ($\Lambda_{SiN} \sim 1.2$ µm & $\Lambda_{Si} \sim 0.65$ µm) entails fewer grating periods for the mode field diameter of the SMF28 (10.4 µm), and so a weaker wavelength dependence. For this reason, SiN grating couplers tend to have a better broadband response vs Si grating couplers (~1.7 times larger) [7].

Due to their high refractive index, Si grating couplers are usually not through-etched, as the strong grating strength (the amount of power diffracted per period) would increase undesirable backreflections. Thus, Si grating couplers usually require a separate mask layer and recipe for a partial RIE etch. With their lower refractive index, SiN grating couplers bypass this issue, allowing the SiO$_2$ beneath to act as a natural etch stop and simplifying the fabrication process [7].

Lastly, Si$_3$N$_4$ has a lower intrinsic material absorption than Si, and no significant nonlinear, free carrier, or two photon absorption effects [68], making it better suited as a waveguiding material. However, Si$_x$N$_y$ has N-H and Si-H bonds which absorb around
1520 nm [67]. PECVD recipe adjustments or circuit designs which avoid 1520 nm will be necessary.

2.4.6 Mirrors

In a theoretical 1-dimensional Bragg condition grating coupler, the power is diffracted equally in the +z and -z direction. 2-dimensional FDTD optimisations of 220 nm SOI grating couplers show that this can be skewed to ~66% for +z and ~44% for -z, as the teeth of the grating coupler are etched in from the top, i.e. vertically asymmetric.

The directionality ratio can be further skewed by adding mirrors between the grating coupler and the bulk silicon substrate to reflect the downward field. These mirrors can be made of metal [5,69,70] like gold [71,72] or aluminium [14,26,73,74] (Fig. 2.4.6.1(c)); single [6,7,75,76] (Fig. 2.4.6.1(a)) or multiple [2,6,10,77–81] (Fig. 2.4.6.1(b)) layers of dielectrics of alternating, contrasting refractive indices like polysilicon/SiNx and SiO2; or high contrast gratings [82] (Fig. 2.4.6.1(d)). Single/multiple dielectric mirrors are referred to as a Bragg Mirror / Distributed Bragg Reflector (DBR) as they operate on the principle of the Bragg condition as well. i.e. thin-film interference. However, the pitch of the scatterers (dielectric interfaces) are in the -z instead of the +x direction.

Gold has been shown to improve the coupling efficiency (directionality & modal field overlap) of SOI grating couplers from 30% to 72% [71]; aluminium improves coupling efficiency from 26.9% to 87.5% [74]; DBRs improve coupling efficiency from 26.9% to 68% [2,78]. Dielectric mirrors tend to have narrower reflectance as their operating principle is wavelength-dependent. In contrast, metals provide broadband reflectance in the infrared regime, with gold being superior to aluminium (cf. Fig. 2.4.6.2) due to its faster plasma frequency.
Fig. 2.4.6.1. Basic 220 nm-thick SOI grating coupler with various bottom mirrors. (a) Single Bragg mirror. Controlling the BOX thickness above the mirror and the mirror’s thickness allows both interfaces to contribute to upwards reflectance. Additionally, controlling the BOX thickness below the mirror allows the mirror and Si substrate to collectively behave as a double DBR. (b) Multiple DBR, usually polySi or SiN. (c) Backside metal. (d) HCG. Images adapted from [6].

Fig. 2.4.6.2 Reflectance of ultrahigh vacuum silver, gold and aluminium films. From [83] ©1965 OSA.
However, gold is avoided in practical designs due to silicon poisoning. Aluminium or DBRs can be deposited as buried structures beneath the SOI layer, or deposited above and then flip-chipped. Either method increases fabrication complexity of the whole wafer for a single device design. A single Bragg mirror can be fabricated on a double SOI (DSOI) substrate [76], though this is an even more expensive substrate than SOI.

Practically speaking, DBRs should be designed around pre-existing mask layers with predetermined thicknesses. However, doing so does not maximise the directionality of the grating coupler as the thin-film interference effect is obviously sensitive to variations in the z dimension. Hence, the best outcome is a compromised design where the DBR is somewhat effective with increasing the directionality without requiring adjustments to the layer stack.

2.4.7 Compact Focusing Grating Couplers

While a coupler’s 2D geometry accounts for most of its efficiency, its lateral geometry plays a significant role as well. For many grating coupler designs, the 2D geometry is invariantly extended into the y-dimension for a fixed length (12–15 µm), usually sufficient to accommodate the mode field diameter of a single mode fibre (10.4 µm). Such a design is called a linear / rectangular grating coupler.

Linear/rectangular grating couplers couple the fibre mode into a broad (12–15 µm) waveguide, which then needs to be tapered in the y-dimension to the width of a single mode waveguide. It is known that linear (straight) tapers perform better at longer lengths and sharper angles [84]. Taper length scales quadratically with width [85] and so are usually \( \approx 500 \ \mu \text{m} \) long to adiabatically convert the fundamental mode of the broad waveguide into the fundamental mode of the single mode waveguide. An adiabacity of 0.9999 requires angles as low as 0.4 mrad [86]. When the reciprocal time-reversed problem is considered, an acute angle ensures that the
taper’s sidewalls expand slower than the diffracting wave from the single mode waveguide, and so effectively confine the fundamental mode without exciting higher order / radiation modes [87].

Theoretically, adiabatic short linear tapers are possible where quasi-periodic mode conversion occurs between the zeroth order mode and usually the symmetric second order mode, and terminating the taper at the right length enables maximum power distribution in the fundamental mode. However, such multi-modal interference (MMI) designs might have a limited bandwidth and tight fabrication tolerances. As most linear taper designs for linear grating couplers require large footprints, there has been research in non-linear (radical, quadratic, Gaussian) [87,88], sinusoidal [89,90], and non-periodic segmented [91] tapers. The latter two design types also operate on MMI, and may be susceptible to similar drawbacks.

Conversely, focusing designs involve curving the grating coupler’s 2D profile into arcs. These arcs are usually elliptical, with a couple of correction factors. The most common formula used is

\[ q\lambda_0 = n_{\text{eff}}^{\text{grat}} \sqrt{x^2 + y^2} + x n_{\text{cladding}} \cos \theta_c , \]  

(2.4.7.1)

where \( q \) is an integer number for each grating line, \( \theta_c \) is the angle between the fiber and the chip surface, \( n_{\text{cladding}} \) is the refractive index of the oxide cladding, \( \lambda_0 \) is the vacuum wavelength, \( x \) and \( y \) are the coordinates of the elliptical curve: \( x \) is parallel to the waveguide; \( y \) is perpendicular, and \( n_{\text{eff}}^{\text{grat}} \) is the effective index of the grating.

Eq. 2.4.7.1 curves the arcs to ensure the diffracted wavefront phase-matches and interferes constructively at the focal point. It has been used in [27,28,92–96]. It is only valid when \( n_{\text{eff}}^{\text{grating}} = n_{\text{eff}}^{\text{taper}} \) which occurs for shallow etch (< ~50 nm) gratings. For deeper etch
gratings, the difference causes aberrations of the light, which results in a larger spot size of the beam and a correction term is added to minimise the aberration errors [15], yielding

$$q\lambda = n^{\text{grating}}_{\text{eff}}(x^2 + y^2)^{1/2} + n_{\text{cladding}}x \cos \theta_c + r(q_a) \times (n^{\text{taper}}_{\text{eff}} - n^{\text{grating}}_{\text{eff}}),$$  \hspace{1cm} (2.4.7.2)

where \( r(q_a) \) represents the correction term, which is weighted with the difference in the effective indices,

$$r(q_a) = q_a\lambda \frac{-xe_a(x^2 + y^2)^{1/2} + x^2 + y^2}{y^2 + (1 - e^2_a)x^2},$$  \hspace{1cm} (2.4.7.3)

with

$$e_a = \frac{n_{\text{cladding}} \cos \theta_c}{n^{\text{grating}}_{\text{eff}}},$$  \hspace{1cm} (2.4.7.4)

where \( e_a \) is the numerical eccentricity of the inner ellipse. Eq. 2.4.7.2 now represents an algebraic equation of the sixth order in \( x \) and \( y \).

Alternatively, [97,98] use another correction factor (expressed in a polar coordinate system):

$$r(q, \alpha) = \frac{q - q_0 \cdot \lambda_0}{n^{\text{grating}}_{\text{eff}} - n_{\text{cladding}} \sin \phi \cos \alpha} + p(q_0, \alpha),$$  \hspace{1cm} (2.4.7.5)

where

$$p(q_0, \alpha) = \frac{\kappa q_0 \lambda_0}{n^{\text{wgr}}_{\text{eff}} - n_c \sin \phi \cos \alpha},$$  \hspace{1cm} (2.4.7.6)

and \( r(q, \alpha) \) represents the trench radius of the grating, \( \alpha \) is the corresponding azimuth, \( q \in \mathbb{N} \) is the index of each line, \( q_0 \in \mathbb{N} \) is the index of the first line in the grating, \( \lambda_0 \) is the central wavelength of light in vacuum, \( \phi \) is the zenith of the coupling direction in free space, \( n^{\text{grating}}_{\text{eff}} \) is

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the effective index of the grating region, \( n_{\text{cladding}} \) is the effective index of the top cladding material, \( p(q_0, \alpha) \) represents the aberration correction factor, \( \kappa \) is a factor to determine the distance \( L \) between the first line and the entrance waveguide. \( \kappa \) is chosen as

\[
\kappa = \frac{n_s - n_c \sin \phi}{n_g - n_c \sin \phi},
\]

so that \( r(q_0, 0) \) is the same as that from the design without aberration correction.

However, it has been established that the aberration correction of the grating lines does not significantly affect the coupling efficiencies [15].

### 2.4.8 Other Advanced Grating Coupler Designs

The remaining design techniques listed here are for the sake of completeness. Generally, they are not compatible with zero-change designs because they require either extra layer masks (extended teeth), modifying the thickness of a given layer (BOX & TOX thickness, HCGs), material substitution (cladding engineering), or were not a primary design goal (polarisation diversity).

#### 2.4.8.1 Extended Teeth

A through-etched grating coupler without a silicon wafer substrate is vertically symmetric. Such a grating coupler diffracts light equally upwards and downwards. Partially etched grating couplers, in addition to modulating the grating strength of the grating coupler, also disrupt this vertical symmetry, thereby diffracting a greater proportion of the outgoing light upwards.

Extended teeth grating couplers operate on the principle of maintaining an optical path length difference of \( 2\pi \) between scattering centres for the upwards scattered light, as seen in Fig. 2.4.8.1. As the teeth are vertically asymmetric, a simultaneous path length difference for the
downward scattered light between scattering centres of \( \pi \) ensures destructive interference to the silicon substrate. Extended teeth grating couplers achieve this by having teeth extended in finely controlled thicknesses and therefore usually require a dedicated mask layer. Designs are usually based on crystalline silicon [100], deposited polysilicon [4,85,99], or silicon nitride [76,77,101]. Such designs can have a directionality of 85% [4].

![Operating principle of extended teeth grating coupler designs](image)

**2.4.8.2 Optimised BOX & TOX Thickness**

In Fig. 2.4.8.2.1, we consider an outgoing grating coupler, the waveguide’s mode encounters the grating and diffracts upwards (black arrow) and downwards (red arrow). The downwards diffracting wave reflects off the buried oxide (BOX) / bulk silicon substrate interface by Fresnel reflection (17.24%), picking up a \( \pi \) phase shift as due to the low-high index transition. When the total optical path length between this reflection (orange arrow) and the original downwards facing wave (red arrow) is \((2n+1)\pi\), i.e. an odd integer of \( \pi \), they undergo destructive interference, and the downwards energy lost to the silicon substrate is minimised. Any remaining energy from the first bottom-up reflection is either reflected downwards (pink arrows) or
diffracted upwards (yellow arrow). Optimum efficiency due to the BOX thickness is a balance between destructive interference between the red and orange arrows, and constructive interference between the black and yellow arrow. The subsequent downward/upward reflections (pink arrows) should similarly experience an odd-integer phase-shift in $\pi$ and also contribute to the desired destructive interference, but their contributions to this effect will be less.

As the BOX thickness is further increased, the phase difference approaches an even integer of $\pi$ ($2n\pi$), causing constructive interference downwards into the silicon substrate. Further increasing the BOX thickness once again causes destructive interference downwards. Fig. 2.4.8.2.2(a) shows how the oxide thickness sinusoidally affects the efficiency of a 220 nm SOI grating coupler optimised for TE-polarised 1550 nm.

Conversely, when we consider the upwards diffracted wave (black arrow), the first reflection (blue arrow) should ideally have a path length difference of an even integer of $\pi$, i.e.
$2\pi n$ to have a maximally efficient grating coupler. At such a phase shift, the top oxide behaves as an anti-reflection layer, where the upwards and downwards waves interfere constructively to produce a standing wave. However, the reflection is much smaller (3.43\%) and therefore the sinusoidal effect of the TOX thickness—compared to the BOX thickness—is less pronounced (cf. Fig. 2.4.8.2.2(b)).

![Graph](image)

**Fig.2.4.8.2.2(a) Grating coupler fibre-to-chip efficiency versus buried oxide (BOX) thickness for a 220 nm-thick SOI grating coupler optimised for 1550 nm, TE-polarised light. (b) Grating coupler fibre-to-chip efficiency versus top oxide (TOX) thickness for a 220 nm-thick SOI grating coupler optimised for 1550 nm, TE-polarised light.**

The first reflection (blue arrow) encounters the grating and part of it is reflected upwards (green arrow, obtaining a $+\pi$ phase shift due to the low/high index interface), while the other part is diffracted downwards (pink arrow).

When both BOX and TOX thicknesses are optimised, the phase differences between the initial upwards diffracted wave (black arrow), the second upwards reflected wave (green arrow), and the second upwards diffracted wave (yellow arrow) should be even integers of $2\pi$, thereby increasing the upwards directionality—and consequently the efficiency—of the grating coupler.
2.4.8.3 Cladding Engineering

The greater the difference in refractive indices between a grating and the cladding, the greater a grating coupler’s scattering strength, $\alpha$. It is also proportional to the grating confinement factor, $\Gamma_g$ [102]:

$$\alpha \propto (n_{\text{grating}}^2 - n_{\text{cladding}}^2) \Gamma_g,$$  \hspace{1cm} (2.4.8.3.1)

where $\Gamma_g$ is an integral of the E-fields of the forward (p) and backward (q) propagating modes,

$$\Gamma_g = \int_{-\alpha}^{0} E_p^*(z) E_q(z) dz,$$  \hspace{1cm} (2.4.8.3.2)

and ‘a’ is the etch depth.

In a high-index-contrast platform like SOI/SiO$_2$ (Fig. 2.4.8.3.1(b)), the $E_p(z)$ is well-confined to the grating layer and the index contrast allows a high $\alpha$, short coupler. By reducing the $n_{\text{cladding}}$ to air (Fig. 2.4.8.3.1(a)), one might expect an even stronger grating coupler. However, the lower $n_{\text{cladding}}$ confines the $E_p(z)$ deeper so less of the mode is exposed to the grating interface, and counter-intuitively leads to a grating with lower directionality as seen in Fig. 2.4.8.3.1.
2.4.8.3.2. The same phenomenon also occurs in low-index-contrast platforms like SOI/InP when the superstrate is replaced with SiO$_2$ (Fig. 2.4.8.3.1(d)–(e)). Similarly, increasing the etch depth may increase grating strength up to a point, but further etching moves the waveguide mode deeper into the grating, and reduces the interaction of the field with the grating.

Medium-index liners have been used to shift the position of the E-field upwards (Fig. 2.4.8.3.1(c), (f)–(g)), thereby increasing the interaction between the mode and the grating interface. In particular, Si$_3$N$_4$ (n = 1.9894 @ 1550 nm) liners have been employed in high-efficiency grating couplers [8,52,53].

Fig. 2.4.8.3.2 shows the upwards directionality of an SOI grating coupler with 2 µm of top cladding as the cladding material is changed with common CMOS dielectrics. The grating coupler’s dimensions were kept constant to give the reader an impression of the effects of changing the waveguide mode E-field profile via $n_{\text{cladding}}$ rather than to determine which cladding material is ‘best’.
2.4.8.4 Polarisation Diversity

Grating couplers are usually designed for either TE or TM polarisation. However, there are circumstances in which having a grating coupler capable of coupling either polarisation would be advantageous. For instance, the fibre could have an axial rotation misalignment which would rotate polarised light off its ideal alignment with respect to the grating coupler. Alternatively, the fibre could be a non-polarisation-maintaining fibre, and random bends in it could cause mechanically-induced birefringence, leading to an unknown polarisation output.

There are two general strategies for designing polarisation diverse grating couplers, as shown in Fig. 2.4.8.4.1.

Of the two, Fig. 2.4.8.4.1(b) is the more common method [23,69,72,95,103–107] whereby two single-polarisation grating couplers are superposed on top of one another with a ~90° rotation. Where the two gratings’ lower index regions intersect, a scattering element (usually a cylinder of SiO₂ of the appropriate radius, though research suggests that other shapes might be more suitable...
for polarisation diverse grating couplers [23,108–111] is placed. Because each individual grating coupler’s scattering region is discontiguous, such designs usually have a poorer performance (-3.75 dB, [103]) for each individual grating coupler compared to dedicated single polarisation grating couplers designed on the same platform.

Fig 2.4.8.4.1(a) depicts a method used in [73] whereby the TE and TM polarised light are diffracted in opposite directions. This design is possible as the polarisations have different effective indices, \( n_{\text{eff,TE}} \) and \( n_{\text{eff,TM}} \). By optimising the \( \theta_m \), \( m \) and \( \Lambda \) from Eq. 2.3, the coupling efficiencies of both polarisations can be equal. This method is also used for duplexing different wavelengths [19,105,112] or for increasing bandwidth [113].

A third option (not shown) involves refractive index manipulation through subwavelength grating structures so that the average mode effective index for both modes is the same [114].

2.4.8.5 High Constrast Gratings

Between the diffraction regime (grating period > \( \lambda \)) and the sub-wavelength regime (grating period \( \ll \lambda \)) is the near-wavelength regime (\( \lambda_0/n_{\text{grating}} \) < grating period < \( \lambda_0/n_{\text{cladding}} \)). Gratings which occupy this near-wavelength regime and have their high-index media fully surrounded by low-index media are High Contrast Gratings (HCGs) and can be engineered to have unique properties such as high Q-factors (Q > 107), broadband high reflectivity (> 99%), and broadband high transmissivity (> 99%) [115], as shown in Fig. 2.4.8.5.1.

Which property an HCG has is determined by the accumulated phase difference between modes propagating in the HCG. When we consider an incident, \( \theta = 0^\circ \) planewave on just an isolated HCG (bottom part of Fig. 2.4.8.5.2), several waveguide array modes are excited in the HCG. The properties arise in the wavelength range where only two modes have real propagation
constants. Higher order modes form evanescent, surface-bound waves [115], which mandate the HCG to be surrounded completely by lower-index media to optically isolate it. The two propagating modes have different lateral profiles and hence different effective indices, $n_{\text{eff}}$'s, and thus propagate downwards through the HCG at different velocities. At the exit plane, the modes reflect back upwards to the entrance plane as well as couple into each other. Both phenomena similarly occur after a round trip at the entrance plane.

The HCG thickness, $t_g$, determines the phase difference and thus which of the three properties the HCG has: destructive interference at the exit plane produces a high reflectivity HCG; constructive interference at the exit plane produces a high transmissivity HCG; constructive interference at both planes produces a high Q-factor resonating HCG.

Fig. 2.4.8.5.1. Three unique properties of HCGs. (a) The high-$Q$ resonances (red) are characterised by very sharp transitions from 0 to $\sim$100% reflectivity and vice versa, as labeled by the black arrows. (b) Broadband high reflection with 99% reflection bandwidth (from 1.344 to 1.922 $\mu$m). (c) Broadband high transmission (green) $>99.68\%$ over a broad spectrum. From [115] © OSA 2012.
Fig. 2.4.8.5.2. High Contrast Grating as reflector. The blue and red oscillating curves represent the E\textsubscript{z} field intensities of the primary and secondary modes of the HCG respectively. The modes have different effective indices and so travel at different speeds. They accumulate a phase difference of $\pi$ as they leave the bottom exit plane of the HCG and so destructively interfere downwards. Conversely, their reflections from the exit plane back up leave the top entrance plane of the HCG with a phase difference of $2\pi$ and so interfere constructively, enabling a near unity reflection coefficient.

The property of concern for this thesis is using the HCG as a reflector [82,116], though using resonant HCGs as grating couplers has also been explored in the literature [117]. Fig. 2.4.8.5.2 shows a reflective HCG being used as a reflector for a standard 220 nm SOI grating coupler. Initially, the waveguide mode diffracts off the diffraction grating. The vertical asymmetry enables more light to be diffracted to the superstrate top oxide (TOX) ($\sim 45\%$) than the bottom oxide (BOX) ($\sim 35\%$). The BOX has to be sufficiently thick above and below the HCG to optically isolate it and avoid evanescent coupling of the waveguide or Si substrate with the higher order surface-bound modes of the HCG.

The downwards diffracted light excites the two propagating modes in the HCG (their E\textsubscript{z} field profiles represented by the oscillating blue (fundamental) and red (first harmonic) lines) which interfere constructively back at the entrance plane after a round-trip reflection. As the incident light is not a planewave and $\theta \neq 0^\circ$, the HCG is not fully reflective and $<35\%$ of the
light is reflected upwards. A secondary diffraction occurs at the 220 nm SOI grating coupler, and the additional light coupled to SMF-28 is less than 35% owing to mode matching and diffraction angle losses. Despite these additional losses, a highly reflective layer such as an HCG will still significantly increase the coupling efficiency of a grating coupler.

Fig. 2.4.8.5.3 Reflectance contours of mono-crystalline silicon (n = 3.48 @ 1550 nm) High Contrast Grating (HCG) embedded in low-index silicon dioxide (n = 1.44 @ 1550 nm). (a) Reflectance as a function of vacuum wavelength and grating thickness, $t_g$ with $\Lambda = 870$ nm & duty cycle = 0.460. Vertical dotted lines separate the diffraction, near wavelength and sub-wavelength regimes. A horizontal dotted line delineates the broadband reflectance for a HCG of $t_g = 0.220$ nm. (b) Broadband reflectance as a function of duty cycle with $\Lambda = 870$ nm & $t_g = 220$ nm. (c) Reflectance vs $\Lambda$ and duty cycle with $t_g = 220$ nm and $\lambda_0 = 1550$ nm. (d) Reflectance vs $\Lambda$ and duty cycle with $t_g = 100$ nm and $\lambda_0 = 1550$nm. (a)-(d) Source was an infinite, TE-polarised, $\theta = 0^\circ$ planewave. (c)-(d) Source was a 1550 nm, 10.4 $\mu$m diameter Gaussian with $\theta = 10^\circ$. 

(a) diffraction regime  
(b) near-wavelength regime  
(c) sub-wavelength regime

Fig. 2.4.8.5.3 Reflectance contours of mono-crystalline silicon (n = 3.48 @ 1550 nm) High Contrast Grating (HCG) embedded in low-index silicon dioxide (n = 1.44 @ 1550 nm). (a) Reflectance as a function of vacuum wavelength and grating thickness, $t_g$ with $\Lambda = 870$ nm & duty cycle = 0.460. Vertical dotted lines separate the diffraction, near wavelength and sub-wavelength regimes. A horizontal dotted line delineates the broadband reflectance for a HCG of $t_g = 0.220$ nm. (b) Broadband reflectance as a function of duty cycle with $\Lambda = 870$ nm & $t_g = 220$ nm. (c) Reflectance vs $\Lambda$ and duty cycle with $t_g = 220$ nm and $\lambda_0 = 1550$ nm. (d) Reflectance vs $\Lambda$ and duty cycle with $t_g = 100$ nm and $\lambda_0 = 1550$nm. (a)-(d) Source was an infinite, TE-polarised, $\theta = 0^\circ$ planewave. (c)-(d) Source was a 1550 nm, 10.4 $\mu$m diameter Gaussian with $\theta = 10^\circ$. 

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As previously mentioned, HCGs are primarily tuned by their $t_g$. Fig. 2.4.8.5.3(a) shows the reflectivity contour of an Si-in-SiO$_2$ HCG with $\Lambda = 870$ nm and duty cycle $= 0.460$. The source is a $\theta = 0^\circ$ TE-polarised planewave. $\Lambda$ and duty cycle values had previously been determined to produce the highest reflection values for a $t_g = 220$ nm @ 1550 nm [82]. Vertical dotted lines delineate the diffraction, near-wavelength and subwavelength regimes. For the broadest broadband reflection, $t_g = 440$ nm would be preferred, and it could be further improved with duty cycle optimisation. However, 220 nm-thick SOI is a more common substrate. Fig. 2.4.8.5.3(b) shows how the reflectivity contour of a $t_g = 220$nm HCG can be further tuned by the duty cycle (peak reflectivity (95.1%) at duty cycle $= 0.425$).

Fig. 2.4.8.5.3(c) shows the reflectance contour of a $t_g = 220$ nm HCG vs $\Lambda$ and duty cycle, when the source is a $10^\circ$-tilted 10.4 $\mu$m diameter Gaussian. The non-planewave profile and oblique angle reduce the reflectivity of the HCG as odd modes are excited [115]. Fig. 2.4.8.5.3(d) shows a similar plot for $t_g = 100$ nm, as both thicknesses were available as pre-existing mask layers. A comparison of both graphs shows that if the SOI is intended to be used as a reflective layer, the preferred $t_g$ is 220 nm, with $\Lambda = 760$ nm and duty cycle $= 0.26$, with a reflection of 71.8%. Note also that due to the tilt and Gaussian profile, the optimum $\Lambda$ and duty cycle values deviate quite significantly from those obtained in Fig. 2.4.8.5.3(b).

