Hybrid Silicon / Lithium Niobate Modulators:

Design and Wafer Bonding

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# Glossary of Acronyms

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<td>AFM</td>
<td>Atomic force microscopy</td>
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<tr>
<td>Ar</td>
<td>Argon</td>
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<tr>
<td>ATR</td>
<td>Attenuated total reflection</td>
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<tr>
<td>BCB</td>
<td>Benzocyclobutene</td>
</tr>
<tr>
<td>CMOS</td>
<td>Complementary metal oxide semiconductor</td>
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<tr>
<td>CO₂</td>
<td>Carbon dioxide</td>
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<tr>
<td>CTE</td>
<td>Coefficient of thermal expansion</td>
</tr>
<tr>
<td>CVD</td>
<td>Chemical vapor deposition</td>
</tr>
<tr>
<td>CW</td>
<td>Continuous wave</td>
</tr>
<tr>
<td>DI</td>
<td>Deionized</td>
</tr>
<tr>
<td>DNFB</td>
<td>Dinitrofluorobenzene</td>
</tr>
<tr>
<td>EAM</td>
<td>Electro absorption modulator</td>
</tr>
<tr>
<td>EOM</td>
<td>Electro optic modulator</td>
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<tr>
<td>FCI</td>
<td>Free-carrier index change effect</td>
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<tr>
<td>FTIR</td>
<td>Fourier transform infrared spectroscopy</td>
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<tr>
<td>FWM</td>
<td>Four-wave mixing</td>
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<tr>
<td>GaAs</td>
<td>Gallium-Arsenide</td>
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<tr>
<td>H</td>
<td>Hydrogen</td>
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<tr>
<td>H₂O₂</td>
<td>Hydrogen peroxide</td>
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<tr>
<td>H₂SO₄</td>
<td>Sulfuric acid</td>
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<tr>
<td>HCL</td>
<td>Hydrochloric acid</td>
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<tr>
<td>He</td>
<td>Helium</td>
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<tr>
<td>HF</td>
<td>Hydrofluoric acid</td>
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<td>IC</td>
<td>Integrated circuits</td>
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IIR  Infinite impulse response
InP  Indium Phosphide
IR   Infrared
LED  Light-emitting diode
LiNbO$_3$  Lithium Niobate
MQW  Multiple quantum well
MZI  Mach-Zehnder interferometer
OTS  Octadecyl-trichloro-silane
QCSE Quantum-confined Stark effect
QW   Quantum well
SAM  Scanning acoustic microscopy
SAM  Self-assembled monolayers
SEM  Scanning electron microscope
Si   silicon
SiCl$_3$  Trichlorosilane
SiO$_2$  Silica
SOA  Semiconductor optical amplifier
SOI  Silicon on insulator
SPM  Self-phase modulation
SRS  Stimulated Raman scattering
TA   Thioacetate
TE   Transverse Electric
TM   Transverse Magnetic
V    volt
XPM  Cross-phase modulation
List of publications

Journal Publications:


Refereed proceedings publications:


Non-refereed presentations:

Abstract

Optical communication has provided the exclusive means for carrying high capacity data over long distances for over three decades. As modern data storage and computing rely increasingly on high-rate sharing of information, optics-based techniques steadily penetrate towards rack-level, board-level and even chip-level communications. The future growth of both computation and communication depends, to a large extent, on the successful integration of optical communication system functionalities alongside electronic integrated circuits on the silicon material platform. Hence, the realization of photonic devices on silicon, or silicon photonics, is a research area of much interest and significance.

While the silicon-on-insulator (SOI) material platform is generally favorable for making passive devices such as waveguides, interferometers and resonators, the properties of silicon raise several challenges to the implementation of active photonic devices such as electro-optic modulators and light sources. The state-of-the-art silicon-photonic light sources, amplifiers, modulators and detectors rely on the hybrid integration of additional electro-optic materials, most often InP-based semiconductors, on top of SOI waveguides. One material drawback of silicon is the absence of a second-order electro-optic effect. This effect is responsible for the change in refractive index through the application of external voltage, and is at the basis of electro-optic modulators, which are key components in optical communication networks. The most widely used material in electro-optic modulators is LiNbO$_3$. LiNbO$_3$ has a high electro optic coefficient, and the fabrication technology of LiNbO$_3$-based devices is mature and well established. The hybrid integration of LiNbO$_3$ alongside silicon in a single device is therefore of much interest and potential significance.

The work presented herein is part of a long-term research program, aiming to realize hybrid electro-optic modulators in LiNbO$_3$ over SOI. More specifically, the work addresses two main
challenges associated with that objective: the bonding of LiNbO$_3$ to silicon, and the design of the hybrid waveguide structure

The most commonly-used technique for bonding dissimilar electro-optic materials is direct bonding. Direct bonding is carried out without any additional intermediate layers. When clean and activated, mirror-polished, flat surfaces are put together subject to pressure and heat hydrogen bonds can initially form across the two surfaces. Following annealing at comparatively high temperatures of 300 – 700 °C, the hydrogen may be released and covalent bonds may form instead. Although this method is successfully employed, for example, in the fabrication of hybrid silicon-InP electro-optic devices, it is not applicable for the bonding of silicon and LiNbO$_3$ due to the mismatch in thermal expansion coefficients between the two materials. Another bonding method relies on the application of relatively thick intermediate adhesive layer. However, the adhesive could disrupt the coupling of light between the two media. Correspondingly, there are only a few reports of bonding LiNbO$_3$ to Silicon in the literature.

A large part of the work is dedicated to a new bonding paradigm, which relies on the deposition of self-assembled monolayers (SAMs) of specially-synthesized organic materials on both surfaces and their subsequent functionalization using chemical reactions. The SAMs modify the surface properties of the two materials in ways that permit their subsequent bonding at low temperatures. The wafer bonding procedure and its monitoring and analysis are described in detail. The advantage of this method is the use of a relatively low temperature of 120°C. Low bonding temperatures reduce the excessive thermal stresses across the bonding interface. The monolayer-based processed was successfully applied to the bonding of two silicon samples to one another.

On the design parts, two geometries are considered. First, a design with large electrodes spacing, on the order of hundreds of microns, is proposed and analyzed. This design is simpler to fabricate, but the large spacing restricts its potential operation of high voltages and low rates. Second, a more advanced device with closely spaced electrodes is also designed. Our analysis and
simulations suggest that hybrid silicon-LiNbO$_3$ modulators should be feasible, with a $V_{\pi}L$ product that is on the same order of magnitude as that of stand-alone LiNbO$_3$ modulators.

The final part of this thesis will discuss the bonding results. Despite several successes, the bonding of silicon to LiNbO$_3$ faced difficulties and most of the attempts did not result in actual bonding, and only showed handling strength. We attribute these difficulties primarily to unfavorable preparation conditions. Potential solution paths for bonding improvements are discussed in the summarizing section. I hope that with certain modifications in place for the bonding process, hybrid LiNbO$_3$ / silicon electro-optic modulators could be realized.
1. Introduction

Silicon photonics is a research subject dedicated to the implementation of electro-optic devices on the silicon material platform[1]. The field is of great significance, due to the promise of monolithic integration of electro-optic devices with silicon electronics [2]. However, silicon suffers from a few drawbacks from optical devices perspective. One such drawback is the absence of a second-order electro-optic effect [3]. This effect is responsible for the change in refractive index through the application of external voltage [4]. The effect is at the basis of electro-optic modulators, which are key components in optical communication networks. The most widely used material in electro-optic modulators is LiNbO$_3$. The electro optic coefficient of LiNbO$_3$ is a high: $30.88 \text{pm/V}$, and the fabrication technology of LiNbO$_3$ based devices is mature and well established [5].

The hybrid integration of LiNbO$_3$ alongside silicon in a single device is therefore of much interest and potential significance. One possible solution path towards silicon-photonic modulators relies on the hybrid integration of additional electro-optic materials, in our case LiNbO$_3$, on top of silicon waveguides. The main method used for bonding dissimilar electro-optic materials is direct bonding. Direct bonding is carried out without any additional intermediate layers. When clean and activated, mirror polished, flat surfaces are put one on top of the other under pressure and heat, hydrogen bonds can initially form across the two surfaces. Following annealing at high temperatures between 300 – 700 $^\circ$C, the hydrogen may be released and covalent bonds may form instead. Although this method is successfully employed, for example, in the fabrication of hybrid silicon-InP electro-optic devices [6,7], only few reports of bonding silicon to LiNbO$_3$ appear in the literature[8–13]. The bonding of LiNbO$_3$ and Silicon is particularly challenging, due to the mismatch in the coefficients of thermal expansion (CTEs) between Silicon and LiNbO$_3$. The mismatch is in the range of 188%–454% at room temperature and depends on the orientation of LiNbO$_3$: The CTE values are $2.6 \mu/K$ for Silicon, $14.4 \mu/K$ for X-cut LiNbO$_3$ and $7.5 \mu/K$ for Z-cut LiNbO$_3$ at 25$^\circ$C [14]. These CTE
levels do not allow for direct wafer bonding at high temperatures due to thermal stresses across the interface.

The thesis focuses on two critical aspects of the silicon / LiNbO$_3$ hybrid technology: the bonding between the two surfaces, and the design and simulation of the hybrid waveguide geometry, as well as the propagation of light in the combined structure.

1.1 Theoretical background:

1.1.1 Why Silicon photonics?

The main driving force behind the modern silicon photonics research is that of optical interconnects among computer boards, among processor chips and even within a single chip. For nearly a decade already, the operating speed of micro-electronic devices is no longer restricted by the switching time of transistor gates themselves, but rather by the delay associated with the electrical wiring inside the processor chip. Every squared centimeter of chip area has an estimated wiring length of 20 km! The complexity that is associated with such wiring length is immense. Even as early as 2003, processor chips had six different metallic layers. Nowadays they have even more. The reduction in dimensions and increase in density of electrical wiring give rise to a plethora of issues, such as prolonged latency and crosstalk among devices. Optical interconnect might, at least in principle, alleviate such problems.
Another major concern of the micro-electronics industry in recent years has to do with heat dissipation. Figure 1.1 shows the increase in the density of generated heat per unit area inside processor chips through the years. Perhaps surprisingly, the generated heat density is fast approaching that of a nuclear reactor! Nowadays, heat dissipation issues restrict the density of micro-electronic devices. Since devices cannot be packed any closer, progress in the operation speed of individual computer processors (the famous Moore’s Law) had stopped to a halt. The solution path that is widely adapted by the micro-electronics industry is based on multi-core architectures, in which the computational task is divided among several processors working in parallel. Efficient parallel processing relies critically on high-speed communication among the cores. With these architectures the significance of interconnects, and the potential benefits of their optical realization, become even more dramatic. Many researchers believe that the future integration of photonics together with silicon electronics is closely linked with the future of micro-electronics itself.

Therefore, the primary motivation for silicon photonic devices is their compatibility with the mature electronic silicon integrated circuits (IC). Silicon wafers have the lowest cost (per unit area) and the highest crystalline quality of any semiconductor material. Industry is able to produce micro-processors with billions of components all integrated into a thumb-size chip, and offer them at such
a low price that they appear in consumer electronics. Creating low-cost photonics for the mass market applications by exploiting the IC industry is a major motivation for silicon photonics.

There are several other advantages to using silicon for photonic purposes. Silicon is boasting a low-propagation-loss window, extending from the wavelength of 1.1 \( \mu \text{m} \) to nearly 7 \( \mu \text{m} \), as can be seen in Figure 1.2[16]. This transparency window includes the telecommunication wavelengths of 1.3 \( \mu \text{m} \) and 1.55 \( \mu \text{m} \), and also the middle-infra-red region that has many sensing and imaging applications. In addition, Silicon has a superior thermal conductivity, compared to most other photonic materials. For example, Gallium-Arsenide (GaAs), a III – V family semiconductor that is particularly suitable for active device applications, has a thermal conductivity that is an order of magnitude lower. Furthermore, the optical damage threshold, denoting the optical intensity for which the material is permanently damaged, is an order of magnitude higher in silicon compared to GaAs.

