Silica High-Mesa Waveguide for Compact Infrared Sensing System

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Acknowledgement
Abstract

The demand for a compact health-check system that can perform routine health-care checks has increased recently. Among many diagnostics methods, breath-content analysis is one of the candidates for daily health-care, as it contains various disease-markers and is non-invasive to human-beings. One of the attractive tools for breath-content analysis is infrared spectroscopy owing to its superior capability in ppm-order sensitivity of various kinds of breath contents. To build a compact breath-sensing system, the gas cell is one of the significantly challenging components to be realized, since the length of a regular gas cell reaches a meter-long optical path length. The compact breath-sensing system that utilizes photonic integrated circuits, such as hollow structure, slot structure, with infrared spectroscopy has been widely researched considering the capability of realizing a small radius of curvature, which is helpful for integrating meter-long optical path length into a compact area. High-mesa waveguide is attractive for its potential of being utilized for infrared absorption, where the evanescent field comes out of its solid core and profiles an optical portion out of the solid waveguide. One critical issue is its propagation loss which limits the sensing capability. In this research, to get lower propagation loss, we proposed silica high-mesa waveguide and extremely low loss of 0.02 dB/cm has been achieved. One of the issues for silica structure lies in its low portion of the optical field-profile out of the waveguide. To get rid of this problem, we have proposed multiple slot silica
high-mesa waveguide. For a quadruple slot silica high-mesa waveguide, a high portion of optical field profiles out of the waveguide of 20.3% has been achieved, and a low scattering loss of 0.06 dB/cm has been confirmed theoretically as well.

In this thesis, the research background and the purpose have been explained in Chapter 1. Breath content detection for easy medical health check-up has been proposed using infrared absorption sensing. Optical waveguide structure for infrared absorption sensing has been proposed and exploited. The estimated required propagation loss criteria have been clarified as well.

In chapter 2, the propagation loss category has been discussed. The propagation loss can be generally attributed to three different mechanisms: scattering losses, radiation losses and absorption losses. For further classification, the scattering losses can be divided into volume scattering and surface scattering; radiation losses can be divided into radiation towards the substrate and the radiation from the waveguide bent; absorption losses can be divided into interband absorption and intraband absorption. Some methods to get low propagation loss have also been discussed in this chapter as well.

In chapter 3, to realize lower propagation loss, silica high-mesa structure is proposed for infrared sensing. Setting under cladding height larger than 5 μm is proposed to suppress the radiation loss. As a result, an extremely low propagation loss of 0.02 dB/cm (@ w = 2.3 μm, λ = 1550 nm) has been achieved.
In chapter 4, the multiple-slot silica high-mesa waveguide structure is proposed. A high portion of 20.3% optical field profiles out of the waveguide has been achieved by quadruple silica high-mesa waveguide structure. Low scattering loss of 0.06 dB/cm has been confirmed theoretically as well.

In Chapter 5, the above results have been summarized and the future view of the proposed waveguide structure has been clarified.
Chapter 1 Introduction

1.1 Background: ageing issue

Population aging was one of the most significant issues of the twentieth century and will surely remain important throughout the twenty-first century\(^1\). The number of elder (age 60 or over) people has been growing at an unprecedented rate. According to official statistics, in 2006 there were 688 million people in the world of aged 60 or over\(^2\). As shown in Fig. 1.1, this number has become 759 million by the end of the year 2010. This age group (60 or over) is now identified as senior citizens. This number is predicted to reach 2 billion at the end of 2050\(^2,3\) as shown in Fig. 1.1. Meanwhile, Fig. 1.1 also predicts that the population of senior citizens will outnumber the population of teenagers who are aged below 14 for the first time in human histories at the year 2050.

One of the consequences of a population aging is its effect on medical care, besides the difficulties it creates for the financing of pension programs. Compare with younger people, older people needs much more medical care\(^1\). Thus, health monitoring for older people will become one of the serious issues for the society in the coming decades. There are a lot of regular health-monitoring methods, such as blood\(^4\), urine\(^5\), cough\(^6\) and other tests, which helps us to identify a disorder or disease. And there are a lot of techniques to identify the presence of microorganism inside the body, like ultrasound\(^7\), magnetic resonance imaging\(^7\), eco-cardiogram\(^8\), and others. These methods
are, however, either expensive or time consuming, and not suitable in routine monitoring mechanism. Moreover, all those methods require professional support to identify a disease. On the other hand, breath content detection, which is detected from the exhaled breath, incurs less stress to human body to collect, and it is real time, and contains massive information of human body 9). Present research on breath-content shows that the contents in the exhaled breath indicate the presence of micro-organism inside the human body or indicate the disorder or infection of any organ inside the body.

We are working on compact breath sensing system that can be integrated on cell phone or other mobile equipment, which makes routine health monitoring much cheaper and easier for senior citizens. What is more, the health condition of senior citizens can be monitored real time.

![World population aging situation and the degree of aging. The projected number is given until 2050.](image)
1.2 Breath sensing: state of the art

Figure 1.2 shows the main content portion in exhaled breath. As shown in the figure, in human breath, 99% are consisted of nitrogen, oxygen and carbon dioxide, and 1% is consisted of a number of volatile organic compounds (VOCs). It is well known that the VOCs found in breath are predominantly exhaled via the blood/breath interface in the lung, which is connected to all of the organs in body.

During 1980s researchers have proved the presence of Helicobacter Pylori inside the stomach by measuring the augmentation of carbon dioxide (CO₂) at the exhaled breath. Helicobacter pylori are micro-aerophilic bacterium,
which are responsible for gastritis, stomach and duodenum cancer. To detect
the presence of the helicobacter pylori inside the stomach, use of “urea breath
test” became popular \(^{10}\). The researchers have detected helicobacter pylori
inside the stomach of human being by using scintillation \(^{11}\) or by using isotope
ratio mass spectrometry \(^{12}\) or by mass correlation spectrometry \(^{13}\) of CO\(_2\). All
these three processes measure the presence of CO\(_2\) in exhaled breath. This
result inspires the researchers to diagnose diseases from the exhaled breath.
Besides “urea breath test”, breath content for other molecules detection and
sensing is now receiving considerable attention by the researchers \(^9\,14-19\), since
breath contents are the disease markers of various diseases \(^9\). Breath contents
that are present in exhaled breath and the disease names that they indicate
are given in table 1.1.

**Table 1.1**: Breath contents with their orders in exhaled breath and the name of
their indicative diseases. (Breath contents can be used to identify disease.)

<table>
<thead>
<tr>
<th>Name of the molecule</th>
<th>Concentration in exhaled breath</th>
<th>Name of the disease</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH(_4) (Methane)</td>
<td>2-10 ppm</td>
<td>Burger disease</td>
<td>[20]</td>
</tr>
<tr>
<td>C(_2)H(_6) (Ethane)</td>
<td>10 ppb</td>
<td>Rheumatic fever, Diabetes mellitus, Chronic obstructive pulmonary disease</td>
<td>[14],  [15]</td>
</tr>
<tr>
<td>C(_5)H(_12) (Pentane)</td>
<td>0-10 ppm</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CO (Carbon monoxide)</td>
<td>1-10 ppm</td>
<td>Lung disease</td>
<td>[9]</td>
</tr>
<tr>
<td>NO (Nitric Oxide)</td>
<td>10-50 ppb</td>
<td>Allergy of trachea system</td>
<td>[21]</td>
</tr>
<tr>
<td>NH(_3) (Ammonia)</td>
<td>0-1 ppm</td>
<td>Kidney and renal failure</td>
<td>[22]</td>
</tr>
<tr>
<td>COS (Carbonyl Sulphide)</td>
<td>0-10 ppb</td>
<td>Lung transfer with acute rejection</td>
<td>[9]</td>
</tr>
<tr>
<td>C(_5)H(_8) (Isoprene)</td>
<td>50-200 ppb</td>
<td>Cholesterol biosynthesis</td>
<td>[23]</td>
</tr>
<tr>
<td>CH(_3)COCH(_3) (Acetone)</td>
<td>0-1 ppm</td>
<td></td>
<td>[14]</td>
</tr>
</tbody>
</table>
As shown in Tab. 1.1, a number of marker molecules have been identified in breath that could be utilized to identify disease. Breath analysis has been widely researched for disease diagnosis or for monitor therapeutic intervention. As shown in the table, however, the concentration of marker molecules is as low as ppb or ppm order. Thus, to detect breath contents, a very high sensitivity is needed. Gas Chromatography and Mass Spectrometry \(^{24}\), which are very precise, have been widely used in modern medical science. But those two methods both take a long time to diagnosis. One of the solutions for high sensitivity and real time is infrared absorption. It is well known that different gases have their unique absorption wavelength and the gas concentration can be deduced through their absorption cross sections through Beer-Lambert law \(^{25}\), which are shown in Tab. 1.2. High sensitivity is available in infrared sensing as long as the optical path is long enough. Actually, the infrared absorption for breath sensing has been widely studied as shown in Tab. 1.3 and a lot of commercial products have been developed as shown in Tab. 1.4. But the size of the instruments are too large for daily use, this study is focus on compact breath sensing system that can be integrated on cell phone or mobile systems finally.
Table 1.2: Breath contents with their absorption wavelength and absorption cross section. (Different gases can be identified by their unique absorption wavelength.)

<table>
<thead>
<tr>
<th>Breath content</th>
<th>Absorption wavelength [μm]</th>
<th>Absorption cross section [cm²]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nitric oxide</td>
<td>NO</td>
<td>5.26</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2.67</td>
</tr>
<tr>
<td>Carbon monoxide</td>
<td>CO</td>
<td>4.6</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2.33</td>
</tr>
<tr>
<td>Ammonia</td>
<td>NH₃</td>
<td>6.15</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3.00</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.51</td>
</tr>
<tr>
<td>Acetone</td>
<td>CH₃COCH₃</td>
<td>2.12</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.69</td>
</tr>
<tr>
<td>Methane</td>
<td>CH₄</td>
<td>3.24</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.651</td>
</tr>
<tr>
<td>Ethane</td>
<td>C₂H₆</td>
<td>3.35</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.7</td>
</tr>
<tr>
<td>Carbon dioxide</td>
<td>CO₂</td>
<td>1.572</td>
</tr>
</tbody>
</table>

Table 1.3: Breath contents analysis reports.

<table>
<thead>
<tr>
<th>Publication year</th>
<th>Name of the institution</th>
<th>Gas type</th>
<th>Worked done</th>
<th>Ref</th>
</tr>
</thead>
<tbody>
<tr>
<td>2003</td>
<td>University of Dusseldorf, Germany</td>
<td>C₂H₆, CO₂</td>
<td>Real time detection</td>
<td>[15]</td>
</tr>
<tr>
<td>2007</td>
<td>Ekips Technologies, USA</td>
<td>CO₂, NO, N₂O</td>
<td>Breath test Infrared sensing</td>
<td>[16]</td>
</tr>
<tr>
<td>2007</td>
<td>Physical Sciences, UK</td>
<td>CO₂</td>
<td>Breath test Infrared sensing</td>
<td>[17]</td>
</tr>
<tr>
<td>2008</td>
<td>Mississippi State University, USA</td>
<td>CH₃COCH₃</td>
<td>Breath test CRDS</td>
<td>[18]</td>
</tr>
<tr>
<td>2009</td>
<td>Physical Sciences, UK</td>
<td>C₂H₆</td>
<td>Breath test ppm order</td>
<td>[19]</td>
</tr>
</tbody>
</table>

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1.3 Sensing waveguide: State of the art

As discussed in section 1.2, breath-contents like carbon monoxide (CO- for lung disease), ammonia (NH₃- for urinary tract infection), and other molecules are the disease-markers \(^9, ^{15}, ^{20-22}\) of various diseases. To detect optical absorption of these molecules \(^{15}\), propagation mode effective index \(^{30}\), extinction of evanescent field \(^{32}\), and other sensing techniques with directional couplers \(^{34-35}\), Mach-Zehnder interferometers \(^{34, 36}\), Bragg gratings \(^{35, 37}\), micro ring resonators \(^{32, 35, 38}\) and other waveguide structures have been exploited. The sensing technique, waveguide structure and the detected substance are shown in table 1.5.
Table 1.5: Reports on waveguide structure and detected substance

<table>
<thead>
<tr>
<th></th>
<th>Detected substance</th>
<th>Main component structure</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Methyl mercaptan (MM: CH3SH)</td>
<td>Optical fiber</td>
<td>[39]</td>
</tr>
<tr>
<td>2</td>
<td>Nano particle detection</td>
<td>Nano cavity</td>
<td>[40]</td>
</tr>
<tr>
<td>3</td>
<td>H₂ Hydrogen</td>
<td>Fabry perot micro cavity</td>
<td>[41]</td>
</tr>
<tr>
<td>4</td>
<td>Acetone, ethanol, dichloromethane</td>
<td>Bragg grating</td>
<td>[42]</td>
</tr>
<tr>
<td>5</td>
<td>Isopropanol, water, cyclohexane</td>
<td>Micro ring resonator</td>
<td>[43]</td>
</tr>
<tr>
<td>6</td>
<td>De-ionized water</td>
<td>Mach-Zehnder interferometer</td>
<td>[33]</td>
</tr>
<tr>
<td>7</td>
<td>Ethanol</td>
<td>High-mesa waveguide</td>
<td>[44]</td>
</tr>
</tbody>
</table>

Fig. 1.3: Schematic of slot waveguide structure. (a) Schematic of cross section, (b) schematic of propagation direction. The light propagates in the slot region (nanometre order) between two cores.