Although a 71.8% reflective HCG mirror would still significantly increase a grating coupler’s efficiency, as the HCG has surface-bound higher order modes, it must be optically isolated to prevent coupling to the grating coupler, which involves a BOX separation on the order of microns. In a zero-change design, such optical isolation may not be a viable option.


2.5 Conclusions

There are a number of techniques to improve apices of the grating coupler performance three-pointed star, most notably, coupling efficiency. Basic grating coupler design can be determined analytically with Eq. 2.3.1.1, the Bragg condition. Individually, most techniques can also be determined analytically. However, when multiple techniques are combined, a multi-variable optimisation space emerges as the variables are interdependent, and the analytically determined values only provide ballpark values for the final gestalt design.

Finally, the advanced techniques are split into two broad categories: zero-change-compatible and zero-change-incompatible. Techniques in the former are used in this work, whereas those in the latter are not.

2.6 Chapter Bibliography

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“Ultra
3. High Positional Freedom (HPF) Grating Coupler

3.0. Chapter Overview

- The $x \times y$ -1 dB lateral misalignment tolerance for:
  - A standard SOI-based grating coupler is $3 \mu m \times 3 \mu m$
  - A HPF grating coupler is $21.4 \mu m \times 10.1 \mu m$.

- The HPF GC has a measured maximum coupling efficiency of -7.49 dB (17.8%), and a -1 dB / -3 dB bandwidth of 14 nm / 29.5 nm respectively.

- Etched: Unetched ratios for $\Lambda_y$ periods of 600 nm were numerically calculated by 3D FDTD and serve as a reference for future designs.

- Scattering element rotation and translation is not explicitly researched in the scientific literature. We have shown that:
  - For elliptical designs, scattering element rotation and translation increased the coupling efficiency by 0.41 dB (9.9%) and the -1 dB area by 12.8%.
  - For circular designs, scattering element rotation and translation decreased the coupling efficiency by -0.75 dB (-15.9%) but increased the -1 dB area by 28.3%. 

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3.1. Introduction

220 nm-thick silicon-on-insulator (SOI) has been a platform for silicon photonics integrated circuits since before 2003 [1]. Although other thicknesses were originally offered, for economic and historical reasons [2], 220 nm SOI has become a standard platform in multi-project wafer (MPW) foundries (e.g. imec, LETI, IME) [3] despite larger thicknesses (250 nm – > 400 nm) being the optimal thickness for photonic MPWs [2].

To ensure high chip yield, optical testing of a wafer at its various process steps is required. This usually involves coupling light from an external laser source via a single mode fibre into the on-chip waveguide. However, there is a large modal mismatch between the mode size of an SMF28 fibre (from Corning, 1550 nm mode field diameter (MFD) of 10.4 μm) and a 450–550 nm × 220 nm SOI single mode strip waveguide.

There are two common methods of mode-size conversion: butt-coupling via tapers / inverse tapers and vertical coupling via grating couplers. (Inverse) taper solutions typically require dicing of the wafer and polishing of the chip edge. This prevents their use in wafer scale testing. Furthermore, their alignment accuracy is about -3 dB for ±1–2.3 μm of misalignment [4–7]. Additionally, in the case of inverse tapers, the tip must be very narrow, e.g. 30 nm [8], resulting in a low-yield of inverse taper devices or in some cases, designs being incompatible with standard CMOS processes. Lastly, the taper’s resulting mode size is still smaller than a cleaved SMF28, requiring a lensed SMF28 to improve modal matching [9,10].

In contrast, grating couplers are not limited to chip-edge real estate, do not require wafer dicing (easily facilitating non-destructive wafer-scale testing) and are compatible with cleaved SMF28 optical fibres. In this sense, optical grating couplers are the equivalent of electrical test pads in the electronics world.
A subwavelength grating (SWG) grating coupler was chosen to fulfil this purpose because it is a single mask, through-etch design where the buried oxide (BOX) acts as a natural etch-stop, which simplifies fabrication and eliminates effects from misaligning multiple masks.

While a regular grating coupler has its duty cycle (etch ratio) in just the x-dimension (parallel to the waveguide) optimised, in an SWG grating coupler also has its duty cycle in the y-dimension (perpendicular to the waveguide) manipulated to produce a metamaterial with the desired equivalent refractive index, \( n_{eq} \), affording another degree of freedom in its design, despite having only one etch level.

Most of the literature regarding SWG grating couplers (see Table 3.1.1) have been designs to maximise the chip-fibre directionality [11]; mode-matching to an SMF28 [12]; polarisation diversity [13–15]; bandwidth [16,17]; and 3D integration [18], and have achieved measured coupling efficiencies of \( \sim -2 \) – \( -6 \) dB.

**Table 3.1.1. A comparison of recent SWG Grating Couplers**

<table>
<thead>
<tr>
<th>Ref.</th>
<th>( \Lambda ) (nm)</th>
<th>Polarisation</th>
<th>SOI thickness (μm)</th>
<th>BOX thickness (μm)</th>
<th>( \Lambda_y ) SWG (μm)</th>
<th>( \Lambda_y ) SWG Uniform/Apodised</th>
<th>Measured Efficiency (dB / %)</th>
<th>Measured -1 dB Bandwidth (nm)</th>
<th>Measured -3 dB Bandwidth (nm)</th>
<th>Remarks</th>
<th>( \theta ) (°)</th>
</tr>
</thead>
<tbody>
<tr>
<td>[13]</td>
<td>1550</td>
<td>TE/TM</td>
<td>0.22</td>
<td>2</td>
<td>0.612</td>
<td>Uniform/Apodised</td>
<td>-5 (31.6%)</td>
<td>30</td>
<td>N/A</td>
<td>Polarisiation</td>
<td>14</td>
</tr>
<tr>
<td>[14]</td>
<td>1550</td>
<td>TE/TM</td>
<td>0.22</td>
<td>2</td>
<td>-0.650</td>
<td>Uniform/Apodised</td>
<td>-4.1 (38.9%)</td>
<td>~35</td>
<td>~72</td>
<td>Scattering shape PDL</td>
<td>10</td>
</tr>
<tr>
<td>[18]</td>
<td>1550</td>
<td>TE</td>
<td>0.22</td>
<td>2</td>
<td>0.5</td>
<td>Uniform/Apodised</td>
<td>-6.02 (25%)</td>
<td>~25</td>
<td>~37</td>
<td>SWG to integrated photodetector</td>
<td>NA</td>
</tr>
<tr>
<td>[19]</td>
<td>1560</td>
<td>TE</td>
<td>0.22</td>
<td>3</td>
<td>0.5</td>
<td>Uniform/Apodised</td>
<td>-4.56 (35%)</td>
<td>~38</td>
<td>~54</td>
<td>Large ( \Lambda_y ) SWG</td>
<td>20</td>
</tr>
<tr>
<td>[15]</td>
<td>1550</td>
<td>TE/TM</td>
<td>0.22</td>
<td>3</td>
<td>0.65</td>
<td>Uniform/Apodised</td>
<td>-5.8 (26.3%)</td>
<td>35</td>
<td>N/A</td>
<td>Polarisiation</td>
<td>10</td>
</tr>
<tr>
<td>[11]</td>
<td>1550</td>
<td>TE</td>
<td>0.22</td>
<td>3</td>
<td>0.45</td>
<td>Uniform/Apodised</td>
<td>-0.69 (85.3%)</td>
<td>~29</td>
<td>60</td>
<td>SWG with mirror</td>
<td>27</td>
</tr>
<tr>
<td>[20]</td>
<td>1550</td>
<td>TE</td>
<td>0.22</td>
<td>3</td>
<td>0.45</td>
<td>Uniform/Apodised</td>
<td>-2.16 (60.8%)</td>
<td>~32</td>
<td>64</td>
<td>High efficiency, large angle SWG</td>
<td>27</td>
</tr>
<tr>
<td>[17]</td>
<td>1550</td>
<td>TE</td>
<td>0.22</td>
<td>3</td>
<td>1D</td>
<td>Uniform/Apodised</td>
<td>-3.2 (47.9%)</td>
<td>36</td>
<td>~58</td>
<td>1D SWG</td>
<td>31</td>
</tr>
<tr>
<td>[16,17]</td>
<td>1550</td>
<td>TE/TM</td>
<td>0.22</td>
<td>3</td>
<td>1D</td>
<td>Uniform/Apodised</td>
<td>-5.5 (28.2%)</td>
<td>90</td>
<td>N/A</td>
<td>1550 Broadband 1D SWG</td>
<td>25</td>
</tr>
<tr>
<td>This work</td>
<td>1550</td>
<td>TE</td>
<td>0.22</td>
<td>2</td>
<td>0.6</td>
<td>Uniform/Apodised</td>
<td>-7.49 (17.8%)</td>
<td>14</td>
<td>29.5</td>
<td>HPF GC</td>
<td>14.5</td>
</tr>
<tr>
<td>[21]</td>
<td>1450</td>
<td>TE</td>
<td>0.22</td>
<td>2</td>
<td>0.400, 0.450, 0.500</td>
<td>Uniform/Apodised</td>
<td>-4.69 (34%)</td>
<td>22</td>
<td>40</td>
<td>circular scatterers</td>
<td>8</td>
</tr>
<tr>
<td>[22]</td>
<td>1310</td>
<td>TE</td>
<td>0.22</td>
<td>3</td>
<td>1D</td>
<td>Uniform/Apodised</td>
<td>-4.5 (35.5%)</td>
<td>30</td>
<td>~65</td>
<td>1310 Broadband</td>
<td>30</td>
</tr>
<tr>
<td>[23]</td>
<td>1310</td>
<td>TE</td>
<td>0.22</td>
<td>2</td>
<td>0.4</td>
<td>Uniform/Apodised</td>
<td>-2.5 (56.2%)</td>
<td>~38</td>
<td>N/A</td>
<td>SWG for O-band</td>
<td>33</td>
</tr>
<tr>
<td>[24]</td>
<td>1550</td>
<td>TE</td>
<td>0.25</td>
<td>3</td>
<td>0.350, 0.300, 0.250</td>
<td>Uniform/Apodised</td>
<td>-5.1 (30.9%)</td>
<td>70</td>
<td>117</td>
<td>Broadband via dispersion engineering</td>
<td>16</td>
</tr>
</tbody>
</table>
Where not stated in the original reference, the -1 dB / -3 dB bandwidth loss was measured from the published data and indicated with a ‘~’. Where such data was unavailable, a ‘N/A’ was used. A thicker horizontal border separates SWG grating couplers based on 0.220 µm SOI from those based on thicker SOI substrates.

Although grating couplers have greater lateral misalignment tolerances than tapers, to ensure consistent results, optical wafer-scale testers should still have lateral alignment accuracies of < 1 µm, height control of < 5 µm, and fibre angle control < 0.2°[37]. Although the lateral misalignment tolerances of 220 nm SOI SWG grating couplers are not generally published, they should be on a similar scale to that of a 220 nm SOI non-SWG grating coupler with a 1 µm BOX, as shown in Fig. 3.1.1(a) [39], i.e. a -1 dB misalignment tolerance of ± 2.5 µm. As another point of comparison, Fig. 3.1.1(b) [40] is the misalignment tolerance of a 250 nm SOI non-SGW grating coupler with a 3 µm BOX.

By increasing the misalignment tolerance, we can reduce the complexity of the machinery (for automated probers) as well as the skill of the technician (for manual probers) in aligning the optical fibre probes needed for wafer scale testing.
A non-SWG grating coupler has been designed to have high positional freedom in z-, the vertical axis, achieving ~ -6 – -8 dB between +50 µm – +300 µm for 1550 nm [41,42]. However, earlier research has shown that for z < 15 µm, the additional coupling loss is negligible, and only -0.5 dB for z = 55 µm [39].

![Fig. 3.1.1(a) Comparison of simulation and measurement results of the lateral alignment tolerances. The smooth curves are simulation results. The normalised coupling efficiency is shown as function of the lateral position of the fibre. The distance between fibre and grating is approximately 10 µm. The -0.5 and -1 dB contour are indicated on the figure. The SOI thickness is 220 nm and the BOX thickness is 1 µm. Reproduced with permission from [39] © 2006 JSAP. (b) The absolute coupling efficiency as a function of the lateral position of the fibre. The SOI thickness is 250 nm and the BOX thickness is 3 µm. Reproduced with permission from [40] © 2011 IEEE. The wavelength is 1550 nm and is TE-polarised in both references.](image-url)

Separately, another non-SWG grating coupler achieved a horizontal misalignment tolerance of ~ -3 dB for ± 4 µm along the direction of the waveguide (x-axis) (y-axis misalignment tolerance not stated) [43].

Lastly, it has been shown that a Si₃N₄-on-SOI grating coupler with a uniform flat-top E-field output as long as a millimetre is possible for applications in optical phased arrays [44]. If used as a grating coupler, it would theoretically have an x-axis misalignment tolerance on the order of a millimetre, though its coupling efficiency would likely be very low.

Thus, this work presents an SWG grating coupler to maximise the lateral positional freedom of the SMF28 while maintaining a reasonable coupling efficiency. This is the first
attempt (to our knowledge) of maximising lateral positional freedom using an SWG. The grating coupler has a peak coupling efficiency of -7.49 dB, -1 dB misalignment tolerance of 21.4 µm × 10.1 µm, and a measured coupling efficiency of -1 dB / -3 dB bandwidth of 14 nm / 29.5 nm respectively.

### 3.2. 2D Design of HPF Grating Coupler

#### 3.2.1. Determining Optimisation/Apodisation Order

The simulation software used for optimising this design was Lumerical FDTD, a commercial-grade simulator based on the finite-difference time-domain method (Lumerical Solutions, Inc., n.d.). Lumerical FDTD utilises ‘Particle Swarm Optimisation’, a population-based stochastic optimisation technique to optimise nanophotonic designs. For the remainder of this thesis, unless otherwise stated, ‘optimisation’ will refer to Lumerical’s ‘Particle Swarm Optimisation’.

Generally, grating couplers are apodised to accept a 5.2 µm-radius Gaussian E-field, which represents an SMF28. In these cases, apodisation order for periods is usually nearest-to-waveguide first. However, it was hypothesised that a high positional freedom grating coupler would require a long (20–30 µm) planewave input, crossing over tens of periods. As the profile of this input E-field is very different from the 5.2 µm-radius Gaussian, initial simulation attempts were undertaken to determine which of the following was the best apodisation methodology to produce a high positional freedom grating coupler:

1. Varying Length Planewave Input, Nearest-to-Waveguide Apodisation
2. Varying Length Planewave Input, Farthest-from-Waveguide Apodisation
3. Constant Length Planewave Input, Nearest-to-Waveguide Apodisation
4. Constant Length Planewave Input, Farthest-from-Waveguide Apodisation
First, 220 nm-thick, 6μm BOX, SOI SWG, with an infinitely tall top oxide was modelled in Lumerical, as shown in Fig. 3.2.1.1. A 2D FDTD computation domain was drawn with Perfectly Matching Layers (PML) as boundary conditions. A ‘frequency domain field and power’ monitor was drawn on the waveguide on the left to monitor the leftwards travelling coupled power. A 26μm long, 1550 nm planewave source with a 10° tilted from the vertical was added 3.8 μm above the polysilicon / buried oxide interface, with the centre 12 μm to the right of the start of the SWG.

The basic SWG above had infinite periods, was unapodised, with variables of $\Lambda_x$, Duty Cycle, and SWG $n_{eq}$. Lumerical’s Particle Swarm Optimisation was then used to maximise the power going leftwards through the power monitor. The resultant SWG GC’s properties are listed in Table 3.2.1.1.
Next, to represent the input from an SMF-28, a 5.2 μm-radius Gaussian source at 1550 nm, 10° tilted from the vertical, 5.8 μm above the polysilicon – buried oxide interface was swept horizontally in the x-axis and the monitor’s power transmission was recorded. This is the ‘original’ SWG’s positional performance against which the remaining 4 apodisation methods’ SWGs will be compared to in Fig. 3.2.1.2.

For the purposes of apodisation, the aforementioned basic design indicated that 32 periods would be sufficient to span the length of the input source: 32 × 0.846 μm ≈ 27 μm. Those periods were grouped as appropriate to reduce simulation intensiveness for this cursory study.

1. **Varying Length Planewave Input, Nearest-to-Waveguide Apodisation:**

   With the first period being a reference of x = 0 μm, the input source was a 26 μm long (-1 μm < x < 25 μm) planewave source while periods 1–4 were optimised in terms of period length, duty cycle and effective SWG etch index to maximise in-coupled light to the power monitor.

   Next, the input source was reduced to 19.29 μm (5.71 μm < x < 25 μm), so that the majority of the source did not impinge on the first 4 periods, and periods 5–8 were optimised to maximise in-coupled light.

   Next, the input source was again further reduced to 17 μm (8 μm < x < 25 μm), so that the majority of the input E-field did not impinge on periods 1–8 and periods 9–12 were then optimised to maximise the in-coupled light into the waveguide power monitor.

   Finally, the input source was reduced to 14 μm (11 μm < x < 25 μm), so that the majority of the input E-field did not impinge on periods 1–12 and periods 13–32 were then optimised to maximise the in-coupled light into the waveguide power monitor.
2. **Varying Length Planewave Input, Farthest-from-Waveguide Apodisation:**

As the reverse of method 1, this method optimised periods 13–32 with a 14 µm input source, then periods 9–12 with a 17 µm source, then periods 5–8 with a 19.29 µm source, and finally periods 1–4 with a 26 µm source.

3. **Constant Length Planewave Input, Nearest-to-Waveguide Apodisation:**

This method utilised a planewave input with a constant length of 26 µm (-1 µm < x < 25 µm). Periods 1–8 were first optimised, followed by 9–16 and finally 17–32.

4. **Constant Length Planewave Input, Farthest-from-Waveguide Apodisation:**

As the reverse of method 3, this utilised a constant length 26 µm planewave input which first optimised periods 17–32, then 9–16 and finally 1–8.

The details of the apodised grating couplers produced from the above four methods are listed in Table 3.2.1.1:

<table>
<thead>
<tr>
<th>Apodisation Method</th>
<th>Variables</th>
<th>Periods 1–4</th>
<th>Periods 5–8</th>
<th>Periods 9–12</th>
<th>Periods 13–32</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Original</strong></td>
<td>Period (µm):</td>
<td>0.847</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Duty Cycle:</td>
<td>0.4583</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>SWG ( n_{eq} ):</td>
<td>2.252</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Varying Length Planewave Input, Nearest-to-Waveguide</strong></td>
<td>Period (µm):</td>
<td>0.792</td>
<td>0.819</td>
<td>0.563</td>
<td>0.936</td>
</tr>
<tr>
<td></td>
<td>Duty Cycle:</td>
<td>0.4066</td>
<td>0.5488</td>
<td>0.3841</td>
<td>0.3622</td>
</tr>
<tr>
<td></td>
<td>SWG ( n_{eq} ):</td>
<td>2.516</td>
<td>2.754</td>
<td>3.016</td>
<td>2.072</td>
</tr>
<tr>
<td><strong>Varying Length Planewave Input, Farthest-from-Waveguide</strong></td>
<td>Period (µm):</td>
<td>0.303</td>
<td>0.357</td>
<td>0.445</td>
<td>0.830</td>
</tr>
<tr>
<td></td>
<td>Duty Cycle:</td>
<td>0.5264</td>
<td>0.4124</td>
<td>0.010</td>
<td>0.6768</td>
</tr>
<tr>
<td></td>
<td>SWG ( n_{eq} ):</td>
<td>3.058</td>
<td>2.896</td>
<td>2.753</td>
<td>1.966</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Apodisation Method</th>
<th>Variables</th>
<th>Periods 1–8</th>
<th>Periods 9–16</th>
<th>Periods 17–24</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Constant Length Planewave Input, Nearest-to-Waveguide</strong></td>
<td>Period (µm):</td>
<td>0.792</td>
<td>0.847</td>
<td>1.034</td>
</tr>
<tr>
<td></td>
<td>Duty Cycle:</td>
<td>0.4636</td>
<td>0.4583</td>
<td>0.3610</td>
</tr>
<tr>
<td></td>
<td>SWG ( n_{eq} ):</td>
<td>2.489</td>
<td>2.253</td>
<td>1.601</td>
</tr>
<tr>
<td><strong>Constant Length Planewave Input, Farthest-from-Waveguide</strong></td>
<td>Period (µm):</td>
<td>0.831</td>
<td>0.903</td>
<td>1.023</td>
</tr>
<tr>
<td></td>
<td>Duty Cycle:</td>
<td>0.3657</td>
<td>0.3960</td>
<td>0.3744</td>
</tr>
<tr>
<td></td>
<td>SWG ( n_{eq} ):</td>
<td>2.405</td>
<td>2.068</td>
<td>1.671</td>
</tr>
</tbody>
</table>

Duty Cycles are reported to 4 decimal places in order to reproduce structures to the nearest nm.
Finally, a 5.2 µm-radius Gaussian source, as previously mentioned, was swept across the x-axis and the input transmission for all the grating couplers was monitored. Fig. 3.2.1.2 shows the grating couplers’ relative performances.

As can be seen from the graph, apodising the periods in a nearest-to-waveguide manner with a constant 26µm planewave input (pink line) produces the best results in obtaining a grating coupler with high positional freedom.

3.2.2. 2D Design: Optimisation

Now that optimal apodisation order has been determined, we refined the optimisation method first using 2D FDTD before moving on to 3D FDTD to reduce computation requirements. First, 220 nm thick SOI SWG was modelled in Lumerical. A 24 µm long, TE-
polarised 1550 nm planewave, 10° tilted off vertical, was used as the input source, the profile of which is below:

![E-field profile](image)

Fig. 3.2.2.1. Input source E-field profile: the input source is a 24 µm long planewave, at 1550 nm with transverse electric (TE) polarisation, 10° tilted from the surface normal.

The grating coupler was first designed 2-Dimensionally in the x-z plane with a 24 µm long, TE-polarised, 1550 nm planewave input with a 10° tilt from the surface normal, as shown in Fig. 3.3.2. 2D placeholders occupied the etched low-index sections of the SWG with an equivalent refractive index, $n_{eq,i}$, which will later determine the dimensions of $l_{y, Si}$ and $l_{y, SiO_2}$ via a combination of Effective Medium Theory (EMT) and 3D FDTD. 2D optimisation occurred at a mesh accuracy setting of 2 (10 mesh points per wavelength) in four stages using a nearest-to-waveguide fashion, through increasingly finer iterations based on powers of 2:

**Stage 1**: the SWG was apodised as a single set of 40 periods. 24 µm spans about 36 periods for most grating couplers based on the 220 nm SOI platform (24 µm / 0.66 µm ≈ 36). 40 periods for this grating coupler was chosen as it is slightly larger than 36 and divisible by powers of 2.

**Stage 2**: periods were apodised as batches of $2^4$: periods 1–16 were optimised, then 17–40.
Stage 3: periods were apodised as batches of $2^3$: periods 1–8 were optimised, followed by 9–16, 17–24, 25–40.

Stage 4: periods were apodised as batches of $2^2$: the grating was optimised as 10 batches of periods of 4.

Ostensibly, a fifth and sixth stage are possible where periods would be apodised as batches of $2^1$ and finally $2^0$, but these were skipped due to exponentially increasing computational demands and diminishing returns in coupling efficiency.

The variables for each optimisation stage were: the centre position of the planewave source from the grating start ($12 \pm 2 \text{ µm}$), a given batch’s period, $\Lambda_x$, ($0.64 \pm 0.2 \text{ µm}$), a given batch’s duty cycle $= \frac{l_{x,\text{Si}}}{\Lambda_x}$, (0.3–0.7) and the equivalent index of the etched section, $n_{\text{eq},i}$, (1.444 – 3.476).