![The linear absorption spectrum of silicon](image)

**Figure 1.2** The linear absorption spectrum of silicon [16].

Silicon has a few nonlinear effects that are relatively strong. One such nonlinear effect is the Kerr effect, in which the refractive index of an optical medium is modified by the optical intensity of a propagating optical field [17]. The optical Kerr effect is responsible for several phenomena that can be used in silicon photonic devices: self-phase modulation (SPM), cross-phase modulation (XPM), four-wave mixing (FWM) and soliton formation [18]. Stimulated Raman scattering (SRS) is also rather pronounced in silicon. SRS is a nonlinear interaction in which the presence of molecular vibration at
THz frequencies ("optical phonons") modifies the effective refractive index of the optical medium and couples between light waves of different frequencies [19].

1.1.2 Passive devices in Silicon

By passive devices we refer to the routing of light in waveguide paths from one point on a photonic chip to another. Waveguide paths may split and combine to form filters, and even close into rings that provide feedback loops, also referred to as resonator structures. Devices in which light undergoes absorption and attenuation at particular locations or wavelengths also qualify as passive. Passive silicon-photonic devices are highly compact, provide low losses, withstand high intensities, and may operate in a broad range of wavelengths. In the following I briefly introduce three examples of passive photonic devices that are commonly realized in silicon:

1. **Directional coupler** — is an optical device that consists of two waveguides in proximity. The inputs of the two waveguides serve as input ports to the entire coupler structure, and the two individual outputs are the output ports. The two waveguides are not necessarily of equal geometry. The transfer of optical field between the two waveguides stems from the fact that part of the transverse profile of the mode propagating in each individual waveguide is in overlap with the core of the other [20].

![Diagram of a directional coupler](image)

Figure 1.3: left – top view of a directional coupler, consisted of two waveguides. The waveguides are in close proximity over a certain region. Right – transverse cross-section of the refractive index geometry of the two waveguides in proximity, $n_a$ and $n_b$ are the refractive indexes of the two waveguides, $n_c$ is the refractive index of the volume in which the two waveguides are places [21].

2. **Mach-Zender interferometer (MZI)** brings together two directional couplers in cascade. The two output ports of the first coupler are linked with the two inputs of the second one. The two
connecting waveguides are not necessarily of equal path lengths. In many cases the interferometer is purposely imbalanced, with one path introducing a delay that is longer than that of the other by a difference $\tau$ sec. The transfer function of cascaded MZIs is equivalent to a finite impulse response (FIR) filter [20].

![Schematic illustration of a Mach-Zender interferometer](image1)

**Figure 1.4 Schematic illustration of a Mach-Zender interferometer [21]**

3. **Ring resonators** Many useful filter architectures require an *infinite impulse response* (IIR). IIR filters include feedback loops that connect an output port back to an input port. The most common implementation of an IIR filter in planar optical waveguides is that of a *ring*. The ring resonator includes a closed-loop waveguide, and one or two couplers for input and output. The radii of the ring waveguides are restricted to tens of microns due to bending loss considerations[22].

![Schematic illustration of a ring resonator](image2)

**Figure 1.5 Left – Schematic illustration of a ring resonator. Right – several examples of fabricated micro-ring resonators on silicon [22].**
1.1.3 **Active devices in Silicon**

The role of silicon is more complex in active photonic devices. These include critical components such as light sources in the forms of light-emitting diodes (LEDs) and laser diodes, semiconductor optical amplifiers (SOAs), electro-optic modulators which imprint information upon a continuous optical field, and detectors. Silicon suffers from fundamental drawbacks which keep it from realizing few of these functionalities in a straight-forward manner. For example, the indirect semiconductor band gap of silicon makes it a poor converter of electrical current to light, a deficiency which makes the realization of silicon light sources very challenging. Also, the electro-optic effect which underlies the operation of modulators in several other materials is practically absent in silicon. Therefore, integration of additional materials is often needed to realize active devices on silicon. In the next section we focus on modulators, which are the objectives of this work.
2. **Electro Optic modulators (EOM):**

   An electro-optic modulator (EOM) is a device which uses an electrical input waveform to modify the amplitude and / or phase of an incoming light wave. The role of an electro-optic modulator in a communication system is to super-impose data, which exists in the electrical domain, onto a continuous wave (CW) optical carrier.

2.1 **Modulation Principles**

   In traditional optical communication, the data is carried as binary on/off keying of the optical amplitude: a logical '1' is represented by some level $P$ of the optical power, whereas a logical '0' is represented by transmitting (ideally) no power. There are two ways to obtain amplitude modulation: The first is *direct* modulation, in which the current driving a laser diode light source is being modified. The advantage in this method is that it doesn't require additional components. However, it imposes severe restrictions upon the modulation rate, and introduces parasitic frequency modulation (referred to as 'chirp') [23]. The second method is known as *external* light modulation, in which an additional component modifies the amplitude of a laser source which is operated in continuous-wave mode.

   Two types of external modulators are widely used commercially:

   a) **Electro-absorption modulators (EAMs)** [24], which directly modify the amplitude of a propagating optical wave. Its principle of operation is based on the Franz-Keldysh effect [25]: an applied electric field changes the bandgap energy, which in turn modifies the absorption spectrum. EAMs make use of a waveguide that is made with a semiconductor material whose bandgap is slightly higher than the energy of incoming photons. Therefore, the material is nominally transparent. However, the material bandgap can become smaller with the application of an external voltage, making the material highly absorptive.
Many EAMs make use of multiple quantum wells (MQWs): thin layers of low-bandgap semiconductor which lie in between barriers of higher bandgap. The spatial confinement leads for discretization of the electron and hole energy levels in the structure. Absorption in MQW is typically stronger than in bulk semiconductor media [26], due to the spatial overlap between the electron and hole wave functions. EAMs in MQWs make use of the quantum-confined Stark effect (QCSE) [27]: an external electric field pulls electrons and holes in opposite directions, thereby reducing their spatial overlap and the absorption efficiency. EAM is effective for photon energies slightly below the medium bandgap. The bandgap of silicon, which corresponds to a wavelength of approximately 1100 nm, is far larger than the energy of photons at the telecommunication wavelength of 1550 nm. Therefore, the effect is inadequate for use in silicon modulators.

b) Electro-optic Mach-Zender interferometer (MZI) modulators, in which the phase in one of the arms is modified in order to switch between constructive and destructive interference at the output. LiNbO₃ is the material of choice in most modulators of this type. Phase modulation in LiNbO₃ through the electro-optic effect is discussed in the following section.

![Figure 2.1 Schematic illustration of a Mach-Zender interferometer electro-optic modulator](image)

**2.2 Linear electro-optic effect (Pockels effect)**

Electro-optic phase modulation relies on the Pockels effect, in which the refractive index of the optical medium is modified by an external voltage. The Pockels effect stems from a second-order nonlinear susceptibility, which can only exist in materials with a non-centro-symmetric crystalline
structure [28]. Silicon, whose crystalline arrangement possesses a center of symmetry, does not support this effect.

The Pockels effect is particularly pronounced in LiNbO$_3$. The extent of refractive index change in a LiNbO$_3$ crystal depends on the relative orientations of the external field, the electric field vector of the optical-frequency wave, and the orientation of the crystal. Different arrangements will be addressed in detail later. An order of magnitude estimate can be obtained as follows. Subject to an external voltage $V$, the electro-optic change in refractive index is given by [29]:

$$\Delta n = \frac{1}{2} n_{\text{LiNbO}_3}^3 \cdot r_{33} \cdot \frac{V}{d}$$

(1)

where $d$ is the distance between the electrodes surrounding the crystal, $n_{\text{LiNbO}_3} = n_0 = 2.21$ is the refractive index for linear propagation, and its numeric value would depend on the polarization and crystalline alignment, and $r_{33} = 30.88 \frac{\text{pm}}{V}$ is an element out of the electro-optic tensor of the crystal (see following sections).

### 2.3 Silicon Modulators

Before we proceed to describe our proposed solution of hybrid silicon and LiNbO$_3$ modulators, let me briefly describe contemporary efforts for the implementation of all-silicon modulators[30,31] and other hybrid configurations. The modulation in silicon relies on the free-carrier index change effect (FCI). Carriers can be introduced either by electrical injection, or via absorption of light at a shorter wavelength. Due to FCI, changes in the number of carriers translate into a change in the refractive index, which in turn leads to a change in the optical phase that is acquired by propagating waveforms. Phase changes can be converted to intensity modulation in either MZI of ring resonator arrangements as described earlier. Several examples are provided below.

One demonstration, which was provided by the group of Prof. Michal Lipson from Cornell University in 2005 [1], makes use of a ring resonator that is located within a p-n junction.
The ring waveguide is made of intrinsic silicon. A bias voltage across the junction introduces carriers which accumulate in the waveguide region and modify its refractive index via FCI. As a result, the periodic transmission notches of the ring resonator through-port shift in frequency. Ring-resonator-based modulators suffer from a major fundamental drawback: they require an input signal at specific discrete wavelengths for their proper operation. Another inherent difficulty is the relatively slow process of carrier injection into silicon junctions, or the order of 1 ns, which is the equivalent to about 1 GHz modulation bandwidth. With some improvements, bandwidths of 5 GHz can be achieved.

The second example was reported by the group of Prof. Yurii Vlasov at the Thomas Watson research center of IBM corp. in 2007[33]. The device once again relies on carrier injection into an intrinsic waveguide that is located within a p-n junction. This time, however, the waveguides are arranged in a MZI layout rather than a ring resonator.
In order to overcome the slow rise time of injected carriers, the analog shape of the pulses was heavily pre-emphasized. Such electronic pre-emphasis might be difficult at higher data rates. The advantage of this modulator is that it supports any incoming wavelength, and it operates at low voltages of 0.3V difference between 'on' and 'off' states. Nonetheless, it is restricted to about 10GHz bandwidth, which isn't enough.

Recently, the bandwidth of all-silicon electro-optic modulators was extended to 40Gbit/s and even 50Gbit/s by the group of G. Reed from University of Surrey, UK [34]. The device is based on a rib waveguide of height 220nm, width 400nm and slab height 100nm. A selfaligned process is used to form the p-n junction that is offset to the edge of the waveguide. The offset of the junction position is significant to the broad bandwidth operation. This p-n junction is connected to coplanar waveguide (CPW) electrodes which are used to drive the device at high speed. Figure 2.4 shows a cross section of the phase modulator.
The phase modulator is incorporated into asymmetric MZI structure with an arm length mismatch of 180μm to convert between phase and intensity modulation. The phase modulator was about 1 cm long, and it was modulated by about 3V. The modulation extinction ratios for 40Gbit/s and 50Gbit/s were in excess of 10dB and 3dB respectively. The losses of the phase shifter were between 2.7dB/mm and 4dB/mm.

Despite the impressive recent progress, the bandwidths of all-silicon modulators are still narrower than those of hybrid devices, which are introduced next.

### 2.4 Hybrid Silicon/InP modulators:

State-of-the-art silicon-integrated modulators rely on hybrid integration of InP-based semiconductor alloys on top of silicon waveguides [24]. Both EAMs and FCI-based MZI modulators have been demonstrated based on this generic strategy. These modulators can be integrated with lasers [35], amplifiers, and photodetectors [27] using quantum well intermixing [36]. A hybrid Silicon/InP EAM consists of a MQW InP region that is bonded on top of a waveguide in a silicon-on-insulator (SOI) wafer.

This structure uses a III-V epitaxial stack originally grown on an InP substrate. InGaAlAs is chosen as the MQW material because it provides a stronger carrier confinement and produces a strong quantum confined stark effect (QCSE) [37] and hence a better modulation efficiency through
The device fabrication process can be divided into three major parts. First, the silicon waveguides and any other desired passive devices are fabricated in a CMOS-compatible fabrication process. Next, the III–V epitaxial layer structure is transferred to the silicon waveguides through an O₂ plasma-assisted, low-temperature bonding process (see later section for a detailed discussion of wafer bonding procedures). Finally, structures in the InP-based layers are defined post-bonding [39].
A hybrid silicon/InP modulator was first demonstrated by the group of J. Bowers at the University of California at Santa Barbara (UCSB). Their devices required only $4V$ over a relatively short length of 1 mm, along with a bandwidth of 100 nm and could handle 20 mW of optical power [40]. The same group recently extended the modulation bandwidth of their hybrid silicon/InP devices to beyond 67 GHz [38].