Fig. 1.4: Schematic of hollow waveguide structure. (a) Schematic of cross section, (b) schematic of propagation direction. The light propagates in the core which is made of air.
Unlike those complex structures (like micro ring resonator or Bragg grating), optical waveguide structures have been proposed for optical absorption sensing, such as slot, hollow, and high-mesa structures as shown in Fig. 1.3, Fig. 1.4, and Fig. 1.5, owing to the evanescent field comes out of the waveguide (solid material) and a certain portion of light profiles out of the waveguide, which can be used for breath sensing. The portion of light profiles out of the waveguide is defined as $\Gamma_{\text{air}}$.

Moreover, for optical absorption sensing in ppm order, meter long or even longer optical path is needed. For example, conventional cavity ring-down spectroscopy systems, which is a well-known technique to realize high sensitivity, usually has kilometre long optical path inside the cavity for optical absorption sensing. This system is, however, not handy, it does not measure in real time, and it is costly. To realize a long optical path in a compact area for
optical absorption sensing device, a gas-cell utilizing an optical waveguide is attractive due to the possibility of long optical path integration in a limited area. We propose optical waveguides based on semi-conductor material to realize an optical waveguide that is able to incorporate meter long or even longer optical path in a limited area. An optical waveguide, which has a small (< 10 µm) radius of curvature helps to realize a meter long or even longer optical path in a compact area. Concept of integrated waveguide in a limited area is shown in Fig. 1.6.

![Concept of integrated waveguide in a limited area.](image)

**Fig. 1.6:** Concept of integrated waveguide in a limited area. (Small radius of curvature helps to integrate a long optical path in a compact area.)

### 1.4 Loss in the waveguide: state of the art

One of the most important characteristics of a waveguide for infrared sensing is the attenuation, or loss. This loss is generally attributed to three difference mechanisms: scattering, radiation and absorption. Scattering loss is usually
 predominates in glass or dielectric waveguides, while radiation loss becomes significant when waveguides are bent through a curve. Table 1.6 shows the current research outcomes about propagation loss on optical waveguide for different structures and materials.

**Table 1.6:** Waveguide propagation loss for different structures and materials. (Extremely low loss has been realized by Si3N4 and silica structures which is promising for infrared sensing.)

<table>
<thead>
<tr>
<th>Structure</th>
<th>Material</th>
<th>Loss [dB/cm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Berried</td>
<td>Si</td>
<td>0.3</td>
</tr>
<tr>
<td>High-mesa</td>
<td>Si</td>
<td>0.3</td>
</tr>
<tr>
<td>Strip</td>
<td>Si</td>
<td>2 ± 1</td>
</tr>
<tr>
<td>Slot</td>
<td>Si</td>
<td>6.5 ± 0.2</td>
</tr>
<tr>
<td>Hollow</td>
<td>Si</td>
<td>0.00006</td>
</tr>
<tr>
<td></td>
<td>Metal</td>
<td>0.05</td>
</tr>
<tr>
<td></td>
<td>As2S3</td>
<td>0.05</td>
</tr>
<tr>
<td></td>
<td>Si3N4</td>
<td>0.007</td>
</tr>
<tr>
<td></td>
<td>Silica</td>
<td>0.001</td>
</tr>
</tbody>
</table>

Currently, optical waveguide has been widely used in optical communication, especially the berried structures due to simplicity itself and low cost. For infrared absorption, low propagation loss is very important because high propagation loss consumes light power which degrades sensing capability. Si-based optical waveguide has been widely reported owning to low cost, mature fabrication technology and low absorption loss at the communication wavelength as shown in Tab. 1.6. But Si3N4 or silica structure is also very promising because extremely low loss has been reported for them.
1.5 High-mesa waveguide: state of the art

For optical absorption sensing, we need optical power portion out of the solid waveguide for the molecules to interact with the optical power. “High-mesa” structure has been proposed \cite{44,55-56} for optical absorption sensing. High-mesa structure has been realized by using SOI (silicon on insulator) wafer, where Si core has been sandwiched by SiO\textsubscript{2} both on the top and at the bottom. Silica high-mesa waveguide has also been proposed for its low propagation loss possibility. Table 1.7 shows the concurrent research on high-mesa waveguide.

**Table 1.7:** Concurrent research on High-mesa waveguide (The lowest propagation loss has been realized by silica high-mesa waveguide.)

<table>
<thead>
<tr>
<th>No.</th>
<th>Optical power portion in air, ( \Gamma_{\text{air}} ) (%)</th>
<th>Propagation loss (dB/cm)</th>
<th>Material Used</th>
<th>Etching process used</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Not mentioned</td>
<td>0.3 (waveguide width 2.5 ( \mu )m)</td>
<td>SOI wafer</td>
<td>Neutral loop discharge plasma and Reactive ion etching</td>
<td>[44]</td>
</tr>
<tr>
<td>2</td>
<td>Not mentioned</td>
<td>0.3 (waveguide width 2.5 ( \mu )m)</td>
<td>SOI wafer</td>
<td>Neutral loop discharge plasma etching</td>
<td>[55]</td>
</tr>
<tr>
<td>3</td>
<td>19 % (waveguide width 0.7 ( \mu )m)</td>
<td>0.3 (waveguide width 2.5 ( \mu )m)</td>
<td>SOI wafer</td>
<td>Neutral loop discharge plasma etching</td>
<td>[56]</td>
</tr>
<tr>
<td>4</td>
<td>2.3 % (waveguide width 2.3 ( \mu )m)</td>
<td>0.02 (waveguide width 2.3 ( \mu )m)</td>
<td>Reactive ion etching</td>
<td></td>
<td>[66]</td>
</tr>
</tbody>
</table>

As shown in Tab. 1.7, propagation loss of 0.3 dB/cm \cite{44,55-56} (@ w = 2.5 \( \mu \)m) has been achieved for Si based high-mesa waveguide. Relatively low propagation loss of 0.9 dB/cm \cite{57} (@ w = 800 nm, \( \Gamma_{\text{air}} \) = 57\%, TE mode) has been realized by
SOI high-mesa waveguide in our lab. What is more, extremely low propagation loss of 0.02 dB/cm \(^{66}\) (@\(w = 2.3 \, \mu m\), \(\lambda = 1550 \, nm\), \(\Gamma_{air} = 57\%\), TE-mode) has been achieved successfully by silica single high-mesa waveguide. Moreover, low bending loss (0.05 dB/90° @ \(w = 2.3 \, \mu m\), \(\lambda = 1550 \, nm\) and TE-mode) with small radius (30 \(\mu m\)) of curvature in bent structure has been calculated \(^{57}\).

We have also proposed a quadruple slot-waveguide structure by using two parallel single high-mesa structures. Using simulation higher (20.3%) optical portion inside the void slot compare with the single high-mesa waveguide has been confirmed. Moreover, low scattering loss of 0.06 dB/cm \(^{67}\) has been predicted theoretically as well.

## 1.6 Estimated required propagation loss criteria

Here we estimate the allowable maximum propagation loss, theoretically, in this part. To estimate the allowable maximum waveguide propagation loss, we assume the following conditions;

1. CRDS (cavity ring-down spectroscopy) \(^{59-61}\) system, that is well-known technique to realize high sensitivity, is utilized.

2. Only one ring-down number difference is detectable (minimum criterion).

Figure 1.7 (a) and (b) show the schematic explanation of ring-down number difference in a conventional CRDS system (a) without gas absorption, (b) with gas absorption. As is shown in the figure, the gas concentration is determined by ring-down time difference (\(\Delta \tau\)) between
the ring-down time of $\tau_{\text{air}}$ (without gas absorption) and $\tau_{\text{gas}}$ (with gas absorption). The ring-down time ($\tau$) is the time that the light intensity falls to $1/e$ of the initial intensity ($I_1$ or $I_1'$); and the pulse number during $\tau$ is called ring-down number, as is shown in Fig. 1.7. The ring-down number difference is the number of pulses during the ring-down time difference ($\Delta \tau$).

**Fig. 1.7:** Schematic of ring-down number difference in a conventional CRDS system. (a) Without gas absorption. (b) With gas absorption. (The gas concentration can be deduced by the ring-down number difference between (a) and (b).)
Target gas is 10 ppm methane (absorption cross section $\sigma = 1.64 \times 10^{-20}$ cm$^2$), which is the same concentration in human breath in case of gut bacterial.

To realize compact system, the gas cavity and the mirrors in conventional CRDS system have been replaced by optical waveguide and coupler, which are integrated on one chip, respectively, as is shown in Fig. 1.8. Here we use 9:1 coupler for example, as is shown in the figure, for each round trip, there is 90% light power goes back to the circle and 10% goes to the detector through the coupler, which means the coupler is an equivalent mirror of which the reflection corresponds to $R = 90\%$.

**Fig. 1.8:** Schematic of compact CRDS system. (All the devices will be integrated on one chip finally.)
(5) Optical amplifier is integrated on one chip with waveguide to compensate the propagation loss. To facilitate the calculation, we assumed complete population inversion for the amplifier, where the noise figure \( NF \approx 3\text{dB} \).

(6) \( \Gamma_{\text{air}} \) (portion of optical field out of the waveguide, which affects the sensitivity) is set to be 80\% \cite{57}. The effective path length of the waveguide is defined as \( L_{\text{eff}} = \Gamma_{\text{air}} \times L \), where \( L \) is the waveguide length which is used for gas absorption (indicated as equivalent gas cell in Fig. 1.8).

Using the assumption above, the output intensity of the 1\textsuperscript{st} pulse, namely, the output light intensity after the 1\textsuperscript{st} round trip, which is seemed as \( I_1 \) and \( I'_1 \) in Fig. 1.7 (a) and (b), respectively, can be deduced through the definition of the system propagation loss and the Lambert-Beer Law \cite{25} as follow:

\[
I_1 = I_0(1 - R)e^{(-\alpha_w L + \alpha_G)}(1 + e^{-\alpha_N}) \quad \text{Without gas} \quad (1.1)
\]

\[
I'_1 = I_0(1 - R)e^{-\sigma n \Gamma_{\text{air}} L}e^{(-\alpha_w L + \alpha_G)}(1 + e^{-\alpha_N}) \quad \text{With gas} \quad (1.2)
\]

Here \( I_1 \) (without gas absorption) and \( I'_1 \) (with gas absorption) are the output light intensity after the first round trip (the 1\textsuperscript{st} pulse), \( I_0 \) is the input intensity, \( \alpha_w \) is the waveguide propagation loss, \( L \) is the waveguide length, \( \alpha_G \) is the gain of amplifier, \( \alpha_N \) is the amplifier noise, \( \sigma \) is the gas absorption cross section, \( n \) is the gas concentration, and the \( \Gamma_{\text{air}} \) is the optical field out of the waveguide.

Repeating the calculation above for each round trip of light, the intensity of the \( N \)\textsuperscript{th} and the \( M \)\textsuperscript{th} pulse, shown in the Fig. 1.7, can be expressed as follow:

\[
I_N = I_0(1 - R)^N e^{N(-\alpha_w L + \alpha_G)}(1 + e^{-\alpha_N})^N \quad \text{Without gas} \quad (1.3)
\]
Here \( I_N \) and \( I_M \) is the intensity of the \( N^{th} \) (without gas absorption) and the \( M^{th} \) (with gas absorption) pulse. For both cases of without gas absorption and with gas absorption, when the parameters of \( L, \alpha_G, \alpha_N, \sigma \) and \( \Gamma_{air} \) are known, the waveguide propagation loss (\( \alpha_w \)) and the output intensity of each pulse \( (I_N & I_M) \) form an equation which can be solved numerically. Comparing the intensity of each pulse to the 1\(^{st} \) pulse, the ring-down number, which is the pulse number when the output intensity falls to \( I_1 \times 1/e \) and \( I_1' \times 1/e \), is obtainable. Then the ring-down number difference is available for different propagation loss. Next we discuss about how to determine \( L, \alpha_G \) and \( \alpha_N \).