Fig. 3.2.2.2. Schematic drawing of the SWG high positional freedom grating coupler. The input source is a 24 µm long, 1550 nm, TE-polarised planewave tilted 10° from vertical (E-field profile shown as black line). The grating coupler was first apodised 2-Dimensionally in the x-z plane, with $n_{\text{eq},i}$ as 2D placeholders for the lower index etched sections of the SWG. $\Lambda_y$, $l_{x,\text{Si}}$ and $l_{x,\text{SiO}_2}$ were later determined by full 3D FDTD that did not use a periodic boundary condition simulation box [12,18,20,23,27]. Adapted from [45]
The completion of the fourth stage of 2D FDTD optimisation yields the following results:

Table 3.2.2.1. 24 µm Planewave High Positional Freedom Grating Coupler dimensions

<table>
<thead>
<tr>
<th>i, Period Number</th>
<th>Λ_x, Period (nm)</th>
<th>Duty Cycle ( \frac{l_{x, \text{Si}}}{\Lambda_x} )</th>
<th>( l_{x, \text{Si}} ) (nm)</th>
<th>( l_{x, \text{SiO}_2} ) (nm)</th>
<th>SWG ( n_{eq,i} )</th>
<th>( l_{y, \text{SiO}_2} ) for ( \Lambda_y = 600 \text{ nm} ) (2nd Order EMT)</th>
<th>( l_{y, \text{SiO}_2} ) for ( \Lambda_y = 600 \text{ nm} ) (3D FDTD – Round 1)</th>
<th>( l_{y, \text{SiO}_2} ) for ( \Lambda_y = 600 \text{ nm} ) (3D FDTD – Round 2)</th>
<th>( l_{y, \text{SiO}_2} ) for ( \Lambda_y = 300 \text{ nm} ) (3D FDTD – Round 2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 – 4</td>
<td>640</td>
<td>0.6301</td>
<td>404</td>
<td>236</td>
<td>2.949</td>
<td>181</td>
<td>128</td>
<td>108</td>
<td></td>
</tr>
<tr>
<td>5 – 8</td>
<td>634</td>
<td>0.5542</td>
<td>351</td>
<td>283</td>
<td>2.996</td>
<td>173</td>
<td>141</td>
<td>102</td>
<td></td>
</tr>
<tr>
<td>9 – 12</td>
<td>642</td>
<td>0.6078</td>
<td>390</td>
<td>252</td>
<td>2.894</td>
<td>190</td>
<td>160</td>
<td>160</td>
<td></td>
</tr>
<tr>
<td>13 – 16</td>
<td>652</td>
<td>0.6333</td>
<td>413</td>
<td>239</td>
<td>2.776</td>
<td>209</td>
<td>165</td>
<td>175</td>
<td></td>
</tr>
<tr>
<td>17 – 20</td>
<td>665</td>
<td>0.6494</td>
<td>432</td>
<td>233</td>
<td>2.635</td>
<td>232</td>
<td>229</td>
<td>227</td>
<td></td>
</tr>
<tr>
<td>21 – 24</td>
<td>669</td>
<td>0.6637</td>
<td>444</td>
<td>225</td>
<td>2.579</td>
<td>242</td>
<td>273</td>
<td>270</td>
<td></td>
</tr>
<tr>
<td>25 – 28</td>
<td>669</td>
<td>0.6566</td>
<td>439</td>
<td>230</td>
<td>2.569</td>
<td>244</td>
<td>237</td>
<td>239</td>
<td></td>
</tr>
<tr>
<td>29 – 32</td>
<td>716</td>
<td>0.6511</td>
<td>466</td>
<td>250</td>
<td>2.095</td>
<td>334</td>
<td>368</td>
<td>363</td>
<td>139</td>
</tr>
<tr>
<td>33 – 36</td>
<td>754</td>
<td>0.6217</td>
<td>469</td>
<td>285</td>
<td>1.794</td>
<td>413</td>
<td>416</td>
<td>409</td>
<td>175</td>
</tr>
<tr>
<td>37 – 42</td>
<td>681</td>
<td>0.6977</td>
<td>475</td>
<td>206</td>
<td>1.444</td>
<td>600</td>
<td>600</td>
<td>600</td>
<td>300</td>
</tr>
</tbody>
</table>

Table 3.2.2.1. SWG Grating Coupler based on maximising the input transmission of a 24 µm long planewave input source. The y-dimensions (rightmost columns, separated by a gap) will be later determined by Effective Medium Theory (EMT) and 3D FDTD. Duty Cycles are reported to 4 decimal places in order to reproduce \( l_{x, \text{Si}} \) and \( l_{x, \text{SiO}_2} \) structures to the nearest nm.

Lastly, a 5.2 µm-radius Gaussian source was swept across the grating coupler in the x-direction and the respective input transmission plotted in Fig. 3.2.3.2. The x-axis misalignment tolerance function was a broad curve, with \( >20\% \) efficiency across 15 µm. In order to obtain a more ideal ‘flat-top’ rectangular misalignment tolerance, 2D SWG designs were based on other E-field input profiles.
3.2.3. 2D Design: Other E-field Input Profiles

Alternative 2D FDTD designs were apodised in order to obtain a more positionally-invariant coupling efficiency curve. This was done by altering the E-fields of the input wave, as are shown in Fig. 3.2.3.1(a) (all input sources are 1550 nm TE-polarised light; fields are vertically displaced for clarity). In order to reduce computation requirements, the respective SWG GC’s periods were only optimised in 4 batches of 2$^3$: periods 1–8, 9–16, 17–24, 25–40. Once the power through the waveguide monitor was maximised, the SWG GCs were excited by a waveguide mode source (1550 nm) and their output E-fields were analysed using an output monitor placed over the grating coupler. The respective SWG GCs’ output E-fields are shown in Fig. 3.2.3.1(b).

![Input E-fields](image1)

![Output E-fields](image2)

Fig. 3.2.3.1(a) Alternative input source E-fields to obtain a more rectangular, ‘flat-top’ coupling efficiency curve. Profiles are displaced vertically for clarity and their intensities are normalised. Fig. 3.2.3.1(b) Corresponding output E-fields from SWG GCs optimised on input E-fields in (a). Profiles are displaced vertically for clarity.
As can be seen, once a grating coupler has been apodised to accept an input E-field—i.e. it is mode-matched—its output E-field will follow a similar profile. When a 5.2 µm-radius Gaussian source was swept along the x-axis, their input coupling efficiencies were:

![Fig. 3.2.3.2. x-axis misalignment tolerances of SWG GCs based on different input source profiles after Stage 3 optimisation (periods of 2^3). An ideal ‘flat-top’ tolerance is represented by a black dotted line. Note the steeper slopes of the x-axis misalignment tolerances of the Horned and Long Horned profiles due to the increased side lobes of their output E-fields in Fig. 3.4.1(b). Input source was a TE-polarised 1550 nm 5.2 µm-radius Gaussian tilted 10° from the surface normal.](image)

The steeper slopes of the Horned and Long Horned designs indicate that they might better suited for producing an ideal ‘flat-top’ misalignment tolerance step function. Both designs were further apodised into groups of 2^2 periods. Their final positional performances were:

![Fig. 3.2.3.3. x-axis misalignment tolerances of SWG GCs based on Planewave, Horned, and Long Horned input source profiles after Stage 4 optimisation (periods of 2^2). Note that in terms of maximum input transmission and side slope steepness, Horned and Long Horned curves are different compared to Stage 3 in Fig. 3.2.3.2. Input source was a TE-polarised 1550 nm 5.2 µm-radius Gaussian tilted 10° from the surface normal.](image)
Both Horned and Long Horned designs deviate from the original planewave design primarily by having an increased E-field amplitude at the ends of the profile. This was intended to increase the modal overlap at the edges and thus produce steeper side-slopes. In the case of the Horned design, we can indeed see this to be so. However, in the Long Horned design, the gradient is not much more significant than the original. From the point of view of an outgoing grating coupler, the most likely explanation is that when the SMF28 is aligned with either ‘long horn’ of the radiated mode, the opposite ‘long horn’ was radiating such a significant amount of power that the transmitted power into the SMF was reduced. As Maxwell’s equations are time-reversible, the explanation would be reversed in, as is the case above, an incoming grating coupler.

This suggests that while increasing the modal overlap at the edges of the radiated mode does increase the steepness/gradient of the final SMF positional performance function, there is indeed a point of regression, as evidenced by the steepness of the Long Horned design.

Another observation was the absence of increased maximum input transmission: Both Horned and Long Horned designs were intentionally made significantly shorter (18 µm long) than the original 24 µm planewave. It was anticipated that this would increase the maximum input transmission from 25% to perhaps 30–35%. However, the Horned design’s maximum is ~25% while the Long Horned design worsened to 21%. Again, this is attributable to the lack of modal overlap caused by the increased amplitudes at the edges of the grating coupler’s radiated mode.
3.3. 3D Design of HPF Grating Coupler

3.3.1. 3D Design: Effective Medium Theory (EMT)

The dimensions for $l_y, SiO_2$ and $\Lambda_y$ were initially determined by 2nd order Effective Medium Theory (EMT), as proposed by Rytov [46]. For the sake of completeness, the formulae for the equivalent effective index for both TE- and TM-polarised light are given.

Below are the equations for zeroth order EMT:

$$
\frac{1}{n_{LTE}^{(0)}} = \left[ \frac{f_y}{n_{hole}^2} + \frac{1 - f_y}{n_{Si}^2} \right]^{\frac{1}{2}},
$$

(3.3.1.1a)

$$
n_{LTM}^{(0)} = \left[ n_{hole}^2 f_y + n_{Si}^2 (1 - f_y) \right]^{\frac{1}{2}},
$$

(3.3.1.1b)

where $n_{LTE}^{(0)}$ and $n_{LTM}^{(0)}$ are the refractive indices of the etched portions for TE and TM polarisation respectively; $f_y$ is the fill factor in the y-direction; $n_{Si}$ is the refractive index of Si; $n_{hole}$ is the refractive index of the in-filled material (SiO$_2$). Zeroth order EMT is considered applicable when $\Lambda_y \ll \lambda/2\pi n_{eff}$ [9,12], where $\lambda$ is the free-space wavelength (here, $\lambda = 1.55$ µm) and $n_{eff}$ is the maximum effective index of the slab waveguide fundamental TE-polarized mode (here, $n_{eff} = 2.8265$), so when $\Lambda_y \ll 87$ nm.

However, the solutions to zeroth order EMT can then be used in 2nd order EMT, also formulated by Rytov, but re-expressed in [33]:

$$
n_{LTE}^{(2)} = n_{LTE}^{(0)} \left[ 1 + \frac{\pi^2}{3} R^2 f_y^2 (1 - f_y) \left( n_{hole}^2 - n_{Si}^2 \right)^2 \times \left( \frac{n_{LTM}^{(0)}}{n_{effTE}} \right)^2 \left( \frac{n_{LTE}^{(0)}}{n_{hole} n_{Si}} \right)^4 \right]^{\frac{1}{2}},
$$

(3.3.1.2a)

$$
n_{LTM}^{(2)} = n_{LTM}^{(0)} \left[ 1 + \frac{\pi^2}{3} R^2 f_y^2 (1 - f_y) \left( n_{hole}^2 - n_{Si}^2 \right)^2 \left( \frac{n_{LTM}^{(0)}}{n_{effTM} n_{LTM}} \right)^2 \right]^{\frac{1}{2}},
$$

(3.3.1.2b)
where $R = n_{\text{eff}} \Lambda_y / \lambda$, $n_{\text{eff}}$ is the mode effective index in the slab waveguide with 220 nm thickness ($n_{\text{eff, TE}} = 2.8265$ and $n_{\text{eff, TM}} = 2.1024$, calculated in 2D FDTD).

2\textsuperscript{nd} order EMT is generally considered more accurate than zeroth order EMT [9,30,33,47], but is only considered applicable when $\Lambda_y$ is sufficiently small to frustrate all but the zeroth diffraction order, i.e. $\Lambda_y < \Lambda_{\text{Bragg}} = \lambda / n_{\text{eff}} [12,23,30]$. In this case, when $\Lambda_y < 548$ nm.

An expression for 4\textsuperscript{th} order EMT is available in [48].

By rearranging Eq. 3.3.1.2a, we can find an expression for $f_y$ and therefore $l_y, \text{SiO}_2$. The range of artificial equivalent indices, $n_{\text{eq}, i}$, required by the period batches of the HPF design ($1.794 < n_{\text{eq}, i} < 2.949$) and the minimum feature size achievable (100 nm) by reactive ion etch (RIE) on a 220 nm-thick SOI substrate mandated that $\Lambda_y \geq 450$ nm, according to 2\textsuperscript{nd} order EMT. However, 3D FDTD optimisations of the resulting designs for $\Lambda_y = 450$ nm, 500 nm, 550 nm showed that the necessary minimum feature sizes for $n_{\text{eq}, i} = 2.949, 2.996$ would be < 100 nm. As a compromise between minimum fabricable dimensions by the RIE process, and preventing higher order diffraction effects, we chose $\Lambda_y = 600$ nm.

Our hypothesis as to 2\textsuperscript{nd} order EMT’s inaccuracy is that the 1550 nm Bloch guided mode, as it transitions from the SOI to the SWG, has a significant portion of its field in the top oxide and BOX, and so encounters an $n_{\text{eq}}$ significantly weighted towards SiO$_2$. Consequently, to achieve the higher $n_{\text{eq}, i}$ required by the design, the corresponding $l_y, \text{SiO}_2$ should be much smaller than the values predicted by EMT.

As $\Lambda_y = 600$ nm > 548 nm—the range beyond which 2\textsuperscript{nd} order EMT is no longer valid—full 3D FDTD simulations were undertaken to maximise the transmission into the waveguide.
3.3.2. 3D Design: Full 3D FDTD Optimisation

Period-batch-by-period-batch, the homogenous $n_{eq}$ placeholders were replaced with discrete etched structures whose $l_{y, \text{SiO}_2}$ lengths were swept in two stages: in 10 nm steps around the values calculated by 2\textsuperscript{nd} order EMT, and then in 1 nm steps. A similar method was used by [19]. $\Lambda_y$ was fixed at 600 nm to obtain etch widths which were $> 100$ nm (i.e. fabricable by industry-standard reactive ion etch (RIE)). Though computationally-intensive, this method was pursued as the numerical method of 3D simulation of only one $\Lambda_y$ period with periodic y-boundary conditions used in [12,18,20,23,27], as shown in Fig. 3.3.2., did not approach the same values as full 3D FDTD.

After all homogenous placeholders were replaced (Round 1), the method was repeated (Round 2), with significant changes in the etch width dimensions. It was repeated once more to confirm that the optimal etch width values had indeed converged.

The final $l_{y, \text{SiO}_2}$ dimensions (to the nearest nm) for Planewave, Horned and Long Horned HPF GCs are shown in Tables 3.2.2.1, 3.3.2.1, and 3.3.2.2 respectively, and are indeed much smaller than otherwise predicted by 2\textsuperscript{nd} order EMT.

| Table 3.3.2.1. 18 µm-Horned High Positional Freedom Grating Coupler dimensions |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| i, Period Number | $\Lambda_x$, Period (nm) | Duty Cycle $\frac{l_{x, Si}}{\Lambda_x}$ | $l_{x, Si}$ (µm) | $l_{x, \text{SiO}_2}$ (µm) | SWG $n_{eq,i}$ | $l_{y, \text{SiO}_2}$ for $\Lambda_y$ = 600 nm (2nd Order EMT) | $l_{y, \text{SiO}_2}$ for $\Lambda_y$ = 600 nm (3D FDTD – Round 1) | $l_{y, \text{SiO}_2}$ for $\Lambda_y$ = 600 nm (3D FDTD – Round 2) | $l_{y, \text{SiO}_2}$ for $\Lambda_y$ = 400 nm (2nd Order EMT) | $l_{y, \text{SiO}_2}$ for $\Lambda_y$ = 400 nm (3D FDTD – Round 1) | $l_{y, \text{SiO}_2}$ for $\Lambda_y$ = 400 nm (3D FDTD – Round 2) |
| 1 – 4 | 0.651 | 0.6682 | 0.435 | 0.216 | 2.804 | 0.205 | 0.184 | 0.192 | 0.089 | 0.089 | 0.091 |
| 5 – 8 | 0.653 | 0.5498 | 0.359 | 0.294 | 2.882 | 0.192 | 0.138 | 0.143 | 0.079 | 0.069 | 0.068 |
| 9 – 12 | 0.670 | 0.5075 | 0.340 | 0.330 | 2.794 | 0.206 | 0.176 | 0.170 | 0.091 | 0.078 | 0.077 |
| 13 – 16 | 0.670 | 0.5567 | 0.373 | 0.297 | 2.682 | 0.224 | 0.196 | 0.197 | 0.106 | 0.098 | 0.097 |
| 17 – 20 | 0.667 | 0.6087 | 0.406 | 0.261 | 2.660 | 0.228 | 0.262 | 0.252 | 0.108 | 0.105 | 0.106 |
| 21 – 24 | 0.754 | 0.5491 | 0.414 | 0.340 | 2.147 | 0.323 | 0.345 | 0.348 | 0.184 | 0.191 | 0.192 |
| 25 – 28 | 0.656 | 0.5305 | 0.348 | 0.308 | 2.580 | 0.242 | 0.241 | 0.241 | 0.119 | 0.111 | 0.108 |
| 29 – 32 | 0.679 | 0.6318 | 0.429 | 0.250 | 1.444 | 0.600 | 0.600 | 0.600 | 0.400 | 0.400 | 0.400 |
| 33 – 40 | 0.704 | 0.7045 | 0.496 | 0.208 | 1.444 | 0.600 | 0.600 | 0.600 | 0.400 | 0.400 | 0.400 |

Duty Cycles are reported to 4 decimal places in order to reproduce $l_{x, Si}$ and $l_{x, \text{SiO}_2}$ structures to the nearest nm.
### Table 3.3.2.2. 18 µm-Long Horned High Positional Freedom Grating Coupler dimensions

<table>
<thead>
<tr>
<th>i, Period Number</th>
<th>( \Lambda_x ), Period (nm)</th>
<th>Duty Cycle ( \frac{l_x,Si}{\Lambda_x} )</th>
<th>( l_s, Si ) (nm)</th>
<th>( l_{s, SiO_2} ) (nm)</th>
<th>SWG ( n_{eq,i} )</th>
<th>( l_{y,SiO_2} ) for ( \Lambda_y = 600 ) nm (2nd Order EMT)</th>
<th>( l_{y,SiO_2} ) for ( \Lambda_y = 600 ) nm (3D FDTD – Round 1)</th>
<th>( l_{y,SiO_2} ) for ( \Lambda_y = 600 ) nm (3D FDTD – Round 2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 – 4</td>
<td>0.625</td>
<td>0.4480</td>
<td>0.280</td>
<td>0.345</td>
<td>2.820</td>
<td>0.202</td>
<td>0.202</td>
<td>0.197</td>
</tr>
<tr>
<td>5 – 8</td>
<td>0.647</td>
<td>0.5626</td>
<td>0.364</td>
<td>0.283</td>
<td>2.782</td>
<td>0.208</td>
<td>0.186</td>
<td>0.195</td>
</tr>
<tr>
<td>9 – 12</td>
<td>0.656</td>
<td>0.5869</td>
<td>0.385</td>
<td>0.271</td>
<td>2.847</td>
<td>0.197</td>
<td>0.157</td>
<td>0.165</td>
</tr>
<tr>
<td>13 – 16</td>
<td>0.656</td>
<td>0.5921</td>
<td>0.389</td>
<td>0.268</td>
<td>2.849</td>
<td>0.197</td>
<td>0.162</td>
<td>0.165</td>
</tr>
<tr>
<td>17 – 20</td>
<td>0.651</td>
<td>0.5668</td>
<td>0.369</td>
<td>0.282</td>
<td>2.872</td>
<td>0.194</td>
<td>0.151</td>
<td>0.157</td>
</tr>
<tr>
<td>21 – 24</td>
<td>0.684</td>
<td>0.5591</td>
<td>0.383</td>
<td>0.302</td>
<td>2.595</td>
<td>0.239</td>
<td>0.246</td>
<td>0.242</td>
</tr>
<tr>
<td>25 – 28</td>
<td>0.671</td>
<td>0.5171</td>
<td>0.347</td>
<td>0.324</td>
<td>2.527</td>
<td>0.251</td>
<td>0.26</td>
<td>0.254</td>
</tr>
<tr>
<td>29 – 32</td>
<td>0.676</td>
<td>0.5459</td>
<td>0.369</td>
<td>0.307</td>
<td>2.420</td>
<td>0.270</td>
<td>0.293</td>
<td>0.294</td>
</tr>
<tr>
<td>33 – 40</td>
<td>0.650</td>
<td>0.5446</td>
<td>0.354</td>
<td>0.296</td>
<td>1.444</td>
<td>0.600</td>
<td>0.600</td>
<td>0.600</td>
</tr>
</tbody>
</table>

Duty Cycles are reported to 4 decimal places in order to reproduce \( l_s, Si \) and \( l_{s, SiO_2} \) structures to the nearest nm.

The numerically calculated \( l_{y,SiO_2} \) dimensions are plotted with their corresponding \( n_{eq,i} \) for \( \Lambda_y = 600 \) nm in Fig. 3.3.2.1, along with those calculated by 0th and 2nd order EMT. At \( \Lambda_y = 600 \) nm, these HPF designs are not strictly within the subwavelength regime, and indeed there are Bragg reflection effects and radiation effects competing with the synthesised subwavelength \( n_{eq} \) [45] while simultaneously generating ±1st order modes [27]. Nevertheless, the numerically calculated \( l_{y,SiO_2} \) dimensions and the fitted fifth order polynomial (Eqs. 3.6.1a, b) serve as a design heuristic for future TE-polarised, 1550 nm, \( \Lambda_y = 600 \) nm subwavelength devices.

![Fig. 3.3.2.1. Equivalent Refractive Index, \( n_{eq} \), for \( \Lambda_y = 600 \) nm for 1550 nm, TE polarised light on a 220 nm SOI substrate, according to 0th order EMT (red dotted), 2nd order EMT (red line) and full 3D FDTD (black crosses).](image-url)
\[ n_{eq} = -4 \times 10^{-14} l_{y, SiO_2}^5 + 1 \times 10^{-10} l_{y, SiO_2}^4 - 1 \times 10^{-7} l_{y, SiO_2}^3 + 4 \times 10^{-5} l_{y, SiO_2}^2 - 0.0075 l_{y, SiO_2} + 3.4701 \] (3.6.1a)

Or re-expressed in a more useful form:

\[ l_{y, SiO_2}(\mu m) = -0.1176n_{eq}^5 + 1.6176n_{eq}^4 - 8.6722n_{eq}^3 + 22.596n_{eq}^2 - 28.823n_{eq} + 14.909 \] (3.6.1b)

### 3.3.3. 3D Design: \( \Lambda_y \neq 600 \text{ nm Designs} \)

Additionally, \( l_y, SiO_2 \) for \( \Lambda_y = 300 \text{ nm} \) were numerically solved for as well. It was hypothesised that since \( \Lambda_y = 600 \text{ nm} \) pushes the regime within which SWG designs function, perhaps designs which mixed \( \Lambda_y = 600 \text{ nm} \) and \( \Lambda_y = 300 \text{ nm} \), where applicable, would:

1) lead to a more homogenous optical medium and consequently have better performance,

2) be more resistant to RIE-lag as the holes were more uniformly sized

In the case of the Planewave SWG GC, periods 29–32 and 33–36 had \( l_{y, SiO_2} \) values of 363 nm and 409 nm respectively—significantly higher than periods 1–28. When solved for \( \Lambda_y = 300 \text{ nm} \), these values became comparable, as shown in Table 3.3.3.1.

<table>
<thead>
<tr>
<th>i, Period Number</th>
<th>( l_{x, SiO_2} ) (nm)</th>
<th>( l_{y, SiO_2} ) for ( \Lambda_y = 600 \text{ nm} ) (3D FDTD – Round 2)</th>
<th>( l_{y, SiO_2} ) for ( \Lambda_y = 300 \text{ nm} ) (3D FDTD – Round 2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 – 4</td>
<td>236</td>
<td>108</td>
<td>102</td>
</tr>
<tr>
<td>5 – 8</td>
<td>283</td>
<td>160</td>
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<td>9 – 12</td>
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<td>13 – 16</td>
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<tr>
<td>17 – 20</td>
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<td>239</td>
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<td>21 – 24</td>
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<td>363</td>
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<td>25 – 28</td>
<td>230</td>
<td>409</td>
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</tr>
<tr>
<td>29 – 32</td>
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<td>300</td>
</tr>
<tr>
<td>33 – 36</td>
<td>285</td>
<td></td>
<td></td>
</tr>
<tr>
<td>37 – 42</td>
<td>206</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
The $\Lambda_y = 300$ nm scattering elements of periods 29–36 had two arrangements, as shown in Fig. 3.3.3.1.: two $\Lambda_y = 300$ nm scattering elements could replace a single $\Lambda_y = 600$ nm one (*Interspersed 300 nm*), or be displaced by $y = 150$ nm such that the centres of every alternate $\Lambda_y = 300$ nm scattering element is in-line with those of $\Lambda_y = 600$ nm (*In-line 300 nm*).

![Diagram showing arrangements of scattering elements](image)

Lastly, for Horned SWG GCs, $l_{y, \text{SiO2}}$ values for $\Lambda_y = 400$ nm were also numerically solved in order to obtain a better performing design than the $\Lambda_y = 600$ nm version. Unfortunately, the corresponding $l_{y, \text{SiO2}}$ values were sub-100 nm and the scattering elements did not fully open, as measurements in Section 3.6 suggest.

### 3.3.4. Planewave Rectangular SWG GC Simulation Results

The final 3D FDTD optimised Planewave Rectangular SWG designs were simulated for their x-axis misalignment tolerances and compared in Fig. 3.3.4.1. The most significant improvement occurs between 2D FDTD and 3D FDTD simulations (both designs have $n_{\text{eq, i}}$...
homogenous placeholders). There is further deprovement when those placeholders were replaced with discrete $\Lambda_y = 600$ nm scattering elements. There is a slight improvement between $\Lambda_y = 600$ nm (3D FDTD – Round 1) and $\Lambda_y = 600$ nm (3D FDTD – Round 2) designs, justifying the additional computational requirements.

Lastly, both $\Lambda_y = 300$ nm designs had slightly poorer tolerances than the original when the Gaussian impinged on those periods due to diffraction effects. However, if a mixed $\Lambda_y$ design is necessary, the in-line arrangement seems superior. In contrast, Xu, Subbaraman et al. 2013 [24] showed that for $\Lambda_y = 400$ nm in-line vs $\Lambda_y = 400$ nm interspersed, both designs had similar maximum coupling efficiencies and -1 dB and -3 dB bandwidths, with $\Lambda_y = 400$ nm interspersed having smaller Fabry-Perot reflections.

![Graph](image)

**Fig. 3.3.4.1.** Planewave SWG GCs’ x-axis Misalignment Tolerances. There is a general drop in efficiency between 2D and 3D (with placeholder) simulations, and a further drop when the homogeneous placeholders are replaced by discrete scattering elements. There is a slight improvement from $\Lambda_y = 600$ nm (3D FDTD – Round 1) to $\Lambda_y = 600$ nm (3D FDTD – Round 2), justifying the additional computation requirements. Both $\Lambda_y = 300$ nm designs performed poorer than the original, but In-line 300 nm is the superior of the two. Input source was a TE-polarised 1550 nm 5.2 $\mu$m-radius Gaussian tilted 10° from the surface normal.