2.5 Hybrid Silicon/LiNbO$_3$ modulators:

As stated earlier, the long-term objective of the research program is to try and carry over the hybrid integration principle described above to the fabrication of silicon/LiNbO$_3$ modulators. In this section I introduce the general architecture of such devices.

Waveguides made of dielectric materials consist of a high-index core, which is surrounded by regions of lower index referred to as cladding. The guiding of light is based on its tendency to "be drawn into" the regions of high refractive index. The optical field propagates in waveguides in the forms of modes, which are solutions to Maxwell's equations that satisfy the appropriate geometric boundary conditions. When the contrast in refractive index between core and cladding is large, the spatial distribution of the guided mode intensity tends to confine itself to the core region.
We use silicon-on-insulator (SOI) wafers as a material platform for the design of a planar waveguide circuit. An SOI wafer consists of a silicon substrate whose thickness is hundreds of μm, a layer of SiO$_2$ (silica), also referred to as buried oxide or BOX, and an upper layer of silicon known as the device layer. The thickness of the silica layer is typically in the range of 1 – 3μm, and the device layer thickness varies between 100nm and 2μm. SOI wafers offer a particularly large contrast index, between that of silicon ($n = 3.45$) and that of SiO$_2$ ($n = 1.45$). This index contrast leads to particularly tight confinement of the modal intensity, which scales down the cross-section of photonic devices to hundreds of nanometers level. The silica layer has a critical role in preventing the leaking of the modal energy into the underlying bulk silicon substrate.

On top of the SOI, we intend to bond a bulk of LiNbO$_3$ ($n_0 = 2.21$), in which electro-optic modulation takes place. The integrated device should be designed to support a single hybrid mode, and to maximize the overlap of the transverse profile of this mode with the LiNbO$_3$ layer. Electrodes are deposited for the application of modulation voltage across the device. The voltage would modify the refractive index of the upper LiNbO$_3$ cladding layer, and hence the effective index of the hybrid mode as a whole and the accumulated phase in propagation along the device. Figure 2.7 shows a schematic illustration of the cross-section of the proposed hybrid device.

![Figure 2.7 A schematic drawing of the cross section of the hybrid modulator](image)

Figure 2.7 A schematic drawing of the cross section of the hybrid modulator
As mentioned above, the combination of mature and well established manufacturing industry and passive waveguides properties of silicon and the electro-optic properties of Lithium Niobate appears an appealing approach towards hybrid electro optic modulators. On the other hand, LiNbO$_3$ and silicon have very different thermal expansion coefficients, which prevent the evaporation of LiNbO$_3$ on silicon [14]. Therefore careful bonding techniques are necessary for such integration.

2.5.1 Bonding techniques for use in silicon photonics

The two main methods for bonding dissimilar electro-optic materials are direct bonding and adhesive bonding using polymers. Direct bonding is carried out without any additional intermediate layers. When clean and activated, mirror polished, flat surfaces are put one on top of the other under pressure and heat, hydrogen bonds can initially form across the two surfaces. Following annealing at high temperatures between $300 - 700^\circ C$, the hydrogen may be released and covalent bonds may form instead [41]. Adhesive-based bonding employs an intermediate thermosetting polymer layer such as benzocyclobutene (BCB) based polymers. In BCB-mediated bonding, a diluted oligomer solution is first spin-coated on the surface of one sample. The solvent is then evaporated, the two samples are attached and the adhesive is cured [42].

Although both methods are successfully employed, for example, in the fabrication of hybrid silicon-InP electro-optic devices, they are not without drawbacks. Direct bonding suffers from out-gassing of by-products such as hydrogen or water which can lead to local de-bonding. It also does not tolerate even modest levels of contamination and surface roughness. In the case of direct bonding of silicon and LiNbO$_3$, the thermal expansion coefficients mismatch between the two materials would induce excessive thermal stresses. BCB-based bonding results in a relatively thick interface which can hinder the coupling of light and the thermal conductivity across the interface. Therefore, new methods should be explored for the bonding of silicon and LiNbO$_3$. 

20
2.5.2 **Reported attempts for bonding silicon and LiNbO$_3$**

There are several reports of bonding these two materials together in the literature [8–13]. The first two use thin layers of LiNbO$_3$ that are transferred onto silicon substrates using ion implantation and subsequent silver diffusion or laser irradiation [8,9]. In one method layer transfer was induced by laser irradiation in conjunction with ion implantation. The technique was developed by the group of Harry A. Atwater from California Institute of Technology [8]. High-dose and high-energy H$^+$ and He$^+$ co-implantation is used to synthesize a buried damage layer in the LiNbO$_3$ bulk crystal, which is bonded to the Si substrate. After bonding, high power CW-CO$_2$ laser-irradiation leads to formation and lateral propagation of gas microcavities at the buried damage layer through the rapid absorption of radiation and heat, eventually leading to localized layer exfoliation from the LiNbO$_3$ donor substrate. Large-area single-crystal LiNbO$_3$ thin films ($6 \, mm^2$, $200 - 800 \, nm$ thick) have been transferred to silicon substrates. However, this method creates cracks along particular orientations of the LiNbO$_3$ thin film. In addition, ion implantation is complex and not always accessible outside specialty foundries.

A second method by the same group was based on silver diffusion bonding and layer transfer of Lithium-Niobate to silicon [9]. A Lithium-Niobate crystal was co-implanted with hydrogen and helium ions. Silver was evaporated on both the implanted Lithium Niobate and silicon substrates and the silvered surfaces were then bonded together at $500\, ^\circ C$. The high temperature anneal caused the silver layers to bond together. Simultaneously, the annealing induced crack formation within the Lithium Niobate at the peak implantation depth. As a result, a layer of Lithium Niobate, whose thickness corresponds to the peak depth of ion implantation, was transferred to the silicon handle substrate. A transmission electron microscopy image of the bonding interface is shown in Figure 2.8. The presence of a metallic silver layer at the interface between silicon and LiNbO$_3$ would disrupt the coupling of light between waveguides each material.
Figure 2.8 Transmission electron image of the extracted lamella. From bottom to top the layers are silicon, the bonded silver layer, Lithium Niobate, and the protective platinum layer[9].

The next two methods use bulk LiNbO₃ that was bonded through the deposition of intermediate Fe layers [11], or using Ar beam sputter etching [12]. One method has been developed by M.M.R Howlader and T. Suga from the University of Tokyo and M.J. Kim from The University of Texas at Dallas [11]. LiNbO₃ wafers were sputtered separately in the processing chamber by a low energy argon ion beam, and deposited with Fe ions. Bonding was performed under a load of 50 kg at room temperature. Figure 2.9 shows the infrared transmission image of Silicon/LiNbO₃ interface: The entire area of LiNbO₃ was bonded completely, and Silicon/ LiNbO₃ interface had no macro- or micro-voids.

Figure 2.9 Infrared transmission image of Si/ LiNbO₃ bonded by the modified SAB process at room temperature[11].

Another technique was developed by H. Takag, R. Maeda and T. Suga from the University of Tokyo [12]. It involves room-temperature wafer bonding of Si to LiNbO₃ by Ar-beam surface activation. The LiNbO₃ wafers undergo cleaning processes, and then placed in high vacuum. Both
silicon and LiNbO$_3$ specimens were sputter etched simultaneously by Ar beam. After sputter etching, the specimens were mated in the vacuum chamber, under applied pressure of 1MPa, however, fracture from the LiNbO$_3$ bulk was observed after preforming tensile tests.

In the next notable example, micron-thick platelets of LiNbO$_3$ were cleaved off a bulk crystal and directly bonded onto SOI waveguides and resonators [10,13]. It has been developed by the group of William H. Steier at the University of Southern California (USC) [10]. The process flow is as follows: He$^+$ ions were implanted into a bulk single crystal LiNbO$_3$ wafer. The implantation energy of 380 keV was selected in order to obtain implantation depth of 1.1μm, where a structural defect layer was formed. The implanted sample was pressed onto a SiO$_2$ coated Si wafer and heated to 170°C in air. Due to the difference in thermal expansion, and because the bonding strength of direct bonding is very weak at 170°C, single crystal LiNbO$_3$ films are separated from bulk LiNbO$_3$ wafer and are not bonded to the substrate. The free standing single crystal platelets are ~1μm thick and they have various widths (15 – 100μm) and lengths (0.4 – 2mm). Many of them are curved at radii between 230μm and 260μm, due to stress caused by the crystal damage in the implanted layer. The platelets can be 'straightened' by high-temperature annealing (1000°C for 3 hours). Individual micro-platelets can be picked up from the surface by the electro-static attraction between an optical fiber tip and the platelet, moved to another substrate, positioned, and subsequently bonded to the new substrate.
Figure 2.10 The procedure for obtaining single crystal LiNbO$_3$ micro-platelets and transferring and integrating them on Si-on-insulator substrate[10].

The micro-platelets were bonded directly on silicon ridge waveguides and on micro-ring structures, at 500°C for 4 hours. Electro-optic modification of the resonator transfer function [13] has been demonstrated. To the best of my knowledge, this is the only example of a hybrid silicon/LiNbO$_3$ electro-optic device. Nonetheless, the splitting and handling of micro-platelets is cumbersome, at best.

Figure 2.11 The integration procedure for the hybrid structure LiNbO$_3$ micro-platelet and silicon micro-ring waveguide[10].

As a major part of this research project, we propose and implement a novel method for wafer bonding of silicon to LiNbO$_3$. It relies on the deposition of self-assembled monolayers (SAMs) on both surfaces and their subsequent functionalization using specific chemical reactions, which allow
for the bonding of the two surfaces at low temperatures. The bonding is formed through covalent bonds across the surfaces, via the monolayers. The bonding interface is only a few nm thick, and does not disrupt optical coupling. Moreover, the relative hydrophobicity of the monolayer coatings is likely to reduce problems associated with the contamination of surfaces with dust particles.
3. Device design

3.1 Device structure

Two phases of goal devices are targeted as a demonstration of the hybrid material integration principle:

- **Phase a**: Bulk LiNbO$_3$ bonded on top of a silicon waveguide in SOI platform (Figure 3.1, left), with electrodes evaporated on the top LiNbO$_3$ surface and the bottom silicon surface. The implementation of this design would be restricted to low-rate, high-voltage electro-optic modulation. The design of the silicon waveguide dimensions aims to optimize the evanescent penetration of the modal transverse profile into the LiNbO$_3$.

- **Phase b**: Same as above, with electrodes evaporated on the exposed silica surfaces (or residual un-etched silicon) to the sides of the waveguide, in order to reduce the required voltage levels (Figure 3.1, right).

Figure 3.1 Potential geometries of hybrid silicon / LiNbO$_3$ electro-optic modulators.
3.2 Hybrid waveguide design

When light is coupled into a waveguide, it propagates with mode profiles that are determined by solutions to Maxwell's equations, subject to the appropriate boundary conditions that are imposed by the geometric design. The waveguide consists of a silicon core of width $b$ and thickness $d$, surrounded by a silica lower cladding and a LiNbO$_3$ upper cladding. The cladding regions to the sides of the waveguide core are air-filled etched trenches. The waveguide cross-section used in numerical simulations is shown in Figure 3.2.