It is well known that the amplifier noise is amplified as well in the each round trip \(^{68}\), which means the ring-down number should be limited in a range that the signal is not affected by the noise. Since about 200-times amplification has been reported \(^{69}\) under the condition that the loss between each amplifier is -12.6 dB and the gain for each amplifier is 13 dB \(^{70}\). Thus, for the calculation result, a ring-down number that less than 200-times is reasonable as long as the whole loss for each round trip is less than -13 dB. On the other hand, the absorption of gas is relatively low, thus it is also necessary to make sure that the gas absorption should not be affected by the noise, either. Namely, the intensity of gas absorption should always higher than that of noise for each round trip before achieving enough ring-down number for gas detection. As to \( L \), since the gain of the amplifier is limited, to get maximum allowable propagation loss, the \( L \) should be as short as possible, but too short.
leads to less gas absorption for each round trip which may cause the noise be higher than the gas absorption before achieving enough ring-down number. Thus during the calculation, adjust the amplifier gain and the waveguide length to determine the maximum allowable propagation loss that meet the conditions above, which are ring-down number less than 200-times; gas absorption higher than the noise; as short as possible $L$. The pulse intensity of $I_1$ and $I_1'$ can be deduced through Eq. (1.1) and (1.2), then the pulse intensity of $I_2 \ldots I_N$ and $I_2' \ldots I_M$ can be deduced through Eq. (1.3) and (1.4), the ring-down number ($N$ & $M$) is decided under the conditions of $I_N \geq I_1 \times 1/e > I_{N+1}$ and $I_M \geq I_1' \times 1/e > I_{M+1}$. Here we set the waveguide length is $L = 50$ cm, the maximum waveguide propagation loss should be about 0.2 dB/cm (the maximum waveguide loss is about -10 dB), since the amplifier gain should not be higher than 13 dB. The losses of the whole system are the waveguide loss and the coupler loss (mirror loss). When the waveguide propagation loss is set as 0.2 dB/cm, the waveguide loss is -10 dB. As to the coupler loss, as mentioned above, a 9:1 coupler has been taken as an example, this means when the light goes through the coupler, there is 90% light power goes back to the circle and 10% goes to the PD, as shown in Fig. 1.9. Namely, there is 10% light loss for each round trip due to the coupler, this 10% light corresponds to about -0.5 dB loss. Thus the whole system loss is about -10.5 dB. The gain was set as 10.2 dB (the noise has been estimated by the gain and the NF), the gain has been set a little lower than the whole system loss to prevent the oscillation in the system, thus here the gain has been set 0.3 dB lower than the whole system loss; and then the calculated ring-down number.
difference is 0, which means a lower propagation loss is necessary. Then when the waveguide loss is set as 0.05 dB/cm, the system loss is about -3 dB, when the gain was set as 2.98 dB (a little lower than the system loss to prevent the oscillation as mentioned above), the ring-down number difference is 8, which indicates a detectable case. This means the maximum allowable waveguide propagation loss is between 0.05 dB/cm and 0.2 dB/cm. Based on the calculation above, the ring-down number difference as a function of the waveguide propagation loss is shown in Fig. 1.9. Figure 1.9 exhibits that when the waveguide propagation loss is 0.09 dB/cm, the amplifier gain was set as $\alpha_G = 4.9$ dB, then the ring-down number difference is 1 (ring-down number N = 74, M = 73), which indicates a detectable case. As is shown in the figure, the ring-down number exceeds 2 when the waveguide propagation loss becomes less than 0.09 dB/cm that corresponds to the maximum allowable waveguide propagation loss.

![Graph](image)

**Fig. 1.9:** Ring-down number difference as a function of waveguide propagation loss. (0.09 dB/cm corresponds to the maximum allowable waveguide propagation loss.)
1.7 Outline of this thesis

Breath sensing realizes painless (unlike, blood and other tests) health check system and breath-content has been detected by using infrared absorption spectroscopy, which requires relatively long optical path (meter-long). To realize a long optical path in a compact area for optical absorption sensing device, a gas-cell, utilizing an optical waveguide is attractive due to the possibility of long optical path integration in a limited area. High-mesa optical waveguide structure has been proposed for optical absorption sensing, as a certain portion of optical field profiles out of the waveguide that is utilized for optical absorption. One of the problems for high-mesa waveguide is its propagation loss since high propagation loss consumes light power which restricts sensing capability. To achieve low propagation loss, silica based high-mesa structure has been studied and low propagation loss of 0.02 dB/cm (@ w = 2.3 μm, λ = 1550 nm) has been confirmed successfully. Further improvement of the proposed silica single high-mesa waveguide structure with a novel design theory of slot waveguide with quadruple high-mesa structure has also been discussed.

In this thesis, the research background and the purpose have been explained in Chapter 1. Breath content detection for easy medical health check-up has been proposed using infrared absorption sensing. Optical waveguide structure for infrared absorption sensing has been proposed and exploited. The estimated required propagation loss criteria have been clarified as well.
In chapter 2, the propagation loss category has been discussed. The propagation loss can be generally attributed to three different mechanisms: scattering losses, radiation losses and absorption losses. For further classification, the scattering losses can be divided into volume scattering and surface scattering; radiation losses can be divided into radiation towards the substrate and the radiation from the waveguide bent; absorption losses can be divided into interband absorption and intaband absorption. Some methods to get low propagation loss have also been discussed in this chapter as well.

In chapter 3, to realize lower propagation loss than SOI structure, silica high-mesa structure is proposed for infrared sensing. Setting under cladding height larger than 5 μm is proposed to suppress the radiation loss. As a result, an extremely low propagation loss of 0.02 dB/cm (@ w = 2.3 μm, λ = 1550 nm) has been achieved.

In chapter 4, the multiple-slot silica high-mesa waveguide structure is proposed. A high portion of 20.3% optical field profiles out of the waveguide has been achieved by quadruple silica high-mesa waveguide structure. Low scattering loss of 0.06 dB/cm has been confirmed theoretically as well.

In Chapter 5, the above results have been summarized and clarified about the future view of the proposed waveguide structure.
1.8 References


41. M. A. Vincenti, M. De Sario, V. Petruzzelli, A. D’Orazio, F. Prudenzano, D. de Ceglia, and M. Scalora, “Fabry-Perot microcavity sensor for H2-


Chapter 2 Propagation loss category in optical waveguides and low loss policy

2.1 Introductory overview

As discussed in section 1.3, for optical absorption sensing of a low concentration gas, meter-long or even longer optical path in air is required for sufficient optical absorption \(^1-^5\)\. High-mesa waveguide is attractive for infrared sensing not only owing to its potential of realizing small radius of curvature, which is helpful for integrating the meter-long optical path length into a compact area \(^6\), but also owing to the fact that a certain portion of the optical field profiles out of the solid material depending on the waveguide width \(^7\), which enables propagating light to be exposed towards volatile gas (breath content). For such a long waveguide structure, we need to focus on its propagation loss. Since high propagation loss consumes the light power which restricts the sensing capability. So far, the high-mesa structure has been fabricated using Si/SiO\(_2\) SOI (Silicon on Insulator) wafer and the propagation loss of 0.9 dB/cm (at 1550 nm) \(^8\) has been confirmed. What is more, we also confirmed that the main cause of the propagation loss in SOI structure is scattering loss \(^8\). As we mentioned in chapter 1, to detect ppm order breath content, at least lower than 0.09 dB/cm propagation loss is needed. To get lower propagation loss structure, a clear loss classification is necessary. In this chapter, a component category of propagation loss and some discussions and
descriptions of each kind of loss will be given. Then some methods to get low propagation loss will be discussed later.

As we mentioned, to get low propagation loss structure, it is necessary to clarify what kinds of losses there are in the propagation loss. A brief category of propagation loss is shown in Fig. 2.1. The propagation loss can be generally attributed to three different mechanisms: scattering losses, radiation losses and absorption losses \(^9\). What is more, there are still several types for each mechanism of loss. Fig. 2.1 shows the main types for each mechanism. For example, scattering losses can be divided into volume scattering and surface scattering; radiation losses can be divided into radiation towards the substrate and the radiation from the waveguide bent; absorption losses can be divided into interband absorption and intraband absorption. The details for each mechanism will be introduced in this section.

![Proposition loss category](image)

**Fig. 2.1:** Propagation loss category. (Propagation loss category is necessary for low loss propagation.)
2.2 Absorption loss

As mentioned, the absorption loss can be divided into interband absorption and intraband absorption. In semiconductors the absorption loss is very significant. Interband absorption indicates that a photon of which the energy is greater than the bandgap energy gives up their energy to the electrons on the valence band to raise them to the conduction band. Intraband absorption indicates that the photons give up their energy to the electrons that are already in the conduction band, or to the holes that are already in the valence band to raise them to higher energy. Usually the electrons are raised out of shallow donor states that near the conduction band edge and the holes are excited into the valence band from shallow acceptor states that near the valence band edge \(^9\). The schematic of electrons transition between energy states for both interband absorption and intaband absorption are shown in Fig. 2.2.

![Fig. 2.2: Electron energy transitions during absorption.](image)

Insert photon

Conduction Band

Valence Band

Electrons

Holes

Interband absorption

Intraband absorption

(Free carrier absorption)
Since the absorption losses is not a big problem of silica based waveguide, we only introduce some possible methods to suppress the absorption loss briefly. The interband absorption is avoidable by using a wavelength that is longer than the waveguide absorption edge wavelength $^{10-12}$. The interband absorption can also be reduced by adding additional elements to a binary compound especially to III-V and II-VI compounds to control the bandgap $^{13}$. As to the free carrier absorption, it can be minimized by choosing the ratio of guide thickness to wavelength properly $^{14}$. The express of intraband absorption coefficient $^{15}$ may inspire some other methods to suppress the free carrier absorption loss. N-type compound semiconductors’ intraband absorption has been studied by Fan $^{16}$ as well.

### 2.3 Radiation loss

Optical energy is able to be lost from the propagated modes through radiation, which means the photons are emitted into the media surrounding the waveguide instead of propagating in the waveguide core. Radiation can happen from almost all types of waveguides like planar waveguides and channel waveguides. The radiation loss can be divided into the radiation towards the substrate and the radiation from the waveguide bent. The radiation towards the substrate becomes significant for the higher-order modes of a waveguide $^{17}$. 
2.3.1 Radiation towards the substrate

The radiation towards the substrate is very important in silica based high-mesa waveguide since the refractive index difference of silica high-mesa waveguide is very small and the waveguide substrate is made of silicon as shown later in Fig. 3.1. Thus, a numerical evaluation method of radiation towards the substrate is helpful to suppress the radiation towards the substrate. The radiation towards the substrate can be evaluated by the imaginary part of effective index \(^{18}\), which has been deduced by perfectly matched layer (PML) boundary condition \(^{19-22}\). This method is also discussed in Chap. 3.

2.3.2 Radiation from the bent waveguide

Radiation loss can be significantly increased when propagated waves go through a bend in a waveguide. This is because the occurrence of the optical field distortions \(^9\). The radiation losses from a bent waveguide must be considered since the waveguide bends are necessary parts for all high density integrated circuits. A general image of radiation from the bent waveguide is shown in Fig. 2.3. As shown in Fig. 2.3, a clear optical energy lost can be observed at the bent area which causes the radiation loss. The physical processes involved in the bent radiation are illustrated by Fig. 2.4. This is a convenient way to analyse the radiation loss called velocity approach developed by Marcatili and Miller \(^23\). The mode field at every point in the
**Fig. 2.3:** General image of the radiation from the bent waveguide.

**Fig. 2.4:** (a) Section of a straight waveguide, (b) section of a waveguide bent into an arc of radius $R$. 

Phase planes

Waveguide
cross-section on a straight waveguide propagates parallel to the waveguide axis with the same phase velocity as shown in Fig. 2.4 (a), and the phase planes are orthogonal to the axis. The fields and phase plane, however, rotate about the centre of bend curvature with an angular velocity, if the waveguide is bent into a curve of radius R, as shown in Fig. 2.4 (b). Thus, the phase velocity that parallel to the waveguide axis must increase linearly with distance from the centre of curvature O otherwise the phase plane could not be preserved. There should be a certain radius $R_c$ beyond which the phase velocity would have to exceed the local speed of light in order to preserve the phase plane. This is impossible, thus the fields in the region beyond $R_c$ must become radiative. As discussed in Chap. 3, the radiation from bent waveguide is not significant in our silica based high-mesa waveguide; we do not discuss its numerical evaluation here. But the numerical evaluation methods has been well developed \(^{24}\). Furthermore, the minimum radius of curvature for radiation loss lower than 0.1 dB/cm for several typical dielectric waveguides has been calculated by Goell \(^{25}\).