### 3.3.5. 3D Design: Rotation & Translation of Scattering Elements of

**Circular and Elliptical Designs**

The SWG GCs had 3 different y-lateral layouts: Rectangular, where $W_{Gr} = 15$ $\mu$m, linear taper length = 1000 $\mu$m; Circular, where the SWG diffracting elements were curved around 50°
concentric arcs; and Elliptical, where the SWG diffracting elements were curved around ellipses as determined by the method in [49] with a minimum grating order of 19. The elliptical equation is presented here for the sake of completeness:

$$q\lambda_0 = n_{\text{eff}}\sqrt{x^2 + y^2} - xn_{\text{cladding}}\sin\theta_c,$$

(3.3.5.1)

where q is an integer for each grating period (i.e. the grating order); $\lambda_0$ is the vacuum wavelength (1550 nm); $n_{\text{eff}} \neq n_{\text{eq}}$ is the effective index of the grating (determined numerically); x and y are the coordinates on the x-y plane of the grating coupler; $n_{\text{cladding}}$ is the refractive index of the cladding ($n_{\text{SiO}_2} = 1.444$); $\theta_c$ is the coupling angle of the fibre with respect to the surface normal (10°).

Generally, for curved SWG GC designs in the scientific literature, scattering elements are either:

- neither rotated nor translated (as shown in Fig. 3.3.5.1(b)) [47] or,
- rotated but not translated (as shown in Fig. 3.3.5.1(c)) [23].

Rotation would be unnecessary if the elements were circles of equivalent area [21], although there is research on the ideal element shape is still ongoing [27,30,47].

On arguments of geometry alone, the elements should be:

- rotated and translated, as in Fig. 3.3.5.1(d).

The farther the diffracting elements deviate from the centreline of the grating coupler, the greater $\Lambda_y$ deviates from 600 nm. At the extreme of ±25°, a lateral step of 600 nm in y produces a $\Lambda_y$ of 656 nm. These curved lateral layout designs performed significantly poorer (cf. Figs. 3.5.2.1(c), 3.5.2.1(d)). Further experiments among ‘not rotated & not translated’ (Fig. 3.3.5.1(b)), ‘rotated & not translated’ (Fig. 3.3.5.1(c)), and ‘rotated & translated’ (Fig. 3.3.5.1(d)) orientations were undertaken to measure their effects on grating coupler performance. Scattering elements were
rotated to the nearest $0.5^\circ$ and translated to the nearest nm where appropriate. All three subvariants were laid out and compared in Section 3.6.

Fig. 3.3.5.1. Comparison of different adjustments of the diffracting elements in a curved SWG grating coupler. (a) The whole circular HPF design with a highlight of the relevant section (b) Diffraction elements neither rotated nor translated. Note $\Lambda_y = 656$ nm. (c) Diffraction elements rotated but not translated, as in . Note $\Lambda_y = 653$ nm. (d) Diffraction elements rotated and translated. Note $\Lambda_y \approx 600$ nm. (e) Diffraction elements translated but not rotated. (f) Diffraction elements skewed but not
translated, similar to [34,35]. (g) Diffraction elements skewed and translated. (h) Diffraction elements radially aligned with different $\Lambda_y$'s, similar to [50].

For the sake of completion, Fig. 3.3.5.1 also covers other ways rectangular scattering elements can be manipulated in curved SWG GCs: ‘not rotated & translated’ (Fig. 3.3.5.1(e)); ‘skewed & not translated’, as in [34,35], (Fig. 3.3.5.1(f)); ‘skewed & translated’ (Fig. 3.3.5.1(g)); ‘radially aligned but with varying $\Lambda_y$’s’(Fig. 3.3.5.1(h)), as in [50].

3.4. Fabrication of HPF Grating Coupler(s)

The devices were fabricated in a state-of-the-art 300mm CMOS foundry using 220 nm-thick SOI wafers. The HPF gratings and waveguides were patterned using an industry-standard ASML 193 nm immersion lithography scanner and then formed using a single reactive ion etch (RIE) step. Approximately 5.14 $\mu$m of SiO$_2$ top cladding was deposited via plasma enhanced chemical vapour deposition (PECVD) tetraethyl orthosilicate (TEOS).

Representative scanning electron microscopy (SEM) images of the rectangular, circular and elliptical layouts of the design are shown in Fig. 3.4.1 below, after the full silicon etch step and before silicon dioxide deposition.
3.5. Manual Measurements of HPF Grating Coupler

A Process of Record (POR) grating coupler was laid out as a pair with a 2 cm-long, 0.22 µm-thick × 0.55 µm-wide strip waveguide connecting them. The insertion loss was measured on an optical bench with a Keysight Technologies (Santa Rosa, CA) 81980A Compact Tunable Laser Source external cavity InGaAsP laser with a wavelength range of 1465 nm – 1575 nm and a N7744A Optical Multiport Power Meter. SMF-28s were tilted at a nominal 9° from surface normal and their x & y positions were optimised to maximise power throughput at a wavelength of 1550 nm (Fig. 3.5.1(a)). Waveguide loss was measured on a separate structure and subtracted from the measured insertion loss. The remaining insertion loss was divided by 2 to obtain the insertion loss per POR grating coupler with an SMF-28 input.

Next, the same structure was measured with a lensed multimode fibre (MMF) (50µm minimumum illumination diameter), and waveguide loss and the insertion loss from an SMF into a
grating coupler—as just previously calculated—were subtracted to obtain the outgoing insertion loss from a POR grating coupler to a lensed MMF (Fig. 3.5.1(b)).

Once the insertion loss from a POR grating coupler outcoupling into a lensed MMF was characterised, the POR grating coupler was measured topologically by stepping the optical wafer in 1.125µm steps in the x- and y-directions (Fig. 3.5.2(a)). As the lensed MMF has a much larger numerical aperture compared to the cleaved SMF (estimated 0.47 vs 0.13), it has a much large
cone of acceptance and therefore is significantly more tolerant to misalignments in x- and y-.

Every 3 steps, the x- or y-position of the lensed MMF output was re-adjusted to obtain maximum throughput, thereby ensuring that any changes in the power throughput was a function of the x- and y-misalignment of the cleaved SMF over the input grating coupler.

In this manner, a topological map of the insertion loss from a cleaved SMF into the POR grating coupler was obtained. Topological maps of the insertion loss of the HPF designs were similarly measured (Fig. 3.5.1(c)). This method was chosen as the fibre micropositioners are analogue devices (micrometre dials), which would make movements in x- and y-difficult to reproduce consistently.

3.5.1. Manual Linear Characterisation

Due to the labour-intensiveness of full topological measurements, Planewave Rectangular SWG GCs devices of several die were measured only with a single raster in x to show device consistency across the wafer (Fig. 3.5.1.1). While the measured values exceed those of the simulation, this is within experimental variances as the coupling efficiency at a specific wavelength is angle-dependent and the fibre tilt is adjusted manually on a Cascade Microtech (Beaverton, OR) Lightwave Probe (LWP).

Fig. 3.5.1.1. Insertion loss of the Planewave Rectangular HPF grating coupler as a function of the x-position of the SMF28 for 1550 nm TE-polarised light. The negative x-direction is towards the waveguide. The SMF28 was tilted to a nominal 14.5° and, as coupling efficiency is angle-dependent, is the likely cause of measured values exceeding the simulation. Device 4 was topologically scanned and the data is presented in Fig. 3.5.2.1(b).
3.5.2. Manual Topological Characterisation

A Process of Record grating coupler, Device 4 from Fig. 3.5.1.1, a Planewave Rectangular HPF SWG GC, as well as curved HPF SWG GC designs from the same chip were topologically scanned. The results of the insertion loss topological scans of the grating couplers are shown in the Figs. 3.5.2.1(a) – (d) in dB.

**Fig. 3.5.2.1.** Topological scans of absolute insertion loss of POR and Planewave HPF SWG GCs with 1550 nm, TE-polarised light. The negative x-direction is towards the waveguide. Peak coupling efficiencies are located at the origins (0, 0) and are stated in the respective graphs. Contours are -1 dB apart. a) Process of Record (POR) grating coupler, b) Rectangular high positional freedom (HPF) grating coupler, c) Circular HPF grating coupler with rotated, but not translated diffracting elements, d) Elliptical HPF grating coupler with rotated, but not translated diffracting elements.
The origins (0, 0) are the points with highest throughputs. The listed loss in dB refers to those peaks. Contour lines are spaced 1 dB apart. Where possible, the x- and y-dimensions have been limited to show the topologies over roughly equal areas, i.e. 40 µm × 40 µm. In all graphs, the waveguide is to the left.

Fig. 3.5.2.2. Topological scans of absolute insertion loss of Horned HPF SWG GCs with 1550 nm, TE-polarised light. The negative x-direction is towards the waveguide. Peak coupling efficiencies are located at the origins (0, 0) and are stated in the respective graphs. Contours are -1 dB apart. For both Circular and Elliptical layouts, there is an increase in loss (~0.30–0.65 dB) when the scattering elements are rotated but not translated.
The further loss caused by curving the SWG GC is not insignificant (~4.5 dB). Further manual measurements were done on Horned SWG GCs, comparing ‘not rotated, not translated’ elements with ‘rotated, not translated’ elements (Fig. 3.5.2.2.).

When the scattering elements are rotated but not translated, both Circular and Elliptical layouts had an increase in loss (~ 0.30–0.65 dB). This is attributed to an increase of the y-z cross-sectional area of the rotated scattering elements increasing the random scattering of the wave as it travels through the HPF GC in the x-direction.

When similar experiments were conducted on curved Horned $\Lambda_y = 400$ nm SWG GC designs, the increase in loss was only ~ 0.1 dB.

### 3.5.3. Manual Bandwidth Measurements

Bandwidth measurements were taken manually with a Keysight Technologies (Santa Rosa, CA) 81980A Compact Tunable Laser Source external cavity InGaAsP laser with a wavelength range of 1465 nm – 1575 nm. Similar to the x- scan in Fig. 3.5.1.1, Device 4 was stepped in x- in 1.125 $\mu$m increments and the laser swept across its wavelength at each position. Bandwidth losses were measured for the waveguide and the output POR grating coupler to MMF on separate structures and subtracted to obtain Fig. 3.5.3.1(b), the absolute bandwidth insertion loss for the Planewave rectangular HPF grating coupler as a function of the SMF28’s x-position. Fig. 3.5.3.1(a) shows the full 3D FDTD simulation result of the same structure. Black lines on both graphs indicate the -1 dB, -2 dB and -3 dB contours. Fig. 3.13.1(c) shows a subset of Fig. 3.5.3.1(b) with the contours marked in clear bands: -1 dB (red), -2 dB (yellow), -3 dB (green).

Bandwidth is a function of several variables, including fibre tilt and position. Generally, for a non-HPF grating coupler, the larger the SMF x Position, the larger the ‘effective interaction area’ (the effective grating area covered by the fibre beam) and consequently, the narrower the
bandwidth [51]. However, for an HPF grating coupler, the ‘effective interaction area’ is constant for most of the SMF’s x-travel, and so the -1 dB bandwidth should be generally unchanged, as shown in Fig. 3.5.3.1(a). The measured structure’s fin-shaped deviation from the ‘rectangular’ bandwidth pattern is hypothesised to be due to RIE lag, as scattering elements farther from the waveguide are bigger and so are likely to be slightly overetched.

Fig. 3.5.3.1. Rectangular HPF grating coupler bandwidth as a function of SMF28 x-position. Black lines indicate -1 dB, -2 dB and -3 dB contours. a) Full 3D FDTD simulated bandwidth, b) measured bandwidth, c) subset of b) with -1 dB (red), -2 dB (yellow) and -3 dB (green) bandwidth contours. The -1 dB and -3 dB bandwidths are 14 nm and 29.5 nm respectively.
Nevertheless, within the range of SMF28 x-position values measured, the -1 dB and -3 dB bandwidths are \~14 nm and \~29.5 nm respectively, which is slightly less than half of other SWG grating couplers built on similar platforms (see Table 3.1.1).

### 3.6. Semi-Automated Measurements of HPF Grating Coupler(s)

As manual measurements were labour-intensive, a semi-automated method was used to map the lateral misalignment tolerance of the various design sub-types (e.g. Planewave vs Horned vs Long Horned; Circular vs Elliptical; ‘not rotated & not translated’ vs ‘rotated & not translated’ vs ‘rotated & translated’). HPF SWG GC sub-type pairs were laid out on a macro compatible with a 20 individual single mode fibre V-Groove assembly by OZ Optics (Ottawa, Ontario). The grating couplers were 127 µm apart and connected by 100 µm long straight waveguide pairs (Fig. 3.6.1). POR grating couplers were used as the outermost pair for the V-Groove assembly optical alignment. As the assembly was polished to 8° and the tilt relatively fixed, the laser wavelength used to characterise the topologies was adjusted to compensate (1603 nm for Planewave, 1580 nm for Horned and 1560 nm for Long Horned SWG GC designs).

![Fig. 3.6.1. Example macro of 8 HPF SWG GC pairs used for automated measurements. Grating couplers are spaced 127 µm apart and are connected by 0.22 µm thick \times 0.55 µm wide strip waveguides with 100 µm straight waveguides. All HPF pairs were measured with the same fibre pair (channel 2) on the V-Groove assembly.](image)

All fibre pairs in the V-Groove assembly were used to measure the same HPF SWG GC sub-type pair to determine which channel (2) had the lowest loss. Channel 2 of the V-Groove assembly was then used to measure all HPF SWG GC sub-type pairs in order to avoid zero-ing issues in loss.
Fig. 3.6.1. Topological scans of absolute insertion loss of Planewave HPF SWG GCs on die: (-1,0) with 1603 nm, TE-polarised light, with the V-Groove assembly polished to 8° and tilted 8° from the surface normal. The negative x-direction is towards the waveguide. Peak coupling efficiencies and the -1 dB areas are stated in the respective graphs. Contours are -1 dB apart. a) Rectangular layout. b) Circular layout with 'not rotated & not translated' scattering elements. c) Circular layout with 'rotated & not translated' scattering elements. d) Circular layout with 'rotated & translated' scattering elements. e) Elliptical layout with 'not rotated & not translated' scattering elements. f) Elliptical layout with 'rotated & translated' scattering elements.
Topological measurements were collected with a Keysight Technologies (Santa Rosa, CA) 81606A Tunable Laser Source and a N7745A Optical Multiport Power Meter. The V-Groove assembly was spiral-rastered in x-y by Physik Instrumente (Karlsruhe, Germany) P-611.3 NanoCube XYZ Piezo System fibre positioners in 0.4 µm steps. Total insertion loss was divided by 2 to obtain fibre insertion loss per HPF GC. Waveguide and bend loss are ignored as the straight waveguides were short (100 µm each) and the bend radii were large (63.5 µm). To show across-wafer repeatability, the 29 HPF SWG GC sub-type pairs were measured over 5 dice.

Figs. 3.6.1(a) – (f) are sample topological measurements of the Planewave $\Lambda_y = 600$ nm HPF GC designs from die: (-1,0).

The maximum coupling efficiencies, -1 dB areas and -3 dB areas of the three Planewave sub-type designs were averaged across 5 dice and their results shown in Table 3.6.1 ($\Lambda_y = 600$ nm), 3.6.2 ($\Lambda_y = 600$ nm & In-line 300 nm), and 3.6.3 ($\Lambda_y = 600$ nm & Interspersed 300 nm).

Table 3.6.1 Effect of Rotation and Translation of Scattering Elements on Curved SWG GCs based on Planewave Input

<table>
<thead>
<tr>
<th></th>
<th>Averaged Max Coupling Efficiency (dB)</th>
<th>% Change</th>
<th>Averaged -1 dB Area (µm²)</th>
<th>% Change</th>
<th>Averaged -3 dB Area (µm²)</th>
<th>% Change</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rectangular</td>
<td>-9.1</td>
<td>0.0%</td>
<td>47.0</td>
<td>0.0%</td>
<td>128.5</td>
<td>0.0%</td>
</tr>
<tr>
<td>Circular – Original (Not Rotated, Not Translated)</td>
<td>-11.7</td>
<td>-45.3% (vs Rectangular)</td>
<td>36.4</td>
<td>-22.5% (vs Rectangular)</td>
<td>113.3</td>
<td>-11.8% (vs Rectangular)</td>
</tr>
<tr>
<td>Circular – Rotated, Not Translated</td>
<td>-12.0</td>
<td>-5.9% (vs Circular Original)</td>
<td>42.6</td>
<td>17.0% (vs Circular Original)</td>
<td>121.2</td>
<td>6.9% (vs Circular Original)</td>
</tr>
<tr>
<td>Circular – Rotated &amp; Translated</td>
<td>-12.5</td>
<td>-15.9% (vs Circular Original)</td>
<td>46.7</td>
<td>28.3% (vs Circular Original)</td>
<td>129.3</td>
<td>14.1% (vs Circular Original)</td>
</tr>
<tr>
<td>Elliptical – Original (Not Rotated, Not Translated)</td>
<td>-11.4</td>
<td>-41.0% (vs Rectangular)</td>
<td>33.4</td>
<td>-29.0% (vs Rectangular)</td>
<td>104.2</td>
<td>-18.9% (vs Rectangular)</td>
</tr>
<tr>
<td>Elliptical – Rotated, Not Translated</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Elliptical – Rotated &amp; Translated</td>
<td>-11.0</td>
<td>9.9% (vs Elliptical Original)</td>
<td>37.6</td>
<td>12.8% (vs Elliptical Original)</td>
<td>111.2</td>
<td>6.7% (vs Elliptical Original)</td>
</tr>
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</table>
Table 3.6.2 Effect of Rotation and Translation of Scattering Elements on Curved SWG GCs based on Planewave Input with periods 29–36 replaced by In-line $\Lambda_y = 300$ nm SWG

<table>
<thead>
<tr>
<th></th>
<th>Averaged Max Coupling Efficiency (dB)</th>
<th>% Change</th>
<th>Averaged -1 dB Area (µm²)</th>
<th>% Change</th>
<th>Averaged -3 dB Area (µm²)</th>
<th>% Change</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rectangular</td>
<td>-9.1</td>
<td>0.0%</td>
<td>37.5</td>
<td>0.0%</td>
<td>126.5</td>
<td>0.0%</td>
</tr>
<tr>
<td>Circular – Original (Not Rotated, Not Translated)</td>
<td>-11.5</td>
<td>-41.9% (vs Rectangular)</td>
<td>33.9</td>
<td>-9.7% (vs Rectangular)</td>
<td>101.7</td>
<td>-19.7% (vs Rectangular)</td>
</tr>
<tr>
<td>Circular – Rotated, NOT Translated</td>
<td>-12.2</td>
<td>-14.3% (vs Circular Original)</td>
<td>28.4</td>
<td>-16.3% (vs Circular Original)</td>
<td>97.7</td>
<td>-3.9% (vs Circular Original)</td>
</tr>
<tr>
<td>Circular–Rotated &amp; Translated</td>
<td>-12.2</td>
<td>-15.1% (vs Circular Original)</td>
<td>31.5</td>
<td>-6.9% (vs Circular Original)</td>
<td>104.3</td>
<td>2.5% (vs Circular Original)</td>
</tr>
<tr>
<td>Elliptical – Original (Not Rotated, Not Translated)</td>
<td>-11.3</td>
<td>-39.4% (vs Rectangular)</td>
<td>29.1</td>
<td>-22.4% (vs Rectangular)</td>
<td>94.2</td>
<td>-25.5% (vs Rectangular)</td>
</tr>
<tr>
<td>Elliptical – Rotated, NOT Translated</td>
<td>-11.7</td>
<td>-9.7% (vs Elliptical Original)</td>
<td>24.9</td>
<td>-14.5% (vs Elliptical Original)</td>
<td>84.0</td>
<td>-10.8% (vs Elliptical Original)</td>
</tr>
<tr>
<td>Elliptical – Rotated &amp; Translated</td>
<td>-11.1</td>
<td>5.9% (vs Elliptical Original)</td>
<td>34.5</td>
<td>18.6% (vs Elliptical Original)</td>
<td>104.1</td>
<td>10.5% (vs Elliptical Original)</td>
</tr>
</tbody>
</table>

Comparing the Rectangular layouts, it is evident that maintaining a consistent $\Lambda_y$ throughout the SWG design results in the highest efficiency and the largest -1 dB area. However, in the case where a 2D SWG $n_{eq}$ is not fabricable within the SWG’s primary $\Lambda_y$, one might use a secondary in-line $\Lambda_{y2} = 2\Lambda_y$.
Comparing the curved (Circular or Elliptical) designs with their Rectangular counterparts, it is evident that curving a SWG GC, while reducing the GC’s footprint, results in significant increases in loss (~2–3 dB). However, this loss seems subdued in designs with shorter $\Lambda_y$, as seen in Table 3.6.4.

Table 3.6.4 Effect of Rotation and Translation of Scattering Elements on Curved SWG GCs based on Horned Input $\Lambda_y = 400$ nm SWG

<table>
<thead>
<tr>
<th></th>
<th>Averaged Max Coupling Efficiency (dB)</th>
<th>% Change</th>
<th>Averaged -1 dB Area (µm²)</th>
<th>% Change</th>
<th>Averaged -3 dB Area (µm²)</th>
<th>% Change</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rectangular</td>
<td>-9.2</td>
<td>0.0%</td>
<td>14.6</td>
<td>0.0%</td>
<td>44.2</td>
<td>0.0%</td>
</tr>
<tr>
<td>Elliptical – Original (Not Rotated, Not Translated)</td>
<td>-10.0</td>
<td>-15.9%</td>
<td>27.0</td>
<td>84.5%</td>
<td>73.3</td>
<td>65.9%</td>
</tr>
<tr>
<td>Elliptical – Rotated, NOT Translated</td>
<td>-9.6</td>
<td>9.0% (vs Elliptical Original)</td>
<td>27.1</td>
<td>0.6% (vs Elliptical Original)</td>
<td>73.7</td>
<td>0.6%</td>
</tr>
</tbody>
</table>

The poor -1 dB area of the Horned $\Lambda_y = 400$ nm SWG GC design is attributed to the small scattering element size (as small as 68 nm), which did not fully open during RIE.

While Circular designs have roughly +10% more -1 dB area, this is usually at a detriment to their maximum coupling efficiency (-2–9%) compared to Elliptical designs.

When considering scattering element rotation and translation, it is evident that rotation without translation leads to poorer performing designs across all curved layouts. However, rotation with translation leads to better performing Elliptical layouts (+6–10% efficiency; +12–19% area) but curiously, not Circular ones (-15–16% efficiency). This suggests that there might be positive consistent $n_{eq}$ benefits from ‘translation only’ being outcompeted by negative scattering effects from ‘rotation only’ of scattering elements. Further research on this would be necessary, specifically comparing how ‘Not Rotated, Translated’ SWG designs compare with their other curved counterparts.
3.7. Conclusions

This chapter covers the design and measurement of a lateral misalignment tolerant, high positional freedom, subwavelength grating grating coupler. The input source design with the best lateral misalignment tolerance was the original planewave design.

To accommodate minimum fabricable dimensions in a 300mm foundry, \( \Lambda_y \) was set to 600 nm. 2\textsuperscript{nd} Order EMT and 3D FDTD with periodic boundaries could not accurately predict the \( l_y, \text{SiO}_2 \) dimensions for this \( \Lambda_y \), so the values were numerically solved using full 3D FDTD, and in doing so, a design heuristic is obtained for other \( \Lambda_y = 600 \text{ nm} \) SWG designs accommodating minimum fabricable requirements.

Of its lateral layouts, Rectangular performed the best, while Circular and Elliptical suffered significant losses. Such losses seem negligible at \( \Lambda_y = 400 \text{ nm} \), but this is a moot point as sub-100 nm scattering elements based in this period failed to fully open up. The Elliptical SWG GCs’ losses at \( \Lambda_y = 600 \text{ nm} \) are ameliorated when the scattering elements are rotated \textit{and} translated. However, Circular SWG GCs counterintuitively deproved in their coupling efficiencies.

The increase in misalignment tolerance was traded for a narrower bandwidth. It was also likely traded for a more stringent tilt misalignment tolerance, as the two are inversely related: a grating coupler with a larger radiated mode has a narrower distribution of power in wave-vector space and so tighter tilt tolerances [52]. Fig. 3.7.1(a) shows 2D FDTD simulation of the HPF GC’s coupling efficiency as a function of position and tilt. Fig. 3.7.1(b) shows the coupling efficiency specifically as a function of tilt when \( x = 15.0 \mu\text{m} \). From Fig. 3.7.1(b), we can see an expected fiber tilt tolerance of \( -0.4 \text{ dB for } \pm 1^\circ \), and \( -2.0 \text{ dB for } \pm 3^\circ \).
However, this grating coupler could potentially be used for inline testing of waveguide loss, where fibre tilts are not often adjusted, as a rapid, single etch design with high reproducability. Alternatively, it could also be used in narrow bandwidth, wafer-to-wafer bonding applications, which require higher misalignment tolerances for high yield.

![Graphs showing coupling efficiency and fiber tilt angle tolerance](image)

Fig. 3.7.1 (a) 2D FDTD simulation of coupling efficiency at $\lambda = 1550$ nm for various fiber tilts as a function of SMF x-position. (b) 2D FDTD simulation of fiber tilt angle tolerance at SMF x-Position = 15 $\mu$m.

Additionally, curved SWG designs were experimentally confirmed to perform better when their scattering elements were ‘Rotated & translated’ compared to ‘Not rotated & not translated’. However, the data suggests that ‘Translated & not rotated’ orientations should have even greater improvement.

### 3.8. References

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4. SiN<sub>x</sub>-only Grating Coupler

4.0. Chapter Overview

- A bilayer grating coupler based only on SiN<sub>x</sub> was designed, fabricated and characterised.
- Theoretical maximum coupling efficiency was 59.1%; theoretical -1 dB bandwidth was 57.7 nm.
- Measured coupling efficiency was -2.56 dB (55.4%), and the measured -1 dB bandwidth was 46.9 nm.
- This design can be used in niche foundry-based applications: bulk Si wafers, interposers, back-end-of-the-line (BEOL).