![Schematic drawing of the hybrid waveguide device cross-section.](image)

Figure 3.2 Schematic drawing of the hybrid waveguide device cross-section. The waveguide consists of a guiding Si layer of thickness $d$ with a refractive index $n_2$, surrounded by LiNbO$_3$ and Silica medias of refractive index $n_1$ and $n_3$ respectively

LiNbO$_3$ is a crystal with anisotropic structure, therefore its refractive index is different depending on the direction in which the optical-frequency electric field is pointing. The coordinate system used to describe the physical properties of LiNbO$_3$ is a Cartesian $x$, $y$, and $z$ system. We follow [43] in the crystallography definition of LiNbO$_3$ $x$, $y$ and $z$ cuts. The crystal planes are presented in Figure 3.3. In our hybrid devices, axis cut is perpendicular to the plane of the bonding.
The $x$ and $y$ axes, for which the refractive index is the same, are referred to as the *ordinary* axes with an *ordinary refractive index* $n_0$, whereas the $z$ axis is known as the *extra-ordinary* axis, with an *extra-ordinary refractive index* $n_e$. The values of the two indices are $n_0 = 2.21, n_e = 2.138@\lambda = 1550\,\text{nm}, T = 300^\circ\text{C}$ [45]. For example, let us assume for the moment that the optical-frequency electric field is in the direction of the $x$ axis of the crystal, and that the mode is propagating along the $z$ axis. The transverse profile of the refractive index within the device would be of the form:

$$n(x, y) = \begin{cases} 2.21 & x > \frac{d}{2} \\ 3.45 & -d/2 < x < d/2, -b/2 < y < b/2 \\ 1 & -d/2 < x < d/2, y < -b/2, y > b/2 \\ 1.45 & x < -d/2 \end{cases}$$

(2)

The exact solution of Maxwell's equations for these boundary conditions cannot be provided analytically. Numeric simulations are used for calculating profiles and effective indices of the propagating modes in the hybrid structure, and their overlap with the various structural layers.
parameters that control the mode profile are the operating wavelength, the polarization of the incoming beam, the thickness and width of the layers, and the crystalline alignment of the LiNbO$_3$ with respect to incoming state of polarization.

Propagating modes may be classified according to the directions of their electric and magnetic field components:

- TE modes (Transverse Electric), which have no electric field in the direction of propagation.
- TM modes (Transverse Magnetic), which have no magnetic field in the direction of propagation.
- Hybrid modes, which have both electric and magnetic field components in the direction of propagation.

Due to the difference in boundary conditions, the propagation constant of a TM mode of a given order is somewhat different from that of the corresponding TE mode. This phenomenon is called birefringence, meaning that electric fields aligned at different directions experience a different effective index inside the waveguide, and hence propagate at different velocities. When the light at the waveguide input consists of a combination of TE and TM components, each component would excite the corresponding mode and propagate accordingly. When the TE and TM components are added together at the output of the waveguide the different phases they had acquired could lead to substantial distortion. In addition, TE and TM modes could experience unequal losses. In principle, it is preferable to excite just one mode, either TE or TM. The choice between the two will take into consideration the strength of the corresponding electro-optic tensor coefficient, as addressed later.

Another design consideration is the modal confinement $\Gamma$, which quantifies the fraction of optical power that is confined to a specific area in the waveguide. The silicon confinement factor refers to the fraction of optical power that is confined to the core, and the LiNbO$_3$ confinement
factor relates to the optical power that is confined to the upper LiNbO₃ cladding. In general, the silicon confinement factor increases as the height or width of the silicon waveguide increases, while the LiNbO₃ confinement factor decreases. We are interested in maximizing LiNbO₃ confinement factor, to achieve a stronger modulation effect. At the same time, confinement in silicon cannot become too small, or else the guided mode would easily diffract into the upper LiNbO₃ cladding. Single mode propagation in the device is also important, since it prevents modal dispersion. Modal dispersion occurs when the incoming light source excites a multiple propagating modes, with each projection propagating at a different group velocity. Differences in accumulated delay lead to waveform distortion. When only a single propagating mode is supported, there is obviously no modal dispersion. The single-mode condition is met when the waveguide’s core size is reduced. The above consideration can be illustrated through the analytic solution for a simplified, one-dimensional asymmetric slab waveguide illustrated below:

![Figure 3.4 illustration of one-dimensional asymmetric slab waveguide](image)

With \( n_1 = n_{LiNbO_3} = 2.21, n_2 = n_{Si} = 3.45, n_3 = n_{SiO_2} = 1.45, \lambda = 1.55 \mu m \).

The single mode condition for TE and TM modes propagation is [21]:

\[
\frac{\lambda}{2\pi \sqrt{n_2^2 - n_1^2}} \times \tan^{-1}\left(\frac{n_2^2 - n_3^2}{\sqrt{n_2^2 - n_1^2}}\right) \leq d_{TE0} \leq \frac{\lambda}{2\pi \sqrt{n_2^2 - n_1^2}} \times \tan^{-1}\left(\pi + \frac{n_2^2 - n_3^2}{\sqrt{n_2^2 - n_1^2}}\right)
\]
Where \( d \) is the height of the core. Using the above numerical values, we find: 21.76nm \( \leq d_{\text{TE}0} \leq 314\text{nm} \), 86.6nm \( \leq d_{\text{TM}0} \leq 379\text{nm} \).

The single-mode condition for the two-dimensional waveguide must be obtained numerically, and it would depend on both height and width of the silicon core. Nevertheless, the above values give an order-of-magnitude estimate for the necessary core thickness. Fortunately, the device layer thickness in most readily-available SOI wafers is 220nm, in good agreement with the above consideration. This is the thickness chosen in my design. The width of the waveguide was taken initially to be 450nm.

Additional key metrics of the devices are mentioned next for completeness, although their quantitative analysis is beyond the scope of this work. These include the coupling of light into the hybrid waveguide, propagation losses along the waveguide, and the modulation extinction ratio. Coupling losses are governed by the flatness and quality of the waveguide facet, and by the dimensions of the core. Coupling losses between standard fibers and SOI waveguides were reduced to 1 dB using annular gratings. Propagation losses depend primarily on the nano-scale roughness of the waveguide sidewalls. Values below 1 dB/cm were obtained. The extinction ratio of the modulator, signifying the ratio between the output power for '1' and '0' states, is primarily determined by the driving electronics.

### 3.2.1 Modulator operation voltage and length calculation

Due to the Pockels effect in LiNbO\(_3\), the application of an electric field changes the refractive index of the material. In the following a quantitative description of the index modification is provided. The effect can be analyzed within the framework of the index ellipsoid formalism. The index ellipsoid is a useful geometric interpretation of the refractive index for the propagation of light in a given medium, as a function of the direction of propagation, state of polarization and crystalline
orientation in the medium. In the most general case, the ellipsoid is a surface in a three-dimensional Cartesian space that is defined by the following equation:

$$\eta_{11}x^2 + \eta_{22}y^2 + \eta_{33}z^2 + 2\eta_{12}yz + 2\eta_{23}xz + 2\eta_{13}xy = 1$$  \hspace{1cm} (5)$$

The index ellipsoid serves to describe the optical propagation properties within an anisotropic material as follows: For a given propagation vector \( \vec{k} \), a plane perpendicular to \( \vec{k} \) is drawn through the center of the ellipsoid. The plane intersects the surface of the ellipsoid, forming an ellipse. The lengths of the long and short axes of this ellipse provide the two possible values for the material refractive index for the given propagation direction. The orientation of these axes represents the states of polarization of the two associated vectors.

In the specific case of the LiNbO\(_3\) crystal, and in the absence of an external field, the index ellipsoid of the is of the simpler form [19]:

$$\frac{x^2}{n_0^2} + \frac{y^2}{n_0^2} + \frac{z^2}{n_e^2} = 1,$$

where the coefficients of the ellipsoid equations are readily identified in relation to the refractive indices for light polarized along each of the axes: \( \eta_1 = \eta_2 = 1/n_0^2 \) and \( \eta_3 = 1/n_e^2 \). The ordinary index \( n_0 \) corresponds to light that is polarized along the \( x \) or \( y \) axes whereas the extra-ordinary index \( n_e \) relates to a \( z \)-polarized field.

Subject to an external electric field vector \( \{E_x, E_y, E_z\} \), the lowest-order modifications to the index ellipsoid coefficients are governed by the coefficients of the \( 6 \times 3 \) electro-optic tensor \( r_{ij} \):

$$\Delta \eta_i = \sum_j r_{ij}E_j$$  \hspace{1cm} (7)$$

The tensor of LiNbO\(_3\) is of the form:
For example, the index ellipsoid index subject to the application of an external field along the $z$-axis becomes:

$$x^2\left(\frac{1}{n_0^2} + r_{13}E_z\right) + y^2\left(\frac{1}{n_0^2} + r_{13}E_z\right) + z^2\left(\frac{1}{n_e^2} + r_{33}E_z\right) = 1$$

(9)

We can recognize in the modified equation new equivalent values for the refractive indices for the three directions of propagating optical fields in the crystal:

$$\frac{1}{n_x^2} = \frac{1}{n_0^2} + r_{13}E_z, \quad \frac{1}{n_y^2} = \frac{1}{n_0^2} + r_{13}E_z, \quad \frac{1}{n_z^2} = \frac{1}{n_e^2} + r_{33}E_z$$

(10)

Where $n_o = 2.21, n_e = 2.138 @ \lambda = 1.55\mu m$ (1)(2), $r_{13} = 9.6\frac{pm}{V}$ and $r_{33} = 30.88\frac{pm}{V}$ [45,46].

Since the modifications to the refractive index are generally small, they can be approximated by:

$$n_z = \frac{n_o}{\sqrt{1 + n_e^2 r_{33} E_z}} \approx n_o \frac{n_e^3 r_{33} E_z}{2}$$

$$\Delta n_z = n_z - n_o = -\frac{1}{2} n_e^3 r_{33} E_z$$

(11)

$$\Delta n_{x,y} = n_{x,y} - n_o = -\frac{1}{2} n_o^3 r_{13} E_z$$

(12)

$$n_{x,y} = n_o - \frac{1}{2} n_o^3 r_{13} E_z$$

(13)
We would choose the alignment of the LiNbO$_3$ crystal and the state of polarization of the incoming optical field so that the electro-optic index modulation is maximized.

Consider a uniform electric field, $E_z = \frac{V}{d}$, where $V$ is the voltage that falls across the LiNbO$_3$, and $d$ is the effective thickness of the LiNbO$_3$ that is between the electrodes. The electro-optic phase modulation following propagation in the waveguide of length $L$ is:

$$\Delta \varphi = \frac{2\pi}{\lambda} \Delta n \times L = -\pi \frac{V}{V_\pi}$$

(14)

Here, $V_\pi$ is defined as the voltage that is required for a $\pi$ phase shift. For the specific example:

$$V_\pi = \frac{\lambda d}{n_e^2 r_{33} L}$$

(15)

The primary figure of merit of an electro-optic modulator is the product $V_\pi L$, which should be made as small as possible. The device geometry will be designed towards that objective. As discussed earlier, a phase modulator can be embedded with a MZI to provide intensity modulation.

![Figure 3.5 - MZI using the electro optic modulator](image)

Two different designs will be considered. In both, as will be addressed shortly, the properties of the optical mode are such that the optical-frequency electric field lies in parallel to the bonding interface. The crystalline alignment, however, would be different between the two designs. In phase $\alpha$ design, where the electrodes are placed on the top and bottom surface of the hybrid device as
shown in Figure 3.6, we choose z-cut LiNbO$_3$, so that the bonding plane is the $xy$ plane. Voltage in this design is applied along the $z$-axis of the crystal. Light will propagate in the waveguide along the $x$ axis, and its electric field would point in the $y$ direction. With these alignments, the $\tau_{13}$ tensor element governs electro-optic modulation. In phase $b$ design, the static electric field is for the most part in parallel with the bonding plane. In order to align this field yet again with the $z$ axis, we choose $x$-cut LiNbO$_3$ in this case. The optical mode would propagate in the $y$ direction, and would now point in the $z$ crystalline axis, just like the external static field. Therefore, the electro-optic effect in this case will be governed by the $\tau_{33}$ tensor element.