### 2.4 Scattering losses

As mentioned, the scattering losses in an optical waveguide can be divided into two types: volume scattering and surface scattering. The volume scattering is caused imperfections in the waveguide, such as contaminant atoms, voids and crystalline defects, as shown in Fig. 2.5. The amount of volume scattering loss is in proportion to the number of imperfections. On the other hand, the
amount of volume scattering loss also strongly depends on the ratio of propagate light wavelength and the imperfections’ relative size. In nowadays, as the waveguide fabrication process becoming more and more mature the volume scattering loss is even negligible compared with the surface scattering loss. This is because the size of volume imperfections are very small compared with the light wavelength and the number is so few. So we will focus on surface scattering loss in this section.

Surface scattering loss (we will refer it as scattering loss below) is caused by sidewall roughness at the interfaces between waveguide core and cladding. Figure 2.6 shows the perspective view and the top view of a high-mesa waveguide under study, of which the sidewalls are considered rough. Here, $n_0$ is the refractive index of cladding material (air), $n_1$ is the refractive index of core material, $w$ is the waveguide width and $\sigma$ is the sidewall roughness. As shown in Fig. 2.6, there are some zigzags along the waveguide sidewall, which is called sidewall roughness. In recent years, the miniaturization of planar lightwave circuits (PLC) has been researched a lot. Meantime, since the scattering loss is generally the dominant loss in dielectric film waveguides (e.g. oxides and glasses), the numerical description of scattering loss has been widely studied, starting with the pioneering work by Marcuse. Suematsu and Furuya, and Miyanaga et al have studied the far-field radiation patterns of light scattered by waveguide surface roughness. In
Fig. 2.5: Schematic of volume scattering.

Fig. 2.6: (a) Perspective view of high-mesa waveguide. (b) Top view of high-mesa waveguide, $n_0$ is the refractive index of cladding material (air), $n_1$ is the refractive index of core material, $w$ is the waveguide width and $\sigma$ is the sidewall roughness.
the recent literature, the waveguide scattering loss analysis has most commonly been based on the Payne-Lacey method \(^{39-43}\). The Payne-Lacey method is very convenient because it provides a relatively simple analytical expression for the scattering loss in planar optical waveguides. Using the parameters and the coordinate system in Fig. 2.7, the scattering loss can be expressed following the well-known Payne-Lacey method \(^{39}\) (details is shown Appendix A)

\[
\alpha = \frac{\sigma^2}{\sqrt{2}k_0 \left(\frac{w}{2}\right)^4 n_1} g(V) f(x, \gamma) \tag{2.1}
\]

Here \(w\) is waveguide core width, \(k_0 = \frac{2\pi}{\lambda}\) is the propagation constant in vacuum, \(g(V)\) is a function depending only on the waveguide geometry, \(f(x, \gamma)\) is linked to the sidewall roughness.

\[
g(V) = \frac{U^2V^2}{1 + W} \tag{2.2}
\]

With

\[
U = d \sqrt{n_1^2 k_0^2 - \beta^2} \tag{2.3a}
\]

\[
V = k_0 d \sqrt{n_1^2 - n_0^2} \tag{2.3b}
\]

\[
W = d \sqrt{\beta^2 - n_0^2 k_0^2} \tag{2.3c}
\]

and
\[ f(x, \gamma) = \frac{x}{\sqrt{2\pi}} \int_0^\pi \exp \left\{ -\frac{x^2}{4} \left[ \left( 1 + \frac{\gamma^2}{2} \right)^{\frac{1}{2}} - \frac{\gamma}{\sqrt{2}} \cos \theta \right]^2 \right\} d\theta \] (2.4)

where

\[ x = W \frac{L_c}{d} \] (2.5a)

\[ \gamma = \frac{n_0 V}{n_1 W \sqrt{\Delta}} \] (2.5b)

\[ \Delta = \frac{n_1^2 - n_0^2}{2n_1^2} \] (2.5c)

Using Eq. 2.1, the scattering loss for most of the waveguide can be calculated numerically. All of the scattering loss in this thesis has been evaluated by the method above.

**Fig. 2.7**: Scattering of light through the rough side-wall of a fabricated waveguide (top view). The coordinate system is shown insets.
2.5 Scattering loss mechanism and reduction scheme in high-mesa waveguide

In this section, we discuss the scattering loss mechanism first. Here, we treat the light as a beam. It is well known that when a beam of light is totally internally reflected in the waveguide, the reflected beam is shifted with a certain amount, which is known as Goos-Hänchen shift \(^4^4\). The shift place, where the light touches the sidewall, can be observed in Fig. 2.8. Here, \(s\) is the amount of the shift, \(w\) is the waveguide width, \(w_e\) is called effective guided width \(^2^4\), which corresponds to the width of a region that the optical field is essentially confined into. Every time the light reflects at the sidewall will result in scattering loss. Therefore, to decrease the scattering loss, it is required to restrain this kind of touches. It is obvious that the loss of each touch can be decreased by smoothing the waveguide sidewall, which is difficult through improving the fabrication procedure of waveguide. Therefore, it is necessary to find other ways to decrease the scattering loss.

**Fig. 2.8:** Total internal reflection from a plane interface showing the Goos-Hänchen shift \(s\) (top view), \(w\) is waveguide width, \(w_e\) is effective guided width.
As it is relatively difficult to decrease the loss of each touch by smoothing the waveguide sidewall, we need to find a way to decrease the number of touch. We propose that increasing the effective guided width \( w_e \), is promising to decrease the number of touch. Figure 2.9 shows that when the effective guided width increases from \( w_{e1} \) (black) to \( w_{e2} \) (red) \( (w_{e1} < w_{e2}) \), the numbers of touch decreased from 8 times to 6 times for the given long waveguide. Therefore, increasing the effective guided width is efficient to decrease the scattering loss. The most intuitive way to increase the effective guided width is to increase the waveguide width. However, one of the critical issues remains for sensing application, since the portion of the optical field out of solid material (we define this portion as optical portion out of the waveguide, “\( \Gamma_{air} \)” of waveguide is decreased as increasing the waveguide width \( w_e \). As the higher optical portion out of the waveguide is one of essential properties for infrared absorption, we need to propose a method that is able to make \( \Gamma_{air} \) increase, which means \( \Gamma_{air} \) need to be increased or at least remain constant when increasing the waveguide width. For this purpose, we propose utilizing mid-infrared light, as well as weakly-confinement in the perpendicular direction are both promising methods to make \( \Gamma_{air} \) increase. Namely, scattering loss is expected to be decreased by using mid-infrared light, as well as weakly-confinement in the perpendicular direction. Next we will confirm the proposal above.
In the aforementioned, scattering loss can be decreased by increasing the effective guided width through applying mid-infrared light and weakly-confinement in perpendicular direction. We will show the simulation and theory calculation results to confirm the proposition above. The finite element (FEM) method and analytical model proposed in Sec. 2.4 provided us useful tools.

2.6 Methods and results on scattering loss reduction

In the aforementioned, scattering loss can be decreased by increasing the effective guided width through applying mid-infrared light and weakly-confinement in perpendicular direction. We will show the simulation and theory calculation results to confirm the proposition above. The finite element (FEM) method and analytical model proposed in Sec. 2.4 provided us useful tools.

2.6.1. Wavelength dependency in scattering loss

Figure 2.10 shows the optical field of FEM simulation results for the same waveguide structure for different wavelengths, from which increasing of \( \Gamma_{\text{air}} \) can be confirmed. From Fig. 2.10 we know that the \( \Gamma_{\text{air}} \) of Fig. 2.10 (b) (@ \( \lambda = 3300 \) nm) is higher than that of Fig. 2.10 (a) (@ \( \lambda = 1550 \) nm), obviously. Therefore, for the same \( \Gamma_{\text{air}} \), the waveguide width of utilizing mid-infrared light
is wider than the waveguide width of utilizing near-infrared light. In other words, compare to using near-infrared light, wider effective guided width is available by using mid-infrared light when the $\Gamma_{\text{air}}$ is fixed. Hence, the scattering loss is expected to be decreased by applying mid-infrared light.

![Optical field profiles](image)

**Fig. 2.10**: Optical field profiles. (a) Wavelength $\lambda_1 = 1550$ nm, (b) wavelength $\lambda_2 = 3300$ nm. Here, in both cases width $w$ is 900 nm.

Figure 2.11 shows the wavelength dependency in scattering loss for different $\Gamma_{\text{air}}$. Black solid line, blue dash line and red dash-dot line are $\Gamma_{\text{air}}$ approximately equal to 20%, 40% and 60%, respectively. It can be seen, in Fig. 2.11, that the
scattering loss is decreased as the wavelength increased as we proposed and the scattering loss is not affected by $\Gamma_{\text{air}}$, seriously. Here we choose $\Gamma_{\text{air}}$ approximately equal to 40% \cite{46}. In addition, the strongest absorption peak of methane exists at approximately 3300 nm \cite{47}. Therefore, we use the wavelength of 3300 nm. When $\Gamma_{\text{air}}$ approximately equal to 40%; wavelength $\lambda$ is 3300 nm, the scattering loss turns out to be 0.2 dB/cm.

![Graph showing scattering loss vs. light wavelength](image)

**Fig. 2.11:** Dependency of the scattering loss and light wavelength for different $\Gamma_{\text{air}}$.

### 2.6.2 Core thickness dependency in scattering loss

Figure 2.12 shows the optical field of FEM simulation results for high-mesa waveguide with different core height in perpendicular direction. It is obvious that the $\Gamma_{\text{air}}$ of Fig. 2.12 (b) (@ h = 200 nm) is higher than that of Fig. 2.12 (a) (@ h = 280 nm). Therefore, as explained above, wider effective guided width is also available by applying weakly-confinement in perpendicular direction when
$\Gamma_{\text{air}}$ is fixed. So, the scattering loss is also expected to be decreased by utilizing weakly-confinement in perpendicular direction.

**Fig. 2.12:** Light field profiles. (a) Core thickness 280 nm, (b) core thickness 200 nm. Here, in both cases width $w$ is 900 nm, wavelength $\lambda = 3300$ nm.
Scattering loss as a function of core thickness for different $\Gamma_{\text{air}}$. Optical wavelength $\lambda = 3300$ nm.

**Fig. 2.13:** Scattering loss as a function of core thickness for different $\Gamma_{\text{air}}$. Optical wavelength $\lambda = 3300$ nm.

Scattering loss as a function of core thickness for different $\Gamma_{\text{air}}$ is illustrated in Fig. 2.13. Wavelength $\lambda$ was set to be equal to 3300 nm. Black solid line, blue dash line and red dash-dot line are $\Gamma_{\text{air}}$ approximately equal to 20%, 40% and 60%, respectively. Figure 2.13 exhibits that the scattering loss is decreased as the core thickness decreased as we assumed and $\Gamma_{\text{air}}$ does not affect the scattering loss seriously, either. We also choose $\Gamma_{\text{air}}$ approximately equal to 40% (~46). In addition, since the effective index of the waveguide becomes lower than the refractive index of SiO$_2$ when core thickness $h < 150$ nm, $\Gamma_{\text{air}}$ approximately equal to 40%, there is no propagation mode any more in the waveguide. Therefore, we adopt core thickness $h = 150$ nm. When $\Gamma_{\text{air}}$ is approximately equal to 40%; wavelength $\lambda$ is 3300 nm; core thickness $h$ is 150 nm, the scattering loss decreased to as low as 0.072 dB/cm. From this result,
we could confirm that the scattering loss of SOI high-mesa waveguide can be decreased to the low lever as enough for sensing application.

2.6.3 Effective index dependency in scattering loss

It is well known that the scattering loss could be affected by effective index significantly. Using Eq. (2.1), the scattering loss as a function of effective index is shown in Fig. 2.14. As shown in Fig. 2.14, the scattering loss will be decreased as the effective index decreased and the scattering loss can be decreased significantly only by changing the material from SOI to silica. This is also a promising method for low propagation loss. So in next chapter, we will study the details of using silica for infrared sensing.