4.1. Introduction

Photonic circuitry is frequently designed and fabricated on silicon-on-insulator (SOI) wafers due to the large difference in refractive indices between silicon and silicon dioxide. However, silicon nitride photonics is also of interest due to several reasons: its transparency reaches as low as 500 nm (Si is only transparent >1.1 µm), which a) enables applications in biophotonics and sensing, in addition to datacom [1–3]; it has a lower index contrast with SiO<sub>2</sub>, which b) enables lower waveguiding losses achievable with the material (lab-based losses of < 0.1 dB/m) [4] as opposed to SOI (0.27 dB/cm) [5]; and c) relaxes fabrication tolerances [3,6–8]; d) silicon nitride has negligible two-photon absorption in the infrared spectrum, enabling nonlinear applications [1–3]; e) it has 5 times better temperature-tolerance [9–11] due to a
thermo-optic coefficient a seventh that of Si [12–14]; finally, f) there is greater design freedom compared to SOI wafers as more than one waveguiding layer can be deposited.

At 1550 nm, low pressure chemical vapor deposition (LPCVD) Si$_3$N$_4$ has a refractive index of $n=1.977$, while plasma-enhanced chemical vapor deposition (PECVD) SiO$_2$—usually its cladding material—has a refractive index of $n = 1.428$ [12]. This difference in index of refraction is significantly less than between silicon ($n = 3.476$) and silicon dioxide, which limits the scattering strength of individual periods in a grating coupler [6]. Additionally, silicon nitride’s lower refractive index (compared to silicon) increases the grating pitch and thus decreases the number of periods (scatterers) that can fit in a given fibre mode width [15]. These reasons unfortunately limit the maximum power that can be diffracted from a single mode fibre (SMF-28, 10.4 µm mode field diameter) into a waveguide; conversely, the fewer periods simultaneously increase the bandwidth of the grating coupler [15,16].

LPCVD Si$_3$N$_4$ requires high temperatures (~800°C) and is stoichiometric, whereas PECVD Si$_N$ can be deposited at lower temperatures (200–400°C), generally induces less stress (particularly in thick films), and depending on the recipe, could result in non-uniform, non-stoichiometric Si$_N$ [2,7,8]. Consequently, Si$_N$’s refractive index can be $> 2$ for Si-rich films and $< 2$ for N-rich films [17,18]. Despite these issues, PECVD Si$_N$’s lower deposition temperature makes it the preferred material for integrated applications which have a limited thermal budget to avoid silicon dopant-diffusion.

Generally, grating couplers based on thicker silicon nitride waveguiding layers (550nm–700nm) have higher grating strengths and thus smaller modal mismatches with the SMF-28, resulting in higher maximum fibre-to-chip efficiencies (32.0% - 70.8%) [19–22]. Indeed, partially-etched Si$_3$N$_4$ grating couplers generally require $> 800$ nm thicknesses to achieve $> 80\%$
upwards directionality [16,23], though this can be bypassed by ingenious design of a two-step staircase-shaped grating profile and forgoing top cladding to increase the grating strength [19]. Conversely, grating couplers based on a thinner (400 nm) waveguiding layer have an increased modal mismatch and a lower maximum fibre-to-chip efficiency (28.8–38.0%) [15,24], as seen in Table 4.2.1 below.

Generally, thicker (400–2500 nm) silicon nitride layers are used to enhance the non-linear response of the material for nonlinear signal processing applications at near infrared (1550–3700 nm) wavelengths, whereas thinner (100–180 nm) layers are used for visible (532–900 nm) wavelength applications. Moderately thick (~ 200–400 nm) layers allow for versatile multi-project wafers with reduced performances for either wavelength extreme, while also avoiding fabrication issues like film cracking [1,3].

### 4.2. Existing Designs from Literature

<table>
<thead>
<tr>
<th>Paper</th>
<th>SiN type</th>
<th>Designed Wave-length (nm)</th>
<th>SiN layer thickness (nm)</th>
<th>SMF-28 angle from normal (°)</th>
<th>Measured Maximum Fibre-to-Chip Coupling Efficiency</th>
<th>1 dB Bandwidth (nm)</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>[22,25]</td>
<td>LPCVD Si$_x$N$_y$ $n=2.022$</td>
<td>1550</td>
<td>700</td>
<td>8</td>
<td>-3.7 dB (42.7%)</td>
<td>54</td>
<td>For non-linear applications in 700 nm Si$_x$N$_y$</td>
</tr>
<tr>
<td>[26]</td>
<td>PECVD SiN</td>
<td>1550 / 1310</td>
<td>700</td>
<td>8</td>
<td>-6.35 dB (23.2%) / -9.2 dB (12.0%)</td>
<td>~39 / ~31</td>
<td>Unidirectional, single-polarisation dual-band GC</td>
</tr>
<tr>
<td>[19,27]</td>
<td>Si$_x$N$_y$ $n=2.0$</td>
<td>1550</td>
<td>600</td>
<td>16.5</td>
<td>-1.5 dB (70.8%)</td>
<td>35</td>
<td>No top oxide to increase grating strength; SMF-28 112 µm above chip surface to diffract over 25 periods</td>
</tr>
<tr>
<td>[20]</td>
<td>PVD SiN$_x$, $n=1.980$</td>
<td>1550</td>
<td>550</td>
<td>0</td>
<td>-4.9 dB (32%) (simulated)</td>
<td>~1 nm</td>
<td>Si$_x$N$_y$ GC between DBR-pair cavity</td>
</tr>
<tr>
<td>[21]</td>
<td>Si$_x$N$_y$, $n=1.9827$</td>
<td>1550</td>
<td>550</td>
<td>-2.9</td>
<td>-2.66 dB (54.2%) (simulated)</td>
<td>80</td>
<td>SMF Gaussian MFD is 20.8 µm</td>
</tr>
<tr>
<td>[15]</td>
<td>LPCVD Si$_x$N$_y$ $n=2.0$</td>
<td>1550</td>
<td>400</td>
<td>8</td>
<td>-4.2 dB (38.0%) (simulated)</td>
<td>67</td>
<td>Through-etch Si$_x$N$_y$ GC with 2.25 µm BOX</td>
</tr>
<tr>
<td>[24,28]</td>
<td>LPCVD Si$_x$N$_y$</td>
<td>1550</td>
<td>400</td>
<td>10</td>
<td>-5.4 dB (28.8%)</td>
<td>~18</td>
<td>Si$_x$N$_y$ GC array for multicore optical fibre</td>
</tr>
<tr>
<td>[29]</td>
<td>Si$_x$N$_y$</td>
<td>1550</td>
<td>400</td>
<td>7</td>
<td>-6.58 dB (22%)</td>
<td>~29</td>
<td>Gold mirror; grating not etched</td>
</tr>
<tr>
<td>[30]</td>
<td>Liquid source CVD Si$_x$N$_y$, $n=1.80$</td>
<td>1550</td>
<td>325</td>
<td>0</td>
<td>-4.5 dB (35.5%)</td>
<td>~35</td>
<td>Si$_x$N$_y$ GC with 10 Si$_x$N$_y$/SiO$_2$ DBR layers</td>
</tr>
<tr>
<td>This work</td>
<td>PECVD SiN$_x$</td>
<td>1550</td>
<td>220</td>
<td>9</td>
<td>-2.73 dB (53.3%)</td>
<td>47.9</td>
<td>Through-etched displaced SiN$_x$ bilayer</td>
</tr>
</tbody>
</table>
Table 4.2.1. Comparison of SiN grating couplers from the literature. Where not explicitly stated in the original reference, the -1 dB bandwidth was extrapolated from the published data and indicated with a ‘~’ symbol; where such data was not available, a ‘?’ symbol was used instead.

Additionally, several nanophotonic devices operating within the C- (1530–1565 nm) and L-bands (1565–1625 nm) use thin-moderate (100–400 nm) silicon nitride layers in their construction: microring filters [37,38], microring bolometers [39], polarisation splitters [40,41], integrated lasers [42–46], and phased antenna arrays [47], further increasing the versatility and importance of thin-moderate silicon nitride layers.

This work presents—to the best of the author’s knowledge—a silicon nitride-only grating coupler design with the highest experimentally confirmed coupling efficiency of 53.3% to a silicon nitride waveguiding layer of only 220 nm. Its primary application is as a medium-efficiency, fast turnaround grating coupler for more rapid measurements on short loop wafers. It is one of three new grating coupler designs compatible with SUNY Poly’s state of the art 300 mm silicon photonics foundry. Emphatically, the grating coupler was fabricated in a 300 mm foundry without the use of high-resolution, low-throughput alternatives like e-beam or focused ion beam (FIB) lithography.

### 4.3. Uniform and Apodised Designs

The grating coupler was built on an American Institute for Manufacturing Integrated Photonics (“AIM Photonics”) multiproject wafer (MPW) with the following layer stack: bulk Si,
2.32 µm SiO₂ (as tetraethoxysilicate (TEOS)), 220 nm PECVD Si₃Nₓ, 100 nm TEOS, 220 nm PECVD Si₃Nₓ, and 5.1 µm of TEOS, as shown in the Fig. 4.3.1.

![Layer stack of the Multi-Project Wafer (MPW) service used for this work.](image)

To reduce the initial modal mismatch, both 220 nm Si₃Nₓ layers, as well as the sandwiched 100 nm TEOS layer in between, were used as a temporary bilayer waveguide, with interlayer coupling facilitated by an interlayer taper of either one of the Si₃Nₓ layers (cf. Fig. 4.4.1(d)).

Three initial designs were simulated: Fig. 4.3.2(a) top-only through-etch, Fig. 4.3.2(b) top-and-bottom parallel through-etches, and Fig. 4.3.2(c) displaced bilayer through-etches. These designs are based on partial-etch [32], through-etch [15,21,24,28,31], and antenna array designs [16,27,48] from literature. The uniform period designs were optimised based upon maximising TE-polarised 1550 nm light from a 9°-tilted SMF-28 into the Si₃Nₓ bilayer waveguide. 2D optimisation was done with Lumerical FDTD, a commercially-available finite-difference time-domain (FDTD) solver, using its in-built particle swarm optimisation algorithm. The maximal fibre-to-chip coupling efficiencies for top-only, top-and-bottom parallel, and displaced bilayer etch designs were 27.8%, 10.4%, and 55.1% respectively, as shown in Fig. 4.3.2.
The details and dimensions of the displaced bilayer etch, design 4.3.2(c), are as shown in Fig. 4.3.3 and Table 4.3.1:

### Table 4.3.1. Uniform Bilayer Design’s Dimensions

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Top layer Period (nm)</td>
<td>1121</td>
</tr>
<tr>
<td>Top layer Duty Cycle (l₁/l₂)</td>
<td>0.5072</td>
</tr>
<tr>
<td>Bottom layer Period (nm)</td>
<td>1085</td>
</tr>
<tr>
<td>Bottom layer Duty Cycle (l₁/l₂)</td>
<td>0.5647</td>
</tr>
<tr>
<td>Bottom layer displacement (nm)</td>
<td>-193</td>
</tr>
</tbody>
</table>

Duty Cycles are reported to 4 decimal places in order to reproduce structures to the nearest nm.

Fig. 4.3.3. Details of the uniform SiNₙ bilayer etch design.
Popović et al. [49,50] showed that offsetting the bottom layer by \( \lambda/4 \) produced ‘array nano-antenna grating couplers’ with unidirectional (99\%) radiation patterns on a crystalline-Si and polysilicon platform, thereby achieving a measured -1.16 dB (76.6\%) fibre-to-chip coupling loss at 1178 nm [48]. Similarly, design 4.3.2(c) (72.4\% upwards directionality according to 2D FDTD, cf. Fig. 4.3.4(a)) confirms that this phenomenon holds for a lower index platform like Si\(_N_x\).

Apodisation was done via maximising the fibre-to-chip coupling efficiency in a nearest-period-to-waveguide-first approach, i.e. period 1’s dimensions were optimised, then period 2’s, and so on. In terms of design simplicity, fibre-to-chip apodisation—also used in [51–53]—is more straightforward as only the optimal x-position of the SMF-28 is varied. In contrast, chip-to-fibre apodisation—used in [54–62]—attempts to match the radiated mode to a 5.2 \( \mu \)m-radius Gaussian, which is further complicated by locating the Gaussian’s optimal position, shape modifications due to fibre tilt, etc.

Apodisation increased the coupling efficiency to 58.2\%. Theoretically, if the optimum coupling efficiency of a uniform grating coupler—with its exponentially decaying diffracted field—is 0.81D, then an apodised grating coupler’s efficiency should approach D [63]. The increase from 55.1\% to 58.2\% may seem underwhelming in light of this, but it should be noted that the uniform grating coupler’s radiated mode is already Gaussian-like as it is composed of \( \text{two} \) grating couplers with different periods, duty cycles and an offset. The apodisation of individual periods is therefore limited in increasing the modal overlap of such a field. The output E-fields of the uniform and apodised designs, along with a fitted Gaussian, are shown in Fig. 4.3.4(b).
Fig. 4.3.4(a). Directionality of uniform 2.32 µm BOX SiNx bilayer etch design. (b) 2D FDTD simulation of the output E-fields of Uniform and Apodised 6 µm BOX designs with a fitted Gaussian and exponential decay to show the modal overlap.

The optimal centre position of the SMF-28 during apodisation was $x = 8.25 \pm 0.25$ µm.

The optimisation boundaries for each period’s four dimensions were the preceeding and succeeding periods’ limiting dimensions ± 0.100 µm as 0.100 µm is the minimum fabricable dimension in this process. Each apodisation step consisted of 20 generations with 40 children per generation, at a mesh accuracy setting of 4 (18 points per wavelength, a variable Lumerical uses to determine the FDTD mesh size). The dimensions of the apodised design, given as the distance from $x = 0$ in Fig. 4.3.3, were:

<table>
<thead>
<tr>
<th>Period</th>
<th>Top layer unetched SiN\textsubscript{x} start (µm)</th>
<th>Top layer unetched SiN\textsubscript{x} end (µm)</th>
<th>Bottom layer unetched SiN\textsubscript{x} start (µm)</th>
<th>Bottom layer unetched SiN\textsubscript{x} end (µm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.000</td>
<td>0.576</td>
<td>0.000</td>
<td>0.535</td>
</tr>
<tr>
<td>2</td>
<td>0.794</td>
<td>1.702</td>
<td>0.745</td>
<td>1.355</td>
</tr>
<tr>
<td>3</td>
<td>2.158</td>
<td>2.785</td>
<td>1.957</td>
<td>2.518</td>
</tr>
<tr>
<td>4</td>
<td>3.367</td>
<td>3.922</td>
<td>3.057</td>
<td>3.612</td>
</tr>
<tr>
<td>5</td>
<td>4.501</td>
<td>4.998</td>
<td>4.106</td>
<td>4.666</td>
</tr>
<tr>
<td>6</td>
<td>5.613</td>
<td>6.134</td>
<td>5.254</td>
<td>5.795</td>
</tr>
<tr>
<td>7</td>
<td>6.727</td>
<td>7.326</td>
<td>6.363</td>
<td>6.901</td>
</tr>
<tr>
<td>8</td>
<td>7.836</td>
<td>8.467</td>
<td>7.437</td>
<td>7.975</td>
</tr>
<tr>
<td>9</td>
<td>8.954</td>
<td>9.580</td>
<td>8.485</td>
<td>9.102</td>
</tr>
</tbody>
</table>
where \( x = 0, 1, 2, \ldots, 27 \).

Both uniform and apodised designs had three lateral layouts: rectangular, circular focusing and elliptical focusing. Rectangular designs were invariant in the \( y \)-direction for 20 \( \mu m \) with a 500 \( \mu m \)-long linear taper which also functions as its interlayer taper. Circular focusing designs were comprised of concentric 50° circular arcs. Elliptical focusing designs were comprised of 50° elliptical arcs curved according to the design procedure from [64] with a minimum grating order of 11. The interlayer taper for both focusing designs is linear, 27 \( \mu m \) long and terminates with a 100 nm tip (cf. Fig. 4.4.1(d)).

While this grating coupler was designed for the AIM MPW layer stack, the same process could be used to design \( \text{SiN}_x \)-only circuits on bulk silicon wafers. Hence, a similar approach was used to design \( \text{SiN}_x \) bilayer grating couplers for 6.0 \( \mu m \) BOX, the results of which are shown in Fig. 4.5.2.

### 4.4. Fabrication of \( \text{SiN}_x \)-only Grating Coupler

The devices were fabricated on AIM MPW runs on a 300 mm SOI wafer using standard CMOS processing techniques. After silicon waveguide formation (not used in this design), 220 nm of near-stoichiometric silicon nitride (refractive index \( \approx 2.0 \)) was deposited via PECVD directly on the silicon waveguide cladding layer. The \( \text{SiN}_x \) was patterned with state of the art ASML 193 nm deep UV argon-fluoride (DUV ArF) immersion lithography and etched with reactive ion etching (RIE). It was then capped with 100 nm of PECVD TEOS. Subsequently, a second layer of 220 nm of \( \text{SiN}_x \) was deposited and patterned as the first \( \text{SiN}_x \) layer. Lastly, a 5.1 \( \mu m \)-thick capping layer of \( \text{SiO}_2 \) was deposited via PECVD TEOS.
Representative scanning electron microscopy (SEM) images of the rectangular, circular and elliptical layouts of the apodised design are shown in Fig. 4.4.1, after each SiNₓ etch step.

Fig. 4.4.1(a)–(b). SEM micrograph of apodised rectangular grating couplers: (a) after first SiNₓ etch, (b) after second SiNₓ etch. (c)–(d) apodised circular: (c) after first SiNₓ etch, (d) after second SiNₓ etch. (e)–(f) apodised elliptical: (e) after first SiNₓ etch, (f) after second SiNₓ etch. Fig. 4.4.1(d) shows the interlayer taper for curved designs which confines the temporary bilayer SiNₓ’s taper mode to just the bottom SiNₓ layer. It is linear, 27 µm long and terminates with a 100 nm tip.
4.5. Experimental Measurements

Grating couplers of the same design were laid out as pairs with a 2 cm-long, 1.5 µm-wide SiN\textsubscript{x} waveguide connecting them. Waveguide loss was measured on a separate structure and subtracted from the measured insertion loss. The remaining insertion loss was divided by 2 to obtain the insertion loss per grating coupler.

The grating coupler pairs were measured on an optical bench with a Keysight Technologies (Santa Rosa, CA) 81980A Compact Tunable Laser Source external cavity InGaAsP laser with a wavelength range of 1465–1575 nm. The single mode fibres (SMF-28s) were tilted at a nominal 9° from surface normal and their x & y positions (cf. Fig. 4.3.3) were optimised to maximise power throughput at a wavelength of 1550 nm. Subsequently, the laser source was swept from 1470–1570 nm to measure the bandwidth performance of the grating coupler with a Keysight Technologies N7744A Optical Multiport Power Meter.

The results of the insertion loss of the grating couplers are shown in Fig. 4.5.1 below, along with the 2D simulated coupling efficiencies from an ideal grating coupler. [64] has shown that elliptical lateral layouts can shorten the taper length while still maintaining similar coupling efficiencies to rectangular layouts. [32] has shown that focusing layouts can sometimes match or even outperform rectangular layouts by as much as 0.7 dB. However, in this bilayer design, elliptical consistently performed best amongst the 3 lateral layouts. It is possible that with the width of the rectangular lateral layout (20 µm) and the thickness of the temporary bilayer SiN\textsubscript{x} waveguide (0.540 µm), the 500 µm-long linear taper does not provide an acute enough taper angle to prevent higher order waveguide modes from being excited and their power subsequently lost when coupling to the single mode 220 nm × 1.5 µm strip waveguide.
Without phase-correction, circular layouts were expected to perform poorer than elliptical ones. However, circular arcs are easier to manipulate in layout programs and in industrial designs, the loss in efficiency could be justified by the footprint reduction (compared to rectangular layouts) and the ease of manipulation (compared to elliptical layouts).

Of the six designs, the apodised elliptical was the most efficient with an experimental efficiency of -2.56 dB (55.4%) and a -1 dB bandwidth of 46.9 nm. The results for other lateral layouts are shown in Fig. 4.5.1. Blue error bars indicate the 1 standard deviation of the elliptical layout’s average insertion loss. Departures from the simulated ideal are attributed to fabrication tolerances and measurement variations.

As previously mentioned, the same process was also used to design grating couplers for SiN$_x$-only circuits on bulk silicon wafers. Uniform and apodised grating coupler versions were re-optimised for bulk silicon with 6.0 µm TEOS. The dimensions for the resulting optimised designs are given in Table 4.5.1 (uniform) and Table 4.5.2 (apodised):

<table>
<thead>
<tr>
<th>Table 4.5.1. Uniform Bilayer (for 6.0 µm TEOS) Design’s Dimensions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Top layer Period (nm)</td>
</tr>
<tr>
<td>Top layer Duty Cycle (L/l)</td>
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<tr>
<td>Bottom layer Period (nm)</td>
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Duty Cycles are reported to 4 decimal places in order to reproduce structures to the nearest nm.

Table 4.5.2. Apodised Bilayer (for 6.0 µm TEOS) Design’s Dimensions

<table>
<thead>
<tr>
<th>Period</th>
<th>Top layer unetched SiNₓ start (µm)</th>
<th>Top layer unetched SiNₓ end (µm)</th>
<th>Bottom layer unetched SiNₓ start (µm)</th>
<th>Bottom layer unetched SiNₓ end (µm)</th>
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<td>12-40</td>
<td>12.309+1.119x</td>
<td>12.903+1.119x</td>
<td>11.836+1.098x</td>
<td>12.374+1.098x</td>
</tr>
</tbody>
</table>

where \( x = 0, 1, 2, \ldots, 27 \).

The apodised design had a simulated efficiency and -1 dB bandwidth of -2.35 dB (58.2%) and 52.1 nm, and an experimental efficiency of -2.73 dB (53.3%) and 54.1 nm for the apodised elliptical layout. The results for other lateral layouts are shown in Fig. 4.5.2.

![Fig. 4.5.2. Simulated and measured coupling efficiencies of SiN, bilayer grating coupler with 6.0 µm bottom oxide for (a) uniform and (b) apodised designs with different lateral layouts (circular, elliptical, and rectangular). Blue error bars indicate the 1 standard deviation of the elliptical layout’s average insertion loss. Variances in the 6 µm BOX designs are attributed to larger variation in deposited oxide thickness as compared to those on the 2.32 µm BOX platform.](image-url)
The 6 µm BOX designs had larger insertion loss variances and are attributed to larger variation in deposited oxide thickness across the wafer as compared to those on the 2.32 µm BOX platform, as shown in Fig. 4.5.3.

![Fig. 4.5.3. Simulated coupling efficiencies for Apodised 6 µm BOX grating couplers with BOX thicknesses variances of ± 3%.

It is known that a grating coupler’s efficiency can be significantly improved by optimising the BOX thickness to obtain a constructive reflection from the BOX-Si interface [31,34,35,55,65–68]. To a lesser extent, efficiency can also be improved by optimising the top oxide thickness to function as an anti-reflective film [31,34,35]. However, in either layer stack reported here, the BOX thicknesses (2.32 µm and 6.0 µm) and top oxide thickness (5.1 µm) were constrained by other photonic devices’ design considerations and were not optimised for a SiNx bi-layer grating coupler. Nevertheless, bi-layer designs of reasonable efficiencies and bandwidths were borne out of the optimisation process discussed in this paper, which is as much as once can hope for in a foundry-compatible design.
4.6. Conclusions

We have demonstrated a bilayer SiNₓ, medium-efficiency, through-etched grating coupler which couples light to a 220 nm-thin SiNₓ waveguiding layer on a bulk Si wafer, with zero change to the AIM MPW layer stack platform. The use of through-etch designs allows the SiO₂ to act as a natural etch-stop, thus ensuring the reliability of the design in a 300 mm foundry without relying on high-resolution, low-throughput e-beam or focused ion beam lithography.

The grating coupler has a theoretical 2D coupling efficiency of -2.28 dB and a -1 dB bandwidth of 57.7 nm. For the uniform designs, the elliptical layout performed the best with a peak coupling efficiency of -2.61 dB and a -1 dB bandwidth of 50.7 nm. For the apodised designs, the best layout was also elliptical with a measured a coupling efficiency of -2.56 dB with a -1 dB bandwidth of 46.9 nm, which demonstrates—to the best of our knowledge—the highest coupling efficiency to a 220 nm-thick SiNₓ waveguide layer.

4.7. Chapter Bibliography


5. High Efficiency SiN$_x$-on-SOI Grating Coupler

5.0. Chapter Overview

- A grating coupler based on SiN$_x$-on-SOI with a high coupling efficiency for 1550 nm TE-polarised light was designed, fabricated and characterised.

- Theoretical maximum coupling efficiency is 85.9%; the highest for a zero-change grating coupler in the literature.

- Out of 15 designs, the top 2 were apodised and their performance metrics are listed:

Table 5.0.1. Summary of Simulated & Measured Characteristics of the Two High Efficiency Designs

<table>
<thead>
<tr>
<th></th>
<th>100 nm SOI DBR Design</th>
<th>100 nm SOI Grating Design</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Uniform</td>
<td>Apodised</td>
</tr>
<tr>
<td>Simulated Max. Coupling Efficiency (dB)</td>
<td>-1.924 (64.2%)</td>
<td>-1.162 (76.5%)</td>
</tr>
<tr>
<td>Measured Max. Coupling Efficiency (dB)</td>
<td>-2.213 (60.1%)</td>
<td>-1.899 (64.6%)</td>
</tr>
<tr>
<td>Simulated -1 dB Bandwidth (nm)</td>
<td>58.7</td>
<td>27.8</td>
</tr>
<tr>
<td>Measured -1 dB Bandwidth (nm)</td>
<td>73.1</td>
<td>52.7</td>
</tr>
<tr>
<td>Simulated -3 dB Bandwidth (nm)</td>
<td>80.5</td>
<td>80.2</td>
</tr>
<tr>
<td>Measured -3 dB Bandwidth (nm)</td>
<td>97.3</td>
<td>93.4</td>
</tr>
</tbody>
</table>

- One utilises a distributed Bragg reflector (DBR); the other utilises a grating.