In the second configuration, since the electrodes are placed in close proximity to the waveguide, additional losses could occur due to potential overlap of the propagating mode and the metals. The electrodes must be separated further than the depth of penetration of the modal profile into the air outside the core, which is relatively small (less than 0.5 microns). Larger electrodes separation would reduce losses due to metal absorption, at the cost of a higher modulation voltage.

![Diagram showing electro-optic modulator configurations](image)

Figure 3.6 – Applied voltage and electrodes orientation of the modulator. The orientation of the axes in both panels relate to the crystalline axes of LiNbO$_3$. 
3.2.2 Waveguide dimensions

I analyzed the profile of the fundamental optical mode for different core widths.

Figure 3.7 and Figure 3.8 show the two-dimensional profiles of the six components of the electro-magnetic field for a hybrid waveguide with a silicon core that is 220 nm thick and 450 nm wide. The axes are labeled as follows: 'longitudinal' is in the propagation direction, 'lateral' is in the bonding plane, and 'perpendicular' is so to the bonding plane. The electric field is predominantly parallel to the bonding interface, in the lateral direction. The magnetic field is zero in the longitudinal direction, therefore the fundamental mode is of the TM category. Simulations suggest that the hybrid structure does not support propagating TE modes. Therefore, it works as an effective polarizer, with TE-polarized incoming light effectively blocked.

Figure 3.7 – Transverse profiles of electric field components. $E_{\text{lateral}}$ left, $E_{\text{perpendicular}}$ middle, $E_{\text{longitudinal}}$ right.
Figure 3.8 – Transverse profiles of magnetic field components. $H_{\text{left}}$ lateral, $H_{\text{middle}}$ perpendicular, $H_{\text{right}}$ longitudinal

The two dimensional electric field strength (in $V/m$) and effective index of the mode for different core widths are presented in Figure 3.9:

Figure 3.9 - Calculated two dimensional electric field strength ($V/m$) mode profiles with different silicon waveguide width of (a) 0.4 μm, (b) 0.45μm, (c) 0.5 μm and (d) 0.6 μm. The silicon waveguide height is fixed at 0.22 μm.

Figure 3.10 shows the silicon confinement factor, LiNbO$_3$ confinement factor, and the modal effective index as a function of the silicon core width. As the width increases, the silicon confinement factor increases as well as the effective index, while the LiNbO$_3$ confinement factor decreases. This trend reduces the efficiency of the electro-optic modulation. At a core width of 1μm, the waveguide can support two propagating modes. The second mode is presented in Figure 3.11. Multimode operation in a wide core is undesirable. On the other hand, a narrow core width would
make it difficult to couple light into the device and collect light out of it. I therefore chose an intermediate width value of 450 nm, which is routinely used in silicon photonics designs.

![Graph](image1.png)

**Figure 3.10** - Calculated confinement factors and effective index of the fundamental TM mode with different silicon waveguide widths.

![Graph](image2.png)

**Figure 3.11** - Calculated two dimensional electric field strength (V/m) mode profile of the second mode, with silicon waveguide width of 1 μm and height of 0.22 μm

### 3.2.3 Operation voltage and length results

We consider first the phase $\phi$ design [Figure 3.6 (a)]. Using a commercial numeric platform (Comsol), we calculated the effective index of the modulator without applied voltage to be
\( n_{\text{eff}} = 2.420373 \). The profile of the external electric field in this configuration resembles that of a dielectric capacitor, and it is expected to be uniform (see Figure 3.12).

![Simulated external electric field through the device in the large electrode spacing configuration](image)

Figure 3.12 – Simulated external electric field through the device in the large electrode spacing configuration

In this configuration, we can make use of the \( r_{13} = 9.6 \text{pm/V} \) tensor element. Since the electric field points in the \( y \)-axis of the crystal, we make use of the ordinary refractive index \( n_{\text{LiNbO}_3} = n_o = 2.21 \). Because of the large electrodes separation, high voltages are necessary. We consider an external voltage of \( 200 \text{V} \). Using an electro-static COMSOL analysis, I estimate the voltage drop across the region in which the optical mode penetrates into the \( \text{LiNbO}_3 \) cladding as \( 1.35V \) over \( d = 0.5\mu\text{m} \), leading to electro-optic index modulation in the cladding of:

\[
\Delta n = \frac{1}{2} n_{\text{LiNbO}_3} r_{33}^3 \frac{V}{d} = \frac{1}{2} 2.21 \cdot 9.6 \cdot 10^{-12} \cdot \frac{1.35}{0.5 \cdot 10^{-6}} = 1.4 \cdot 10^{-4}
\]

At this stage I repeated the numerical solution of the optical mode in the waveguide, albeit with a modified refractive index in the upper \( \text{LiNbO}_3 \) cladding. Since the mode is only in partial overlap with the \( \text{LiNbO}_3 \), the modification to the effective index is smaller than that of the upper cladding:

\[
\Delta n_{\text{eff-new}} = 2.8 \cdot 10^{-5}
\]
The estimated device length that is required for the given voltage is \( L = \frac{\lambda}{2\Delta n} = 2.8\text{cm} \), or \( V_\pi L \sim 560\text{Volt cm} \).

I repeated the electro-static analysis for the phase b design [Figure 3.6 (b)], having close electrodes spacing. In this configuration, we make use of the \( r_{33} \) tensor element, and since the electric field points in the z-axis of the crystal the relevant refractive index is now \( n_{Linbo_3} = n_e = 2.138 \). Figure 3.13 shows the distribution of an external static electric field, applied across the electrodes. Within the region that is in overlap with the optical mode, this field is predominantly aligned in parallel with the bonding interface plane. The external voltage in this configuration is much smaller due to the close spacing of the electrodes. A value of 5\( V \) was chosen. The electro-static analysis suggests that about 0.105\( V \) drop across the 0.45 \text{micron} lateral extent of the optical field. The corresponding device length for \( \pi \)-phase modulation is 5.5\( cm \), or \( V_\pi L \sim 27.5\text{Volt cm} \). The close spacing of the electrodes allows for an improvement in the device metrics by over a factor of 20. For comparison, the value of \( V_\pi L \) in standard LiNbO\(_3\) modulators is between 4.7 – 25.5\( \text{Volt cm} \), depending of the orientation of the crystal [5,47]. The tight modal confinement in a high-index-contrast SOI waveguide allows, in principle, for a closer electrodes separation than that of standard devices. That close spacing might be offsetting, to a large extent, the degradation due to the relatively small penetration of the mode profile into the LiNbO\(_3\) cladding.
Figure 3.13 – Comsol simulations of the voltage and electric field through the device in the close electrode spacing configuration. The colors present the voltage and the arrows show the electric field directions.
4. Wafer bonding using self-assembled monolayers

4.1 Bonding between silicon and LiNbO$_3$

In addition to the design and simulation of hybrid modulator performance, the work also addressed the main fabrication challenge of hybrid devices: the bonding of LiNbO$_3$ to silicon. The bonding must meet several requirements:

- The interface has to be strong and durable for a long time. It must also withstand the post-bonding processes of waveguide fabrication (evaporation of contacts etc.).

- The process should have potential for commercial scaling.

- A thin bonding interface is necessary (<50nm), to allow for effective coupling of light between structures in both materials.

As discussed at length in the previous section, the bonding between the two materials is difficult and challenging. Only few reports are provided in the literature, and only a single report describes the making of a hybrid device. Even that work required the splitting of micro-platelets of LiNbO$_3$ in a cumbersome procedure that is difficult to scale. In particular, use of direct bonding procedures with relatively high annealing temperatures is prohibited due to large thermal stresses.

Alternatively, we proposed and attempted a new paradigm for the bonding process, which is assisted by the deposition of single molecular layers of specially-synthesized organic materials on the surfaces of both substrates. The deposition occurs spontaneously in a solution which contains the monolayer-making molecules, in a process that is referred to as self-assembly [48]. Hence the term self-assembled monolayers (SAMs) is used in the following in relation to the bonding mechanism. While one terminus of the molecule is designed to attach to the substrate, the functional chemical group at the opposite terminus remains free-standing and defines the chemistry of a modified surface. The resulting dense and orderly array of these functional groups can be regarded as a
specialized form of surface activation. Following deposition, the functional groups are modified through chemical reaction, and brought into a form that readily attaches to the opposite modified substrate.

Before addressing the details of the deposition and activation processes, I will briefly introduce the field of SAMs, and the specific molecule that is underlying our procedures.

### 4.2 Self-assembled Monolayer (SAM):

Self-assembly is a process by which an organized structure can spontaneously form from simple parts on a variety of surfaces [49]. Self-assembled monolayers (SAMs) are highly ordered two-dimensional structures that are strongly anchored to a surface. Although these films are extremely thin (typically 2nm), they are able to completely change the surface properties. The most common adsorbate/substrate combinations are alkylsilanes on oxide surfaces [50], and sulfur-containing molecules on gold [51].

Since the first report on SAMs in 1983 by Lucy Netzer and Jacob Sagiv [50], the field of SAMs on Silicon oxide surfaces has grown immensely. Self-assembled monolayers on silicon oxide constitute ordered molecular platforms which can be employed in surface patterning and nanofabrication techniques, as well as for bio-chemical sensing [32],[33], lubrication[54], electrochemistry[55], photochemical mechanism[56], and electrical conduction[57].

The interaction between two monolayers deposited on opposing solid substrates, in order to form covalent bonds between the two organic monolayers, was studied by the group of Prof. U. Gosele at Max Plank Institute in Halle, Germany. The group reported the SAM-assisted bonding of two silicon wafers [58]. We demonstrate herein a modification of this methodology which takes advantage of controlled surface chemistry on well-defined functionalized monolayers and extends this bonding paradigm to non-silicon, optically active, materials, such as LiNbO₃ [59].
Components of SAMs

The SAM structure is usually divided into three parts: the anchoring group, the alkyl chain, and the free-standing surface functional group.

The anchoring group:

This group attaches to the oxidized surfaces, and forms an ordered, well-packed array of molecular chains. The choice of anchoring group is determined by the type of substrate onto which the chain will be deposited. The anchoring group used in our experiments is trichlorosilane (SiCl₃)[60] - a molecule containing silicon, hydrogen, and chlorine, that creates strong covalent bonds with the oxidized surface of SiO₂. Figure 4.1 below illustrates the molecular structure of SiCl₃.

![Figure 4.1 molecule structure of Trichlorosilane (SiCl₃).](image)

The alkyl chain:

This is an organic chain, that connects between the anchoring group and the functional group at the end of the molecule. Alkyl chains[61] consist of \( n \) CH₂ units: hydrogen and carbon atoms that are bonded exclusively by single bonds. The chains contribute to the packing of the monolayers, based on short-range van-der-Waals interactions among them, resulting in tightly packed arrays. The quality of the monolayer depends on the chain length. In most bonding experiments \( n = 9 \) was used, although successful bonding was achieved using \( n = 14 \) as well.
The functional group:

The functional group exposed on the outer edge of the monolayer determines the chemical and physical properties of the modified surface. We used two different functional groups:

1. **OTS (Octadecyl-trichloro-silane)**. As an initial stage, deposited monolayers consisted of octadecyl-trichloro-silane or OTS molecules, a commercially-available material comprised of a long hydrocarbon chain and the trichloro-silyl anchoring group, but with no other chemical functional group. The anchoring group is suitable for linking with the surface of either LiNbO₃ or the thin SiO₂ that naturally forms on the surface of silicon substrates. OTS is an ideal material for practicing the deposition of siloxane-anchored monolayers since it is more cost effective, while having the same deposition method and similar behavior to the more advanced monolayer used afterwards. Therefore, we preferred practicing the establishment of stable, uniform self-assembled monolayers (SAMs) on LiNbO₃ and silicon wafers, using OTS [59]. Figure 4.2 below illustrates the molecular structure of OTS:

![Molecular structure of OTS](image)

Figure 4.2 Molecular structure of Octadecyl-trichloro-silane(OTS).