![Graph showing scattering loss as a function of effective index](image)

**Fig. 2.14**: Scattering loss as a function of effective index. (The scattering loss can be suppressed a lot by changing the material from SOI to silica.)
2.7 Conclusions

In this chapter we first gave a brief category of propagation loss and some low loss policies for the losses that we are interested in. Since scattering loss is unavoidable for all types of waveguides, the scheme and the numerical evaluation method of scattering loss has been discussed as well. We proposed that applying mid-infrared light and weakly-confinement in perpendicular direction is helpful in decreasing scattering loss. We also confirmed the proposition above, theoretically, by the analytical model suggested by Payne and Lacey. As a result, the scattering loss can be decreased to 0.2 dB/cm (@ $\lambda = 3300$ nm) by applying mid-infrared and further decreased to 0.072 dB/cm (@ $\lambda = 3300$ nm, $h = 150$ nm) by applying weakly-confinement in the perpendicular direction when $\Gamma_{\text{air}}$ approximately equal to 40%. Moreover, we also investigated the relation between the scattering loss and the effective index and found that the scattering loss can be significantly decreased by decreasing the effective index. So we will discuss the possibility of utilizing silica high-mesa waveguide for infrared sensing in next chapter.
2.8 References


47. HITRAN Database: http://www.cfa.harvard.edu/hitran/
Chapter 3 Low loss silica high-mesa waveguide for infrared sensing

3.1 Introductory overview

As mentioned in Sec. 1.3, for breath content sensing by using infrared absorption, the propagation loss must be less than 0.09 dB/cm. On the contrary, as shown in Chap. 2, the lowest propagation loss we got for SOI based high-mesa waveguide was 0.9 dB/cm \(^{1,2}\) (@ SOI base, \(\lambda = 1550\ nm, w = 800\ nm\)). We gave some theoretical methods to suppress the scattering loss for SOI structure in Sec. 2.6.1 and 2.6.2, but those methods have not been confirmed experimentally yet. As mentioned in Sec. 1.4, extremely low propagation for \(\text{Si}_3\text{N}_4\) \(^{3,4}\) or silica \(^{5-8}\) structures had been reported which should be very promising for breath infrared sensing. We also verified that the scattering loss can be suppressed a lot by changing the material from SOI to silica in Sec. 2.6.3, For this reason, we have started to investigate the silica high-mesa waveguide owing to its low propagation loss potential. The fabricated waveguide, however, showed not so low loss (0.65 dB/cm). Thus, we have analysed the cause. As a result, the major cause of the high propagation loss was the radiation towards the substrate. Further improvement was made in the under cladding layer structure (thickness optimization) to suppress the radiation loss towards the substrate. As a result, a low propagation loss of 0.02 dB/cm (@ \(\lambda = 1572\ \text{nm}, w = 2.35\ \mu\text{m}\)) has been achieved.
3.2 Propagation loss analysis

As mentioned in Chap. 2, the main cause of the propagation loss in SOI structure was scattering loss \(^1,2\). This was because its high index contrast (\(\Delta n = 46\%\)) between the air and the core that lead to much suffering from the sidewall roughness than that of SOI structure. Instead of utilizing a Si/SiO\(_2\) waveguide, we research the silica high-mesa waveguide for its lower propagation loss potential due to its relatively low horizontal index contrast (\(\Delta n = 27\%\)), compared to the SOI (\(\Delta n = 46\%\)) structure, between the air and the core. Since the propagation loss has been reported to be as low as 0.001 dB/cm \(^5\) in the case of a buried silica waveguide, we expected less than 0.1 dB/cm propagation loss for the silica high-mesa waveguide.

![Schematic of silica high-mesa waveguide cross section.](image)

**Fig. 3.1:** Schematic of silica high-mesa waveguide cross section.
Figure 3.1 shows the waveguide cross section of the silica high-mesa waveguide. As shown in the figure, it consists of a GeO$_2$-doped SiO$_2$ core with SiO$_2$ cladding. We set the thickness of the cover cladding layer, the core, and the under cladding layer to be 3, 3.5, 3.8 μm, respectively. For the actual implementation, the layer structure was formed by flame deposition and the high-mesa structure was formed by the regular reactive ion etching technique. The evaluated propagation loss as a function of waveguide width at $\lambda = 1550$ nm is shown in Fig. 3.2. The reason we chose $\lambda = 1550$ nm is that a lot of absorption peaks in the breath content, such as ammonia at 1520 nm, methane at 1650 nm, and others, exist at approximately 1550 nm in the range of ±100 nm. As shown in the figure, less than 0.1 dB/cm propagation loss was achieved in case of a wider width of more than 3.2 μm. In addition, the optical portion out of the waveguide decreases as the waveguide width increases, as shown in Fig. 3.3. Thus, 2.3 μm width is more preferable than 3.2 μm width. The propagation loss, however, was 0.65 dB/cm in the case of 2.3 μm width, as is also shown in Fig. 3.2, and further loss reduction was needed. Since the refractive index difference between the core and the cladding was only 2.5% and the substrate is made of silicon as shown in Fig. 3.1, we suspected that radiation loss towards the substrate might account for a large part of the propagation loss.
It is well known that increasing the wavelength is equivalent to decreasing the effective index of the waveguide, which means that the confinement of the
waveguide will be weakened, and in the meantime, the radiation will increase. Figure 3.4 shows excess loss as a function of wavelength (red line: experiment, blue line: calculation) in the case of \( w = 2.3 \) μm. The evaluated excess loss increased as the optical wavelength increased, as shown in the figure. The optical field profiles simulated by using the finite element method (FEM) when the wavelength \( \lambda = 1400 \) nm and \( \lambda = 1800 \) nm are shown as insets in the figure, respectively. As can be seen in the simulated optical field, radiation towards the substrate is observed in the case of \( \lambda = 1800 \) nm while it remains in case of \( \lambda = 1400 \) nm. Thus, the excess loss is considered to be corresponded to the radiation loss towards the substrate. Figure 3.4 also exhibits that the results of both the experiment and theory show that the radiation loss is approximately 0.45 dB/cm (@ \( \lambda = 1550 \) nm, \( w = 2.3 \) μm), which means that the radiation loss takes almost 70% of the propagation loss. This result is in accordance with our assumption. In addition, as shown in this paper later, the waveguide width affects the radiation loss as well. As the waveguide width increases, the radiation loss will be decreased, as shown in Fig. 3.5, the simulated optical field profiles when waveguide width \( w = 2 \) μm and \( w = 3.5 \) μm are shown as insets. We believe that this is because increasing the waveguide width minimizes the total modal intensity at the cladding interfaces which leads to the radiation loss reduction. This is also supported by the optical field profiles. Compared with the optical field of \( w = 2 \) μm, there are more mode power profiles in the horizontal direction of \( w = 3.5 \) μm, which leads to the mode power at the cladding interfaces being less than that of \( w = 2 \) μm. This causes the radiation loss increasing as the waveguide width decreasing. The radiation loss has been
calculated by the imaginary part of effective index \(^{13}\), which has been deduced by perfectly matched layer (PML) boundary condition \(^{14-17}\).

**Fig. 3.4:** Radiation loss as a function of wavelength. Optical field profiles of \(\lambda = 1400\) nm and \(\lambda = 1800\) nm are shown as insets.

**Fig. 3.5:** Radiation loss as a function of waveguide width. Optical field profiles of \(w = 2\) \(\mu m\) and \(w = 3.5\) \(\mu m\) are shown as insets.
In addition, we also analysed further causes besides the radiation loss towards the substrate, and suspected scattering loss. For this reason, we theoretically calculated the scattering loss as a function of waveguide width to carry out curve fitting on the experimental results. The result is shown in Fig. 3.6 (\(\lambda = 1550\) nm); and the curve fitting was done by the method gave in Sec. 2.4. The circle mark (o) denotes the experimental results (propagation loss) including radiation loss towards the substrate, and the triangle mark (Δ) denotes the propagation loss derived by extracting the experimental radiation loss towards the substrate. The solid-line (—) denotes the fitting-curve based on scattering loss with an assumption of 40 nm side-wall roughness. As is shown in the figure, the triangle-marks (Δ) were fitted very well to scattering loss.
loss curve. So the scattering loss is also one of the main components of the propagation loss.

What is more, we also investigated the effect of higher modes to the propagation loss. Because multi-modes might be excited in a high-mesa waveguide once the waveguide width is wider than 0.8 μm. We excited the fundamental mode at the input end, thus the higher mode effects are mainly concentrated at the bent area. We simulated the bending loss by using two dimension finite-difference time-domain (FDTD) technique. We have simulated 90-degree-bent waveguide connecting to a certain length of straight waveguides. To minimize the connecting loss between the straight waveguides and the bent waveguide, proper offset is introduced in the simulation and the radius of curvature is R as shown in Fig. 3.7 (a). The simulated bending loss as a function of radius of curvature for different waveguide widths are shown in Fig. 3.7 (b). As shown in the figure, a low bending loss of 0.05 dB/90° is realized at $R = 30 \, \mu m \, (@ \, w = 2.3 \, \mu m)$ and the bending loss slightly increases as the waveguide width increases. This is because the mode-mismatch of a higher mode between the bent end and the connecting straight waveguides, and a wider width is beneficial to higher mode excitation. In this simulation, the obvious radiation is confirmed only at $R < 10 \, \mu m$ especially when $w = 5 \, \mu m$ as shown in Fig. 3.7 (b). This is also confirmed in Fig. 3.7 (c) and (d). Thus, according to the analysis above, the higher mode does not affect the propagation loss significantly as long as the waveguide width $w < 5 \, \mu m$ and the radius of curvature $R > 30 \, \mu m$. In our case, the interested waveguide width $w = 2.3 \, \mu m$ and the implemented radius of curvature $R = 500 \, \mu m$, so we consider
Fig. 3.7: Calculated bending loss. (a) Waveguide layout with offset configuration, (b) theoretical bending loss as a function of the curve radius for different waveguide widths, (c) typical optical field profiles at $w = 2.3$ μm, and (d) typical optical field profiles at $w = 5$ μm.
that the higher mode does not impact the propagation loss significantly. On the basis of these analyses shown above, we concluded that the propagation loss was caused by the radiation loss towards the substrate and the scattering loss. On the basis of the discussion above, we discuss how to suppress the propagation loss in the next section.

3.3 Scheme to suppress the propagation loss

It is well known that the cladding height affects the effective refractive index; then, the waveguide confinement will be influenced. Furthermore, increasing the under cladding height makes the optical field far away from the silicon substrate. Thus, we consider that increasing the under cladding height may contribute to the radiation loss reduction. Figure 3.8 shows the calculated radiation loss towards the substrate as a function of under cladding mesa height. As shown in the figure, the radiation loss decreased as the under cladding mesa height increased. In the case that the under cladding mesa height exceeds 5 μm, the radiation loss becomes less than 0.03 dB/cm, and the radiation loss is no longer affected by the under cladding mesa height significantly once the under cladding mesa height exceeds 5 μm, as shown in the figure. In addition, a larger mesa height may cause worse sidewall roughness owing to the longer etching time. Thus, here we chose the under cladding mesa height of 5 μm, the extra loss (target is 0.09 dB/cm) will be occupied by scattering loss. For further improvement, the scattering loss
should be suppressed as well. For scattering loss reduction, wet etching and heat treatment after dry etching may be useful.

![Graph showing radiation loss as a function of under cladding mesa height.](image)

**Fig. 3.8:** Radiation loss as a function of under cladding mesa height.

### 3.4 Results and discussion

For further improvement of the implementation, we set the thickness of the under cladding mesa height to be 5 μm to suppress the radiation loss towards the substrate, while the thickness of the cover cladding and the core were set to be 5 and 3.5 μm, respectively. We evaluated the propagation loss by the cut-back method at 1572 nm. The reason we chose this wavelength was that 1572 nm is one of the peak wavelengths of CO₂, which is one typical breath component for infrared absorption. Figure 3.9 shows the evaluated
propagation loss as a function of the waveguide width. An extremely low loss of 0.02 dB/cm was achieved when $w = 2.35 \ \mu m$.

We analysed the remaining propagation loss causes. We did not find any radiation loss at $w = 2.35 \ \mu m$ for the newly fabricated waveguide, experimentally, as shown in Fig. 3.10. Figure 3.10 shows the spectrum of the newly fabricated waveguide when the waveguide width was 2.35 and 1.85 $\mu m$. As mentioned in Sec. 3.2, the radiation loss increases as the wavelength increases and the waveguide width decreases, which means that the spectrum should collapse for the longer wavelength, as the 1.85-$\mu m$-width waveguide shows in the case that the wavelength exceeds 1550 nm. On the other hand, the 2.35-$\mu m$-width waveguide did not show this kind of collapse, which means no radiation loss exists. This means that our proposal of using an under cladding of 5 $\mu m$ suppresses the radiation loss effectively. The obtained propagation loss was fitted to the scattering loss curve perfectly with an

![Graph showing propagation loss as a function of waveguide width.](image)

**Fig. 3.9:** Propagation loss as a function of waveguide width.
assumption of 10 nm sidewall roughness, which means that the sidewall roughness has also been improved successfully. Figure 3.11 (b) shows the SEM image of the implemented waveguide. For comparison, one of the previously fabricated waveguides is shown in Fig. 3.11 (a). The estimated sidewall roughness was 19.3 nm on average for the implemented waveguide, while it was 35.4 nm on average for the previous waveguide.