- Such grating couplers can be used in high-efficiency applications where ultra-wide bandwidth is not necessary.
5.1. Introduction

Although grating couplers can be designed to emphasise more than one apex of the grating coupler star of performance (cf. Chapter 1), the most common denominator across which grating couplers are compared is coupling efficiency. In the literature, it is almost a point of pride to design a grating coupler of near-unity coupling efficiency [1–4].

The purpose of the grating coupler designs presented in this chapter is to maximise fibre-to-chip coupling efficiency for 1550 nm light without changing a given layer stack, i.e. with zero-change to the pre-existing layer stack for which the grating coupler will be used.

To achieve high coupling efficiencies, some grating couplers utilise metal mirrors [5,6] (Au [7], Al [8–11]), others use single [6,12] or multiple dielectric Bragg mirrors [6,13–15] (c-Si, a-Si), or high contrast gratings (HCG) [3,16] mirrors with an optimised reflection distance. Other designs utilise optimised BOX [9,16–21] heights, which is extremely effective as there is a strong reflection at the Si substrate-oxide interface, and the correct optical path length can create a constructive reflection upwards back to the grating coupler. To a lesser extent, TOX heights can be optimised [9,17,20,21]) to act as an antireflection layer to the incoming wavefront of a hovering SMF-28. Other designs use extended teeth, usually of SiNx [13,17,22] or polysilicon [23–26], while others use multiple etch depths [27] to disrupt the vertical symmetry of a grating coupler. Many of these solutions involve using layer thicknesses or mask layers which are unique only to the grating coupler, and so would be untenable on an integrated platform.

5.2. Existing Designs from Literature

Specifically with regards to SiNx-on-SOI platforms, there has been recent work to develop grating couplers which mostly maximise efficiency. Table 5.2.1 compares these designs. Designs which require unique layers/thicknesses are marked with an asterix (*).
Table 5.2.1. A comparison of other SiN$_x$-on-SOI grating couplers in the literature

<table>
<thead>
<tr>
<th>Paper</th>
<th>SiN type</th>
<th>Designed Wave-length (nm)</th>
<th>SOI thickness (µm)</th>
<th>BOX thickness (µm)</th>
<th>SiN waveguiding layer thickness (nm)</th>
<th>SMF-28 angle from normal (°)</th>
<th>Measured Maximum Fibre-to-Chip Coupling Efficiency (dB)</th>
<th>1dB Bandwidth (nm)</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>[22,28]</td>
<td>PECVD SiN$_x$, n= 1.9896</td>
<td>1550</td>
<td>0.220</td>
<td>2.0</td>
<td>600</td>
<td>-8</td>
<td>-2.5 (56.2%)</td>
<td>65</td>
<td>SiN$_x$-on-SOI; single etch; SiN extended teeth; No top oxide;</td>
</tr>
<tr>
<td>[29,30]</td>
<td>LPCVD Si$_3$N$_4$, n = 2.0</td>
<td>1550</td>
<td>0.065 / 0.150 / 0.220</td>
<td>2.0</td>
<td>400</td>
<td>21</td>
<td>-1.3 (74.1%)</td>
<td>82</td>
<td>SiN$_x$-on-SOI; bilayer design</td>
</tr>
<tr>
<td>[16]*</td>
<td>Si$_3$N$_4$, n=2.0</td>
<td>1550</td>
<td>0.220</td>
<td>2.0</td>
<td>400</td>
<td>8</td>
<td>0.88 (81.7%) (simulated)</td>
<td>40</td>
<td>SiN$_x$-on-SOI; special oxide separation layer height layer stack</td>
</tr>
<tr>
<td>This work</td>
<td>PECVD SiN$_x$, n=1.9894</td>
<td>1550</td>
<td>0.100 / 0.100 / 0.220</td>
<td>2.0</td>
<td>220</td>
<td>9</td>
<td>-1.259 (74.8%) (simulated)</td>
<td>48.8</td>
<td>Trilayer SiN$_x$-on-SOI; zero-change</td>
</tr>
<tr>
<td>[31]*</td>
<td>LPCVD Si$_3$N$_4$, n=2.0</td>
<td>1490</td>
<td>0.108 / NA / NA</td>
<td>2.6</td>
<td>400</td>
<td>8</td>
<td>-2.5 (56.2%)</td>
<td>53</td>
<td>Si$_3$N$_4$ GC with 2 a-Si DBR layers</td>
</tr>
<tr>
<td>[17]*</td>
<td>Si$_3$N$_4$</td>
<td>1550</td>
<td>0.220</td>
<td>2.16</td>
<td>220 nm Si</td>
<td>10</td>
<td>-1.19 (76%) (simulated)</td>
<td>75</td>
<td>SiN$_x$-on-SOI with 2 Si DBR; SiN extended teeth</td>
</tr>
<tr>
<td>[13]</td>
<td>SiN</td>
<td>1492</td>
<td>0.320</td>
<td>?</td>
<td>320 nm Si</td>
<td>?</td>
<td>-0.75 (84.1%)</td>
<td>~29</td>
<td>SiN$_x$-on-SOI; SiN extended teeth; double SOI DBR</td>
</tr>
<tr>
<td>[32,33]</td>
<td>PECVD SiN$_x$, n=1.873</td>
<td>1310</td>
<td>0.150 / 0.300 / 0.300</td>
<td>2.0</td>
<td>600</td>
<td>29</td>
<td>-2.1 (61.7%)</td>
<td>72</td>
<td>SiN$_x$-on-SOI; bilayer design</td>
</tr>
</tbody>
</table>

Table 5.2.1. Comparison of SiN$_x$-on-SOI grating couplers from the literature. Designs requiring unique layers/thicknesses are marked with an asterix (*). Where not explicitly stated in the original reference, the -1 dB bandwidth was extrapolated from the published data and indicated with a ‘~’ symbol; where such data was not available, a ‘?’ symbol was used instead.

5.3. Layer Stack

The grating coupler is based on the standard layer stack developed for AIM Photonics, which shown below in Fig. 5.3.1:

![Fig. 5.3.1. Available mask layers / layer stack for the high efficiency designs.](image-url)
5.4. Initial Designs

Given the layer stack, 15 initial designs were optimised 2-Dimensionally. They can be divided into 3 groups, shown in Fig. 5.4.1: (row 1) displaced bilayer through-etches, (row 2) top-only through-etch, and (row 3) top-and-bottom parallel through-etches. These designs are based on antenna array [2,30,34], partial-etch [35,36], and through-etch [36–39] designs, from literature.

Within each row, there are 3 columns which utilise different SOI thicknesses: no SOI structures, 220 nm-thick SOI structures, and 100 nm-thick SOI structures. The latter 2 columns have a further sub-division between a distributed Bragg reflector (DBR) or a grating.

All initial designs were of uniform period and optimised based on maximising TE-polarised 1550 nm light from a 9°-tilted SMF-28 into the SiNx temporary bilayer waveguide instead of directly into the bottom layer SiNx waveguide. This strategy was found to have a slightly higher coupling efficiency (~+6%) as the temporary bilayer waveguide has a smaller mode size mismatch with the SMF-28 source. Interlayer coupling from the top SiNx waveguide to the bottom layer was facilitated via an interlayer taper farther on down the line.

2D optimisation was done with Lumerical FDTD, a commercially-available finite-difference time-domain (FDTD) solver, using its in-built particle swarm optimisation algorithm. Generally (but not always), 100 nm-thick SOI structures improved the coupling efficiencies more so than 220 nm-thick SOI structures. The displaced bilayer etch already had a moderate coupling efficiency of 55.1% (a), and was improved to 64.2% with the addition of a 100 nm DBR (j) and 72.3% with the addition of a 100 nm grating (k). Top-only etch (b) and Parallel etch (c) both improved as well, but not to the same extent.
The details of design (j) and (k) are covered in sections 5.4.1 and 5.4.2 respectively.

**5.4.1. Uniform 100 nm SOI DBR Design**

Design (j)’s dimensions are as reported in Table 5.4.1.1 and Fig. 5.4.1.1. It should be noted that the 100 nm SOI DBR terminates well before the bilayer waveguide and does *not* constitute part of a temporary tri-layer waveguide. Earlier designs with a trilayer waveguide (less modal mismatch, ∼+10% coupling efficiency improvement over monolayer waveguide) had abysmal measured efficiencies. 3D FDTD simulations showed that as silicon has a much higher refractive index compared to SiNₓ (3.47 vs 1.99), the mode would quickly confine itself to the bottom 100 nm SOI layer of the trilayer waveguide and required non-trivial interlayer taper design optimisation to transfer the mode to the bottom SiNₓ waveguide. During measurements of earlier designs, straightforward linear tapers failed to accomplish interlayer transfer efficiently.
Table 5.4.1.1. Uniform SOI DBR Design’s Dimensions

<table>
<thead>
<tr>
<th></th>
<th>Period (µm)</th>
<th>Duty Cycle</th>
<th>Offset (µm)</th>
<th># periods</th>
</tr>
</thead>
<tbody>
<tr>
<td>Top SiN&lt;sub&gt;x&lt;/sub&gt; layer</td>
<td>1.135</td>
<td>0.5974</td>
<td>0</td>
<td>40</td>
</tr>
<tr>
<td>Bottom SiN&lt;sub&gt;x&lt;/sub&gt; layer</td>
<td>1.093</td>
<td>0.6121</td>
<td>-0.196</td>
<td>40</td>
</tr>
<tr>
<td>100 nm SOI layer</td>
<td>NA</td>
<td>NA</td>
<td>-3.158</td>
<td>NA</td>
</tr>
</tbody>
</table>

Duty Cycles are reported to 4 decimal places in order to reproduce structures to the nearest nm.

Fig. 5.4.1.1. Overview of design (j) SiN<sub>x</sub>-bilayer with 100 nm SOI DBR.

5.4.2. Uniform 100 nm SOI Grating Design

Design (k)’s dimensions are as reported in Table 5.4.2.1 and Fig. 5.4.2.1.

Table 5.4.2.1. Uniform SOI Grating Design’s Dimensions

<table>
<thead>
<tr>
<th></th>
<th>Period (µm)</th>
<th>Duty Cycle</th>
<th>Offset (µm)</th>
<th># periods</th>
</tr>
</thead>
<tbody>
<tr>
<td>Top SiN&lt;sub&gt;x&lt;/sub&gt; layer</td>
<td>1.140</td>
<td>0.6272</td>
<td>0</td>
<td>40</td>
</tr>
<tr>
<td>Bottom SiN&lt;sub&gt;x&lt;/sub&gt; layer</td>
<td>1.092</td>
<td>0.6063</td>
<td>-0.135</td>
<td>40</td>
</tr>
<tr>
<td>100 nm SOI layer</td>
<td>1.136</td>
<td>0.5238</td>
<td>-3.105</td>
<td>16</td>
</tr>
</tbody>
</table>

The SOI grating had an optimum number of 16 periods for improving coupling efficiency. Duty Cycles are reported to 4 decimal places in order to reproduce structures to the nearest nm.
The 100 nm SOI grating functions as a third diffracting layer, i.e. a tri-layer grating [40] which operates on a principle similar to the displaced bilayer design in Chapter 4, but whose design was arrived at independent of first principles. Its function is indicated by its period being close to that of the SiN$_x$ layers (~1.1 µm). If it were instead functioning as a high contrast grating (HCG), a 100 nm SOI high contrast grating (HCG) would have an optimal reflectance of 54.6% at 0.760 µm and 0.40 duty cycle (Fig. 5.4.2.2(a)). Ostensibly, a design with a 220 nm-thick HCG (design (e)) should have a better overall performance as a 220 nm-thick HCG has an optimal reflectance of 71.8% at 0.760 µm, 0.26 duty cycle (shown in Fig. 5.4.2.2(b)). Both the longer period and the superior performance of design (k) over (e) indicate the function of the SOI layer as a diffracting layer.

Fig. 5.4.2.1. Overview of design (k) SiN$_x$-bilayer with 100 nm SOI grating.
5.5. Apodised Designs

Finally, designs (j) and (k) were apodised to obtain (p) (76.8%) and (q) (85.8%) respectively. They were apodised in a period-by-period, nearest-to-waveguide manner, with a ±1 μm of play in the SMF-28’s x position to ensure optimum modal overlap. The mesh accuracy was set to 4 (18 mesh points per wavelength) for all apodisation steps. A mesh accuracy of 2 (10 mesh points per wavelength) is the most common balance between computation requirements and accuracy.

5.5.1. Apodised 100 nm SOI DBR Design

Lumerical’s particle swarm optimisation algorithm was used to individually optimise periods 1–15, then batch-optimise 16–40 together in two rounds. After round 1, (j) improved from 64.2% to 71.7%. After round 2, (j) further improved to 75.7%.
Fig. 5.4.2.3. 2D Optimisation & Apodisation of the 100 nm SOI DBR Design. In the Uniform Design Phase, the design was optimised with 151 generations of 100 children per generation at Mesh Accuracy 4 (black line). Next, each Uniform Design’s parameter was swept (periods, offsets and SMF-28 x-position to the nearest nm; duty cycles to the nearest 0.001) for highest efficiency (red line). During the Apodised Design Phase, each period’s top & bottom start/end dimensions and SMF-28 x-position were optimised in a period-nearest-to-waveguide fashion. Optimisation of the first few periods led to the greatest improvement in coupling efficiency. Periods 1–15 were individually optimised once (blue line), and then individually optimised again, along with group optimisation of periods 16–40 (green line) as a back reflector. Finally, each period’s top & bottom start/end dimensions and SMF-28 x-position were swept to the nearest nm for high efficiency (pink line). The improvement in coupling efficiency was 76.8 % (apodised) vs 64.2 % (uniform) (+ 0.778 dB).

Finally, a given period’s start (µm) and end (µm) dimensions were swept, to the nearest nm, to maximise coupling efficiency. (p), the apodised version of (j), had a final efficiency of 76.8%. Table 5.5.1.1 shows (p)’s final dimensions, as a distance from x = 0 µm (where the first period’s SiNx layers’ unetched sections start).

<table>
<thead>
<tr>
<th>Period</th>
<th>Top layer unetched SiNx start (µm)</th>
<th>Top layer unetched SiNx end (µm)</th>
<th>Bottom layer unetched SiNx start (µm)</th>
<th>Bottom layer unetched SiNx end (µm)</th>
<th>100 nm SOI layer start (µm)</th>
<th>100 nm SOI layer end (µm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.000</td>
<td>0.623</td>
<td>0.000</td>
<td>0.584</td>
<td>-2.586</td>
<td>NA</td>
</tr>
<tr>
<td>2</td>
<td>1.182</td>
<td>1.906</td>
<td>1.015</td>
<td>1.756</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>2.109</td>
<td>3.069</td>
<td>1.945</td>
<td>2.606</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>3.332</td>
<td>4.104</td>
<td>3.028</td>
<td>3.637</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>4.533</td>
<td>5.217</td>
<td>4.122</td>
<td>4.790</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>5.761</td>
<td>6.294</td>
<td>5.146</td>
<td>5.863</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>6.875</td>
<td>7.515</td>
<td>6.419</td>
<td>7.042</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>8.014</td>
<td>8.639</td>
<td>7.470</td>
<td>8.089</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
10 10.244 10.890 9.720 10.424
11 11.309 12.026 10.789 11.537
12 12.361 13.019 11.880 12.499
13 13.578 14.103 13.217 13.727
15 15.874 16.708 15.644 15.796
16–40 17.014 +0.559x 17.354 +0.559x 16.206 +1.130x 17.073 +1.130x NA 46.000

where x = 0, 1, 2, …, 24. The 100 nm thick SOI DBR was extended to underlie the 40th period, at 46.000 µm.

Periods 16–40 have a very short top layer period (559 nm). This value was initially obtained through Lumerical’s particle swarm optimisation algorithm and finally swept to the nearest nm. It functions as a back-reflector for any evanescent waves travelling in the +x direction [41–44] and improved the efficiency by ~2.5%.

5.5.2. Apodised 100 nm SOI Grating Design

Periods 1–19 were individually optimised via particle swarm optimisation. After round 1, (k) improved from 72.3% to 80.7%. After round 2, (k) further improved to 84.1%.

Fig. 5.4.2.3. 2D Optimisation & Apodisation of the 100 nm SOI Grating Design. In the Uniform Design Phase, the design was optimised with 80 generations of 100 children per generation at Mesh Accuracy 4 (black line). Next, each Uniform Design’s parameter was swept (periods, offsets and SMF-28 x-position to the nearest nm; duty cycles to the nearest 0.001) for highest efficiency (red line). During the Apodised Design Phase, each period’s top/bottom/SOI start/end dimensions and SMF-28 x-position were optimised in a period-nearest-to-waveguide fashion. Optimisation of the first few periods led to the greatest improvement in coupling efficiency. Periods 1–19 were individually optimised once (blue line), and then individually optimised again, along with group optimisation of periods 20–40 (green line) as a back reflector. Finally, each
period’s top/bottom/SOI start/end dimensions and SMF-28 x-position were swept to the nearest nm for high efficiency (pink line). The improvement in coupling efficiency was 85.8 % (apodised ) vs 72.3 % (uniform) (+ 0.744 dB).

After nm-scale sweeping, (q), the apodised version of (k), had a final efficiency of 85.8%. Table 5.5.2.1 shows (q)’s final dimensions, as a distance from x=0 µm.

<table>
<thead>
<tr>
<th>Period</th>
<th>Top layer unetched SiNx start (µm)</th>
<th>Top layer unetched SiNx end (µm)</th>
<th>Bottom layer unetched SiNx start (µm)</th>
<th>Bottom layer unetched SiNx end (µm)</th>
<th>100 nm SOI layer start (µm)</th>
<th>100 nm SOI layer end (µm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.000</td>
<td>0.656</td>
<td>0.000</td>
<td>0.654</td>
<td>-6.257</td>
<td>NA</td>
</tr>
<tr>
<td>2</td>
<td>1.227</td>
<td>1.892</td>
<td>0.993</td>
<td>1.827</td>
<td>NA</td>
<td>NA</td>
</tr>
<tr>
<td>3</td>
<td>2.283</td>
<td>2.892</td>
<td>1.965</td>
<td>2.712</td>
<td>NA</td>
<td>NA</td>
</tr>
<tr>
<td>6</td>
<td>5.685</td>
<td>6.360</td>
<td>5.073</td>
<td>5.922</td>
<td>5.416</td>
<td>6.081</td>
</tr>
<tr>
<td>11</td>
<td>11.412</td>
<td>12.139</td>
<td>10.894</td>
<td>11.583</td>
<td>11.068</td>
<td>11.642</td>
</tr>
<tr>
<td>16</td>
<td>16.995</td>
<td>17.760</td>
<td>16.042</td>
<td>17.032</td>
<td>17.030</td>
<td>17.709</td>
</tr>
<tr>
<td>17</td>
<td>18.073</td>
<td>18.893</td>
<td>17.307</td>
<td>18.294</td>
<td>18.025</td>
<td>18.718</td>
</tr>
<tr>
<td>19</td>
<td>NA</td>
<td>20.244</td>
<td>19.685</td>
<td>21.100</td>
<td>20.080</td>
<td>21.100</td>
</tr>
<tr>
<td>20–40</td>
<td>20.492 +0.556x</td>
<td>20.800 +0.556x</td>
<td>21.437 +1.123x</td>
<td>22.223 +1.123x</td>
<td>NA</td>
<td>NA</td>
</tr>
</tbody>
</table>

where x = 0, 1, 2, …, 20. During optimisation, the end of certain periods merged with the start of succeeding periods, resulting in NA values.

A back-reflector of 556 nm was independently optimised in design (q). It improved (q)’s coupling efficiency by −1.4%.
5.6. Lateral Layout

The 2D designs had 3 lateral layouts: Rectangular designs were invariant in the y-direction for 20 µm with a 510 µm-long linear taper. Circular focusing designs were comprised of concentric 50° circular arcs with a 12 µm radius waveguide taper. Elliptical focusing designs were comprised of 50° elliptical arcs curved according to the design procedure from [45,46] with a minimum grating order of 11.

5.6.1. Elliptical Dimensions

The phase-matching condition in [45] states that the plane wave wavefront from an almost vertical SMF-28 can be curved into a cylindrical wavefront to focus on the origin (0, 0) when the grating curves are expressed as

\[ q\lambda_0 = n_{eff}^{grating} \sqrt{x^2 + y^2} - xn_{cladding} \sin \theta_c, \]

(5.6.1.1)

where q is an integer number for each grating line, \( \theta_c \) is the angle between the fiber and the surface normal, \( n_{cladding} \) is the refractive index of the oxide cladding, \( \lambda_0 \) is the vacuum wavelength, x and y are the coordinates of the elliptical curve: x is parallel to the waveguide; y is perpendicular, and \( n_{eff}^{grating} \) is the effective index of the grating.

In the context of a multimode waveguide, \( n_{eff} \) is the weighted average refractive index for a mode of a given order, depending on its field distribution between the core and the cladding (see Fig. 5.6.1.1(a)). Higher order modes are more distributed throughout the cladding. Since \( n_{cladding} < n_{core}, n_{eff, 0^{th}} > n_{eff, 1^{st}} > n_{eff, 2^{nd}} \).

In the context of a grating coupler, usually only the 0th order mode is considered, and the effective index of the grating, \( n_{eff}^{grating} \), is the weighted average of the effective indices the
fundamental mode experiences between the etched and unetched regions of the grating coupler (see Fig. 5.6.1.1(b)). Generally, $n_{\text{eff}, b} < n_{\text{eff, grating}} < n_{\text{eff}, a}$.

Fig. 5.6.1.1(a) effective index, $n_{\text{eff}}$, of $0^\text{th}$, $1^\text{st}$ and $2^\text{nd}$ order modes in a multimode waveguide. Higher order modes have a greater proportion of their field in the cladding. As $n_{\text{cladding}} < n_{\text{core}}$, so $n_{\text{eff}, 0^\text{th}} > n_{\text{eff}, 1^\text{st}} > n_{\text{eff}, 2^\text{nd}}$. Fig. 5.6.1.1(b) effective index, $n_{\text{eff, grating}}$ of $0^\text{th}$ order mode in a grating coupler. The $0^\text{th}$ order mode has a lower effective index in the etched b regions, i.e. $n_{\text{eff}, b} < n_{\text{eff}, a}$. The effective index of the grating, $n_{\text{eff, grating}}$, can be approximated as the weighted average of the effective index of the etched ($n_{\text{eff}, b}$) and unetched ($n_{\text{eff}, a}$) regions.

However, in more sophisticated grating coupler designs—such as the two covered in this chapter—determining the $n_{\text{eff, grating}}$ is not as straightforward. We can extrapolate from Fig. 5.6.1.1(b) that $n_{\text{eff, grating}}$ should be a roughly constant value for uniform grating couplers. Re-expressing Eq. 5.6.1.1, we get

$$
n_{\text{eff, grating}} = \frac{1}{\sqrt{x^2 + y^2}} \left[ q \lambda_0 + x n_{\text{cladding}} \sin \theta_c \right],
$$

and setting $y = 0$, we obtain
In Eq. 5.6.1.3, ‘$x_{\text{ellipse}}$’ has been partially determined by the 2D designs from Sections 5.4 (Uniform Designs) and 5.5 (Apodised Designs), where $x_{2D} = 0$ was arbitrarily defined as the start of the first period of the grating coupler. In an elliptically focusing design, (0,0) is defined as the focal origin, so the $x_{2D}$-values from Sections 5.4 and 5.5 must be shifted by a constant ‘Initial Radius’, i.e. $x_{\text{ellipse}} = x_{2D} + \text{‘Initial Radius’}$. 

To accommodate an SMF-28 in the y-dimension, the minimum q-integer (grating order) is set to ‘11’: $11 \times \sim 1.1 \text{ µm (period)} \approx 12.1 \text{ µm} > 10.4 \text{ µm}$. For each 2D design, the Initial Radius was swept in 0.100 µm steps around 12.1 µm until the average $n_{\text{eff}}^{\text{grating}}$ between the inner and outer elliptical curves of a given layer was roughly constant across the periods (cf. Fig. 5.6.1.2). 

![Graphs showing $n_{\text{eff}}^{\text{grating}}$ for different Initial Radii](image)

Fig. 5.6.1.2. $n_{\text{eff}}^{\text{grating}}$ of the Uniform 100 nm SOI DBR 2D design for periods 1–48 for q = 11 and a) Initial Radius = 11.5 µm, b) Initial Radius = 12.0 µm, c) Initial Radius = 12.5 µm. As can be seen from the graphs, Initial Radius = 11.5 µm has an average $n_{\text{eff}}^{\text{grating}}$ between the inner and outer ellipses which is decreasing across the periods. In contrast, Initial Radius = 12.5 µm has a *increasing* average $n_{\text{eff}}^{\text{grating}}$ across the periods. Initial Radius = 12.0 µm was found to have a roughly constant averaged $n_{\text{eff}}^{\text{grating}}$ across the periods, for this 2D design as well as separately for the remaining three 2D designs for $q = 11$.

In both apodised designs, the top SiNx layer has a rapidly increasing $n_{\text{eff}}^{\text{grating}}$ for the periods of the back reflector (cf. Fig. 5.6.1.3). This effect is not considered when selecting the
Initial Radius as those periods are not involved in directly diffracting the SMF-28 mode but on back-reflecting scattered E-fields in the +x direction.

The SMF-28 mode impinges primarily on periods 1–10, so the Initial Radius was swept till the averaged $n_{\text{eff}}^{\text{grating}}$ for those periods was roughly constant.