2. **TA (Thioacetate)**. The next phase of the research was dedicated to the synthesis and deposition of more elaborate monolayers, bearing specific chemical functional groups on both LiNbO₃ and silicon wafer surfaces [62]. Thioacetate (TA) [63] is a functional group that allows, after a few additional chemical reactions, for the bonding between monolayers that are deposited on both surfaces.
4.3 **Wafer bonding procedure, based on self-assembled monolayers:**

The silicon samples used in this study were taken from n-type, $1 - 10 \ \Omega \cdot cm$, (100) oriented commercially-available wafers. The root-mean-squared micro-roughness of the polished wafer surfaces was verified by atomic-force microscopy to be on the order of 0.3 nm. The sizes of the samples were approximately $1 \times 1 \ cm^2$. The LiNbO$_3$ samples used were taken from commercially-available x-cut wafers. The root-mean-squared micro-roughness of the polished wafer surfaces was verified by atomic-force microscopy to be on the order of $0.3 - 0.4 \ nm$. The sizes of the samples were also approximately $1 \times 1 \ cm^2$.

The procedure was first established and demonstrated in the bonding of two silicon samples. The process is described below in much detail, while specific adjustments that were necessary for the bonding of LiNbO$_3$ will be addressed afterwards. The procedure consists of the following primary steps:

1. Cleaning and preparation of both surfaces using organic solvents and a ‘piranha’ acidic solution ($H_2SO_4$ (sulfuric acid) : $H_2O_2$ (hydrogen peroxide)), that yields a 1nm thick oxide layer on the treated surface:
   - The wafers are cleaned in chloroform ($CHCl_3$), acetone, and ethanol. Following each of these organic solvents, the substrates are rubbed with swab handles and then blown dry in a filtered nitrogen stream.

![Figure 4.3 Structure of the monolayer-forming molecule, with thioacetate group on the other end.](image-url)
A ‘piranha’ solution (H$_2$SO$_4$ (sulfuric acid) : H$_2$O$_2$ (hydrogen peroxide)) at a ratio 7:3 is prepared.

The wafers are immersed in the piranha solution test tube for 20 minutes, in a temperature of 80°C. This treatment cleans the surface from organic contaminants.

After the wafers are taken off the piranha solution, they are rinsed three times with deionized (DI), distilled water.

The wafers are immersed in 4% Hydrofluoric acid (HF) solution for 5 minutes followed by DI water rinse and blown dry using filtered nitrogen. The HF solution removes native oxide layer from the Si surface.

The wafers are again immersed in Piranha for additional 15 minutes to regrow an oxide layer. This treatment guarantees that the oxide layer is of known width and enables better examination by ellipsometry.

After the wafers are taken off the piranha solution, they are rinsed three times with deionized, distilled water.

The wafers are blown dry under a filtered nitrogen stream.

2. The deposition of the monolayer on both surfaces. The monolayer-forming molecule was introduced in detail earlier. The molecule and the assembly are illustrated in Figure 4.4.
The deposition phase details are:

- The synthesized monolayer-making molecules are mixed with dicyclohexyl in a dried test tube, at a ratio of 50 μL: 10mL.

- The wafers are put in this solution for 1 hour at room temperature.

- The wafers are cleaned in chlorophorm, blown dry under a filtered nitrogen stream, placed in ultrasonic cleaning in chlorophorm for 15 minutes, rubbed with chloroform and blown dry again under a filtered nitrogen stream.

- The wafers are cleaned in n-Hexane at a temperature of 80 °C for 6 minutes, put in a room-temp n-Hexane and blown dry with nitrogen.

- This cleaning process ensures that there are no leftovers from the monolayer solution on the coated Si surface.

The successful deposition is verified through measurements of the contact angle of a water droplet on the wafer surface, ellipsometry, and the infra-red absorption spectrum. These surface analysis methods will be presented in details in later sections.

3. A hydrolysis reaction for the modification of the terminating functional group on both surfaces. The reaction takes place in a mixture of hydrochloric acid (HCL) in methanol, at a
ratio of 1:9. It cleaves the thio-acetate group, leaving a thiol group instead [64]. The reaction is described in Figure 4.5.

![Chemical reaction diagram]

The reaction conditions are:

- The coated samples are put in the hydrolysis solution overnight (12 hours), at a temperature of 80 °C.
- The wafers are cleaned in chlorophorm, blown dry under a filtered nitrogen stream, placed in ultrasonic cleaning in chlorophorm for 15 minutes, and blown dry again under a filtered nitrogen stream.
- The wafers are cleaned in n-Hexane at a temperature of 80 °C for 6 minutes, put in a room-temp n-Hexane and blown dry with nitrogen.

The indication of a successful hydrolysis is seen both in the IR measurements and also by observing no change in contact angle.

4. A second chemical reaction is then carried out on either one or both silicon samples. A solution of 30 mg of iodine in 2 ml of methanol converts the thiol groups at the end of
some fraction of the molecules to disulphide groups instead [65]. The reaction is illustrated in Figure 4.6:

\[
\begin{array}{c}
\text{SH} & \text{SH} & \text{SH} & \text{SH} \\
\vdots & \vdots & \vdots & \vdots \\
\text{SiO}_2 \\
\end{array}
\quad \xrightarrow{\text{MeOH:I}_2} \quad \begin{array}{c}
\vdots \\
\text{S-S} & \text{S-S} & \text{S-S} \\
\vdots \\
\text{SiO}_2 \\
\end{array}
\]

\(n=9,14\)

Figure 4.6 A reaction for converting Thiol terminating groups to disulphide groups.

The reaction conditions are:

- The wafers are put in this solution for 15 minutes at room temperature.
- The wafers are rinsed in methanol, inserted to ultrasonic cleaning for 10 minutes in methanol, and blown dry under a filtered nitrogen stream.
- The wafers are cleaned in \(n\)-Hexane at a temperature of 80 °C for 6 minutes, put in a room-temp \(n\)-Hexane and blown dry with nitrogen.

5. Bonding of the two wafers. The bonding takes place within a home-made bonding press, shown in Figure 4.7.

Figure 4.7 The bonding press closed (left) and the bonding press open (right).
The samples are blown dry by nitrogen and placed on top of one another inside the press. A load of $\sim 160$ kPa is applied overnight at a temperature of 120°C. The bonding relies on the chemical reaction of disulfide exchange [65], illustrated in Figure 4.8:

![Illustration of a wafer bonding process, based on a disulphide exchange reaction among monolayers on both surfaces.](image)

Figure 4.8 Illustration of a wafer bonding process, based on a disulphide exchange reaction among monolayers on both surfaces.

### 4.4 Surface analysis

After the deposition of the monolayer, there is a need to characterize it. There are a number of ways to analyze and characterize the surface coatings. They are summarized in Table 4.1.
<table>
<thead>
<tr>
<th>Technique</th>
<th>Principle</th>
<th>Determination</th>
</tr>
</thead>
<tbody>
<tr>
<td>Contact angle measurement [62]</td>
<td>Characterization of surface properties by the interaction of a liquid drop with the surface.</td>
<td>Film packing and homogeneity, measure of the surface polarity.</td>
</tr>
<tr>
<td>Atomic force microscopy (AFM) [69]</td>
<td>Scanning probe microscopy based on non-covalent forces between probe tip and surface</td>
<td>Surface topography</td>
</tr>
<tr>
<td>Spectroscopic Ellipsometry [70]</td>
<td>Changes in polarization of the light due to reflection from a surface.</td>
<td>Films thickness and optical properties.</td>
</tr>
</tbody>
</table>

Table 4.1 Surface analysis techniques

**Contact Angle Measurement** is a simple method for characterizing the interfacial tension between a solid, a liquid, and a vapor. When a droplet of a high surface tension liquid (water) rests on a solid of low surface energy, the liquid surface tension will cause the droplet to form a spherical shape (lowest energy shape). Conversely, when the solid surface energy exceeds the liquid surface tension, the droplet is flatter. By viewing small droplets of liquid on a surface in profile, the effects of interfacial tension can be readily observed. In order to define these droplet profiles, a line tangent to the curve of the droplet is drawn at the point when the droplet intersects the solid surface. The angle formed by this tangent line and the solid surface is called the contact angle [62].
A bare silicon surface is naturally oxidized. Such a surface is normally hydrophilic, meaning that the contact angle of a water droplet on that surface would be small. After depositing OTS, the surface becomes hydrophobic, and a water droplet forms a large contact angle. Figure 4.9 shows a contact angle measurement of a droplet on an OTS-coated silicon. A large angle of 108° is observed, which is characteristic of a hydrophobic surface. The large contact angle is in contrast with angle of a droplet on an untreated Silicon surface, which is close to zero.

Figure 4.9 Contact angle measurement of a water droplet on an untreated Silicon surface (left) and on an OTS-coated Silicon surface (right).

**FTIR spectroscopy** [66] is based on absorption by molecular vibration levels in the mid-IR region. Implemented using attenuated total reflection (ATR), FTIR-ATR detects the organic molecules on the surface and shows absorptions that correspond to the vibrations characteristics of specific functional groups. The peak positions and intensities in the FTIR spectrum also provide information about the order, tilt and packing of the thin organic films. The IR spectrum is obtained by plotting absorbance versus the IR frequency, usually in units of wavenumber [cm\(^{-1}\)] [67,68].

Figure 4.10 Schematic illustration of an ATR-FTIR measurement of thin organic films
**Spectroscopic ellipsometry.** The most important application of ellipsometry is to study thin films. In the context of ellipsometry a thin film is one that ranges from essentially zero thickness to several thousand Angstroms, although this range can be extended in some cases. If a film is thin enough that it shows an interference color then it will probably be a good ellipsometric sample. The sensitivity of an ellipsometry is such that a change in film thickness of a few Angstroms is usually easy to detect [70]. Ellipsometry measures the change in polarization state of light reflected from the surface of a sample as shown in Figure 4.11.

In order to describe the ellipsometry operation, we will use a coordinate system that relates to the plane made by the propagation direction and a vector perpendicular to the plane of a reflecting surface. This is known as the plane of incidence. The component of the electric field within this plane is termed \( p \)-polarized and the component perpendicular to this plane is termed \( s \)-polarized. In Figure 4.11, a linearly polarized input beam is converted to an elliptically polarized reflected beam. For any angle of incidence greater than \( 0^\circ \) and less than \( 90^\circ \), \( p \)-polarized light and \( s \)-polarized will be reflected differently. In the figure \( E \) is vector of electric field, \( \theta_i \) is the angle of incidence relative to normal to the surface, and the refractive index, absorption coefficient and thickness of layer \( i \) are donated as \( n_i, k_i \) and \( d_i \) respectively.

Figure 4.11 schematic drawing of Ellipsometry measurement
The measured values are represented in terms of two so-called ellipsometric angles: $\psi$ and $\Delta$. These angles are related to the ratio of the total Fresnel reflection coefficients, $R_p$ and $R_s$ for $p$ and $s$-polarized light, respectively.

\[
\tan \psi = \frac{|R_p|}{|R_s|} \quad (16)
\]

\[
\tan(\psi)e^{i\Delta} = \frac{R_p}{R_s} \quad (17)
\]

For an Air/Film/Substrate interface case described in Figure 4.12, the Fresnel coefficients become:

\[
R_p = \frac{r_{ab}^p r_{bc}^p e^{-i\beta}}{1 + r_{ab}^p r_{bc}^p e^{-i\beta}} \quad (18)
\]

\[
R_s = \frac{r_{ab}^s r_{bc}^s e^{-i\beta}}{1 + r_{ab}^s r_{bc}^s e^{-i\beta}} \quad (19)
\]

\[
\beta = 2\pi(d/n_b - ik_b) \cos \theta_b \quad (20)
\]
Because Ellipsometry measures a ratio of two values, it can be highly accurate and very reproducible. From Eq. (16) the ratio is seen to be a complex number, thus it contains phase information expressed in Δ, which makes the measurement very sensitive. With knowledge of the refractive index of the organic film, we can estimate its thickness based on measurements of the complex-valued $R_p$ and $R_s$ for multiple angles of incidence. Usually, we use the value of 1.45 as the refractive index for organic monolayers.