According to our calculation, the optical portion out of the waveguide is expected to be 2.2% for a 2.3-μm-width silica high-mesa waveguide. 10 ppm methane detection, for instance, is possible when the optical portion out of the waveguide exceeds 20%; therefore, further improvement is needed in obtaining not only a lower propagation loss but also a higher optical portion out of the waveguide.

![Graph](image)

**Fig. 3.10:** Spectroscopy of new waveguide when waveguide widths at 2.35 μm and 1.85 μm.
Conclusions

We proposed silica high-mesa waveguide for infrared sensing. Under cladding mesa height of 5 μm was effective to suppress the radiation loss towards

Fig. 3.11: SEM pictures of waveguide sidewall roughness comparison for different under-cladding thicknesses.

3.5 Conclusions

We proposed silica high-mesa waveguide for infrared sensing. Under cladding mesa height of 5 μm was effective to suppress the radiation loss towards
substrate, then an extremely low propagation loss of 0.02 dB/cm has been achieved successfully.
3.6 References


10. HITRAN Database: http://www.cfa.harvard.edu/hitran/.


Chapter 4 Proposal of multiple-slot silica high-mesa waveguide

4.1 Introductory overview

As mentioned in Sec. 1.3, for breath content sensing by using infrared absorption, the propagation loss must be less than 0.09 dB/cm. Instead of SOI structure, we have proposed silica based high-mesa waveguide for infrared sensing owing to its low propagation loss in Chap. 3. And an extremely low propagation loss of 0.02 dB/cm\(^1\) (\(\lambda = 1550\) nm, \(w = 2.3\) μm) has been achieved. Another issue for silica structure lies, however, in its low portion of light profiles outside of the waveguide (\(\Gamma_{\text{air}}\)), which is used for sensing. The estimated \(\Gamma_{\text{air}}\) of single silica high-mesa waveguide was only 2.2\% (\(\lambda = 1550\) nm, \(w = 2.3\) μm) as shown in Sec. 4.4. This is because the small difference in the refractive indices of silica high-mesa and air leads to a low electric field discontinuity at the high-mesa-air interface, and thus a relatively low \(\Gamma_{\text{air}}\) for single high-mesa structures. Low \(\Gamma_{\text{air}}\) leads to less light power being used for sensing, thus limiting the sensing capability. In this chapter we propose a multiple-slot silica high-mesa waveguide for the possibility of realizing higher \(\Gamma_{\text{air}}\)\(^2\). In the meantime, low propagation loss is expected as well by using silica material, since high propagation loss consumes light power, thus restricting sensing capability. The simulated results showed a higher \(\Gamma_{\text{air}}\) of 20.3\%
for a quadruple structure under a wavelength of 1550 nm. In addition, a low scattering loss of 0.06 dB/cm was confirmed theoretically.

4.2 Estimation of $\Gamma_{\text{air}}$ for single high-mesa waveguide

As mentioned above, the $\Gamma_{\text{air}}$ affects the sensing capability as well. Thus a theoretical evaluation method of $\Gamma_{\text{air}}$ is necessary for further study. In this section we use a single high-mesa waveguide as an example to introduce the theoretical evaluation method of $\Gamma_{\text{air}}$. The $\Gamma_{\text{air}}$ is defined as the portion of optical field out of the waveguide, as shown in Fig. 4.1 (a). In Fig. 4.1 (a), the optical field can be divided into three parts A, B and C, the $\Gamma_{\text{air}}$ is defined as follow

$$\Gamma_{\text{air}} = \frac{B + C}{A + B + C}$$

Fig. 4.1: (a) Schematic of silica high-mesa waveguide optical field dispersion; (b) simulated optical field dispersion by FEM.
So the $\Gamma_{\text{air}}$ can be evaluated as long as the optical field dispersion is known. The optical field dispersion can be evaluated by finite element method (FEM) as shown in Fig. 4.1 (b). All the $\Gamma_{\text{air}}$ have been evaluated by this method in this thesis.

4.3 Concept of multiple-slot high-mesa waveguide

Figure 4.2 shows the waveguide cross-sections of different waveguide structures, namely, (a) single silica high-mesa waveguide, (b) double high-mesa waveguide, (c) triple high-mesa waveguide, and (d) quadruple high-mesa waveguide. The geometry parameters of all structures were set as 5 $\mu$m, 3.5 $\mu$m, and 5 $\mu$m for the cover cladding layer, core, and under cladding layer, respectively. As shown in Fig. 4.2 (a), for the single structure, most of the optical power is confined in the solid material, and only a few optical profiles can be detected outside of the solid material. This leaves a low amount of light power for infrared sensing. In contrast, compared with the single structure, the slot structures shown in Figs. 4.2 (b), (c), and (d) show a great number of optical power profiles out of the waveguide, especially in the slot regions. This is because multiple-slot high-mesa structures comprise several parallel conventional single high-mesas adjacent to each other, and the slot width between mesas is only of the order of nanometers. Thus, the near-field effect enhances the optical power portion inside the slot region, and higher $\Gamma_{\text{air}}$ can be expected from the multiple structure. The optical fields were simulated using the finite element method.
Fig. 4.2: Schematics of waveguide cross-sections and simulated optical profiles. The parameters are shown on set of the figures. (a) Single silica high-mesa, (b) double high-mesa, (c) triple high-mesa, (d) quadruple high-mesa.
The TE mode was used for obtaining all simulation results in this study.

4.4 Results and analysis

4.4.1 $\Gamma_{air}$ improvement of multiple-slot high-mesa waveguide

Figure 4.3 shows the $\Gamma_{air}$ as a function of the numbers of mesa (the maximum of $\Gamma_{air}$ for each number of mesas is shown). As shown in Fig. 4.3, the $\Gamma_{air}$ of the multiple-slot high-mesa is higher than that of the single high-mesa, as we expected, and the highest $\Gamma_{air}$ appears with the quadruple high-mesa structure. In addition, Fig. 4.3 shows that the $\Gamma_{air}$ of an even number of mesas is higher than that of an odd number of mesas. This is further confirmed in Fig. 4.2. Compared with the double and the quadruple structures, there are considerably more power profiles inside the middle mesa than in the slot regions in the triple structure, as shown in Fig. 4.2 (c), which results in a low $\Gamma_{air}$. For a multiple-slot waveguide, internal waveguides (e.g., $w$ for triple structures, $w_1$ for quadruple structures) and slot regions can be considered as an equivalent inter-slot sandwiched between the two external waveguides. Thus, altering the numbers of internal waveguides is equal to changing the effective index of this equivalent inter-slot. Owing to the symmetry of the propagation mode, the effective indices of this equivalent inter-slot of an odd number of mesas are higher than those of an even number of mesas. Therefore, the effective indices of an even number of mesas are lower.
than those of an odd number of mesas. This leads to the lower $\Gamma_{\text{air}}$ when using an odd number of mesas. In addition, Fig. 4.4 shows the effective refractive indices as a function of numbers of mesa. As shown in Fig. 4.4, it is expected that the effective refractive indices of even number of mesa are lower than that of odd number of mesa. This implies that for even number of mesa, much higher power propagates in the slot regions than that of odd number of mesa. This is the reason why the $\Gamma_{\text{air}}$ of even number of mesa are higher than that of odd number of mesa. Figure 4.4 also exhibits that the quadruple structure shows the lowest effective refractive index. This explains why the highest $\Gamma_{\text{air}}$ appears at qaudruple structure.

Considering the analysis mentioned above, we propose a quadruple struture given its possibility of achieving the highest $\Gamma_{\text{air}}$. Given that the optical field profile depends on the waveguide geometry of the waveguide width $w$ and the slot widht $d$, $\Gamma_{\text{air}}$ should be estimated depending on these parameters. Figure 4.5 shows a theoretical estimation of $\Gamma_{\text{air}}$ as a function of the slot width (the maximum $\Gamma_{\text{air}}$ for each slot width is shown). From Fig. 4.5, the highest $\Gamma_{\text{air}}$ appears when the slot width $d = 400$ nm. The region of $d = 400$ nm ± 20% is marked in Fig. 4.5 as well. This region is a reasonable tolerance range for a slot width in actual fabrication. Compared with the peak, the difference in the maximum and minimum $\Gamma_{\text{air}}$ in this region is less than 2%. This could be very helpful for facilitating the etching procedure. For the slot width of $d = 400$ nm, the results of altering $w_1$ (0.8 μm ~ 1.3 μm) and $w_2$ (1 μm ~ 1.4 μm) are summarized in Tab. 4.1. The maximum $\Gamma_{\text{air}}$ reaches 20.3%, which is almost ten times the value of the single structure for $w_1 =$
**Fig. 4.3:** \( \Gamma_{air} \) as a function of numbers of mesa. \( \lambda = 1550 \) nm and TE mode have been used.

**Fig. 4.4:** Effective indices as a function of numbers of mesa for a conventional and multiple slot high-mesa waveguides. The geometry parameters are the same as those of the maximum \( \Gamma_{air} \) for each structure.
Fig. 4.5: $\Gamma_{\text{air}}$ as a function of the slot width for quadruple structure. We have used TE mode.

Table 4.1: $\Gamma_{\text{air}}$ of quadruple structure high-mesa.

(Slot width $d = 400$ nm, $\lambda = 1550$ nm, TE mode)

<table>
<thead>
<tr>
<th>$w_1$ (μm)</th>
<th>$w_2$ (μm)</th>
<th>1</th>
<th>1.1</th>
<th>1.2</th>
<th>1.3</th>
<th>1.4</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.8</td>
<td></td>
<td>17.2%</td>
<td>13.7%</td>
<td>11.1%</td>
<td>9.2%</td>
<td></td>
</tr>
<tr>
<td>0.9</td>
<td></td>
<td>18.1%</td>
<td>14.1%</td>
<td>11.3%</td>
<td>8.9%</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td></td>
<td>20.3%</td>
<td>15.3%</td>
<td>11.7%</td>
<td>9.5%</td>
<td></td>
</tr>
<tr>
<td>1.1</td>
<td></td>
<td>19.1%</td>
<td>19.2%</td>
<td>16.1%</td>
<td>12.2%</td>
<td>9.7%</td>
</tr>
<tr>
<td>1.2</td>
<td></td>
<td>15.7%</td>
<td>15.9%</td>
<td>15.8%</td>
<td>11.4%</td>
<td>13.3%</td>
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<tr>
<td>1.3</td>
<td></td>
<td>13.0%</td>
<td>13.1%</td>
<td>13.3%</td>
<td>13.3%</td>
<td>10.9%</td>
</tr>
</tbody>
</table>
1 μm and \( w_2 = 1.1 \mu m \). There are no propagation modes when \( w_1 \leq 1 \mu m \) and \( w_2 = 1 \mu m \).

### 4.4.2 Comparison to the single silica high-mesa structure

In addition, we theoretically estimated the scattering loss of the quadruple structure waveguide using the beam propagation method (BPM) with the sidewall roughness was set to 10 nm, which is the sidewall roughness value realized using the single structure \(^1\). A scattering loss of 0.06 dB/cm is estimated for the quadruple structure. To identify the better alternative between the single high-mesa structure and the quadruple structure based on the above results, we consider the following criterion for evaluating waveguide performance in infrared sensing.