The process was repeated for the 100 nm SOI Grating 2D design, and the ideal Initial Radius was also found to be Initial Radius = 12.0 μm for $q = 11$ (cf. Fig. 5.6.1.4).
Finally, with the values of $n_{eff,grating}$ solved for each period, Eq. 5.6.1.1 is re-expressed to solve for $y$,

$$y_{\text{ellipse}} = \left[ \frac{1}{n_{eff,grating}^2} \left( q \lambda_0 + x_{\text{ellipse}} n_{\text{cladding}} \sin \theta_c \right)^2 - x_{\text{ellipse}}^2 \right]^{1/2}, \quad (5.6.1.4)$$

where $q = 11$ for period 1, 12 for period 2, 13 for period 3, and so on; $n_{eff,grating}$ has already been solved for period 1, 2, 3, and so on, as shown in Figs. 5.6.1.1–4; and $x_{\text{ellipse}} = \text{Initial Radius} (= 12.0 \ \mu m) + x_{2D} - x_{\text{sweep}}$, where $x_{\text{sweep}}$ is a value between 0.000–6.500 \mu m.

The final calculated elliptical curves (red) of the SOI layer of the Apodised 100 nm SOI Grating Design are contrasted against circular curves (black) in Fig. 5.6.1.5(a). As can be seen, the elliptical curves have a tighter bend the farther they are from the focal origin (0,0) to maintain the phase-matching condition of Eq. 5.6.1.1.

![Fig 5.6.1.5. a) Circular arcs (black) vs elliptical arcs where $\theta_e = 9^\circ$ (red) of the SOI layer of the Apodised 100 nm SOI Grating Design based on Eq. 5.6.1.4. The elliptical arcs have tighter bends than circular ones the farther they are from the focal origin (0,0). b) $\theta_e = 9^\circ$ elliptical arcs (red) vs $\theta_e = 6.2^\circ$ elliptical arcs (blue) of the SOI layer of the Uniform 100 nm SOI Grating Design. $\theta_e = 9^\circ$ elliptical arcs have slightly tighter bends. When $\theta_e = 0^\circ$, elliptical arcs would correspond to the black circular arcs in Fig. 5.6.1.5(a) [47].](image-url)
5.6.2. \( \theta_c \): Coupling Angle versus Fibre Tilt

In [46], \( \theta_c \) is called the ‘coupling angle’ which from the diagrams is defined as the angle at which the incoming beam impinges on the grating coupler. In contrast, [45], whose design is based on [46], defines \( \theta_c \) as the fibre tilt. For a cleaved SMF-28, the two definitions of \( \theta_c \) are not synonymous, as Fig. 5.6.2.1, a screenshot of the x-z plane of the Lumerical interface for the Apodised 100 nm SOI Grating Design, shows. As a default—and for clarity—the z-dimension is expanded ten times, but otherwise the diagram is to scale. According to Snell’s Law, a fibre tilt of 9° will result in a coupling angle of 6.2° at the top oxide-SiN\(_x\) interface.

Consequently, a different set of ellipses will be produced from Eq. 5.6.1.4 based on \( \theta_c = 6.2^\circ \). Fig. 5.6.1.5(b) contrasts elliptical arcs based on \( \theta_c = 9^\circ \) (red) and \( \theta_c = 6.2^\circ \) (blue). Both sets of ellipses were laid out in the Uniform 100 nm SOI DBR as well as Grating designs to compare their experimental coupling efficiencies.
5.6.3. Interlayer Taper Optimisation

The Rectangular designs have a 510 µm-long linear interlayer taper (Fig. 5.6.3.1). The top SiN, (blue) layer has a 510 µm-long linear taper terminating in a 0.100 µm tip, while the bottom SiN, layer (red) is a 500 µm-long linear taper with an extended 10 µm-long, 1.5 µm-wide straight waveguide so that the termination of both tapers do not coincide, therefore easing the transition of the mode to the bottom layer waveguide.

![Fig. 5.6.3.1. Interlayer taper of the Rectangular layout. The bottom SiN, layer is drawn in red. The top SiN, layout is drawn in purple.](image)

Both focusing designs originally have a 27 µm-long linear interlayer taper. To improve the taper shape, it was modeled in 3D FDTD instead of Lumerical Solution’s MODE 2.5D variational FDTD solver as it was not invariant in z. Due to the demand on computational resources, the mesh accuracy was set to 2, which corresponds to 10 mesh points per wavelength in the structure.

The top nitride taper was parameterised with the following equation [48]:

$$w(x) = \alpha(L - x)^m + w_2,$$  \hspace{1cm} (5.6.3.1)

where

$$w(0) = w_1 = 0.100 \mu m,$$  \hspace{1cm} (5.6.3.2)

$$w(L) = w_2 = 1.5 \mu m,$$  \hspace{1cm} (5.6.3.3)

and
\[
\alpha = \frac{(w_1 - w_2)}{L^m}.
\] (5.6.3.4)

This expression is given as is, where the taper width is proportional to \( x^m \). When \( m = 0.5 \), the taper is radical; when \( m = 1 \), the taper is linear; when \( m = 2 \), the taper is parabolic [49]. As can be seen, Eq. 5.6.3.1 covers a wide range of general taper designs. A view of the taper structure along the \( z \)-axis is shown in Fig. 5.6.3.2(a).

![Fig. 5.6.3.2. Top-down view of the interlayer taper optimisation. The bottom SiNx 1.5 \( \mu \)m-wide straight waveguide is drawn in red. The top SiNx taper is drawn in blue. Orange lines indicate the power monitors placed throughout the interlayer taper. The bilayer taper is excited by the fundamental TE mode at 1550 nm (indicated by the green curve) at \( x = 41 \) \( \mu \)m. (a) Single interlayer taper optimising the length \( L \) with \( m = 1 \), then single taper optimising \( m \) with \( L = 30.45 \) \( \mu \)m. (b) Double interlayer taper optimising \( m_2 \) with \( m_1 = 3.0 \), \( L_1 = 25.68 \) \( \mu \)m, \( L_2 = 8.87 \) \( \mu \)m and \( w_{1.5} = 0.482 \) \( \mu \)m.](image)

\( w_0 = 0.100 \) \( \mu \)m as that is the smallest reliably printable dimension by 193 nm DUV lithography. \( w_2 = 1.5 \) \( \mu \)m, the width of the bottom SiNx waveguide. \( \alpha \) is then determined by \( L \) and \( m \), so the overall shape of the taper is thus determined by only 2 parameters, reasonably limiting the parameter space.

First, we simulate the optimal length for a linear taper by setting \( m = 1 \) and sweeping length of the taper, and obtain Fig. 5.6.3.3(a). We observe an improvement of power transmission through the last power monitor, \( T_0 \), as \( L \) of the linear interlayer taper increases. However, one of the main benefits of a focusing grating coupler design, compared to the
rectangular design, is the reduction in footprint area, and increasing L detracts away from this. The original design was $m = 1, L = 27 \, \mu m$, and we can see that we lose significant power (78.3% transmission at $T_0$). As a compromise between L and $T_0$ transmission, $L = 34.5 \, \mu m$ was chosen, where $T_{25 \, \mu m}$ just starts to dip away from $T_{35 \, \mu m}$. $m$ was then swept from 1–6 to improve transmission at $T_{15 \, \mu m}$ and $T_0 \, \mu m$, the results of which are shown in Fig. 5.6.3.3(b).

It is interesting to note that $T_{15 \, \mu m}$ and $T_{25 \, \mu m}$ actually have higher power throughputs than $T_{35 \, \mu m}$ at larger values of $m$. This is likely a simulation artefact caused by the lower mesh accuracy (2) and the tight simulation space ($y$-span = 3.0 $\mu m$, $z$-span = 1.3 $\mu m$) as compromises for 3D FDTD simulation speed. Nevertheless, if we consider only individual power monitors, we can see how the $m$ value (curve of the taper) affects transmission. $T_0 \, \mu m$ plateaus at $m \approx 4.5$ (87.7%), which would be an appropriate value for a single interlayer taper design. However, significant power is still lost between $T_{15 \, \mu m}$ and $T_0 \, \mu m$ (8.4%).

If the reciprocal time-reversed problem is considered, i.e. the fundamental mode is travelling to the right, [50,51] suggest that the spreading of the taper’s sidewalls must be slower.
than the diffraction spreading of the lowest order mode to confine it in the taper without conversion to higher order or radiation modes. Thus, we can reduce the power lost between $T_{15\,\mu m}$ and $T_{0\,\mu m}$ by means of a second interlayer taper starting at $x = 15\,\mu m$ with a more acute ($m < 1$) curve. This constrains the length of the first taper, $L_1 = 25.68\,\mu m$. Subsequently, $L_2 = 8.87\,\mu m$ (cf. Fig. 5.6.3.2(b)).

With two interlayer tapers, $m_1$ (the $m$ value for the first taper) should be as low as possible, as that will reduce the curve mismatch with $m_2$. From Fig. 5.6.3.3(b), $m_1 = 3$ as $T_{15\,\mu m}$ just starts to dip, which constrains the taper width where both tapers meet, $w_{1.5} = 0.482\,\mu m$. $m_2$ was then swept across values $0.2 < m_2 < 1.5$ and the 1550 nm transmission through power monitor $T_{0\,\mu m}$ shown in Fig. 5.6.3.4(a). The 1550 nm transmission through power meter $T_{0\,\mu m}$ is optimal (86.85%) at $m_2 = 0.6$.

Finally, a wavelength sweep of the double interlayer taper design is compared to the original 27 $\mu m$-long linear interlayer taper in Fig. 5.6.3.4(b). At 1550 nm, there is an efficiency improvement of 10.3%.
5.6.4. Lateral Taper Optimisation

Farther up the grating coupler, a similar optimisation strategy was pursued to optimise the lateral taper. Fig. 5.6.4.1(a) shows the optimisation set up a single lateral taper where both the bottom and top SiN$_x$ layers share the same taper profile. However, despite both layers sharing the same profile, a quicker 2.5D FDTD simulation program (such as Lumerical MODE) was not used as the SiN$_x$ bilayer lateral taper is not invariant in $z$—it has a 100 nm SiO$_2$ layer sandwiched between, a bottom Si substrate which acts as a reflecting layer, and a 100 nm SOI layer which either acts as a DBR or a third grating layer. Hence, Lumerical FDTD was utilised for this optimisation process.

![Fig. 5.6.4.1. Top-down view (along the z-axis) of the optimisation of the lateral taper. Blue indicates both the first SiN$_x$ and second SiN$_x$ layers, as both profiles are to be determined by the same taper values. Orange lines indicate the power monitors placed throughout the lateral taper. The bilayer lateral taper is excited by the fundamental TE mode at 1550 nm (indicated by the green curve) at $x = 20 \mu m$. The pink dotted line indicates the outline of the bottom 100 nm SOI layer. (a) Optimisation of a single lateral taper. (b) Optimisation of a double lateral taper (green). The outline of the single lateral taper is indicated by blue dotted lines.](image)

Power monitor $T_0 \mu m$ was placed 5 $\mu m$ down the 1.5 $\mu m$-wide bilayer waveguide to ensure it would measure only the guided fundamental mode. Other power monitors were placed 1 $\mu m$ apart near the lateral taper convergence as the previous section has shown that to be an area for significant optimisation. Lastly, one was placed at $x = 15 \mu m$ to confirm appropriate launch conditions of the fundamental mode. A fundamental mode source for TE-polarised 1550 nm light (represented by the green curve) was placed at $x = 20 \mu m$ in lieu of an out-of-plane SMF-28
source to limit the simulation space in z. A pink dotted line indicates the bottom 100 nm SOI structure which was left unchanged in order to limit the parameter space for optimisation. The reduction of possible optimisation parameters is even more crucial here as the lateral taper’s simulation volume (and hence memory requirements and simulation time) is 5.2 times larger than the interlayer taper’s.

As per Eq. 5.6.1–4, \( w_1 = 1.5 \mu m \) (to connect to the interlayer taper) while \( w_2 = 10.5 \mu m \) (the chord length of the first period as determined in section 5.6.1. Elliptical Dimensions). In the original linear lateral taper design, \( L_1 = 10.5 \mu m \). To see if \( L_1 \)’s optimal value might be significantly different, \( L_1 \) was swept for a linear lateral taper (\( m_1 = 1.0 \)), to obtain Fig. 5.6.4.2(a). Unsurprisingly, increasing \( L_1 \) leads to a more gradual taper and therefore better transmission. However, \( L_1 \) cannot be infinitely long as that would obviate the smaller footprint feature of a focusing design. As a compromise, \( L_1 = 15.0 \mu m \), where \( T_{6 \mu m} \) starts to dip.

![Fig. 5.6.4.2. Single lateral taper optimisation. (a) \( L_1 \) sweep with \( m_1 = 1.0 \). (b) \( m_1 \) sweep with \( L_1 = 15.0 \mu m \).](image)

To see if efficiency can be further improved, \( m_1 \) was swept from 0.5–1.5 to obtain Fig. 5.6.4.2(b). A more radical taper (\( m_1 < 1.0 \)) results in increases in \( T_{0 \mu m} \), but there are mode
conversion losses occurring in the earlier power monitors, suggesting that just manipulating $m_1$ to increase $T_0 \mu m$ might not be an optimal solution.

At $m_1 = 1.0$, we can see a significant mode conversion loss occurring between $T_5 \mu m$ and $T_0 \mu m$. The losses between $T_5 \mu m$ and the earlier power monitors is not of significant concern as the source used in this truncated 3D FDTD simulation is the fundamental mode of the bilayer taper where it is 10.5 $\mu m$ wide. For such a mode, the sidewalls of the converging linear taper would indeed scatter the energy to higher order modes. However, we must bear in mind that the actual source is an out-of-plane Gaussian SMF-28 whose wavefront has already been focused by the elliptical curves determined in section 5.6.1. Elliptical Dimensions. Such a source, with an already converging wavefront, would likely not be significantly scattered by the linear taper’s sidewalls, and so the crucial juncture where a second lateral taper (the green trapezoid in Fig. 5.6.4.1(b)) should be optimised remains the transition between $T_5 \mu m$ and $T_0 \mu m$. Nevertheless, as a precautionary measure, the second taper was placed 1 $\mu m$ before $T_{10} \mu m$. This corresponded to a $w_{1.5} = 3.058 \mu m$.

While maintaining $m_2 = 1.0$, i.e. the second lateral taper is linear, $L_2$ was swept to produce Fig. 5.6.4.3(a). $L_2 = 2.4 \mu m$ corresponds to an unmodified single lateral taper of $L_1 = 15.0 \mu m$, and we can clearly see an improvement in the modal confinement at $T_0 \mu m$ as $L_2$ is increased. $T_0 \mu m$ plateaus at $L_2 > 6.0 \mu m$ at 43.6%, so it was fixed for $L_2 = 6.3 \mu m$, which does not significantly increase the length of the lateral taper.

Similar to the process for the interlayer taper, it should stand to reason that the second lateral taper should be radical ($m < 1.0$) to have (again, considering the reciprocal problem of the fundamental mode travelling from left to right) the taper sidewalls spread slower than the
diffraction spreading of the fundamental mode. Thus, while maintaining $L_2 = 6.3 \, \mu\text{m}$, $m_2$ was swept from $0.5 < m_2 < 1.0$ to produce Fig. 5.6.4.3(b).

Curiously, Fig. 5.6.4.3(b) suggests that $T_{0 \mu\text{m}}$ would increase if $m_2 > 1.0$, but we should bear in mind that the source is the fundamental mode of the $10.5 \, \mu\text{m} \times 0.550 \, \mu\text{m}$ taper, and not an SMF-28 Gaussian focused by the elliptical arcs, which accounts for the only ~40% efficiency at $T_{0 \mu\text{m}}$. A secondary taper with a large $m_2$ value would indeed benefit the former $10.5 \, \mu\text{m}$-broad fundamental mode as it is basically a straight waveguide, but does not efficiently confine a source with an already converging wavefront, as in the latter case. Thus the source was changed to a $10.4 \, \mu\text{m}$ MFD Gaussian source diffracting off of the elliptical arcs and the $m_2$ value swept from $0.2 < m_2 < 2.0$, to produce Fig. 5.6.4.4(a). To accommodate the arcs and Gaussian source, the simulation space increased by 3.4 times. The Gaussian source was located within the top oxide, $1.5 \, \mu\text{m}$ above the top SiN$_x$ layer, with a tilt of $6.2^\circ$ to account for refraction at the air-top oxide interface of a $9^\circ$-tilted SMF-28 source. Its central position was $x = 6.0 \, \mu\text{m}$ (estimated to be
similar to the SMF-28 source in its ideal position). If the latter source were used, the simulation space would have increased by 9.7 times.

We can see from Fig. 5.6.4.4(a) that $T_{0\,\mu m}$ peaks at $m_2 = 0.4$ with an efficiency of 69.0%. Although $T_{5\,\mu m} - T_{10\,\mu m}$ straddled the second lateral taper, they do not seem significantly affected by $m_2$, except for $T_{5\,\mu m}$ where $m_2 < 0.4$. There seems to be a ~1.4% loss between $T_{10\,\mu m}$ and $T_{8\,\mu m}$, and this might be improved by optimising a third lateral taper between the two power monitors.

Finally, the Gaussian source was swept across $1480 < \lambda < 1570$ nm and the transmission through $T_{0\,\mu m}$ was compared between the improved and original lateral tapers as shown in Fig. 5.6.4.4(b). At 1550 nm, there is an improvement of 3.2%.

5.7. Fabrication of SiN$_x$-on-SOI Grating Coupler(s)

The devices were fabricated on AIM MPW runs on a 300 mm wafer with 220 nm-thick SOI using standard CMOS processing techniques. Both 2D designs (DBR and Grating) utilise
the same mask level used during silicon rib waveguide formation to thin the 220 nm-thick SOI down to 100 nm. 220 nm of PECVD TEOS was then deposited as cladding.

Next, 220 nm of near-stoichiometric silicon nitride (refractive index \( \approx 2.0 \)) was deposited via PECVD directly on the silicon waveguide cladding layer. The Si\( \text{N}_x \) was patterned with state-of-the-art ASML 193 nm deep UV argon-fluoride (DUV ArF) immersion lithography and etched with reactive ion etching (RIE). It was then capped with 100 nm of PECVD TEOS.

Subsequently, a second layer of 220 nm of Si\( \text{N}_x \) was deposited and patterned as the first Si\( \text{N}_x \) layer. Lastly, a 5.1 \( \mu \text{m} \)-thick capping layer of SiO\(_2\) was deposited via PECVD TEOS.

Optical microscopy of the general layout is shown in Fig. 5.7.1, while representative scanning electron microscopy (SEM) images of the rectangular, circular and elliptical layouts of the apodised design are shown in Fig. 5.7.2 below, after the SOI and each Si\( \text{N}_x \) etch step.

![Fig. 5.7.1. Optical microscopy of the general layout of the grating coupler designs. Grating couplers of the same design are paired and connected with a 2 cm-long, 1.5 \( \mu \text{m} \)-wide bottom Si\( \text{N}_x \) waveguide. (a) Rectangular grating couplers have a 500 \( \mu \text{m} \)-long, linearly tapered, temporary Si\( \text{N}_x \) bilayer waveguide to confine the mode to the bottom Si\( \text{N}_x \) waveguide. The top Si\( \text{N}_x \) taper starts at 20 \( \mu \text{m} \) wide but tapers to 0.100 \( \mu \text{m} \). (b) The temporary Si\( \text{N}_x \) bilayer waveguide in circular and elliptical focusing grating couplers is 27 \( \mu \text{m} \) long. The top Si\( \text{N}_x \) layer has an optimised taper which starts at 1.5 \( \mu \text{m} \) wide and tapers to 0.100 \( \mu \text{m} \).](image)
Fig. 5.7.2(a) – (c) SEM micrographs of 100 nm DBR apodised rectangular grating couplers: (a) after first SiN$_x$ etch, (b) close up of first three periods after first SiN$_x$ etch, (c) after second SiN$_x$ etch. (d) – (f) SEM micrographs of 100 nm DBR apodised elliptical grating couplers with a lateral layout inspired by [30], which had a two-stage taper to laterally confine the spot size in the y-dimension: (d) after SOI thinning etch, (e) after first SiN$_x$ etch. (f) after second SiN$_x$ etch. (d) is based on an earlier, unsuccessful 2D design with a temporary trilayer waveguide (100 nm SOI + 220 nm SiN$_x$ + 220 nm SiN$_x$), and is presented here solely to give an impression of what the 100 nm SOI DBR layer might look like in the device based on the successful 2D design. (g) – (h) SEM micrographs of 100 nm DBR apodised circular grating couplers: (g) after first SiN$_x$ etch, (h) after second SiN$_x$ etch. (h) shows a 27 µm-long interlayer taper which confines the temporary bilayer SiN$_x$’s taper mode to just the bottom SiN$_x$ layer.
5.8. Experimental Measurements

Grating couplers of the same design were laid out in pairs on a macro compatible with a 20 individual SMF V-Groove assembly by OZ Optics (Ottawa, Ontario) for in-circuit testing (ICT). The grating couplers were 127 µm apart and connected by straight 100 µm-long, 1.5 µm-wide strip waveguide pairs (Fig. 5.8.1).
and the same lateral layout (Rectangular, Circular, 6.2° Elliptical, 9° Elliptical). Grating couplers were 127 µm apart and connected by 100 µm-long, 1.5 µm-wide strip SiN₅ waveguides.

All fibre pairs in the V-Groove assembly were used to measure the same high efficiency grating coupler pair to determine which channel (3) had the lowest loss. Channel 3 of the V-Groove assembly was then used to measure all high efficiency pairs in order to avoid zero-ing issues in loss.

The outermost pair POR SiN₅ grating couplers were used for the initial V-Groove assembly optical alignment. However, as channel 3 was stepped across each GC pair, the V-Groove assembly was further aligned using channel 3 over said specific GC pair. Ostensibly, the best wavelength to perform this further alignment at is 1550 nm. However, as the assembly was polished to 8° and the tilt relatively fixed at 8°, leading to an incident angle of 11.6°, the laser wavelength was adjusted to compensate. Empirically, 1525 nm was found to produce the alignment with the highest coupling efficiency, and differed from the 1550 nm alignment position by ~ -2 µm in x.

Bandwidth measurements were collected with a Keysight Technologies (Santa Rosa, CA) 81606A Tunable Laser Source, an N7786B Polarisation Synthesiser, and a N7745A Optical Multiport Power Meter. The full light path was 81606A Tunable Laser Source → 81595B 1 × 4 Optical Switch → N7786B Polarisation Synthesiser → N7734A 1 × 13 Optical Switch → ADAFC4 Mating Sleeve → High Efficiency Grating Coupler pair with 2 63.5 µm-radius 90° bends and 2 100 µm-long strip waveguides → ADAFC4 Mating Sleeve → N7731A 1×4 Optical Switch → N7745A Optical Multiport Power Meter. The polarisation synthesiser re-normalises the lost power prior to—and including—itself, so only the components after it were calibrated for their losses.
The losses from the waveguide bends and straight waveguides were measured on a separate structure and they—along with calibrated losses from the relevant optical components along the light path—were subtracted from the total insertion loss. The remaining insertion loss was divided by 2 to obtain the SMF insertion loss per high efficiency GC. To show across-wafer repeatability, the 18 high efficiency GC type pairs were measured over 6 dice.

The results of the insertion loss of the grating couplers are shown in Figs. 5.8.1–2 below, along with the simulated 2D FDTD in-line (8° polish, aligned at 1525 nm—black dotted line) and manual (cleaved SMF, aligned at 1550 nm—red dotted line) coupling. Departures from the simulated ideal are attributed to fabrication tolerances and measurement variations.

![Fig. 5.8.1. Measured and simulated bandwidth of (a) Uniform and (b) Apodised 100 nm SOI DBR designs.](image)
Between the two 2D designs: 100 nm SOI DBR and 100 nm SOI Grating, the Grating design had better performance but slightly poorer resistance to fabrication tolerances. The latter is not surprising as it is a more complex structure than the bilayer grating coupler of the SOI DBR design, requiring tight alignment and etch tolerances between three mask levels rather than two.

The former can be quantified by comparing the performances of the best lateral layout (9° elliptical with modified taper), i.e. comparing the purple lines of Fig. 5.8.1(b) and 5.8.2(b): (-1.259 vs -1.814 dB). The efficiency improvement of 0.555 dB (8.98%) will have to be weighed against the more stringent fabrication tolerances. Of note, earlier experiments have shown that the SOI Grating performed significantly poorer than the SOI DBR design (-4.306 vs -
2.757 dB) when the SiN$_x$ bake temperature and duration was adjusted, highlighting how sensitive a specialised high efficiency design like the trilayer SOI Grating is to fabrication variances.

Amongst the three main lateral layouts, elliptical designs performed the best, followed by rectangular and lastly circular layouts. As previously mentioned, circular curves coincide with $\theta_c = 0^\circ$ elliptical ones. As the circular curves did not accommodate the phase-matching condition of a tilted fibre, it is unsurprising that they were the poorest performers.

Between rectangular and elliptical layouts, [45] has shown that elliptical lateral layouts can shorten the taper length while still maintaining similar coupling efficiencies to rectangular layouts (~ 30 %). [35] has shown that focusing layouts can sometimes match or even outperform rectangular layouts by as much as 0.7 dB. It is possible that with the width of the rectangular lateral layout (20 µm) and the thickness of the temporary bilayer SiN$_x$ waveguide (0.540 µm), higher order waveguide modes are excited that—even with the 500 µm long linear taper—are not adiabatically coupled to the fundamental mode of the 220 nm × 1.5 µm strip waveguide, resulting in poorer performance than expected of the rectangular layouts. Additionally, it is likely that in the outgoing grating coupler, the ground mode of the single mode waveguide expands to a larger beam inside the 20 µm-wide taper than is acceptable by the fibre mode [51].