### 4.5 Bonding interface characterization

Several methods are available for bonding characterization. They are summarized in Table 4.2:

<table>
<thead>
<tr>
<th>Technique</th>
<th>Principle</th>
<th>Determination</th>
</tr>
</thead>
<tbody>
<tr>
<td>IR transmission microscopy [71]</td>
<td>Reflected light from unbonded areas will be shown as interference fringes</td>
<td>Wafer bonding failures as unbonded areas/voids</td>
</tr>
<tr>
<td>Scanning electron microscope (SEM) [72]</td>
<td>Imaging a sample by scanning it with a high-energy beam of electrons.</td>
<td>Characterization of a cross section of the bonding interface</td>
</tr>
<tr>
<td>Pull-Off Adhesion Test [73]</td>
<td>A load is increasingly applied to the surface until the bonded samples are pulled apart. The force required yields the tensile strength in mega Pascals (MPa).</td>
<td>Determines the tensile strength of the bonding.</td>
</tr>
<tr>
<td>Scanning acoustic microscopy (SAM) [74]</td>
<td>focused sound is used to image an object</td>
<td>Failure analysis and non-destructive evaluation of bonding interface</td>
</tr>
</tbody>
</table>

Table 4.2 bonding characterization techniques
**IR transmission microscopy.** Infrared (IR) void imaging is used for analyzing materials that are IR transparent, such as silicon and LiNbO$_3$. The measurement equipment consists of an infrared lamp as a light source and an infrared video system. Unbonded areas appear as interference fringes, if the void opening is $\geq 1$ nm [71]. Figure 4.13 presents an illustration of the IR imaging setup.

![Figure 4.13 Schematic infrared transmission microscopy setup.](image)

**Scanning electron microscope (SEM).** The scanning electron microscope (SEM) [72] uses a focused beam of high-energy electrons to generate a variety of signals at the surface of solid specimen. The signals that derive from electron-sample interactions reveal information about the sample including external morphology (texture), chemical composition, and crystalline structure and orientation of materials making up the sample. SEM can also map the interface of bonded samples, and measure the gap between them. Data is collected over a selected area of the surface of the sample, and a two-dimensional image is generated that displays spatial variations in these properties. Figure 4.14 presents an illustration of a SEM imaging.

The spatial resolution of the SEM depends on the size of the electron spot, which in turn depends on both the wavelength of the electrons and the electron-optical system that produces the scanning beam. Depending on the instrument, the resolution can fall somewhere between less than 1 nm and 20 nm.
Preparation of samples for SEM imaging includes lapping using Struers Labopol-6 standard lapping machine with low-medium pressure. A SiC paper (grit 500) and ethyl-glycol lapping solution were used as the abrasive materials for 5 minutes. This aggressive procedure removes more than 300 microns from the top wafer. The sample is then cleaved with a diamond pen, and the facet is cleaned using a focused ion beam.

Figure 4.14 schematic drawing of the electron and x-ray optics of a SEM

Pull-off adhesion test. A commercial adhesion tester, Defelsko Positest AT-A, was used. The bonded samples were glued to a metal holder on one side and to a transparent window from the other side, in order to avoid dripping of the slow cure epoxy. The force measurement error corresponded to an uncertainty of ±0.5 MPa. A tensile force, perpendicular to the bonding interface, is applied to the metal holder until it is detached. The tensile bond strength (in MPa) is calculated as the force at failure divided by the bonded area [73]. Figure 4.15 shows the Pull-off adhesion test equipment
Figure 4.15 Pull-off adhesion test equipment
5. Characterization of deposited monolayers on silicon and LiNbO₃ and subsequent bonding.

5.1 Monolayer deposition

5.1.1 Octadecyltrichlorosilane (OTS) terminated SAM:

Ellipsometry measurements on OTS coated Silicon samples provided an estimate of 2.2 ± 0.25 nm for the monolayer thickness. This results corresponds to < 5 nm-thick bonding interface, that should not disrupt the transfer of light between the substrates or the electrical conductivity across the interface [75].

Infra-red spectroscopy measurements yielded the following absorption spectra (Figure 5.1), which indicate the success of the deposition of the monolayer on both silicon and LiNbO₃ wafers. The two absorption peaks at 2850 and 2917 cm⁻¹ are characteristic of the CH₂ groups of OTS on Silicon. Their frequency is that which would be expected for a well-packed, highly organized monolayer in which all of the molecular chains are in an extended conformation and aligned parallel to each other. Less well ordered films would give higher frequency absorptions (approaching 2855 and 2925 cm⁻¹ for liquid like films). The peak at 2959 cm⁻¹ is due to the terminal CH₃ group.
Contact angle measurements confirm that the monolayer deposition turns the originally hydrophilic surface ($\sim 30^\circ$) of the sample to a hydrophobic one ($\sim 105^\circ$). These measurements indicate that we have a well-established OTS monolayer on top of both Silicon and Lithium Niobate.
Thioacetate (TA) terminated SAM:

Ellipsometry measurements on TA coated Silicon samples provided an estimate of $1.9 \pm 0.25 \text{ nm}$ for the monolayer thickness. Ellipsometric measurements of monolayers on LiNbO$_3$ could not be performed, in lack of the appropriate materials parameters in the database of the instrument.

The following absorption IR absorption spectra (Figure 5.3) indicate the success of the deposition of a silane-anchored, thio-acetate terminated SAM on silicon wafers. The absorption peak at $1695 \text{ cm}^{-1}$ is characteristic of the thio-acetate group.
Infra-red absorption measurements of the monolayer on LiNbO$_3$ could not be performed, in absence of double side polished LiNbO$_3$ wafers.

Contact angle measurements of a typical thio-acetate terminated SAM is $73 - 75^\circ$, indicating a successful deposition on both silicon and LiNbO$_3$.
5.2 Thiols-forming hydrolysis

As already explained in the bonding procedure, a hydrolysis reaction modifies the terminating functional group on both surfaces. It cleaves the thioacetate group, leaving a thiol group instead. This is a crucial stage of the bonding procedure. Silicon wafers endure the process, leaving the monolayer on top intact. Unfortunately we have found that the same process on x-cut LiNbO₃ strips off the monolayer. Next we will present the characterization of hydrolysis: its success on silicon and its failure on LiNbO₃.

Figure 5.5 shows the ATR-FTIR trace of a SAM-deposited silicon slab following hydrolysis. An absorption peak that is characteristic of the thioacetate group is evident prior to the reaction, whereas it is eliminated following the reaction. The thickness of the hydrolyzed monolayer is estimated as 1.9 ± 0.25 nm. Figure 5.6 shows water droplets on the treated silicon surface, before and after the hydrolysis reaction. The contact angle remains unchanged at 75°, indicating that the reaction did not degrade the monolayer.

![Infra-red absorption spectra of a monolayer-coated silicon sample. Following deposition (red) and following successful hydrolysis (blue).](image)
In contrast, the contact angle of a water droplet on top of a monolayer-coated LiNbO$_3$ decreased from 73 ° to 50 °, indicating a significant degradation of the monolayer (see Figure 5.7).

As a potential solution path, we proposed to modify the surface of the LiNbO$_3$ surface so that it better replicates that of the silicon surface, in hope that it could better sustain the monolayer following hydrolysis. To that end, the LiNbO$_3$ surface was pre-deposited by a 20 $\text{nm}$-thick layer of silica using chemical vapor deposition. The surface of the deposited sample is now close to that of an oxidized silicon wafer (see the process details above for the oxidization of the silicon samples in the 'piranha' solution). As expected, the SAM on top of a silica-coated LiNbO$_3$ sample remained intact following hydrolysis (Figure 5.8). The contact angle retained its value of 75 °.
5.3 Conversion of thiols to disulfides

A fundamental problem in developing this surface chemistry is the need for analytical methods that distinguish between interfacial thiols and disulfides, since they have similar surface wetting properties (i.e. contact angle), and they can’t be distinguished using conventional methods of FTIR and ellipsometry. A new method for distinguishing between thiols and disulfides was developed by the group of C.N Sukenik from the department of chemistry, Bar Ilan University, Israel [76]. The method uses Sanger’s reagent, (2,4-dinitrofluorobenzene, 2,4-DNFB) [77], that readily reacts with thiols but does not react with disulfides. This reaction can be later on be observed using FTIR. Based on this work, and in collaboration with Prof. Sukenik group, we have proved that the method we use for converting thiols to disulfides and was previously described in 4.3, indeed works properly.

5.4 Wafer bonding attempts based on disulfide exchange reaction

The bonding of pairs of silicon samples using disulfide exchange as proposed above was undertaken 32 times. Remarkably, the vast majority of these bonded pairs, about 85% of the samples, were strong enough to withstand rough handling, even though the bonding experiments
were carried out without the benefit of a clean-room environment. Figure 5.9 shows an example of two silicon samples bonded together.

![Image](image_url)

*Figure 5.9 A sample of two bonded silicon pieces (~1 X 1 cm²)*

Pull strength tests were carried out in order to quantify the strength of the bonding. A weak bonding is defined as one that its strength is less than 1MPa, whereas a strong bonding is over 2MPa [78]. The unfavorable preparation conditions lead to some variations in the pull-test strengths of silicon-to-silicon bonded samples. The strength of 10% of the samples was extremely high and in the range of 3 – 5 MPa. 20% were in the range of 1 – 2 MPa, whereas the strengths of the rest was on the order of 1 MPa or lower. As a control experiment, we have tried to use different combinations of monolayers for bonding, and also the conventional method of direct bonding under these relatively modest temperatures, followed by pull test strengths measurements. The results are summarized in Table 5.1.

<table>
<thead>
<tr>
<th>Bonding samples</th>
<th>Number of successes</th>
<th>Number of strong bonding</th>
<th>Highest strength measurement(MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thiols coated Si to Disulfide coated Si</td>
<td>27 out of 32</td>
<td>3</td>
<td>5</td>
</tr>
<tr>
<td>OTS coated Si to OTS coated Si</td>
<td>2 out of 8</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>Thiols coated Si to clean Si</td>
<td>0 out of 5</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Thiols coated Si to Thiols coated Si</td>
<td>9 out of 17</td>
<td>2</td>
<td>1.2</td>
</tr>
<tr>
<td>Disulfide coated Si to Disulfide coated Si</td>
<td>6 out of 14</td>
<td>1</td>
<td>1.5</td>
</tr>
<tr>
<td>Direct bonding - clean Si to clean Si</td>
<td>5 out of 8</td>
<td>2</td>
<td>2.1</td>
</tr>
</tbody>
</table>

*Table 5.1 Pull strength test measurement statistics and control experiments*
Our suggested method of bonding was consistently successful, and provided the highest strength measurements over the control experiments. We suggest that the relative hydrophobicity of the SAM treated surface minimizes surface contamination and combines with the modest flexibility introduced by the monolayer chains to provide a robust, readily generalizable process.

Fourteen attempts for bonding silicon-to-LiNbO$_3$ that had been pre-deposited with silica were undertaken. Unfortunately, most of these attempts did not result in actual bonding, with the two samples separated as soon as they were removed from the bonding press. Six attempts, however, did show handling strength. One such bonded pair is shown in Figure 5.10. The small number of successful attempts did not allow for a quantitative assessment of the bonding strength. We hypothesize that the low success rate has to do with the thermal stresses that are associated with the application of a 120 °C thermal load to the bonded interface. Although the process is carried out at a substantially lower temperature than that of direct bonding techniques, it may still be too high due to the large mismatch between the thermal expansion coefficients of the two materials (more on that matter in the conclusions section).

![Image](image.jpg)

**Figure 5.10** A sample of Si and LiNbO$_3$ bonded pieces using Silica as a mediated layer

For completeness, two more methods for the characterization of bonded samples are demonstrated below for a different material system: InP bonded to silicon. This particular combination is very significant for the making of hybrid-silicon light sources, amplifiers, modulators
and detectors as discussed in chapter 2. This bonding process was developed in parallel with the silicon/LiNbO₃ bonding procedure in the same working group, and its details are beyond the scope of this thesis. Figure 5.11 presents a scanning electron microscope (SEM) image of the cross-section of the bonding interface (made using a focused ion beam). Analysis of high-resolution SEM images of such cross-sections provided an upper limit of 6 nm for the thickness of the bonding interface (which includes both the silicon oxide and the SAM).