As mentioned above, the sensitivity of infrared absorption is influenced by both the propagation loss and the \( \Gamma_{\text{air}} \). To compare the proposed quadruple structure with the single structure, we presented a new criterion that takes into account both the propagation loss and the \( \Gamma_{\text{air}} \) for waveguide evaluation. According to the definition of propagation loss and the Lambert-Beer law \(^8-13\), the intensity of incident light and transmitted light can be written as follows:

\[
I = I_0 e^{-\sigma n L \Gamma_{\text{air}}} e^{-\alpha L}
\]

Here, \( I_0 \) and \( I \) denote the intensities of the incident light and the transmitted light, respectively, \( \sigma \) denotes the cross section of light absorption by a single particle, \( n \)
denotes the density (number per unit volume) of the absorption particles, \( L \) denotes the waveguide length, \( \alpha \) denotes the propagation loss, and \( \Gamma_{\text{air}} \) denotes the portion of optical field profiles outside the solid material. \( e^{-\sigma nL\Gamma_{\text{air}}} \) and \( e^{-\alpha L} \) correspond to the infrared absorption attenuation and propagation loss attenuation, respectively. We define a new variable \( A \) as follows:

\[
A = \frac{e^{-\alpha L}}{e^{-\sigma nL\Gamma_{\text{air}}}} = e^{\alpha L(\sigma n\Gamma_{\text{air}} - 1)}
\]  

(4.3)

\( A \) can be used for evaluating the waveguides’ performance; a higher \( A \) favours higher infrared absorption sensitivity. \( \alpha L \), on the right side of Eq. 4.3, denotes the propagation loss of the entire waveguide and can be controlled by adjusting the waveguide length; therefore, it can be considered as a constant. For a certain concentration gas, \( \sigma \) and \( n \) can also be considered as constants. Then, \( A \) is decided by \( B = \frac{\Gamma_{\text{air}}}{\alpha} \). The higher the \( B \) value, the higher is the value of \( A \). The waveguide can be evaluated by substituting the parameters into \( B \). For instance, for the single silica high-mesa waveguide, \( \alpha = 0.02 \, \text{dB/cm} \) and \( \Gamma_{\text{air}} = 2.2\% \), thus leading to \( B_{\text{single}} = 1.1 \). For the proposed quadruple structure, \( \alpha = 0.06 \, \text{dB/cm} \) and \( \Gamma_{\text{air}} = 20.3\% \), thus leading to \( B_{\text{quadruple}} = 3.4 \). From this view-point, the proposed quadruple structure is better for infrared absorption. Furthermore, the sidewall roughness of the silica structure was 10 nm \(^1\), which is considerably high compared with that of the SOI structure (1 nm) \(^14\). Therefore, we believe that for this multiple-slot silica high-mesa structure, a further reduction of the propagation loss is possible.
through improvement of sidewall roughness. For a sidewall roughness of 1 nm, the propagation loss of the proposed quadruple silica structure has been confirmed to be as low as 0.005 dB/cm through BPM simulation. Concurrently, an extremely high $B_{\text{quadruple}}$ of 40.6 can be achieved.

4.5 Conclusions

We proposed a multiple-slot silica high-mesa waveguide and found that the $\Gamma_{\text{air}}$ when using an even number of mesas is always higher than that when using an odd number of mesas. Theoretically, a high $\Gamma_{\text{air}}$ of 20.3% was achieved with the proposed quadruple structure. Furthermore, it was confirmed that the highest $\Gamma_{\text{air}}$ appears at $d = 400$ nm and a tolerance range of $\pm 20\%$, wherein the difference of $\Gamma_{\text{air}}$ is less than 2%, which is helpful for facilitating etching. Meanwhile, a low scattering loss of 0.06 dB/cm was estimated theoretically. The proposed quadruple structure high-mesa waveguide can realize future high-sensitivity devices for optical absorption spectroscopy.
4.6 References


Chapter 5 Conclusions and outlook

5.1 Conclusions

As mentioned in Chap. 1, high-mesa waveguide is attractive for infrared sensing owing to not only its possibility of small curvature of radius, which is useful to realize high density integration on a compact area, but also a portion of light profiles out of the waveguide, which enables propagating light to be exposed towards volatile gas (breath content). The propagation loss, however, prevents the high sensing capability since it consumes the light power. Therefore, in this study, we discussed several proposals to suppress the propagation loss.

In Chap. 2, the propagation loss category has been discussed. The propagation loss can be generally attributed to three different mechanisms: scattering losses, radiation losses and absorption losses. For further classification, the scattering losses can be divided into volume scattering and surface scattering; radiation losses can be divided into radiation towards the substrate and the radiation from the waveguide bent; absorption losses can be divided into interband absorption and free carrier absorption. Some methods to get low propagation loss have also been discussed in this chapter as well.

In Chap. 3, we proposed silica high-mesa waveguide for infrared sensing owing to its low propagation loss possibility. And found that the radiation towards the
substrate takes a large part of propagation loss due to the low refractive index
difference between the core and the cladding. Under cladding mesa height of 5
μm was effective to suppress the radiation loss towards substrate, then an
extremely low propagation loss of 0.02 dB/cm (@ λ = 1550 nm, w = 2.3 μm) has
been achieved successfully.

In Chap. 4, we discussed how to increase the portion of optical field profiles out of
the waveguide (Γair). Because although extremely low propagation loss has been
achieved by silica high-mesa waveguide, the Γair of silica structure is as low as 2.2%
(@ λ = 1550 nm, w = 2.3 μm), which leads to less light power being used for
sensing and limits the sensing capabilities. To solve this problem, in this chapter,
we proposed multiple-slot silica high-mesa structure in the light of its possibility
of realizing higher Γair. As a result, we found that the Γair when using an even
number of mesas is always higher than that when using an odd number of mesas.
Theoretically, a high Γair of 20.3% was achieved with the proposed quadruple
structure. Furthermore, it was confirmed that the highest Γair appears at d = 400
nm and a tolerance range of ± 20%, wherein the difference of Γair is less than 2%,
which is helpful for facilitating etching. Meanwhile, a low scattering loss of 0.06
dB/cm was estimated theoretically. The proposed quadruple structure high-mesa
waveguide can realize future high-sensitivity devices for optical absorption
spectroscopy.
5.2 Outlook

We hope and believe that this concept will contribute to realize compact and highly sensitive waveguide-cell in future. Especially, for silica high-mesa waveguide, although extremely low loss has been achieved, the sidewall roughness is not very low compared with that of SOI structure. Thus, lower propagation loss is expected through the improvement of fabrication. Moreover, we have proposed multiple-slot silica high-mesa waveguide to enhance optical portion out of the waveguide up to 20.3% for quadruple structure and low scattering loss of 0.06 dB/cm has been confirmed as well. For multiple-slot silica high-mesa waveguide, lower scattering loss is expected through sidewall roughness improvement as well. Therefore, it is expected that high sensitivity for optical absorption sensing can be realized by multiple-slot silica high-mesa waveguide in the future.
Appendix

A: Theory calculation of scattering [1]-[5]

The critical issue for infrared sensing by high-mesa waveguide is propagation loss, which is mainly consists of scattering loss in SOI structure. To analyse the scattering loss and give possible methods to suppress the scattering loss, a mathematical scattering loss evaluation method is necessary. In this section we introduce a scattering loss theoretical evaluation method which has been used widely.

Scattering loss is caused by sidewall roughness at the interfaces between waveguide core and cladding. Figure A.1 shows the perspective view and the top view of a high-mesa waveguide, of which the sidewalls are considered rough. Here, \(n_0\) is the refractive index of cladding material (air), \(n_1\) is the refractive index of core material, \(w\) is the waveguide width and \(\sigma\) is the sidewall roughness. As shown in Fig. A.1, there are some zigzags along the waveguide sidewall, which is called sidewall roughness.
Fig. A.1: (a) Perspective view of high-mesa waveguide. (b) Top view of high-mesa waveguide, $n_0$ is the refractive index of cladding material (air), $n_1$ is the refractive index of core material, $w$ is the waveguide width and $\sigma$ is the sidewall roughness.

Fig. A.2: Scattering of light through the rough side-wall of a fabricated waveguide (top view). The coordinate system is shown insets.
The description of the scattered light from the waveguide is shown in Fig. A.2, the coordinate system is shown insets. As shown in Fig. A.2, the waveguide core width is \( w \), a random function \( f(z) \) can be used to describe the vertical deviations of the interfaces from their mean position, \( x = \frac{w}{2} \) and \( x = -\frac{w}{2} \). The waveguide length is considered \( L \to \infty \) in this chapter. Both walls are assumed randomly distorted, and the distributions of the distortions on opposite walls are identical. The refractive index distribution can be written as:

\[
 n^2 = n_0^2 + (n_1^2 - n_0^2)U\left[\frac{w}{2} + f(z) - |x|\right] \quad \text{(A.1)}
\]

where \( U\left[\frac{w}{2} + f(z) - |x|\right] \) is the unit step function, i.e.:

\[
 U[\alpha] = \begin{cases} 
 0 & \alpha < 0 \\
 1 & \alpha > 0 
\end{cases}
\]

so that:

\[
 n^2 = n_0^2 \quad |x| > \frac{w}{2} + f(z)
\]

\[
 n^2 = n_1^2 \quad |x| < \frac{w}{2} + f(z)
\]

the wave equation can be written as:

\[
 \nabla^2 E_y(x, z) + k_0^2 n_0^2 E_y(x, z) = k_0^2 (n_0^2 - n_1^2)U\left[\frac{w}{2} + f(z) - |x|\right] E_y(x, z) \quad \text{(A.2)}
\]

the solution of the equation above can be assumed as:

\[
 E = E_y(x, z) \exp(i\omega t)
\]

so that
Eq. A.2 cannot be analytically solved, although it is an exact description of the radiation process. An approximate form of Eq. A.1, which can be solved analytically, however, is possible. It can be written as:

\[ E = E_{y0}(x, z) \exp(i\omega t) = \Phi(x)\exp[i(\omega t - \beta z)] \]  

(A.3)

This is the solution of Eq. A.2 by considering the field from a single mode waveguide without sidewall roughness. Techniques for obtaining the field \( \Phi(y) \) and \( \beta \) has been well established by Yariv. The right side of Eq. A.2 depends only upon the field inside the waveguide, because of the presence of the step function \( U\left[\frac{w}{2} + f(z) + |x|\right] \). The Eq. A.2 can be solved to give an approximation for the radiated field outside the waveguide, if the field is approximated by the smooth-walled waveguide modal field \( E_{y0}(x, z) \). Therefore, replace \( E_y(x, z) \) in the right hand of Eq. A.2 by the smooth-walled waveguide field \( E_{y0}(x, z) \), to give:

\[ \nabla^2 E_y(x, z) + k_0^2 n_0^2 E_y(x, z) = k_0^2 (n_0^2 - n_1^2) U\left[\frac{w}{2} + f(z) - |x|\right] E_{y0}(x, z) \]  

(A.4)

This approximation has been referred by Kuznetsov.

Regarding the waveguide as an antenna is a useful way of discussion Eq. A.4. The term on the right side of the equation, consists of the field \( E_{y0}(x, z) \) (known) and the random function \( f(z) \), describing the current which is the
source of the radiation of the waveguide. The field $E_y(x,z)$ on the left side is the solution of Eq. A.4 which describes the resulting field in space.

The so-called near field is a standard result from antenna theory. It is well known that the near field consists of not only the radiated field in which we are interested, but also the exponentially decaying of the waveguide guided modes (evanescent field). To simplify the calculation, only the far field will be considered. Green function technique is a convenient way to solve Eq. A.4.

Green function $G(x,x',z,z')$ for Eq. A.4 is defined as:

$$\nabla^2 G(x,x',z,z') + k_0^2 n_0^2 G(x,x',z,z') = \delta(z-z')\delta(x-x') \quad (A.5)$$

then the solution to Eq. A.4 is given by

$$E_y(x,z) = (n_0^2 - n_1^2)k_0^2 \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} U(x',z')E_{y0}(x',z') G(x,x',z,z') dx'dz' \quad (A.6)$$

To evaluate the integrals in Eq. A.6 is our task now. Using the conventional antenna theory again, it is reasonable to assume that the solution consists of a superposition of monochromatic plane waves. In this case, the analysis will be simplified if we work in the wavenumber $(k_x,k_z)$ domain. Thus it will be convenient to utilize the Fourier transform of the Green function. The Fourier transform of $F(x,z)$, which is $\tilde{F}(k_x,k_z)$, is defined as:

$$\tilde{F}(k_x,k_z) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} F(x,z)\exp(-ik_xx)\exp(-ik_zz) \, dx \, dz \quad (A.7)$$

We take the Fourier transform of Eq. A.5 to obtain an expression of $\tilde{G}(k_x,x',k_z,z')$, the Fourier transform of the Green function $G(x,x',z,z')$:
\[ \tilde{G}(k_x, x', k_z, z') = \frac{\exp(-ik_x x)\exp(-ik_z z')}{(k_0^2 n_0^2 - k_x^2 - k_z^2)} \]  

(A.8)

Inserting the function \( U[\frac{w}{z} + f(z) - |x|] \) into Eq. A.6 above, we have

\[ E_y(x, z) = (n_0^2) \]

(A.9)

\[ - n_1^2 k_0^2 \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} U[\frac{w}{z} + f(z) - |x|] \]

\[ \times E_{y0}(x', z') G(x, x', z, z') dx' dz' \]

The integral with respect to \( x' \) can be divided into halves, from \( x' \in (-\infty, 0) \) and \( x' \in (0, \infty) \). Because the integrand is an even function, then we get

\[ E_y(x, z) = \sqrt{2}(n_0^2 - n_1^2)k_0^2 \]

\[ \times \int_{-\infty}^{\infty} dz' \int_{0}^{\infty} dx' U[\frac{w}{z} + f(z') - x'] \times E_{y0}(x', z') G(x, x', z, z') \]