Comparing $\theta_c = 9^\circ$ versus $\theta_c = 6.2^\circ$ elliptical layouts in Figs. 5.8.1(a) and 5.8.2(a), we can see a finite improvement of ~ 0.188–0.218 dB (4.42–5.15%) in the uniform designs when $\theta_c = 9^\circ$. The incident angle is 11.6° while the coupling angle is 8.0° to the surface normal. Despite the greater difference (11.6° - 9° = 2.6° vs 1.8°), the $\theta_c = 9^\circ$ elliptical outperformed the $\theta_c = 6.2^\circ$ elliptical layout. This suggests that it is sufficient to interpret $\theta_c$ as the incident angle (in the case of a polished SMF) or the angle between the fibre and the surface normal (in the case of
a cleaved SMF) instead of the coupling angle for the purposes of accommodating the phase-matching condition of the measurement setup.

This could be because while [46] had intended \( \theta_c \) to be the coupling angle rather than the fibre tilt, it also included an aberration correction factor for grating etch depths > 50 nm, which both 2D designs indeed have. Eq. 5.6.1.1 is valid assuming \( n_{\text{eff}}^{\text{grating}} = n_{\text{eff}}^{\text{waveguide}} \). When \( n_{\text{eff}}^{\text{grating}} \neq n_{\text{eff}}^{\text{waveguide}} \),

\[
q\lambda_0 = n_{\text{eff}}^{\text{grating}} \sqrt{x^2 + y^2} - x n_{\text{cladding}} \sin \theta_c + r(q_a) \times \left( n_{\text{eff}}^{\text{waveguide}} - n_{\text{eff}}^{\text{waveguide}} \right),
\]

where \( r(q_a) \) represents the correction term, which is weighted with the difference in the effective indices,

\[
r(q_a) = q_a \lambda_f \frac{-xe_a (x^2 + y^2)^{\frac{1}{2}} + x^2 + y^2}{y^2 + (1 - e_a^2)x^2}, \text{ and}
\]

\[
e_a = \frac{n_{\text{cladding}} \cos \phi_c}{n_{\text{eff}}^{\text{grating}}}. \tag{5.8.3}
\]

e_a is the numerical eccentricity of the inner ellipse. With the aberration correction, Eq. 5.8.1 becomes a 6\(^{th}\) order polynomial in \( x \) and \( y \), complicating the drawing of the elliptical arcs.

Between the uniform and apodised designs, there are significantly bigger Fabry-Perot resonances in the latter. The likely cause of this are the back reflectors of the apodised designs, which weren’t detected in simulation as only a single apodised grating coupler was simulated. In an application requiring high efficiency but less noise across the bandwidth, the back reflector’s contribution to efficiency (~ 1.4–2.5\%) would have to be weighed against the introduction of noise in the form of Fabry-Perot resonances.
Comparing the 9° elliptical apodised designs with and without a gradual lateral and interlayer tapers (Section 5.6.4), we see a modest improvement of 0.131–0.133 dB (3.06–3.11%) as the transition between the grating taper and the grating waveguide is smoothed out.

Regarding bandwidth performances, the 9° elliptical layouts (green lines) across the four types (100 nm Grating/DBR, uniform/apodised) are compared and summarised in Table 5.8.1.

| Table 5.8.1. Bandwidth Comparisons of 2D Designs using 9° Elliptical Layouts |
|---------------------------------|-----------------|-----------------|-----------------|-----------------|
|                                 | 100 nm SOI DBR Design | 100 nm SOI Grating Design |
|                                 | Uniform | Apodised | Uniform | Apodised |
| Simulated Max. Coupling Efficiency (dB) | -1.924 (64.2%) | -1.162 (76.5%) | -1.345 (73.4%) | -0.662 (85.9%) |
| Measured Max. Coupling Efficiency (dB) | -2.213 (60.1%) | -1.899 (64.6%) | -1.672 (68.0%) | -1.351 (73.3%) |
| Simulated -1dB Bandwidth (nm) | 58.7 | 27.8 | 51.3 | 26.8 |
| Measured -1dB Bandwidth (nm) | 73.1 | 52.7 | 57.2 | 47.2 |
| Simulated -3dB Bandwidth (nm) | 80.5 | 80.2 | 73.2 | 68.6 |
| Measured -3dB Bandwidth (nm) | 97.3 | 93.4 | 83.6 | 75.2 |

The coupling efficiencies were slightly lower than the theoretical maxima because—aside from lateral layout losses—the grating couplers were characterised with an 8° polished SMF, which changes the incident angle and the Gaussian-like E-field profile of the fibre. This difference causes a shift in peak coupling efficiency and peak coupling wavelength as seen between the red dotted (original cleaved SMF) and black dotted (polished 8° SMF) lines in Figs. 5.8.1 and 5.8.2.

**5.9. Conclusions**

Overall, this chapter outlines the general design process and measurement of a high efficiency grating coupler with zero change to the layer stack:

- Starting with a given layer stack and etch levels, established design strategies which can operate within those parameters are combined, and the most successful of those designs are
• (with a reasonably high mesh accuracy) Apodised, apodised again, and then have back
  reflectors added, then
• Swept to the nearest nm to obtain the best possible 2D design. Next,
• The 3D design is curved using focusing ellipses,
• The interlayer taper optimised to reduce insertion losses from the temporary SiN_x
  bilayer waveguide to just the bottom SiN_x waveguide,
• And finally, the lateral-taper-to-interlayer-taper transition smoothed out

Each step is carefully optimised to maximise the final efficiency of the grating coupler.

Between the two final 2D designs, the trilayer 100 nm SOI Grating had higher simulated
and measured efficiency, but also poorer fabrication tolerances.

Between uniform and apodised designs, apodised designs had higher efficiencies but
poorer bandwidths. Apodised designs also suffered from larger Fabry-Perot resonances which
may be undesirable in certain applications.

Due to computational requirements, 3D lateral layout designs were not wholly optimised
in simulation, but instead laid out based on principles established by earlier research, partially
optimised, then fabricated and their relative performances compared. In terms of efficiency, 9°
elliptical layouts with improved lateral and interlayer tapers performed the best amongst the
present designs. However, the elliptical 3D lateral layouts can still be further refined, for
example, in parameters of arc angle, minimum period order, multiple taper sections, or period 1
SOI profile shape (pink dotted line in Fig. 5.6.4.1), and would be a suitable area for further
research.

5.10. Chapter Bibliography

1. A. Michaels and E. Yablonovtich, “Inverse design of near unity efficiency perfectly vertical grating couplers,”


6. Conclusions

6.1 Research Objectives

At the outset of this thesis, the research objects were threefold:

- to design a high misalignment tolerance, single-etch grating coupler;
- to design a SiN$_x$-only grating coupler; and
- to design a maximally-efficient grating coupler which couples into an SiN$_x$ waveguiding layer

To be industry-applicable, these three different styles of grating couplers were limited to the pre-existing American Institute for Manufacturing Integrated Photonics (“AIM Photonics”) layer stack, and thereby forewent incompatible design techniques.

6.2 Achieved Results

In Chapter 1, the grating coupler problem was illustrated as an overlay of a performance three-pointed star (blue) and a design hexagram (red) (cf. Fig. 1.2.1.1) as a communicative device to the reader. Any physical grating coupler must try to balance the three apices of the performance star, as the Bragg Condition—the basic physical principle on which a grating coupler operates—prevents a grating coupler from having 100% efficiency, infinite bandwidth and infinite alignment tolerances. Any practical grating coupler must also balance the 6 apices of the design hexagram, of which zero-change and minimum feature size are non-negotiable.
Chapter 3 covered the design, fabrication and measurement of a grating coupler with an -1 dB x × y lateral misalignment tolerance of 21.4 µm × 10.1 µm, which is 24 times the area of a regular grating coupler based on the 220 nm SOI platform. However, maximising the lateral misalignment apex of the blue performance star necessitated sacrificing its coupling efficiency (-7.49 dB / 17.8%), -1 dB bandwidth (14 nm) and tilt misalignment tolerance (-1.0 dB: ± 2°). If the design’s complexity is to continue being constrained to a single through-etched mask, then a balancing act will have to be struck between the apices: by reducing the lateral misalignment tolerance (primarily by using a shorter planewave source), one can expect an accompanying improvement in efficiency, bandwidth and tilt misalignment tolerance.
Chapter 4 covered the design, fabrication and measurement of a bilayer SiN$_x$-only grating coupler with a coupling efficiency of -2.56 dB (55.4%), and a -1 dB bandwidth of 46.9 nm. When compared to other industry-compatible SiN$_x$-only designs, namely,

table

<table>
<thead>
<tr>
<th>Paper</th>
<th>SiN type</th>
<th>Designed Wavelength (nm)</th>
<th>SiN layer thickness (nm)</th>
<th>SMF-28 angle from normal (°)</th>
<th>Measured Maximum Fibre-to-Chip Coupling Efficiency</th>
<th>-1 dB Bandwidth (nm)</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>[1,2]</td>
<td>LPCVD Si$_3$N$_4$ n=2.022</td>
<td>1550</td>
<td>700</td>
<td>8</td>
<td>-3.7 dB (42.7%)</td>
<td>54</td>
<td>For non-linear applications in 700 nm Si$_3$N$_4$</td>
</tr>
<tr>
<td>[3]</td>
<td>PECVD SiN</td>
<td>1550 / 1310</td>
<td>700</td>
<td>8</td>
<td>-6.35 dB (23.2%) / -9.2 dB (12.0%)</td>
<td>~39 / ~31</td>
<td>Unidirectional, single-polarisation dual-band GC</td>
</tr>
<tr>
<td>[4]</td>
<td>PVD SiN, n = 1.980</td>
<td>1550</td>
<td>550</td>
<td>0</td>
<td>-4.9 dB (32%) (simulated)</td>
<td>~1 nm</td>
<td>SiN GC between DBR-pair cavity</td>
</tr>
<tr>
<td>[5]</td>
<td>LPCVD Si$_3$N$_4$ n = 2.0</td>
<td>1550</td>
<td>400</td>
<td>8</td>
<td>-4.2 dB (38.0%)</td>
<td>67</td>
<td>Through-etch Si$_3$N$_4$ GC with 2.25 μm BOX</td>
</tr>
<tr>
<td>[6,7]</td>
<td>LPCVD Si$_3$N$_4$</td>
<td>1550</td>
<td>400</td>
<td>10</td>
<td>-5.4 dB (28.8%)</td>
<td>~18</td>
<td>SiN GC array for multicore optical fibre</td>
</tr>
<tr>
<td>This work</td>
<td>PECVD SiN, n=1.9894</td>
<td>1550</td>
<td>220</td>
<td>9</td>
<td>-2.73 dB (53.3%)</td>
<td>47.9</td>
<td>Through-etched displaced SiN$_x$ bilayer</td>
</tr>
<tr>
<td>[8]</td>
<td>PECVD Si$_3$N$_4$</td>
<td>900</td>
<td>220</td>
<td>8</td>
<td>-5.7 dB (26.9%)</td>
<td>25</td>
<td>Si$_3$N$_4$ GC for NIR</td>
</tr>
<tr>
<td>[9]</td>
<td>LPCVD SiN</td>
<td>850</td>
<td>220</td>
<td>10</td>
<td>-9 (12.6%)</td>
<td>?</td>
<td>SiN$_x$-on-SOI MSM photodetector</td>
</tr>
<tr>
<td>[10,11]</td>
<td>SiN n=1.87</td>
<td>660</td>
<td>100</td>
<td>5</td>
<td>-2.29 dB (59%) / -4.20 dB (38%) (w/o metal reflector)</td>
<td>?</td>
<td>SiN grating couplers with AlCu/TiN reflectors</td>
</tr>
</tbody>
</table>

Designs which required special layer heights [12] or non-CMOS compatible mirror/reflector layers [13], non-standard sources/fibres [14–16], special z-height placement of the fibre [17,18], or low-throughput fabrication techniques like e-beam [13] or focused ion beam (FIB) lithography were truncated from this list.

It has the second highest coupling efficiency (the highest without a reflector [10,11]) and the third broadest -1 dB bandwidth. When we consider the thickness of the SiN$_x$ layer it is coupling to (220 nm), it is in a class of its own. Within the context of the blue performance star, this grating coupler has comparable efficiency and bandwidth to a higher index 220 nm SOI grating coupler, making it a suitable industry workhorse replacement for SiN$_x$-only photonic circuitry.

Additionally, we repeated the design process for a 6 μm BOX layer and measured an experimental efficiency of -2.73 dB (53.3%) and a -1 dB bandwidth of 54.1 nm, suggesting that
the general design and design process is adaptable to different BOX thicknesses. Interestingly, the dimensions between both BOX thickness designs are quite comparable.

Table 4.3.1. (2.32 µm BOX) and Table 4.5.1. (6.0 µm BOX) Uniform Bilayer Design’s Dimensions

<table>
<thead>
<tr>
<th></th>
<th>2.32 µm BOX</th>
<th>6.0 µm BOX</th>
</tr>
</thead>
<tbody>
<tr>
<td>Top layer Period (nm)</td>
<td>1121</td>
<td>1119</td>
</tr>
<tr>
<td>Top layer Duty Cycle (L_i/L_b)</td>
<td>0.50719</td>
<td>0.53083</td>
</tr>
<tr>
<td>Bottom layer Period (nm)</td>
<td>1085</td>
<td>1098</td>
</tr>
<tr>
<td>Bottom layer Duty Cycle (L_i/L_b)</td>
<td>0.56469</td>
<td>0.48998</td>
</tr>
<tr>
<td>Bottom layer displacement (nm)</td>
<td>-193</td>
<td>-221</td>
</tr>
</tbody>
</table>

which suggests that replicating these designs on an arbitrary BOX thickness will produce a near-optimal uniform grating coupler, while an optimally maximised design could be quickly obtained by using Lumerical’s particle swarm algorithm near these values.

Chapter 5 covered the design, fabrication and measurement of two designs of high efficiency SiNx-on-SOI grating couplers.

Table 5.0.1. Summary of Simulated & Measured Characteristics of the Two High Efficiency Designs

<table>
<thead>
<tr>
<th></th>
<th>100 nm SOI DBR Design</th>
<th>100 nm SOI Grating Design</th>
</tr>
</thead>
<tbody>
<tr>
<td>Simulated Max. Coupling Efficiency (dB)</td>
<td>-1.924 (64.2%)</td>
<td>-1.345 (73.4%)</td>
</tr>
<tr>
<td>Measured Max. Coupling Efficiency (dB)</td>
<td>-2.213 (60.1%)</td>
<td>-1.672 (68.0%)</td>
</tr>
<tr>
<td>Simulated -1 dB Bandwidth (nm)</td>
<td>58.7</td>
<td>51.3</td>
</tr>
<tr>
<td>Measured -1 dB Bandwidth (nm)</td>
<td>73.1</td>
<td>57.2</td>
</tr>
<tr>
<td>Simulated -3 dB Bandwidth (nm)</td>
<td>80.5</td>
<td>73.2</td>
</tr>
<tr>
<td>Measured -3 dB Bandwidth (nm)</td>
<td>97.3</td>
<td>83.6</td>
</tr>
</tbody>
</table>

The coupling efficiency of the Apodised 100 nm SOI Grating design with Modified Taper exceeds the best zero-change SiNx-on-SOI grating couplers in the literature.

Table 6.2.2. Industry-Compatible SiNx-on-SOI Grating Couplers Designs (Truncated Version of Table 5.2.1)

<table>
<thead>
<tr>
<th>Paper</th>
<th>SiN type</th>
<th>Designed Wave-length (nm)</th>
<th>SOI thickness (µm)</th>
<th>BOX thickness (µm)</th>
<th>SIN waveguiding layer thickness (µm)</th>
<th>SMF-28 angle from normal (°)</th>
<th>Measured Maximum Fibre-to-Chip Coupling</th>
<th>1dB Bandwidth (nm)</th>
<th>Remarks</th>
</tr>
</thead>
</table>

165
166

<table>
<thead>
<tr>
<th>Ref.</th>
<th>Description</th>
<th>n=</th>
<th>Thickness (nm)</th>
<th>Height (nm)</th>
<th>Efficiency (dB)</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>[19,20]</td>
<td>PECVD SiN, n=1.9896</td>
<td>1550</td>
<td>0.220</td>
<td>2.0</td>
<td>600</td>
<td>-8</td>
</tr>
<tr>
<td>[21,22]</td>
<td>LPCVD Si$_3$N$_4$, n=2.0</td>
<td>1550</td>
<td>0.065 / 0.150 / 0.220</td>
<td>2.0</td>
<td>400</td>
<td>21</td>
</tr>
<tr>
<td>This work</td>
<td>PECVD SiN, n=1.9894</td>
<td>1550</td>
<td>0.100 / 0.100 / 0.220</td>
<td>2.0</td>
<td>220</td>
<td>9</td>
</tr>
<tr>
<td>[23]</td>
<td>SiN</td>
<td>1492</td>
<td>0.320</td>
<td>?</td>
<td>320 nm Si</td>
<td>?</td>
</tr>
<tr>
<td>[24,25]</td>
<td>PECVD SiN, n=1.873</td>
<td>1310</td>
<td>0.150 / 0.300 / 0.300</td>
<td>2.0</td>
<td>600</td>
<td>29</td>
</tr>
</tbody>
</table>

Designs which required special layer heights [26–28] were truncated from this list. [23]’s efficiency is ~ -1.35 dB if built on a single SOI substrate, and could rightfully be considered an SOI grating coupler with SiN extended teeth rather than an SiN$_x$-on-SOI grating coupler since it coupled into 320 nm Si instead of SiN$_x$.

Additionally, it couples to the thinnest SiN$_x$ waveguiding layer (220 nm). However, in maximising coupling efficiency, and without having choice of coupling angle unlike [21,22,24,25], the designs have a -1 dB bandwidth between the ranges normally associated with SiN$_x$-on-SOI (60–80 nm) and pure SOI grating couplers (41 nm). Again, we encounter the limitations of balancing the blue performance star.

However, a significant fact about the designs in this thesis is that they are all industry-applicable, constrained not only in mask layers but also in characterisation angles used; and their general design methodologies can be adapted to other industrial applications.

### 6.3 Contributions to the Field of Grating Couplers

Through the design of these grating couplers, several techniques were developed or proven to work:

#### 6.3.1 Method of Apodising Unique E-field Grating Couplers

When designing large coupling length grating couplers, a computationally-efficient method of apodising it is in gradually smaller groups of $2^x$: This produces a grating coupler...
which broadly matches the incoming source, with increasingly finer adjustments which can be
terminated if the anticipated improvement does not justify the computational cost.

This apodisation method also works for input sources with unique profiles (cf. Fig.
3.2.3.1), and so could be applied to applications which require non-Gaussian outputs.

6.3.2 Numerically Solved Etched: Unetched ratios for $\Lambda_y = 600$ nm

The SWG GC designs from Chapter 3 set $\Lambda_y = 600$ nm to comply with the minimum
fabricable dimensions of the foundry-level process, even if this was an unusually large $\Lambda_y$ for
1550 nm SWG devices. It is known that 2$^{nd}$ order EMT does not effectively predict $l_{y, \text{SiO}_2}$ at such
a large $\Lambda_y$. However, 3D FDTD simulations using periodic y-boundary conditions (as in [29–
33]) did not converge on the same solutions as full 3D FDTD simulations with regular PML
boundary conditions. As full 3D FDTD takes into account the finite boundaries of the grating
coupler’s width, its solutions should be more valid. The $l_{y, \text{SiO}_2}$ for several designs from numerous
3D FDTD numerical solutions were compiled into Fig. 3.3.2.1 and the resulting 5$^{th}$ order
polynomial (Eq. 3.6.1(b)) will be a useful design guide—either as a rule of thumb or as an
optimisation starting point—for other SWG devices that must be fabricated in processes with
similar minimum feature size restrictions.

Fig. 3.3.2.1. Equivalent Refractive Index, $n_{eq}$, for $\Lambda_y = 600$ nm for 1550 nm, TE polarised light on a 220 nm SOI substrate,
according to 0$^{th}$ order EMT (red dotted), 2$^{nd}$ order EMT (red line) and full 3D FDTD (black crosses).
\[ l_{y, \text{SiO}_2}(\mu\text{m}) = -0.1176n_{eq}^5 + 1.6176n_{eq}^4 - 8.6722n_{eq}^3 \\
+ 22.596n_{eq}^2 - 28.823n_{eq} + 14.909 \]  

(3.6.1b)

More generally, when designing an SWG device where \( \Lambda_y > \Lambda_{\text{Bragg}} = \lambda/n_{\text{eff}} \), the recommended approach is to use 2nd order EMT to estimate if the extreme \( l_{y, \text{SiO}_2} \)'s are within fabricable limits for a given \( \Lambda_y \); confirm that they are indeed fabricable using 3D FDTD; and then determine the remaining \( l_{y, \text{SiO}_2} \) values of the design.

Unfortunately, higher order EMT is still an active area of research, and there is no straightforward expression of 4th order EMT refractive index for TE polarisation, \( n_{\text{LTE}}^{(4)} \) or if there is consensus on such construal [34–41].

### 6.3.3 Interspersed vs In-line SWG elements

A study was done between in-line and interspersed scattering elements when the \( n_{\text{eff}} \) was suitable to half the \( \Lambda_y \). To the author’s knowledge, this is the first time this has been experimentally measured in SWG grating couplers. Initially, this was done as a method to combat anticipated RIE lag from bigger holes opening up before smaller ones, but this study also applies in cases where one might have to double \( \Lambda_y \) to reach \( n_{\text{eff}} \)'s not otherwise attainable by the minimum fabricable dimensions of a given technology/process.

Comparisons between Table 3.6.1–3 show that an in-line arrangement does not significantly decrease coupling loss, but an interspersed arrangement can increase loss by -1.3 dB.

### 6.3.4 Effect of Scattering Elements Orientation

Scattering element rotation and translation in SWG grating couplers are not explicitly researched in the scientific literature. For the first time their effects were measured. We have shown that:
• For elliptical designs, scattering element rotation and translation increased the 
coupling efficiency by 0.41 dB (9.9%) and the -1 dB area by 12.8%.

• For circular designs, scattering element rotation and translation decreased the 
coupling efficiency by -0.75 dB (-15.9%) but increased the -1 dB area by 28.3%.

Interestingly, ‘Rotated, not Translated’ arrangements increased losses by -0.7 – -0.4 dB, which suggests that ‘not Rotated, Translated’ would have even better efficiency improvements over ‘not Rotated, not Translated’ arrangements.

### 6.3.5 Designing within Zero-Change Parameters

A general design methodology has been established that is capable of producing world-class zero-change grating couplers. Multiple design principles can be explored rapidly in the initial design phase to gauge their efficiencies using fibre-to-chip (instead of chip-to-fibre) optimisation, which obviates modal matching and tilt-based shape modifications. The best designs can then be optimised with nm-scale sweeps and further improved with apodisation and the addition of back-reflectors.

For designs which utilise multiple layers, such as in Chapters 4 and 5, coupling to temporary multi-layer waveguides increased coupling efficiencies by a non-insignificant 5–7% (a strategy not generally used in the literature), though eventually confining power to just one waveguiding layer required further lateral taper and interlayer taper optimisation in 3D space.

### 6.4 Research Limitations and Future Directions

The three types of grating couplers were designed for manual measurements on an optical bench. However, measuring the subtle differences in performance depending on the SWG sub-types (as in Chapter 3) or the effects of taper modification (as in Chapter 5) necessitated the use of a semi-automated In-circuit tester with a different fiber end (8° polish and 8° tilt).
Similar industry-compatible designs can be carried out for 1310 nm, with designs for manual optical benching (nominal 9° tilt, cleaved SMF-28), and semi-automated optical benching (8° tilt, 8° polished SMF-28).

The rectangular HPF design was the best performing lateral layout for $\Lambda_y = 600$ nm. Further research could be undertaken to find compromises between lateral misalignment tolerances and coupling efficiencies. Improvement in the taper design would help to reduce its footprint and make it more useful as a process-monitoring grating coupler.

Additionally, it is known that a smaller $\Lambda_y$ will improve efficiency as the material is more homogenous. Experiments could be carried out to compare in-line arrangements of scattering elements with mixed values of $\Lambda_y$. Some practical design rules might then be extrapolated on using mixed $\Lambda_y$ values to accommodate minimum fabricable dimensions in a given process/fab.

If designing a HPF grating coupler for wafer-to-wafer bonding applications, the incoming source’s tilt might be changed to vertical, and the optimum planewave length adjusted to compromise coupling efficiency and x-misalignment tolerance. y-misalignment tolerance could also be explored through specialised or multiple tapers which utilise multi-modal interference [42,43].

At $\Lambda_y = 600$ nm, curved designs generally performed ~ -2 dB (36.9%) poorer than their rectangular counterparts, but in small $\Lambda_y$ designs (usually requiring high resolution e-beam / focused ion beam lithography) this penalty is minimised, and the ~0.4 dB improvement from scattering element orientation becomes more significant. Thus, further research could be undertaken to measure these effects. In addition to what has been summarised in Section 6.3.4, combinations of a third ‘skew’ transformation could be compared, and the effect of all these arrangements compared to rotation- and skew-invariant circular scattering elements.
Fig. 4.3.4(b) shows that the Si\textsubscript{N\textsubscript{x}}-only grating couplers had a significant portion of their upward radiated field beyond the 5.2 µm-radius Gaussian, indicating that the through-etched SiNx bilayers did not provide a strong enough scattering strength. The addition of a back-reflector would reflect the outward travelling wave backwards through the first ten or so periods again and therefore increase the coupling efficiency. However, as we have seen in Chapter 5, such back reflectors would also introduce Fabry-Perot reflections which may not be desirable in the applications the Si\textsubscript{N\textsubscript{x}}-only grating couplers would be used for.

In Chapter 5, further research could be undertaken to improve efficiency: varying grating arc angles of 25–60° GC angle [44,45]; lateral taper designs, either in the form of even more multi-stage lateral tapers or sinusoidal [46,47]/multi-mode interference [48] designs; variations in minimum grating order.

6.5 Chapter Bibliography