![Figure 5.11 SEM image of the interface of Si bonded to InP](image)

The quality of the bonding was evaluated using infra-red microscopy. Figure 5.12 (a) shows Bonded InP and silicon samples. Figure 5.12 (b) shows an image of the bonding interface between a silicon sample and an InP sample. The InP piece was cut out of the edge of the wafer, so that a region on the right-hand side could not be bonded. Interferometric rings are evident in the area that is not bonded, whereas the bonded region is free of such rings. The image illustrates the formation of a continuous bonded interface in the flat part of the sample. InP samples taken from the center of the wafer exhibited a uniform bonding to their entire surface.
Figure 5.12 (a) Bonded InP and silicon samples. (b) Infra-red microscopy image of an InP sample and a silicon sample bonded together. Rings appear in a corner region that was taken from the edge of the InP wafer and could not be bonded. An illustration of the partially bonded samples is shown above the microscopy image. IR image of the interface of Silicon bonded to InP

5.5 Alternative bonding procedure: thiols-to-platinum.

Due to the difficulties encountered in the bonding of silicon to LiNbO₃ via disulfide exchange, and in particular due to the challenges facing the hydrolysis of SAMs on LiNbO₃, and alternative bonding procedure was proposed and attempted as well. In this modified procedure, the silicon sample was deposited with the monolayer as before, and the free-standing functional groups of the monolayers were cleaved to thiols using hydrolysis as described above. Unlike the previous bonding scheme, the thiol form was used directly for bonding, and the further conversion of the functional groups into disulfides was not carried out.

Thiol-terminated molecules are known to attach to platinum in solution [79]. The underlying principle for the proposed bonding mechanism was to try and carry over this known reaction into the solid state. To that end, the LiNbO₃ sample was pre-deposited by a 25nm thick platinum layer using a chemical vapor deposition (CVD) process. The coated sample was then cleaned in a plasma cleaner for 30 min. The silicon and LiNbO₃ samples were then placed on top of one another inside the press, in a similar manner to the disulfide-exchange processes discussed earlier. Here too, a load of ~160 kPa was applied overnight at a temperature of 120 °C.
As occurred with the disulfide-exchange-based process, the majority of platinum-mediated bonding attempts were unfortunately unsuccessful: six attempts in total. A quantitative assessment of the bonding strength could not be performed. Nevertheless, handling strength was achieved in two of the occasions. A pair of a silicon sample and a LiNbO$_3$ sample bonded together via monolayer-to-platinum interface is shown in Figure 5.13:

![Image](image.png)

Figure 5.13 A sample of Si and LiNbO$_3$ bonded pieces using platinum as a mediated layer.
6. Summary and Conclusions

In this work, I have presented a technology for the vertical integration between LiNbO3 and silicon-on-insulator (SOI) substrates, for the future fabrication of integrated hybrid electro-optic modulators. Thus type of hybrid-silicon photonics is of major potential importance and interest, since although silicon is the material of choice for the mature and developed electronic integrated circuits industry, realization of modulators and other active devices in silicon is difficult. The two specific objectives of my work over the last two years were the following key aspects of such devices: The geometric design and the bonding technology.

On the design part, our analysis and simulations suggested that hybrid silicon-LiNbO3 modulators should be feasible, with a $V_{th} L$ product that is on the same order of magnitude as that of stand-alone LiNbO3 modulators. Two designs were discussed: 1) a far spaced electrode configuration, which is easier to fabricate but requires high voltages, and should serve for a proof-of-principle; and 2) a more advanced device with closely spaced electrodes.

On the bonding parts we proposed a new bonding paradigm of SAM-assisted bonding. The advantage of this method is the usage of a relatively low temperature of 120°C. It potentially reduces the thermal stresses that stem from the mismatch between the thermal expansion coefficients of silicon and LiNbO3. Our process relies on the deposition of SAMs of organic material on either one or both surfaces to be bonded, and their subsequent functionalization using specific chemical reactions which allow for the bonding of the two surfaces at low temperatures. The wafer bonding procedure was addressed in detail and the chemical processes were described. During the development of the process, I became familiar not only with the area of SAM, but also with many fabrication procedures and analytic and characterization tools such as AFM, FTIR, contact angle measurements, SEM, IR imaging and pull strength tests.

The bonding of silicon-to-silicon was successful, while the application of the process to the bonding of silicon to LiNbO3 faced difficulties, such as the stripping of the monolayer on LiNbO3.
pieces after the hydrolysis reaction. As a potential solution path, we modified the surface of the LiNbO$_3$ so that it better replicates that of the silicon surface, and used LiNbO$_3$ that had been pre-deposited with silica. A bonding of silicon-to-LiNbO$_3$ that had been pre-deposited with silica was attempted a number of times. Most of these attempts did not result in actual bonding, and only showed handling strength when removed from the bonding press. A second variant of the process, using platinum coated LiNbO$_3$, also showed limited success to-date.

We hypothesize that the low success rate has to do with the thermal stresses that are associated with the application of a 120 °C thermal load to the bonded interface. Although the process is carried out at a substantially lower temperature than that of direct bonding techniques, it may still be too high due to the large mismatch between the thermal expansion coefficients of the two materials. LiNbO$_3$ and Silicon expend differently under 120 °C. The bonding occurs after a few hours when the two surfaces have reached this temperature, and each had expended accordingly. When taken out of the bonding press, the samples are cooled down to room temperature, and each of the materials contract back. If a bonding has occurred, the molecules that bond the two surfaces may be torn away because of these thermal stresses leading to bonding failure. In addition, the lack of clean room environment may also be a cause to the failure of bonding attempts.

Future work could see an improvement in bonding success, first and foremost, through working in cleanroom environments that are now becoming available to us. In addition, alternative bonding procedures, which may take place at room temperature or close to it, could be attempted. These include different types of monolayer based reactions, direct bonding via oxygen plasma activation, or the electro-static attraction between polymer chains of opposite charge [80,81].

In summary, the goal of generating a hybrid silicon-LiNbO$_3$ electro-optic modulator is still a notable one with great potential importance. Furthermore, the concept of SAM-assisted bonding is worth pursuing from the fundamental material science standpoint as well. I expect considerable progress towards that objective in the next few years.
References


תקציר

תקשורת אופטית

הינה האמצעי הכהה ביותר ל_traibilit של תקשורת נתונים על פני מרחקים ארוכים, זה למעלה משלושה עשורים. בעידן המודרני, ככל שהאחסון והדרישה להעלאת קצב שיתוף המידע גדלים, טכנולוגיות תקשורת מבוססות אופטיקה חודרות בהדרגה אל רמת הלוח, השבב ואף המעבד. עד_namespace של תקשורת נתונים הממשים גם הם זהالت, בידור, יבוא ויצוא האפקטיביות של מערכות תקשורת אופטיות ליצת נתונים אלקטרוניות, באמצעות אלכטרומטרים משולבים, לאורך פיטופטרות מתווך. לפיכך, מימין של התקני פוטונים על-גב סיליקון הוא תחום מחקר בעל חשיבות רבה.

בامعةパイון החומרים של סיליקון על-גב משולב (SOI), מהווה פלטפורמה מוצלחת בכל תחומי תקשורת והמחשוב. בзыיסון февраיג פוטוניםstoffים נמוכים, אינטגרר- כלומר, סיליקון ואטום- mostra את התכונות הנוחות של הסיליקון. דוגמא לצ関わ מספק את הأنشطة במוסדות בנAscii. אפקט זה התאים את מחזור של התוכן האפקטים, ומ ula-אופטיים, שמשתמש בהם במערכות תקשורת אופטיות. השיטה הרווחת ביותר בחיבור חומרים אלקטרו אופטיים שונים נקראת "direct bonding" או הדבקה ישירה. השיטה מובילה לחיבור בין שני חומרים חיסול ניאובט (LiNbO₃) וליהם שתי מטריות פוטוניות נוספים. השיטה מיושמת בהצלחה ביצור תכניות אינדיום-פוספיד (InP) וסיליקון, לדוגמה, אך ל_exist החומרים שונים, בזווית של 3-300 מעלות צלזיוס. שיטה של הגتطוגина הרביעית של ליטו בחומרים רבים, מתאימה Lagele, גם באשר לשתי התרוממות מקrome של החומרים הביניים. הקבע בין מימין ו-ליצין וניבובים, ליצין ניאובט, החומרים האופטיים של התקני ההיברידיים.

לקריאת העד: אופט הלוח ובין ליצין ו-ליצין ובין ניוובט, החומרים האופטיים של התקני ההיברידיים.
היאמר המתאים תרומתי Каגמיו על הממשק שבין החומריםသבנית ביניהם לשימור, או השבכה三层�ב עיבוד升降 ו 의사 עד_fhכל השכבתם, שיתות האזון בטרם והשבכה בידידות בין
השכבת. התוכנאה מכש,キーים אידטיו מתווספים בחבף בשכבות החיבור בין ליתם ניאובט לייקולינו.

הצחק עליה, היא מתודהgy contemplated Light 있어بت מדרשה שמדLayoutPanel על יצירシェבך-חרנקלירית,_ser
מתוחה באואף spécialisé מתצר תמסכם "(Self-assembled monolayers)" על פי יש התממשים. לאחר
הפעולה של השכבה הדח_externalית באמצעות תقوانين ייחודי שפטייה, מתאpatible השכבה של שיני
משטחים בטרם תומך סמור. התדריך ייצד השכבות, התבניות הכימיות התلازمויות והחזרה
מתוחמות בטרם תומך רב העבודה.жить וחווית של השיטה מתמשכת על פי השיטה הקימית, או
הישווט בטרם תומך נמוכה יסוד של 120 מעלה. איש מת硔ית את התממשים הכימיות הנדרשים לע-פי
הمسؤولת השכבה.

בחוק הממקדש לתוך הגיאומטריה, שטח trường על הרביע לשכבה הבטוח,dear ששברשה מרחק רב ב-
האלקטרודות ממותג גודל של שאות מיקרונים. תוצרת זו الكل יתר למידה או דרישה העמדה מתוחם גביה
ומתחמות לקに向けて ב짢ים. התנודה החשניה מประสงך יוצר מתבשות על מרחק של מיקרונים בודד,ב
האלקטרודות. סימושיונית גאומטריה המתמשכות יובלים למסקנה כי מIMITו מודולטויםibbeanшимו hip אברקר
והם שעוני השטח they תועדים את התממש יסוד של המสะดวกות לרמת מודולטוים ליימי מובסם,ליימונ
 giveaways.

הפרק אחרון בדחה עסוק בשכבות החיבור. לתרומת מסמר رمضמות של האזון ראגמיו, עיבוד שליתים
אין גובט לייקולינו מpng פברית תבניות ליימות אל התמשכים ביניהם בירוח דקатурתן להטעות תך
הנדבירת מתוחמות בבודא. בין מייסום את הקשיות חלול בשיך להטעות תת-אידאליים. פתרונות
אפשריו לשיפור השכבה במה בים העבודה. בין מקוות כי לאחר שיבוצעו מסמר שוניים בשיטה
הказан, מדליילר מודולטוים היברידיים של ליתם ניאובט לייקולינו.
המחק לתזה בוצע תחת הנהגתו של "ר' אבי צדוק מהפקולטה
לנדסה באוניברסיטת בר-אילן.
מודולטור אלקטרואופטי היברידי בסיליקון ולייטום

גיוסט: תכנון גיאומטרי וטכניות להרבה בין מצעים

טלי אילוביץ

עבודה זו מוצעת כחלק מהדרישות لنשיאות קבלת תואר מוסמך

בפקולטה להנדסה של אוניברסיטת בר-אילן

רמט ג'אלול תשע"ב