(A.10)

Because \( U[\frac{w}{z} + f(z') - x'] = 0 \) for \( x' > \frac{w}{z} + f(z') \), we get

\[ E_y(x, z) = \sqrt{2}(n_0^2 - n_1^2)k_0^2 \int_{-\infty}^{\infty} dz' \int_{0}^{\frac{w}{z} + f(z')} dx' E_{y0}(x', z') G(x, x', z, z') \]

(A.11)

The integral with respect of \( x' \) can be split into integrals \( x' \in (0, \frac{w}{2}) \) and \( x' \in (\frac{w}{2}, \frac{w}{2} + f(z')) \) again. In Appendix A we show that the far field is not affected by the first integral \( x' \in (0, \frac{w}{2}) \). Hence, we need only consider the second
integral \( x' \in \left( \frac{w}{2}, \frac{w}{2} + f(z') \right) \). We assume that \( |f(z')| \ll \frac{w}{2} \) to evaluate this integral,

\[
\int_{\frac{w}{2}}^{\frac{w}{2} + f(z')} p(x')dx' \approx p\left(\frac{w}{2}\right) f(z')
\]  \hspace{1cm} (A.12)

(a first order Taylor expansion), so

\[
E_y(x, z) \approx \sqrt{2} \Phi\left(\frac{w}{2}\right) \left(n_0^2 - n_1^2\right) k_0^2 \int_{-\infty}^{\infty} \exp(-i\beta z') G\left(y, \frac{w}{2}, z, z'\right) f(z')dz'
\]  \hspace{1cm} (A.13)

Using \( E_{y0}(x', z') = \Phi(x') \exp(-i\beta z') \) in Eq. A.3. Namely, we demonstrate that only the current on the antenna surface or the waveguide core-cladding interface, contributes to radiation. Then we take the Fourier transform of Eq. A.13. Since \( G(x, \frac{w}{2}, z, z') \) is the only function of \( y \) and \( z \) in Eq. A.13, applying Fourier transform operator to it directly, we get

\[
\tilde{E}_y(k_x, k_z) = \frac{\sqrt{2} \Phi\left(\frac{w}{2}\right) \left(n_0^2 - n_1^2\right) k_0^2 \exp(-ik_x \frac{w}{2}) \tilde{F}(\beta + k_z)}{(n_0^2 k_0^2 - k_x^2 - k_z^2)}
\]  \hspace{1cm} (A.14)

where the \( \tilde{F}(\beta + k_z) \) is the Fourier transform of \( f(z) \), the result for the Fourier transform of the Green function in Eq. A.8 has been used. It is obvious that the radiated field depends on the Fourier transform of the roughness function \( f(z) \) by translating to the wavenumber \((k_x, k_z)\) domain utilizing the Fourier transform.

Now transform Eq. A.14 back to the spatial \((x, z)\) domain from the wavenumber domain, using the inverse Fourier transform relation.
\[ E_y(x, z) \equiv \frac{1}{4\pi^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \tilde{E}_y(k_x, k_z) \exp(i k_x x) \exp(i k_z z) \, dk_x \, dk_z \]  

(A.15)

which gives

\[ E_y(x, z) \equiv \frac{1}{4\pi^2} \sqrt{2} \Phi \left( \frac{w}{2} \right) (n_0^2 - n_1^2) k_0^2 \]

\[
\times \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{\tilde{F}(\beta + k_z) \exp[i k_x (x - \frac{w}{2})] \exp(i k_z z) dk_x \, dk_z}{(n_0^2 k_0^2 - k_0^2 - k_z^2)} 
\]

the integral in Eq. A.16 can be evaluated as

\[ E_y(x, z) \equiv \frac{i \sqrt{2}}{4\pi} \Phi \left( \frac{w}{2} \right) (n_0^2 - n_1^2) k_0^2 \]

\[
\times \int_{-\infty}^{\infty} \tilde{F}(\beta + k_z) \exp\{i[k_z z - (x - \frac{w}{2}) Q(k_z)]\} \, dk_z 
\]

(A.17)

where

\[ Q(k_z) = (n_0^2 k_0^2 - k_z^2)^{\frac{1}{2}} \quad |k_z| < n_0 k_0 \]

\[ Q(k_z) = -i(k_z^2 - n_0^2 k_0^2)^{\frac{1}{2}} \quad |k_z| > n_0 k_0 \]

This expression is a summation of plane waves of which amplitudes are proportional to the Fourier transform of \( f(z) \), and of which directions of propagation are \( \theta \), where \( \cos \theta = k_z / n_0 k_0 \). To evaluate the integral in Eq. A.17, the substitution of follow is made:

\[ k_z = n_0 k_0 \sin \omega \]
We also transform to a polar co-ordinate system, with its origin at the waveguide surface, at \( x = \frac{w}{2} \), so that

\[
\begin{align*}
z &= r \cos \theta \\
x - \frac{w}{2} &= rsin \theta
\end{align*}
\]

thus the Eq. A.17 becomes

\[
E_y(r, \theta) = \frac{i \sqrt{2}}{4\pi} \Phi(\frac{w}{2})(n_0^2 - n_1^2)k_0^2 \\
\times \int_{-\infty}^{\infty} \tilde{F}(\beta + k_0n_0 \sin \omega) \times \exp[in_0k_0r \sin(\omega - \theta)] \, d\omega
\]

Eq. A.18 is valid for all values of \( k_z \). Using the method of steepest descents, the Eq. A.18 can be approximately evaluated as:

\[
E_y(r, \theta) = \frac{i \Phi(\frac{w}{2})(n_0^2 - n_1^2)k_0^2}{(4\pi n_0 k_0 r)^{\frac{1}{2}}} \tilde{F}(\beta - k_0n_0 \cos \theta) \exp[i(\frac{\pi}{4} - n_0k_0r)]
\]

Eq. A.19 is a general result that describes the field radiated from two-dimensional waveguides with any type of wall roughness, as long as the Fourier transform of the roughness exists.

Next we evaluate a more practically useful quantity that is the exponential radiation loss coefficient \( \alpha \) using Eq. A.19. \( \alpha \) is defined as:

\[
P(z) = P(0)exp(-\alpha z) \tag{A.20}
\]

\( P(z) \) is the guided power in the core at a distance \( z \) along the waveguide. \( P(z) \) is launched at \( z = 0 \). To find \( \alpha \), the ensemble average of the magnitude squared of the radiated field is necessary, which is given as:
\[ \langle |E_y(r, \theta)|^2 \rangle = \Phi^2 \left( \frac{W}{2} \right) (n_0^2 - n_1^2) \frac{k_0^3}{4\pi n_0 r} \langle |\tilde{F}(\beta - k_0 n_0 \cos \theta)|^2 \rangle \]  \hspace{1cm} (A.21)

If we define the power spectral density of \( f(z) \) is \( W(k) \), then the \( W(k) \) is given as:

\[ W(k) \equiv \langle \lim_{L \to \infty} \left| \frac{1}{2L} \int_{-L}^{L} f(z)e^{-ikz} \, dz \right|^2 \rangle \]  \hspace{1cm} (A.22)

then

\[ \langle |\tilde{F}(k)|^2 \rangle = \langle \lim_{L \to \infty} \left| \int_{-L}^{L} f(z)e^{-ikz} \, dz \right|^2 \rangle = 2LW(k) \]  \hspace{1cm} (A.23)

It is well known that \( W(k) \) is equal to \( \tilde{R}(\theta) \) that is the Fourier transform of the autocorrelation function \( R(u) \), where the autocorrelation function is defined as:

\[ R(u) \equiv \langle f(z)f(z+u) \rangle \]  \hspace{1cm} (A.24)

This means that

\[ \langle |\tilde{F}(k)|^2 \rangle = 2L\tilde{R}(\theta) \]  \hspace{1cm} (A.25)

Therefore the ensemble average of the magnitude squared of the field radiated per unit length of waveguide is given by:

\[ \frac{\langle |E_y(r, \theta)|^2 \rangle}{2L} = \Phi^2 \left( \frac{W}{2} \right) (n_0^2 - n_1^2) \frac{k_0^3}{4\pi n_0 r} \tilde{R}(\beta - n_0 k_0 \cos \theta) \]  \hspace{1cm} (A.26)

The exponential radiation loss coefficient can be expressed as:
\[ \alpha = \frac{P_r/2L}{P_g} \quad (A.27) \]

where \( P_r/2L \) is the total power radiated per unit length of waveguide, given by:

\[ \frac{P_r}{2L} = \frac{n_0}{2} \left( \frac{\varepsilon_0}{\mu_0} \right) \int_0^{\pi} \frac{\left| E_y(r, \theta) \right|^2}{2L} r \, d\theta \quad (A.28) \]

and \( P_g \) is the total guided power, given by

\[ P_g = \frac{n_1}{2} \left( \frac{\varepsilon_0}{\mu_0} \right) \int_{-\infty}^{\infty} \Phi^2(x) \, dx \quad (A.29) \]

Thus the radiation loss coefficient \( \alpha \) is given by:

\[ \alpha = \Phi^2 \left( \frac{W}{2} \right) (n_0^2 - n_1^2) \frac{k_0^3}{4\pi n_1} \int_0^{\pi} \tilde{R}(\beta - n_1 k_0 \cos \theta) d\theta \quad (A.30) \]

for many waveguides, the roughness function \( f(z) \) can be described by a Gaussian autocorrelation function:

\[ R(u) = \sigma^2 \exp \left( -\frac{u^2}{L_c^2} \right) \quad (A.31) \]

Where \( R(0) = \sigma^2 \) is the mean square perturbation, \( L_c \) is the correlation length. Substituting this into Eq. A.30, we obtain:

\[ \alpha = \frac{\sigma^2}{\sqrt{2} k_0 \left( \frac{W}{2} \right)^4 n_1} g(V) f(x, \gamma) \quad (A.32) \]
here \( g(V) \) is a function depending only on the waveguide geometry, \( f(\chi, \gamma) \) is linked to the sidewall roughness.

\[
g(V) = \frac{U^2 V^2}{1 + W} \quad (A.33)
\]

with

\[
U = d \sqrt{n_1^2 k_0^2 - \beta^2} \quad (A.34a)
\]

\[
V = k_0 d \sqrt{n_1^2 - n_0^2} \quad (A.34b)
\]

\[
W = d \sqrt{\beta^2 - n_0^2 k_0^2} \quad (A.34c)
\]

and

\[
f(x, \gamma) = \frac{x}{\sqrt{2\pi}} \int_0^\pi \exp \left\{ -\frac{x^2}{4} \left[ \left( 1 + \frac{\gamma^2}{2} \right)^{\frac{1}{2}} - \frac{\gamma}{\sqrt{2}} \cos \theta \right]^2 \right\} d\theta \quad (A.35)
\]

where

\[
x = \frac{W L_c}{d} \quad (A.36a)
\]

\[
\gamma = \frac{n_0 V}{n_1 W \sqrt{\Delta}} \quad (A.36b)
\]

\[
\Delta = \frac{n_1^2 - n_0^2}{2n_1^2} \quad (A.36c)
\]

Using Eq. A.32, the scattering loss for most of the waveguide can be calculated numerically. All of the scattering loss in this thesis has been evaluated by the method above.
B: Finite Element Method (FEM)

Finite element method (FEM) is usually used for waveguide analysis. FEM is convenient to find the solution of Maxwell’s equations for the homogeneous-core planner optical waveguide. FEM is very handy for the waveguides that have complicated cross-section waveguide geometries but homogeneous core such as rib structure, ridge structure, strip structure and others. FEM is a numerical method to find approximate solutions of boundary value problems. Several boundary conditions can be applied to FEM, such as PML (perfectly matched layer) and PEC (perfect electrical conductor). We used FEM to evaluate the modes inside the strip, high-mesa, rib and other waveguides. PML boundary condition has also been exploited to evaluate the leak mode.

Fig. B1: Step index multi-layer waveguide and its FEM simulation optical field profile.
C: Finite Difference Time Domain method (FDTD)

The finite difference time domain (FDTD) method is an exact solution to Maxwell’s equations. It does not have any theoretical restrictions or approximations. FDTD is widely utilized as a propagation solution method in integrated optics, especially when the adequate solutions are not obtainable by other methods, such as BPM (Beam Propagation Method). As shown in Fig. C1, small curvature of radius of our proposed waveguide is one of the situations to utilize FDTD. FDTD can cancel the round-off errors which could happen in BPM. FDTD could do this calculation in tow or in three dimensional processes.

Fig. C1: Bending loss calculation using FDTD simulation.
References


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